

ELECTRONIC SUPPLEMENTARY INFORMATION

FOR

**Molybdenum and Tungsten Complexes with Carbon Dioxide and
Ethylene Ligands**

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Table of Contents

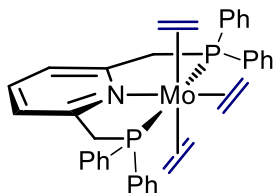
General Considerations	S2
Synthesis of complexes 1-3, characterization by NMR and IR spectra, and attempts to induce coupling of ethylene and CO₂	S2
Solid state reactivity	S19
Computational Methods	S20

General Considerations

All air and moisture-sensitive manipulations were carried out using standard Schlenk techniques with an inert atmosphere of argon or in a glovebox containing an atmosphere of nitrogen. All reactants were purchased from Sigma-Aldrich or Across and used without further purification. Solvents were dried using a SPS-MBraun system with the exception of toluene which was distilled in the presence of sodium under argon. The compounds PNP (PNP = 2,6-(CH₂PPh₂)₂-C₅H₃N),^[1] MoCl₃(PNP)₃^[2] and WCl₃(thf)₃^[3] were prepared according to literature procedures. NMR spectra were recorded on Agilent 400 MR or Agilent 500 DD₂, ¹H and ¹³C NMR shifts are reported relative to tetramethylsilane. FT-IR spectra were collected on a Nicolet IR200 FTIR spectrometer. Elemental analyses were performed on a Perkin-Elmer Series II CHNS/O Analyzer 2400. Crystal structure determinations were carried out using a BRUKER D8 FIXED-CHI diffractometer equipped with an Oxford Cryosystem low-temperature device.

Experimental Procedures, NMR and IR spectra

Complex 1a. *mer*-Mo(C₂H₄)₃(PNP) (PNP = 2,6-(CH₂PPh₂)₂-C₅H₃N).



Following a previously described method for MoCl₃(PNP),² a mixture of PNP ligand (1.9 g, 4 mmol) and [MoCl₃(thf)₃] (1.67 g, 4 mmol) in THF (20 mL) was stirred at 40 °C for 12 h. The resulting yellow suspension was filtrated and the solid washed with Et₂O (3 x 5 mL), and dried under vacuum to give a yellow solid in 98% yield. In a 250 mL Schlenk flask, Na-Hg amalgam (0.5 wt %, 0.55 g Na in 110 g Hg) was prepared under argon and THF (100 mL) was added. Complex MoCl₃(PNP) was incorporated onto the amalgam as a suspension (2.71 g, 4 mmol in 60 mL of THF) via canula under an ethylene atmosphere, and ethylene was bubbled for 45 min until the mixture turned dark red. The mixture was further stirred at room temperature for 16 h under a closed ethylene atmosphere. After that time the mixture was decanted, and the supernatant solution was centrifuged under argon (2500 rpm, 5 min). The red solution was then transferred into a flask before removing volatiles under reduced pressure. The residue was extracted with benzene (2 x 20 mL) and the filtrates were combined before evaporation under vacuum. The resultant solid was dissolved in THF (20 mL) and hexane (1 mL). Concentration and cooling at -30 °C afforded dark red crystals of the complex **1a** in 90% yield (combined crops). Crystals contained some THF of crystallization. The sample for the elemental analysis was submitted to vacuum for several hours to obtain a completely dried material.

1 B. M. Cochran and F. E. Michael, *J. Am. Chem. Soc.*, 2008, **130**, 2786-2792.

2 K. Arashiba, K. Sasaki, S. Kuriyama, Y. Miyake, H. Nakanishi and Y. Nishibayashi, *Organometallics*, 2012, **31**, 2035-2041.

3 E. Kim, A. L. Odom and C. C. Cummins. *Inorg. Chim. Acta*, 1998, **278**, 103-107.

Anal. Calcd. for $C_{37}H_{39}MoNP_2$ (**1a**): C, 67.8; H, 6.0; N, 2.1. Found: C, 67.1; H, 5.7; N, 2.0. 1H NMR (500 MHz, THF- d_8): δ 0.49 (t, 8H, $^3J_{H-P}$ = 5 Hz, $CH_{2ethylene}$), 0.95 (br s, 4H, $CH_{2ethylene}$), 4.47 (t, 4H, $^2J_{H-P}$ = 4 Hz, CH_2-P), 7.2-7.27 (m, 12H, $CH_{aromatic}$), 7.44 (m, 3H, $C-H_{pyr}$), 7.64 ppm (br s, 8H, CH_{Ph}). $^{31}P\{^1H\}$ NMR (202.4 MHz, THF- d_8): δ 59.3 ppm. $^{13}C\{^1H\}$ NMR (125 MHz, THF- d_8): δ 39.7 (t, $^2J_{C-P}$ = 5 Hz, $CH_{2ethylene}$), 43.2 (t, J_{C-P} = 8 Hz, CH_2-P), 48.9 (t, $^2J_{C-P}$ = 5 Hz, $CH_{2ethylene}$), 120.2 (t, $^3J_{C-P}$ = 5 Hz, CH_{pyr}), 127.2 (t, $^3J_{C-P}$ = 4 Hz, CH_{Ph}), 127.8 (s, CH_{Ph}), 131.6 (t, $^2J_{C-P}$ = 4 Hz, CH_{Ph}), 133.4 (s, CH_{pyr}), 138.7 (t, $^2J_{C-P}$ = 14 Hz, C_{qPh}), 160.7 (t, 2J = 6 Hz, C_{qpyr}).

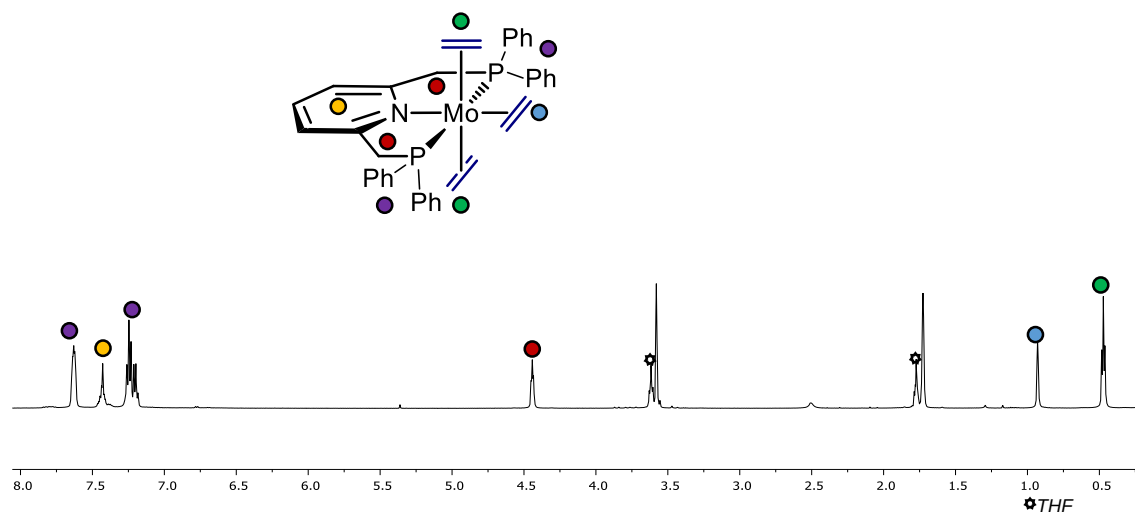


Figure S1: 1H NMR (500 MHz, THF- d_8) of complex **1a**.

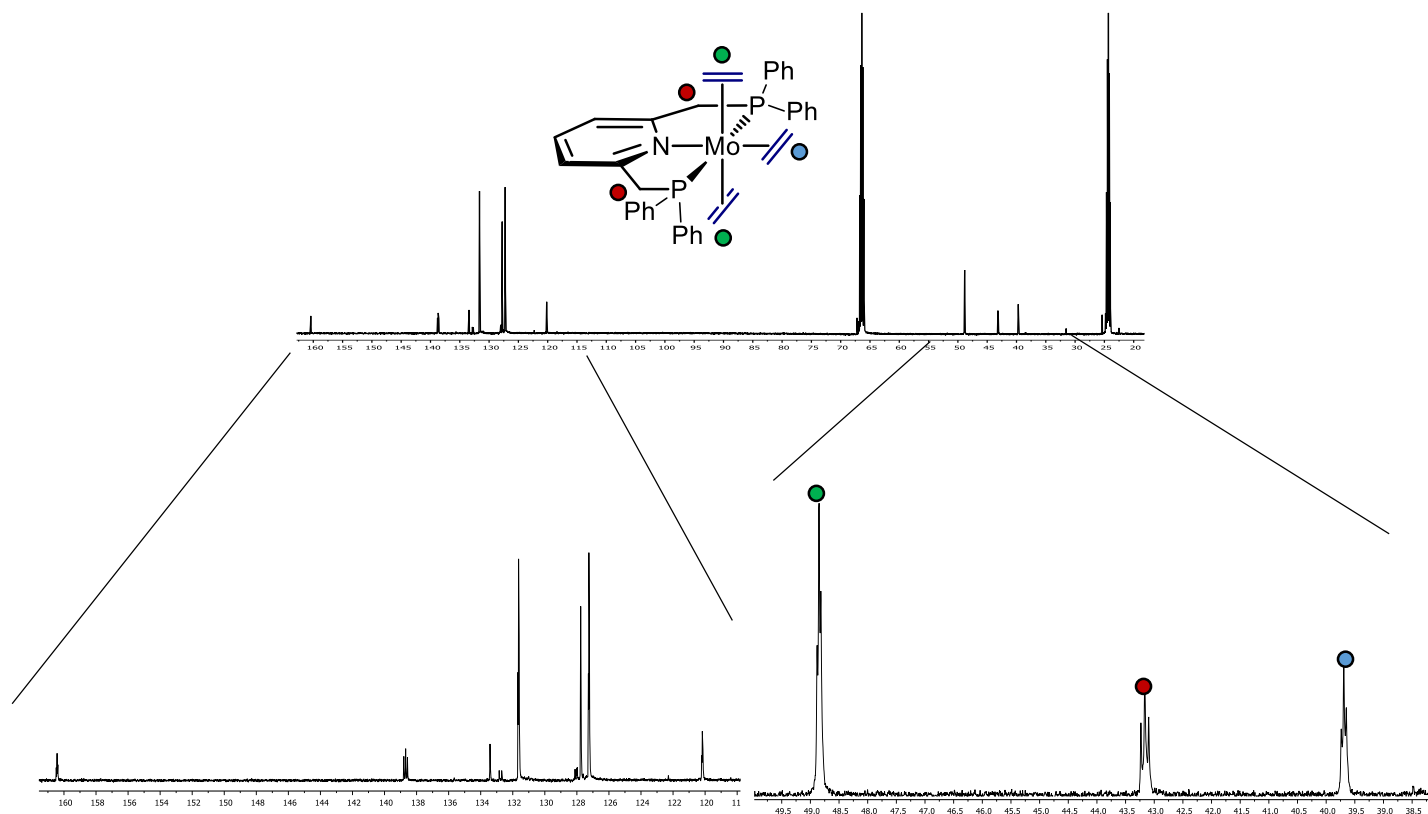


Figure S2: $^{13}C\{^1H\}$ NMR (125 MHz, THF- d_8) of complex **1a**.

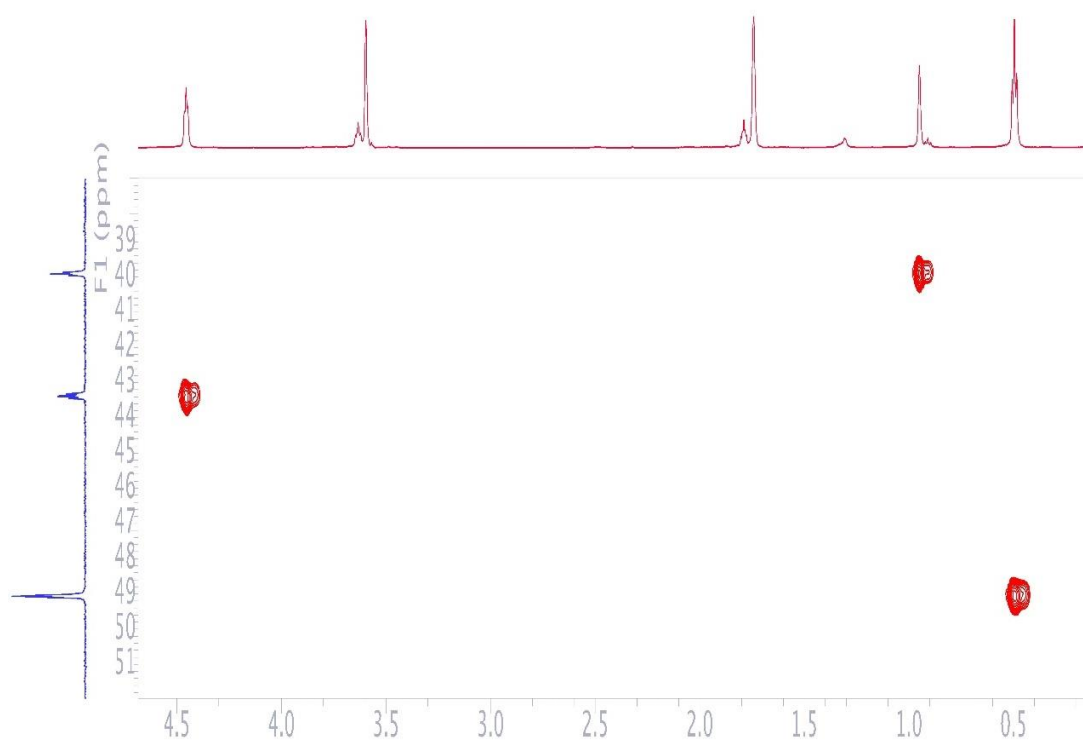


Figure S3: HMQC (methylene region) of complex **1a** (THF- d_8).

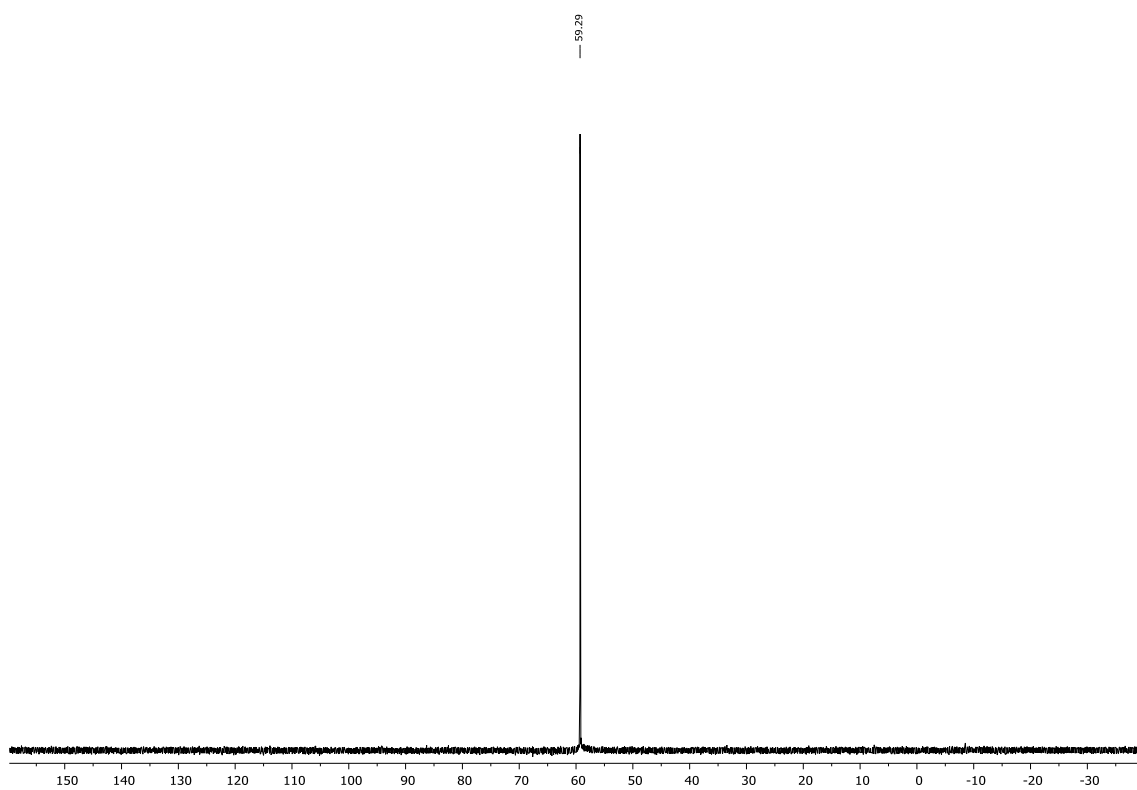
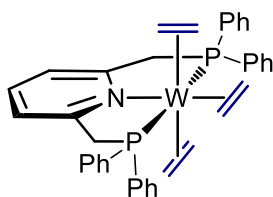


Figure S4: $^{31}\text{P}\{^1\text{H}\}$ NMR (202.4 MHz, THF- d_8) of complex **1a**

Complex 1b. mer-W(C₂H₄)₃(PNP)

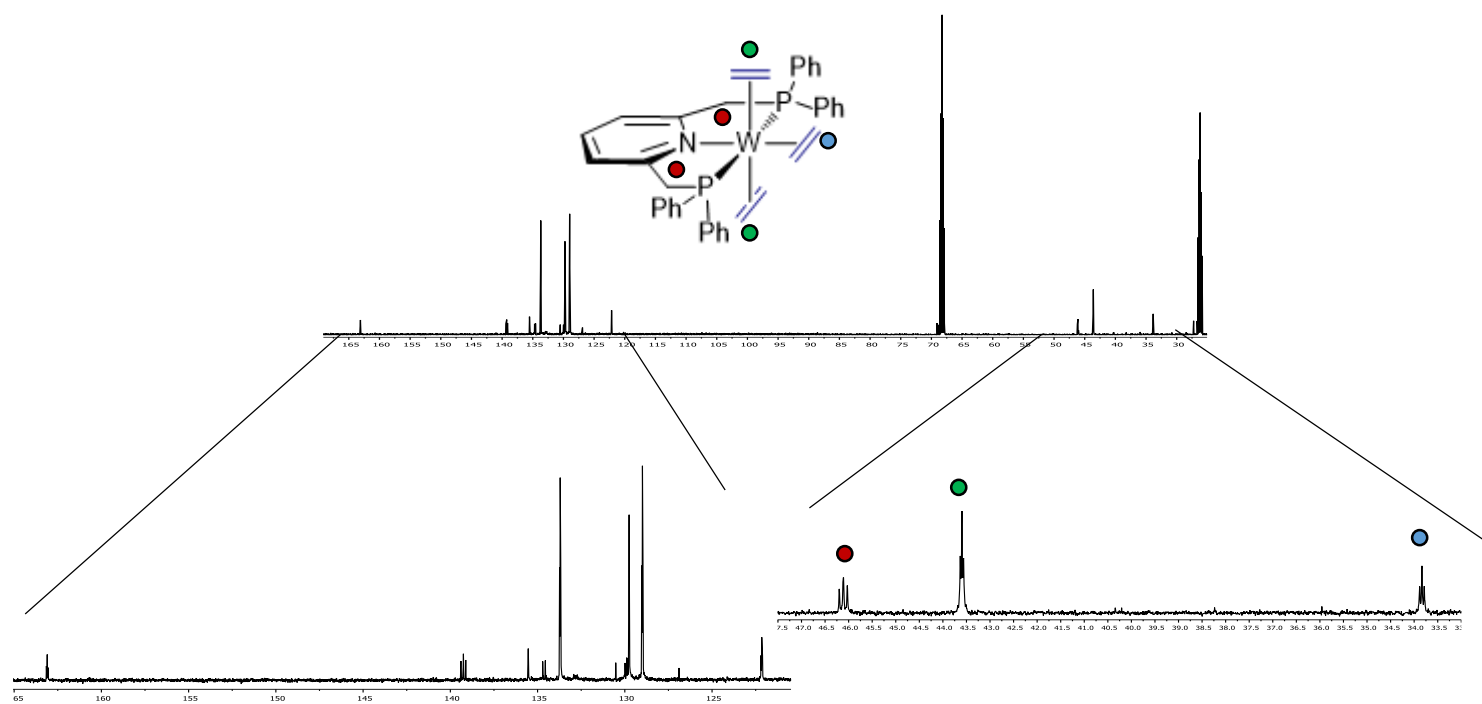
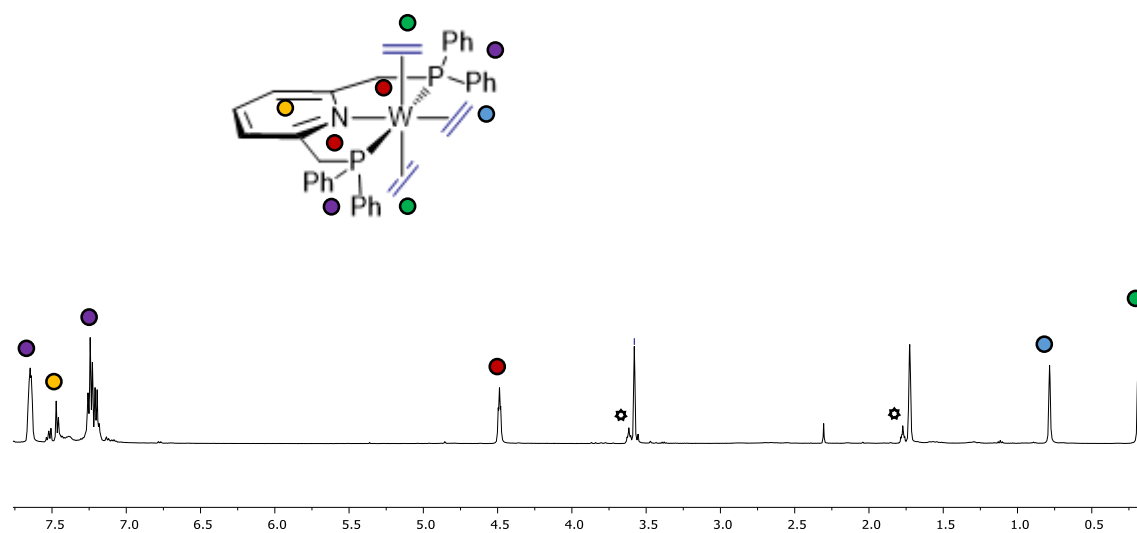


In a 250mL Schlenk flask Na-Hg amalgam (0.5 wt %, 0.55 g Na in 110 g Hg) was prepared under argon and THF was added (100 mL). Complex WCl₃(PNP) (see below) was incorporated onto the amalgam as a suspension (3.06 g, 4 mmol in 60 mL THF) via canula under ethylene, and ethylene was bubbled for 45 min until the solution turned into dark red. The mixture was stirred at room temperature for 20 h under a closed ethylene atmosphere. After that time the mixture was decanted and the supernatant solution was centrifuged under argon (2500 rpm, 5 min). The red solution was then transferred into a flask prior to removal of volatiles under reduced pressure. The residue was extracted with benzene (2 x 30 mL), and the solution filtered. The filtrates were combined and volatiles were again removed, the resulting solid being dissolved in THF (25 mL) and hexane (3 mL). Concentration under reduced pressure and cooling at -30°C gave red crystals of the complex **1b** in 65 % yield (combined crops).

Synthesis of WCl₃(PNP). A mixture of PNP (1.42g, 3 mmol) and WCl₃(thf)₃ (1.52 g, 3 mmol) in THF (20mL) was stirred at 40 °C for 20 h. The resultant purple suspension was filtrated and washed with Et₂O (3 x 5mL), and dried in vacuum affording a purple-pink solid in 60% yield. Anal. Calcd. for C₃₁H₂₇WCl₃NP₂: C, 48.6; H, 3.5; N, 1.8. Found: C, 48.1; H, 3.6; N, 1.7.

Data for **1b**:

Anal. Calcd for C₃₇H₃₉WNP₂ (**2b**): C, 59.8; H, 5.3; N, 1.1. Found: C, 59.4; H, 5.4; N, 1.8. ¹H NMR (500 MHz, THF-d₈): δ 0.18 (t, 8H, ³J_{H-P} = 6 Hz, CH_{2ethylene}), 0.78 (br s, 4H, CH_{2ethylene}), 4.49 (t, 4H, ²J_{H-P} = 4 Hz, CH_{2-P}), 7.23 (m, 12H, CH_{Ph}), 7.46 (d, 2H, ³J = 7 Hz, CH_{pyr}), 7.52 (t, 1H, ³J = 7 Hz, CH_{pyr}), 7.65 (m, 8H, CH_{Ph}). ³¹P{¹H} NMR (202.4 MHz, THF-d₈): δ 27.3 ppm (s; J_{P-W} = 115 Hz, W-satellites). ¹³C{¹H} NMR (125 MHz, THF-d₈): δ 33.8 (t, ²J_{C-P} = 5 Hz, CH_{2ethylene}), 43.6 (t, ²J_{C-P} = 5 Hz, CH_{2ethylene}), 46.1 (t, J_{C-P} = 10 Hz, CH_{2-P}), 122.1 (t, ³J_{C-P} = 5 Hz, CH_{pyr}), 129.0 (t, ³J_{C-P} = 4 Hz, CH_{Ph}), 129.7 (s, CH_{Ph}), 133.7 (t, ²J_{C-P} = 4 Hz, CH_{Ph}), 135.5 (s, CH_{pyr}), 139.3 (t, ²J_{C-P} = 17 Hz, C_{qPh}), 163.1 (t, ²J_{C-P} = 6 Hz, C_{qpyr}).



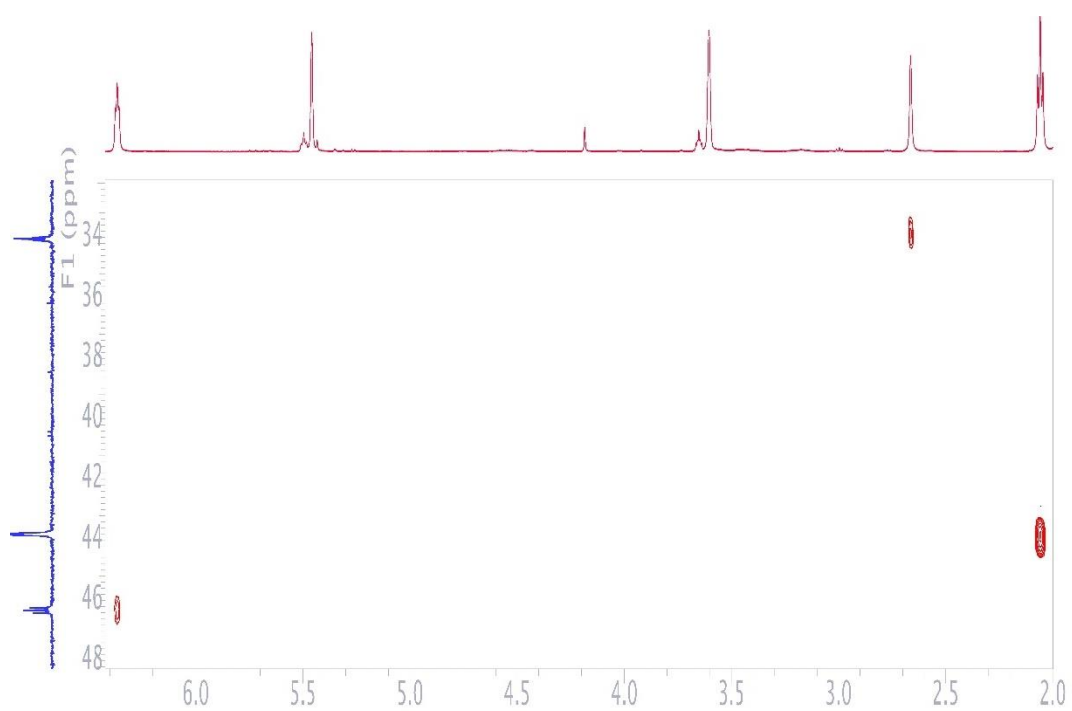


Figure S7: HMQC (methylene region) of complex **1b** (THF- d_8).

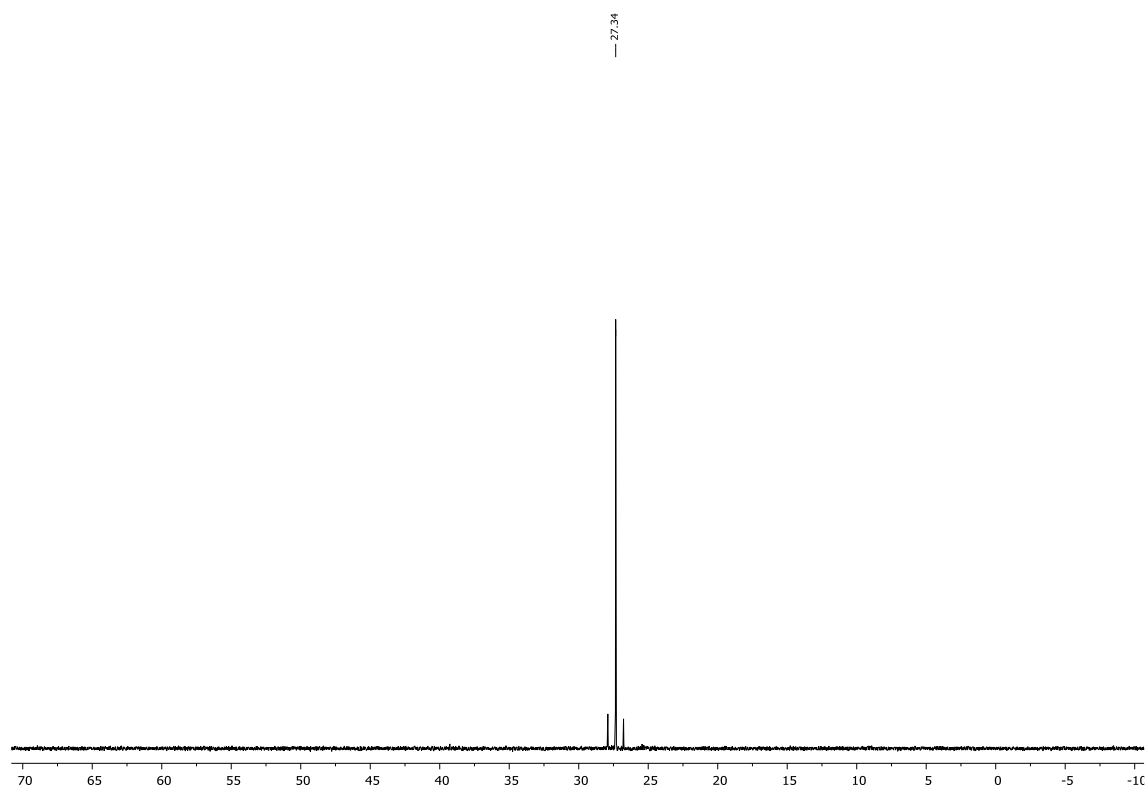
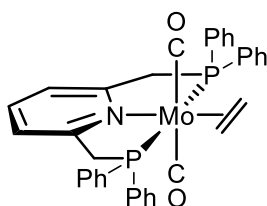


Figure S8: $^{31}\text{P}\{^1\text{H}\}$ NMR (202.4 MHz, THF- d_8) of complex **1b**.

Complex 2a. *trans*-Mo(CO)₂(C₂H₄)(PNP)



Complex **1a** (0.3 g, 0.484mmol) was dissolved in THF (15 mL) in a Fisher-Porter vessel under argon. The system was charged with 2 atm of carbon monoxide and the mixture was stirred at 60°C overnight. The resultant intense orange solution was transferred to a Schlenk tube, concentrated under reduced pressure before hexane was added dropwise until cloudiness. Cling at -30 °C gave orange crystals of complex **2a** in 86% yield.

Anal. Calcd. for C₃₅H₂₁MoO₂NP₂: C, 64.1; H, 4.8; N, 2.1. Found: C, 64.9; H, 5.7; N, 1.8. IR(nujol mull): $\nu(\text{CO})$, 1807 cm⁻¹. ¹H NMR (400 MHz, C₆D₆): δ 1.77 (br, 4H, CH_{2ethylene}), 3.64 (t, 4H, ²J_{H-P} = 3.6 Hz, CH_{2-P}), 6.41 (d, 2H, ³J = 7.6 Hz, CH_{pyr}), 6.56 (t, 1H, ³J = 7.6 Hz, CH_{pyr}), 6.96 (t, 4H, CH_{Ph}), 7.07 (t, 8H, J_{H-P} = 7. Hz, CH_{Ph}), 7.66 (m, 8H, CH_{Ph}); ³¹P{¹H} NMR (161.9 MHz, C₆D₆): δ 65.4 ppm ¹³C{¹H} NMR (100 MHz, C₆D₆): δ 27.09 (t, ²J_{C-P} = 5 Hz, CH_{2ethylene}), 46.9 (t, J_{C-P} = 9 Hz, CH_{2-P}), 119.8 (t, ³J_{C-P} = 5 Hz, CH_{pyr}), 128.2 (t, ³J_{C-P} = 5 Hz, CH_{Ph}), 128.9 (s, CH_{Ph}), 131.7 (t, ²J_{C-P} = 6 Hz, CH_{Ph}), 132.1 (s, CH_{pyr}), 138.6 (t, ²J_{C-P} = 16 Hz, C_{qPh}), 160.3 (t, ²J_{C-P} = 6 Hz, C_{qpyr}), 218.8 (t, ²J_{C-P} = 10 Hz, CO).

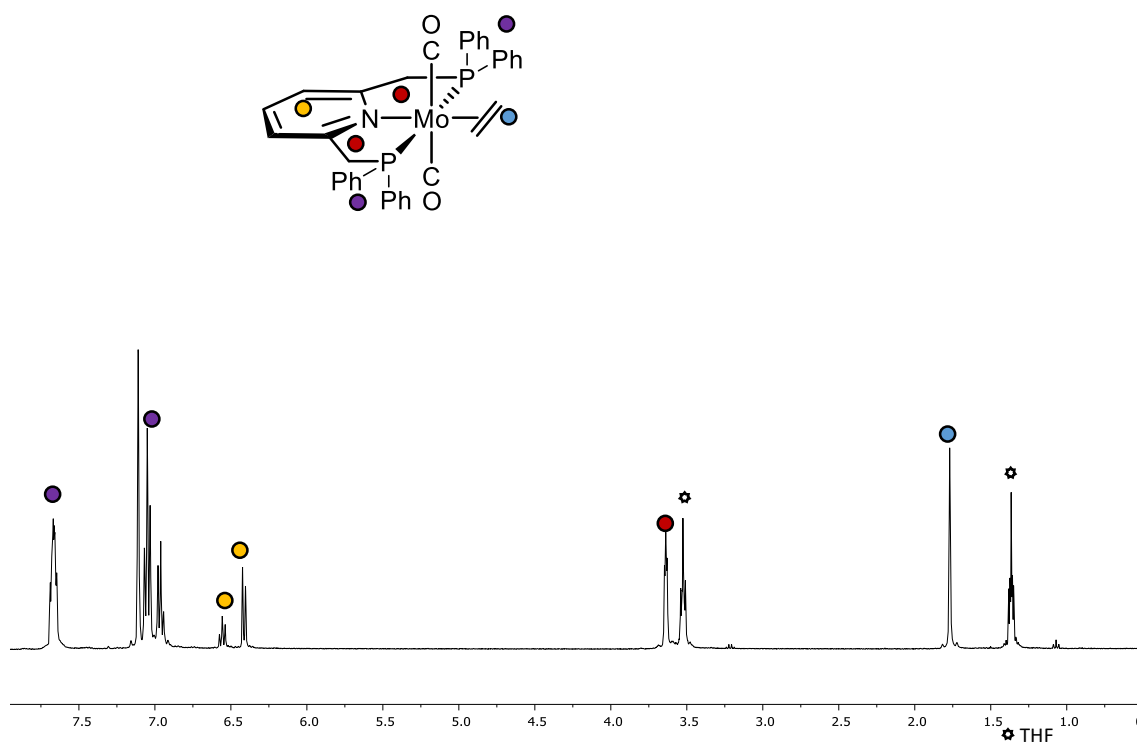


Figure S9: ¹H NMR (400 MHz, C₆D₆) of complex **2a**.

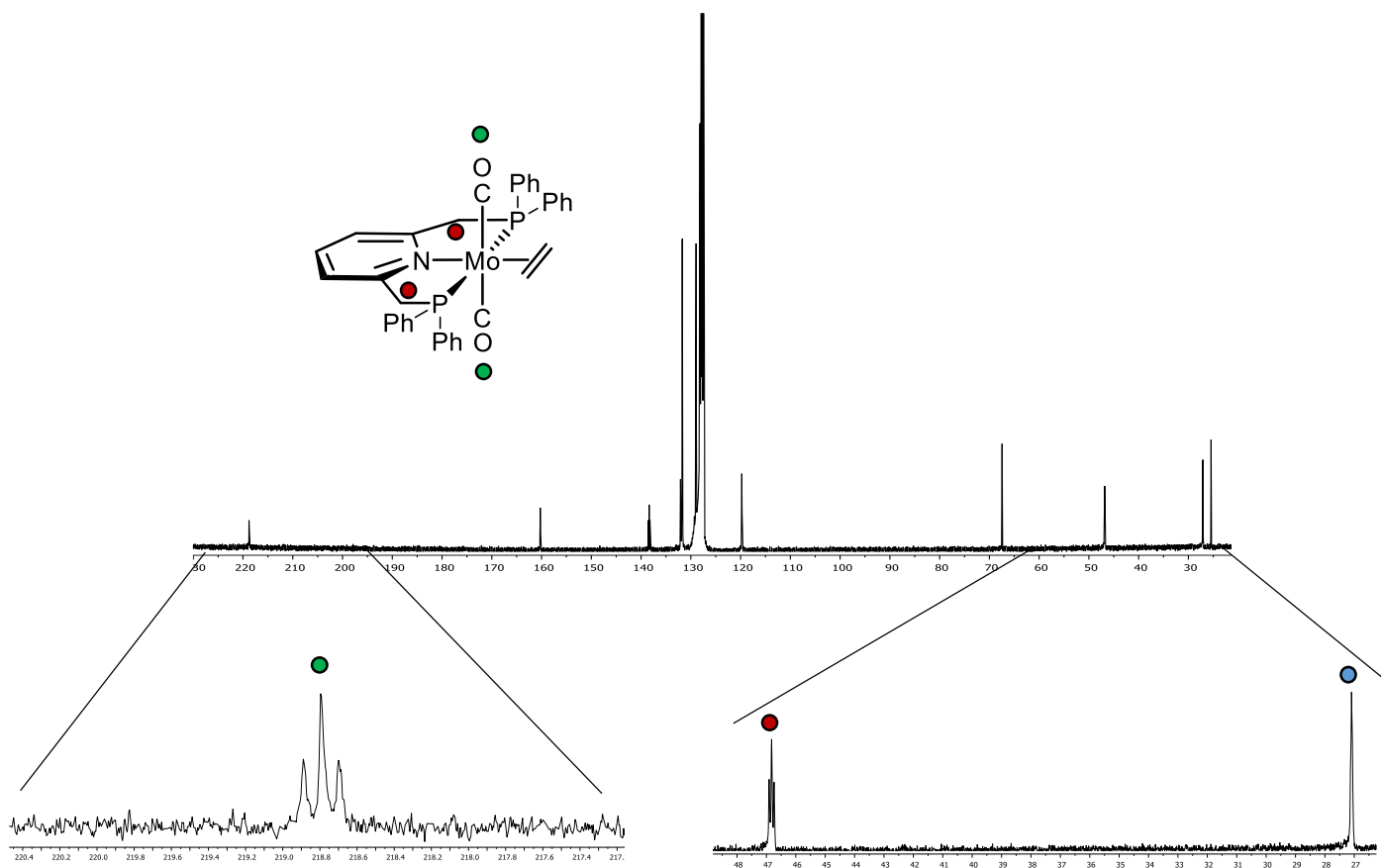


Figure S10: $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6) of complex 2a.

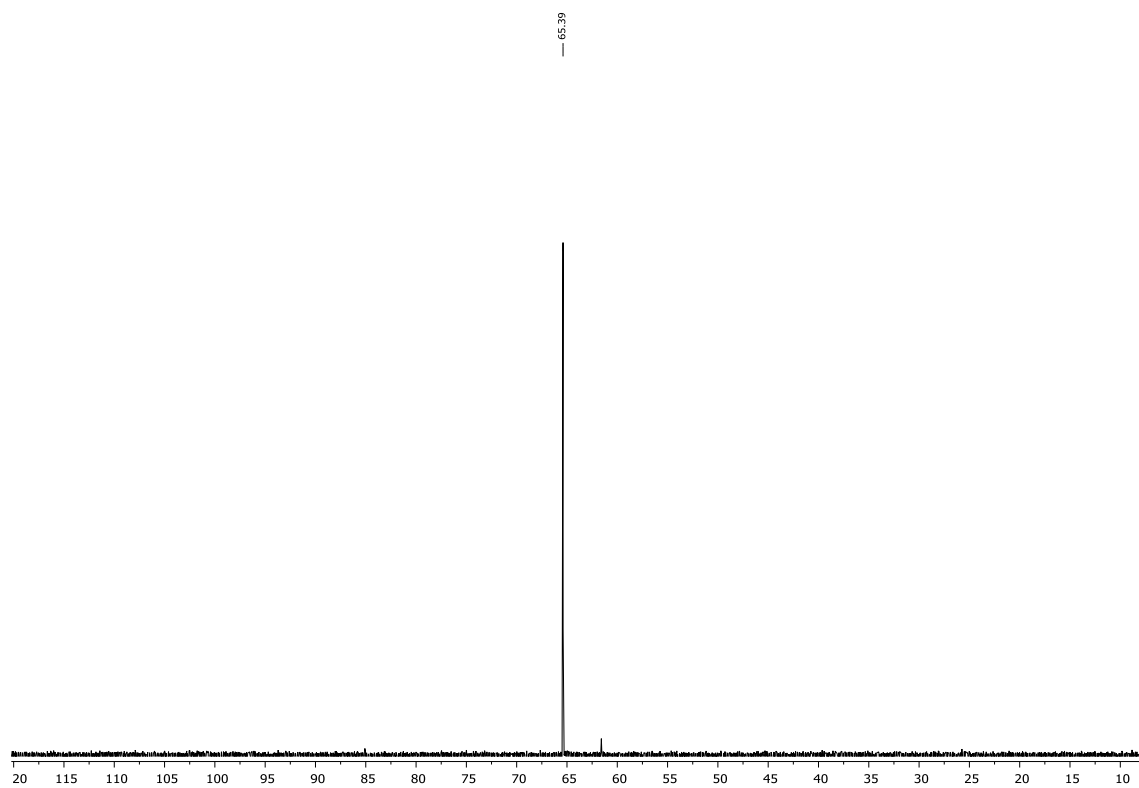


Figure S11: $^{31}\text{P}\{^1\text{H}\}$ NMR (161.9 MHz, C_6D_6) of complex 2a.

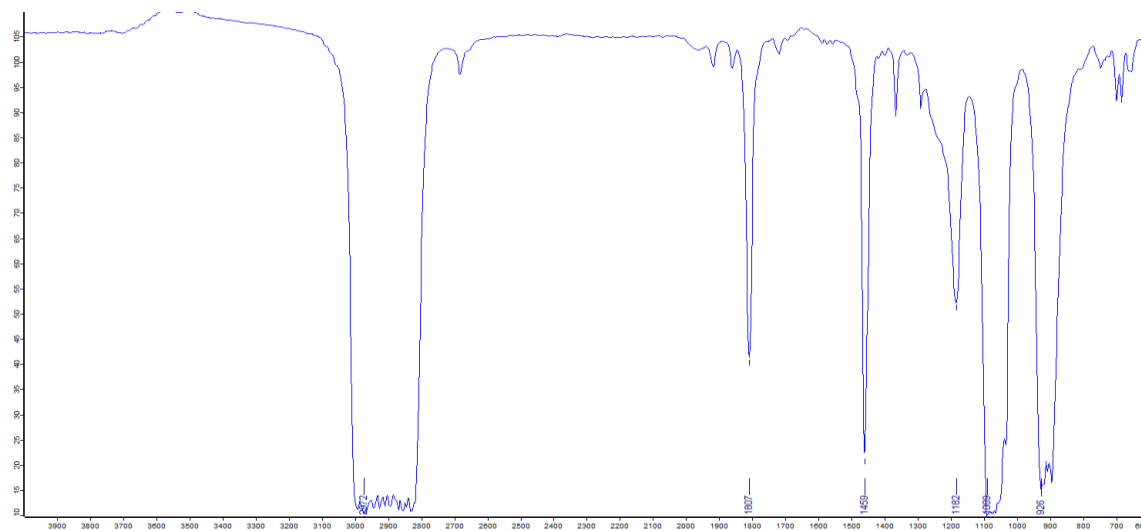
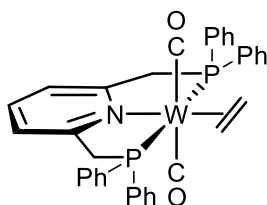


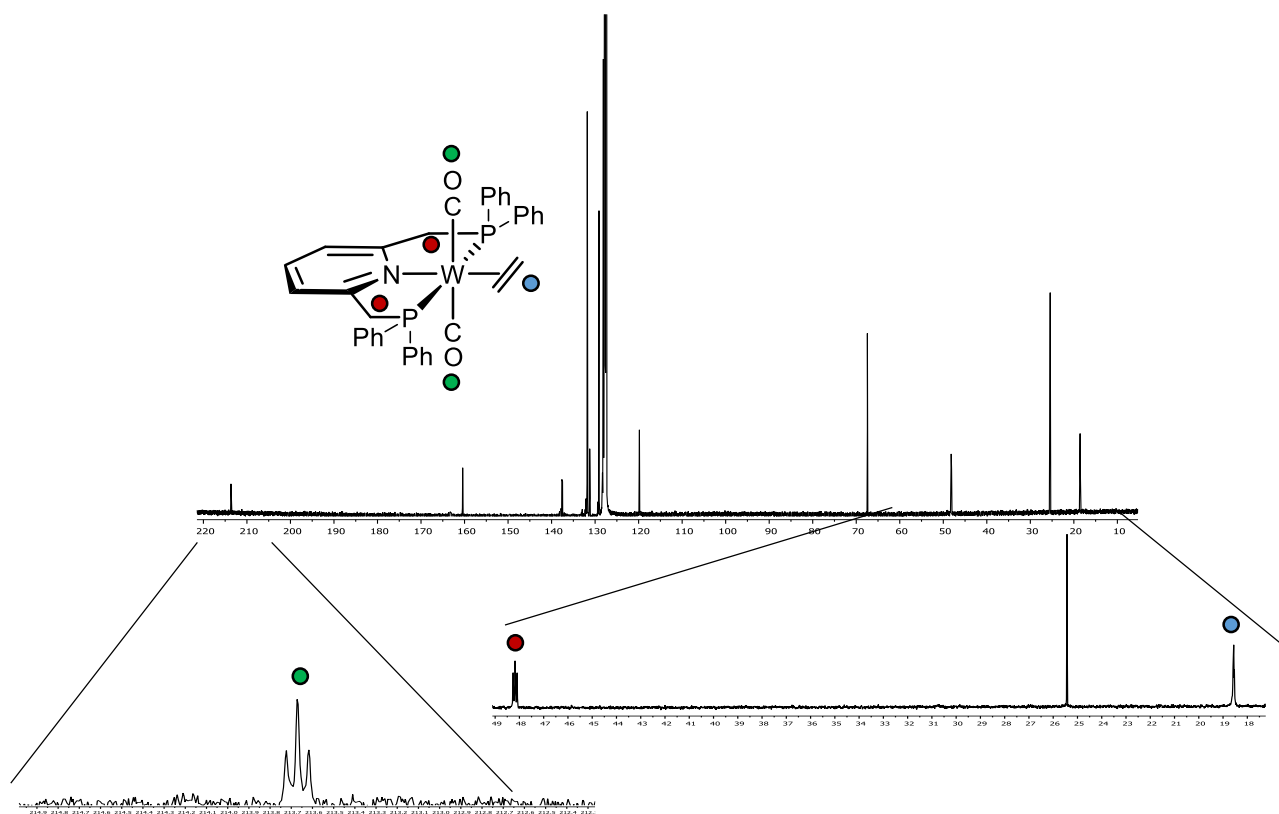
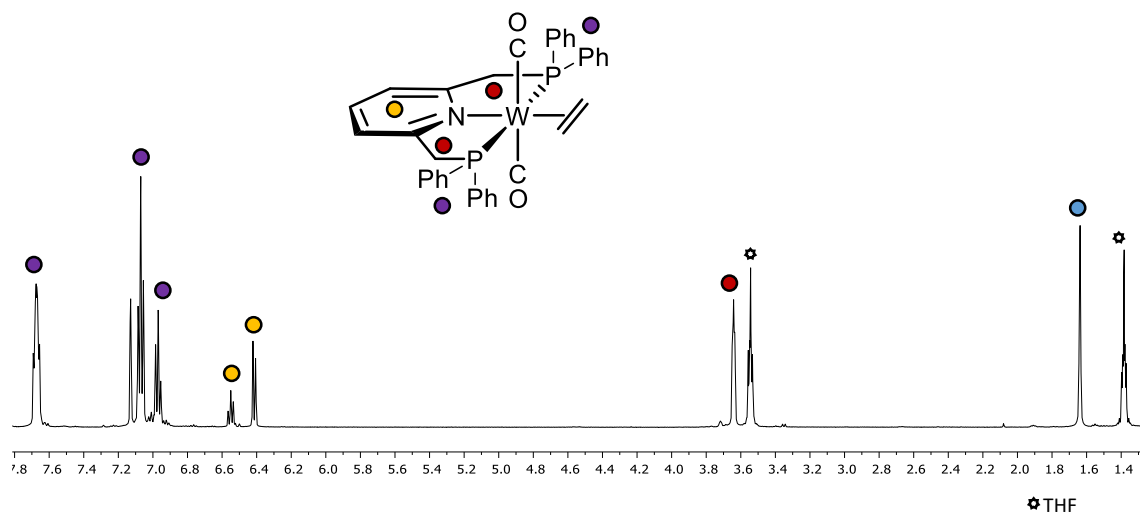
Figure S12: IR spectrum complex **2a** (nujol mull).

Complex 2b. *trans*-W(CO)₂(C₂H₄)(PNP)



Following the previous procedure for **2a**, complex **1b** (0.15 g, 0.212 mmol) was converted into **2b** in 75% yield.

Anal. Calcd for C₃₅H₂₁WO₂NP₂ (**2b**) C, 56.5; H, 4.2; N, 1.9. Found: C, 56.6; H, 4.4; N, 1.9. IR(nujol mull): $\nu(\text{CO})$, 1781 cm⁻¹. ¹H NMR (400 MHz, C₆D₆): δ 1.64 (br, 4H, CH_{2ethylene}), 3.64 (t, 4H, ²J_{H-P} = 3.6 Hz, CH_{2-P}), 6.41 (d, 2H, ³J = 7.6 Hz, CH_{pyr}), 6.55 (t, 1H, ³J = 7.6 Hz, CH_{pyr}), 6.97 (t, 4H, CH_{Ph}), 7.07 (t, 8H, ³J = 7 Hz, CH_{Ph}), 7.67 (m, 8H, CH_{Ph}). ³¹P{¹H} NMR (161.9 MHz, C₆D₆): δ 45.4 ppm (s; J_{P-W} = 141 Hz, W-satellites). ¹³C{¹H} NMR (100 MHz, C₆D₆): δ 18.6 (t, ²J_{C-P} = 5 Hz, CH_{2ethylene}), 48.2 (t, J_{C-P} = 10 Hz, CH_{2-P}), 119.8 (t, ³J_{C-P} = 5 Hz, CH_{pyr}), 128.1 (t, ³J_{C-P} = 5 Hz, CH_{Ph}), 129.1 (s, CH_{Ph}), 131.2 (s, CH_{pyr}), 131.8 (t, ²J_{C-P} = 6 Hz, CH_{Ph}), 137.6 (t, ²J_{C-P} = 19 Hz, C_{qPh}), 160.4 (t, ²J_{C-P} = 6 Hz, C_{qpyr}), 213.7 (t, ²J_{C-P} = 7 Hz, CO).



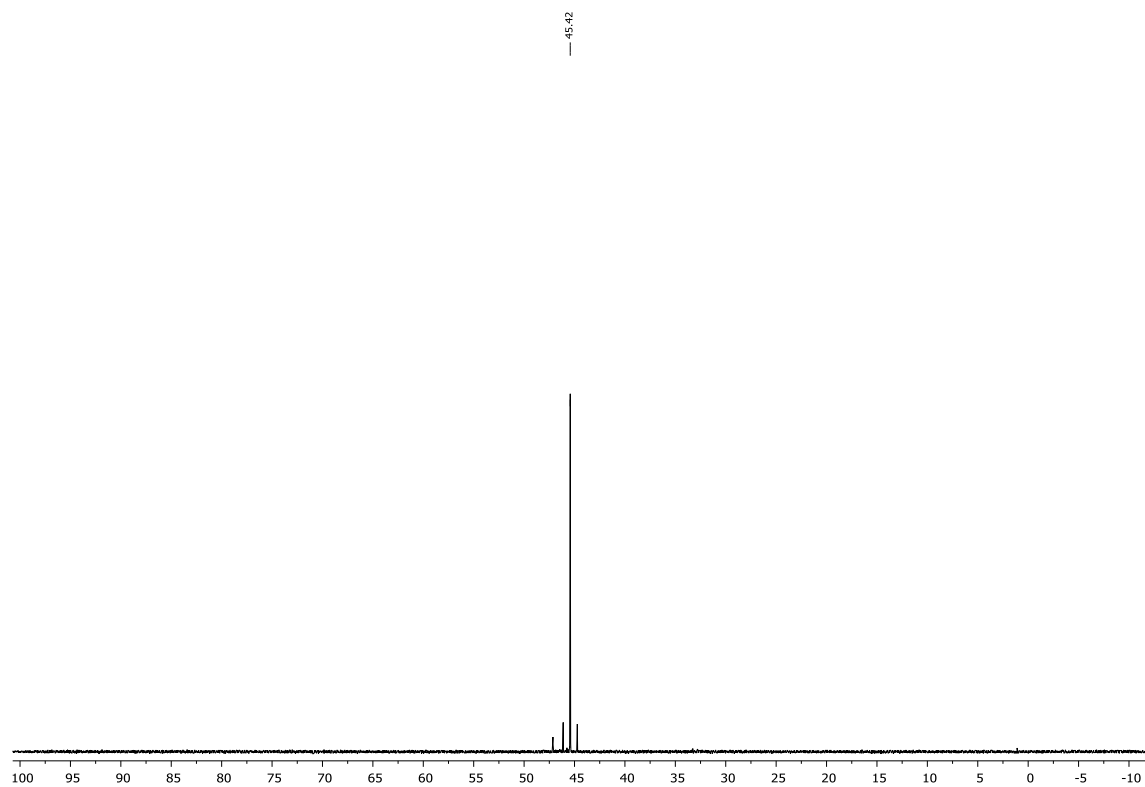


Figure S15: $^1\text{P}\{^1\text{H}\}$ NMR (161.9 MHz, C_6D_6) of complex **2b**.

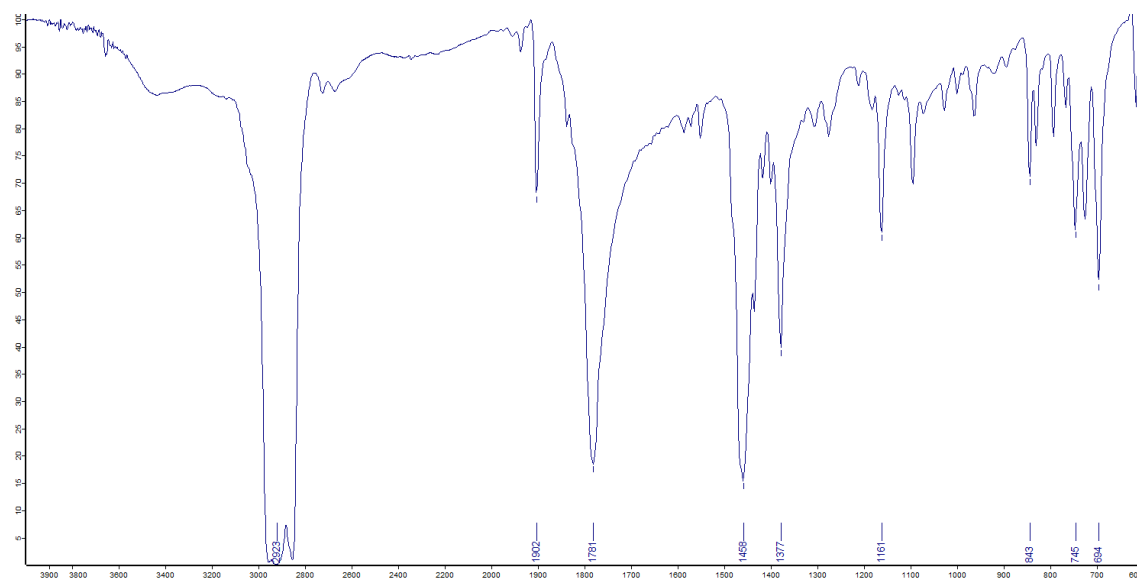
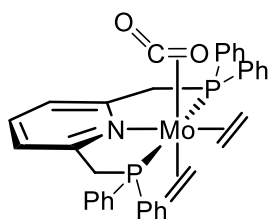


Figure S16: IR spectrum complex **2b** (nujol mull).

Complex 3a. *cis*-Mo(CO₂)(C₂H₄)₂(PNP)



Complex **1a** (0.5 g, 0.813 mmol) was placed in a Schlenk tube under a carbon dioxide atmosphere, and toluene (40 mL) was added. After 15 min of stirring, a brown solid precipitated out, being filtered off. The resulting solution was left at room temperature overnight, affording brown crystals, that were separated by filtration. Concentration and cooling of the filtrate led to a second crop of brown crystals. Yield: 68 % yield. The initially separated brown solid showed identical spectroscopic properties than the crystalline materials.

Anal. Calcd. for C₃₆H₃₆MoO₂NP₂ (**3a**): C, 64.3; H, 5.4; N, 2.1. Found: C, 63.5; H, 5.7; N, 1.8. IR (nujol mull): $\nu(\text{CO}_2)$, 1701 cm⁻¹. ¹H NMR (500 MHz, THF-d₈): δ -0.01 (br, 2H, CH_{2ethylene}), 0.07 (br, 2H, CH_{2ethylene}), 0.68 (d, 2H, ³J_{H-P} = 10 Hz, CH_{2ethylene}), 1.98 (d, 2H, ³J_{H-P} = 10 Hz, CH_{2ethylene}), 4.65 (dd, 4H, ²J_{H-P} = 18 Hz, CH_{2-P}), 7.21-7.71 (m, 23H, CH_{aromatic}). ³¹P{¹H} NMR (202.4 MHz, THF-d₈): δ 46.9 ppm. ¹³C{¹H} NMR (100 MHz, THF-d₈): δ 42.8 (t, J_{C-P} = 11 Hz, CH_{2-P}), 43.8 (s, CH_{2ethylene}), 50.6 (t, ²J_{C-P} = 4 Hz, CH_{2ethylene}), 121.3 (t, ³J_{C-P} = 5 Hz, CH_{pyr}), 127.4 (t, ³J_{C-P} = 4 Hz, CH_{Ph}), 127.6 (t, ³J_{C-P} = 4 Hz, CH_{Ph}), 128.6 (s, CH_{Ph}), 131.3 (t, ²J_{C-P} = 4 Hz, CH_{Ph}), 133.6 (t, ²J_{C-P} = 4 Hz, CH_{Ph}), 135.9 (s, CH_{pyr}), 138.4 (t, ²J_{C-P} = 13 Hz, C_{qPh}), 139.6 (t, ²J_{C-P} = 21 Hz, C_{qPh}), 160.0 (t, ²J_{C-P} = 6 Hz, C_{qpyr}), 200.8 (t, ²J_{C-P} = 14 Hz, CO₂).

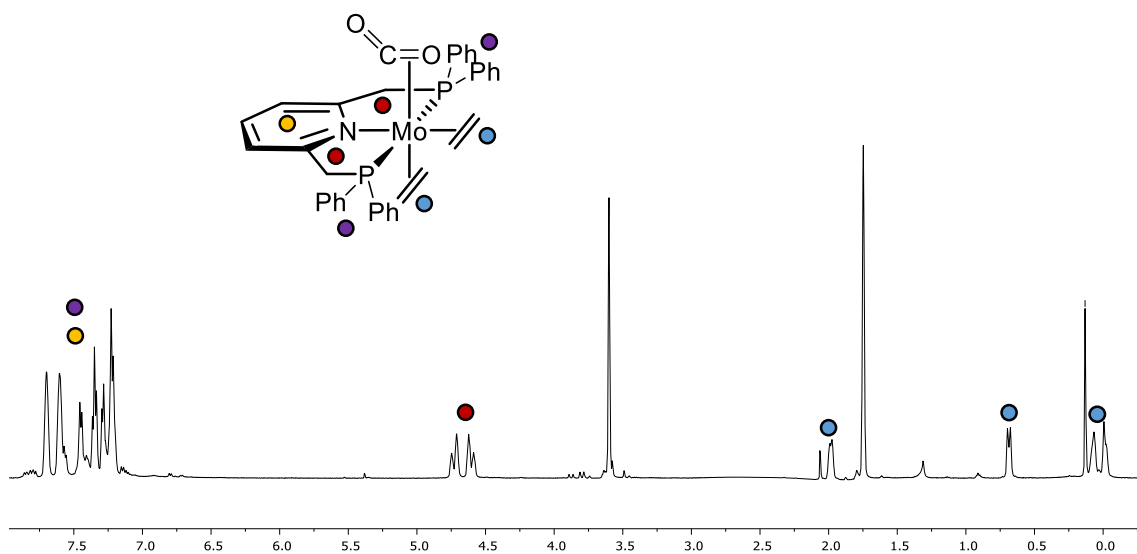


Figure S17: ¹H NMR (500 MHz, THF-d₈) of complex **3b**.

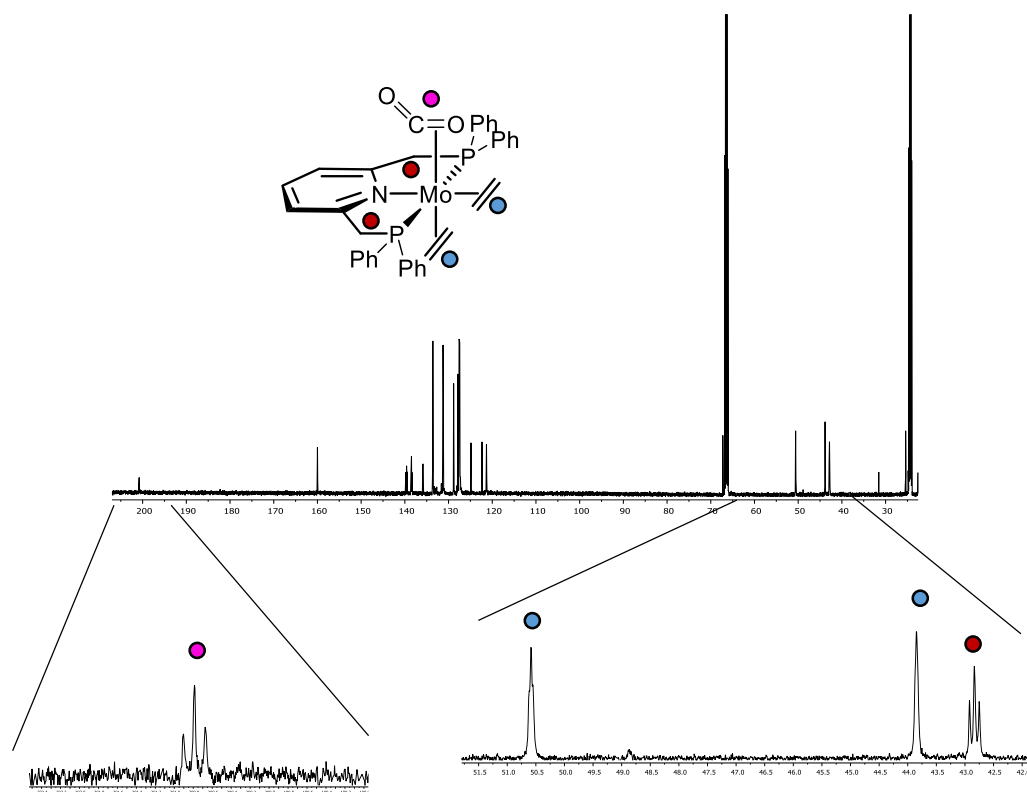


Figure S18: $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, THF-d_8) of complex **3a**.

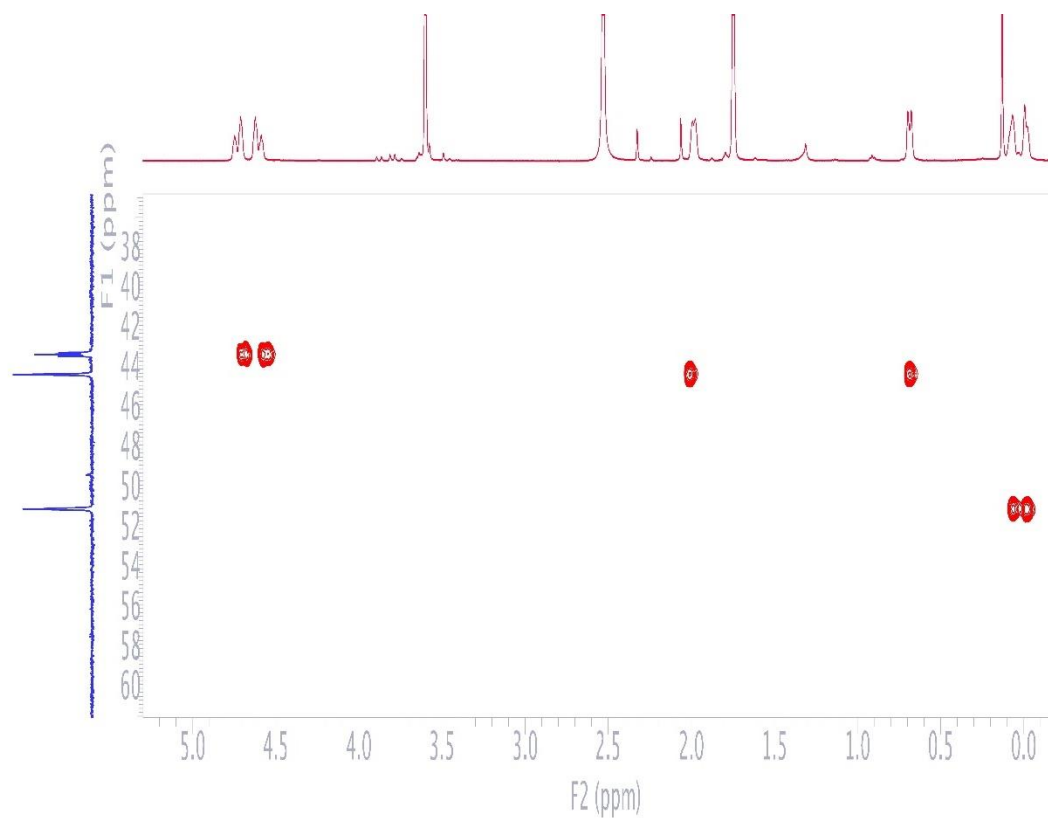


Figure S19: HMQC (methylene region) of complex **3a**(THF-d_8).

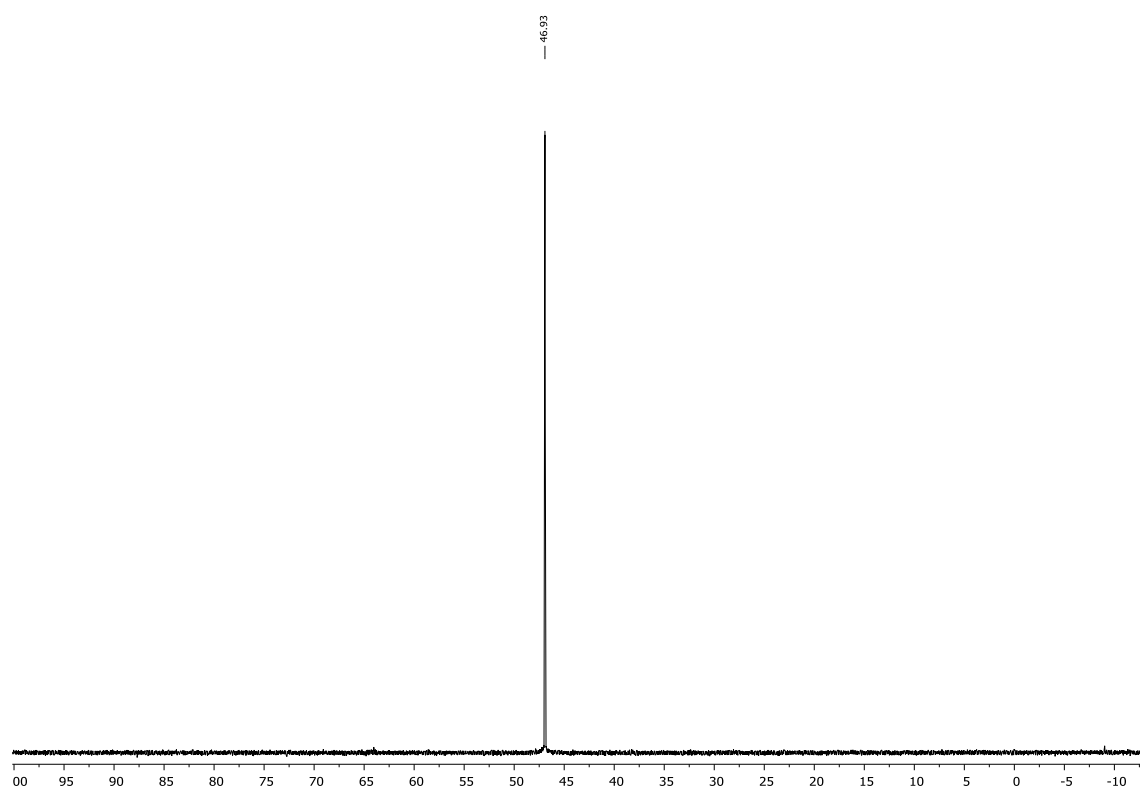


Figure S20: $^{31}\text{P}\{^1\text{H}\}$ NMR (202.4 MHz, THF-d_8) of complex **3a**.

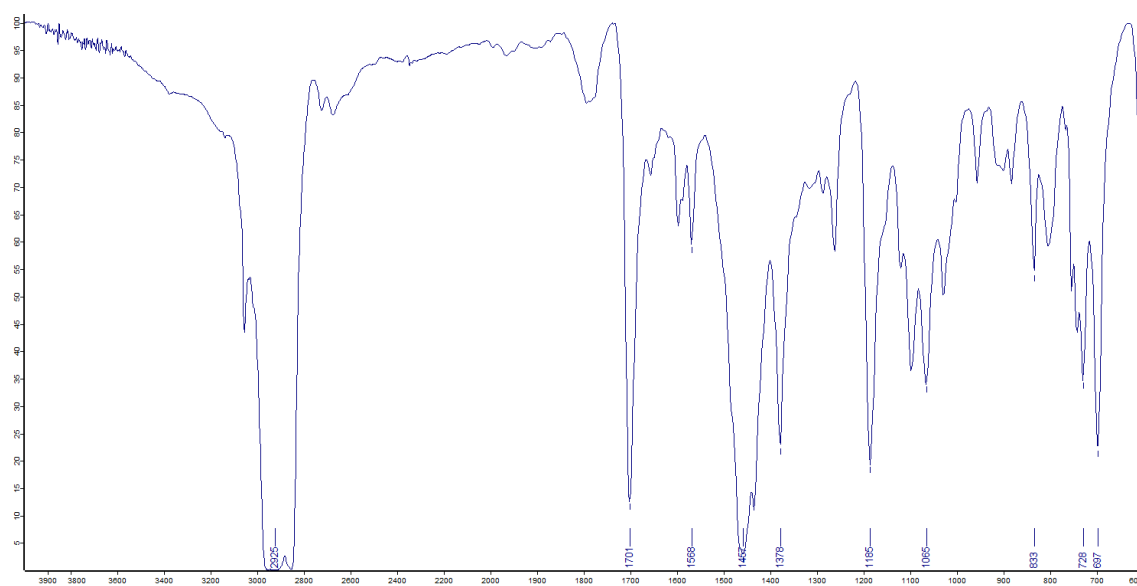
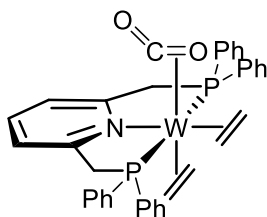


Figure S21: IR spectrum of complex **3a**.

Complex 3b. *cis*-W(CO₂)(C₂H₄)₂(PNP)



Complex **1b** (0.5 g, 0.672 mmol) was placed in a Schlenk tube under an atmosphere carbon dioxide, toluene was then added (20 mL) and the red solution was heated at 80 °C for 4h. The reaction was cooled down, and the yellow-brown crystals of complex **3b** were filtered off. The filtrate was concentrated under reduced pressure and cooled at -30 °C to give a second crop of yellow-brown crystals. Yield: 48 % (combined crops).

Anal. Calcd. for C₃₆H₃₆WO₂NP₂ (**3b**): C, 56.9; H, 4.8; N, 1.8. Found: C, 56.0; H, 4.4; N, 1.8. IR(nujol mull): $\nu(\text{CO}_2)$, 1789 cm⁻¹. ¹H NMR (500 MHz, THF-d₈): δ -0.53 (br s, 2H, CH_{2ethylene}), -0.01 (br, 2H, CH_{2ethylene}), 0.15 (d, 2H, ³J_{H-P} = 8 Hz, CH_{2ethylene}), 1.8 (br, 2H, CH_{2ethylene}), 4.01 (dd, 4H, ²J_{H-P} = 18 Hz, CH_{2-P}), 7.16-7.31 (m, 23H, CH_{aromatic}). ³¹P{¹H} NMR (202.4 MHz, THF-d₈): δ 46.9 ppm (s; J_{P-W} = 107 Hz, W-satellites). ¹³C{¹H} NMR (100 MHz, THF-d₈): δ 37.8 (t, J_{C-P} = 11 Hz, CH_{2-P}), 44.0 (s, CH_{2ethylene}), 45.4 (t, ²J_{C-P} = 4 Hz, CH_{2ethylene}), 121.7 (t, ³J_{C-P} = 5 Hz, CH_{pyr}), 127.6 (t, ³J_{C-P} = 4 Hz, CH_{Ph}), 127.9 (t, ³J_{C-P} = 4 Hz, CH_{Ph}), 129.3 (s, CH_{Ph}), 131.9 (t, ²J_{C-P} = 4 Hz, CH_{Ph}), 134.0 (t, ²J_{C-P} = 4 Hz, CH_{Ph}), 136.4 (s, CH_{pyr}), 138.0 (t, ²J_{C-P} = 15 Hz, C_{qPh}), 139.3 (t, ²J_{C-P} = 25 Hz, C_{qPh}), 161.6 (t, ²J_{C-P} = 5 Hz, C_{qpyr}), 210.2 (t, ²J_{C-P} = 13 Hz, CO₂).

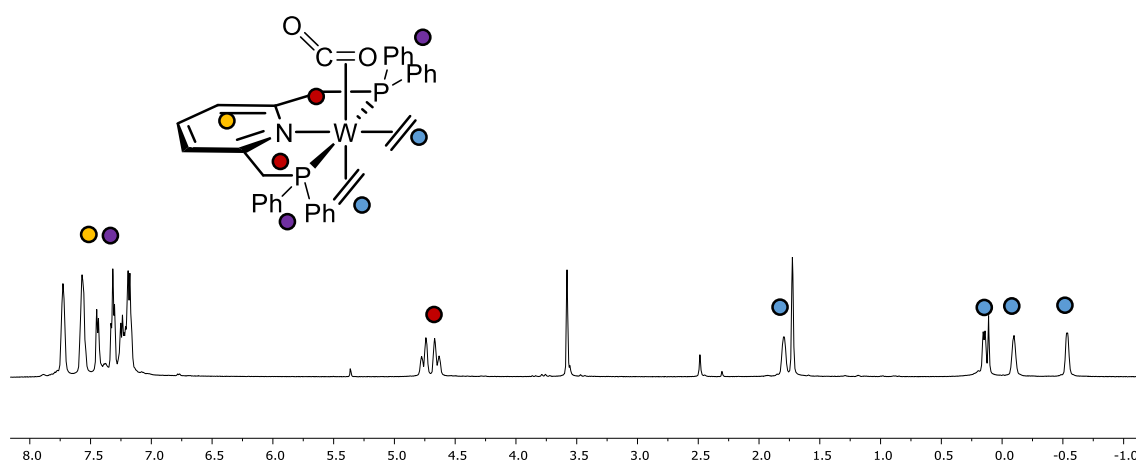


Figure S22: ¹H NMR (500 MHz, THF-d₈) of complex **3b**.

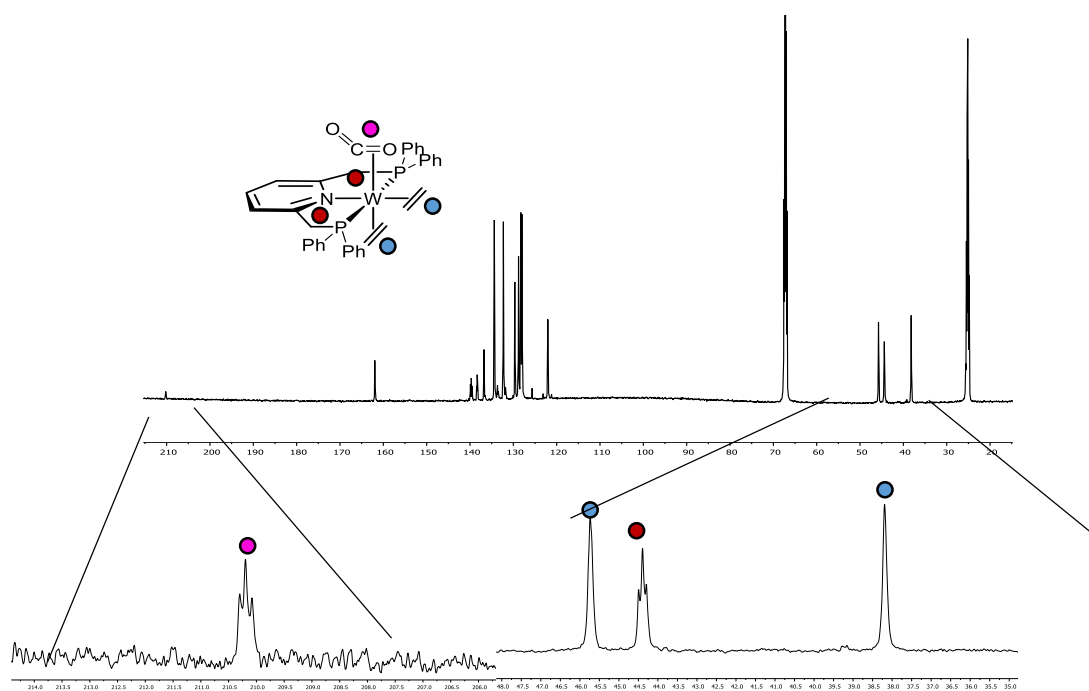


Figure S23: $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, THF-d_8) of complex **3b**.

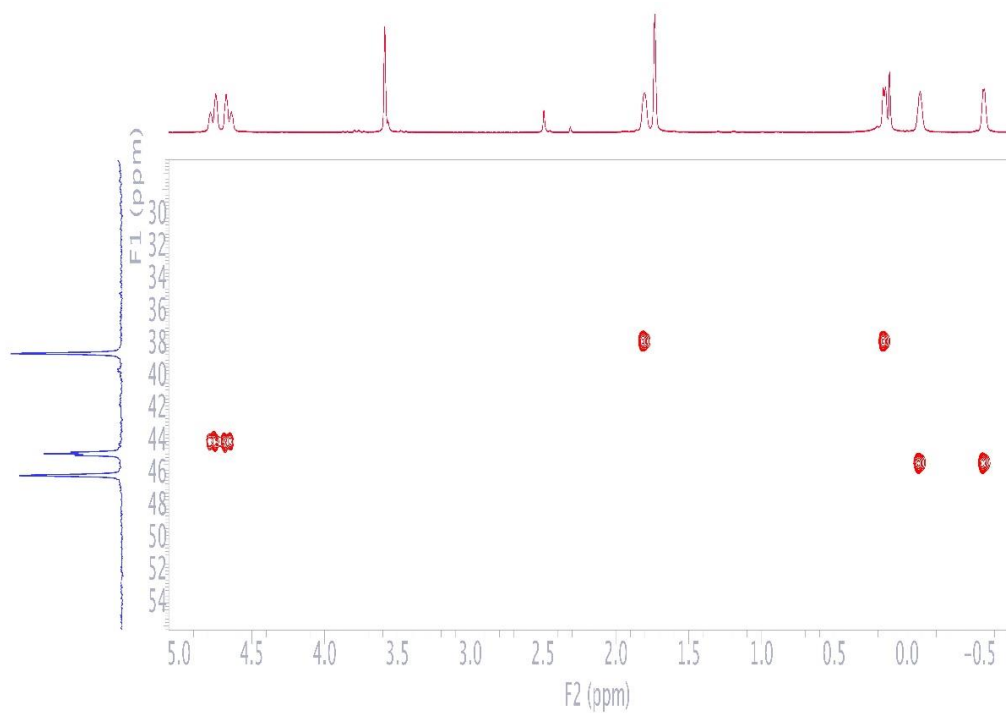


Figure S24: HMQC (methylene region) of complex **3b**(THF-d_8).

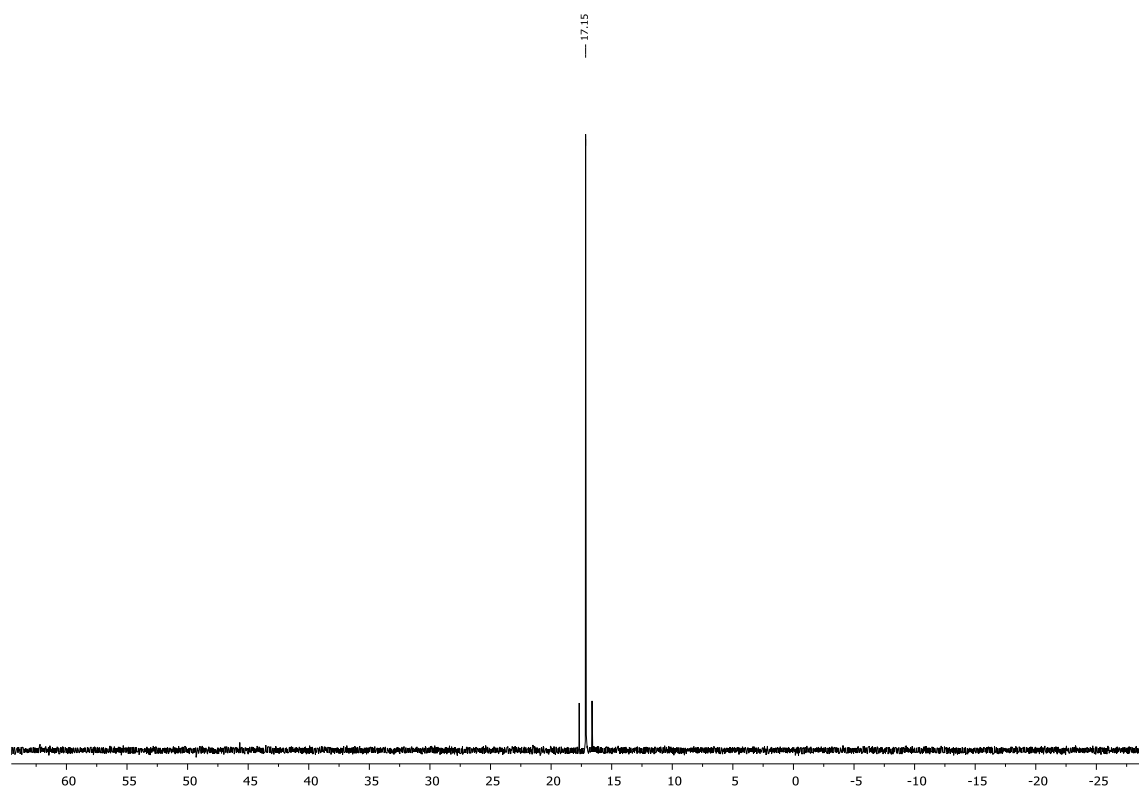


Figure S25: $^{31}\text{P}\{^1\text{H}\}$ NMR (202.4 MHz, THF-d_8) of complex **3b**.

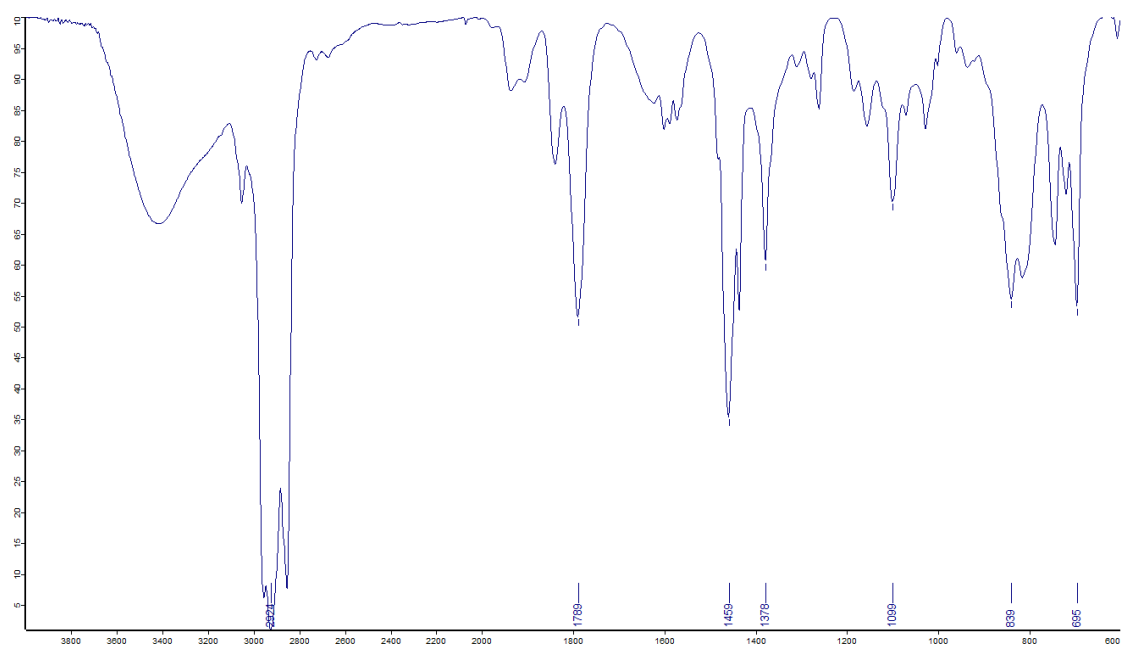


Figure S26: IR spectrum of complex **3b**.

Attempts to induce the ethylene-carbon dioxide coupling.

At the NMR scale, in a pressure NMR tube, and using $^{13}\text{CO}_2$ labelled samples of **3a** and **3b**, the following experiments were carried out, in all cases observing no reaction and gradual decomposition, as inferred for the appearance of the signal of free PNP. The experiments were recorded under Ar, under ethylene, under carbon dioxide, or mixtures of ethylene/carbon dioxide.

- Heating within the range 100-140 °C.
- Addition of bases (KOH, alkaline phenolates).
- Addition of Lewis acid (AlCl_3).

Solid state reactivity

Complexes **1a** y **1b** in a pressure NMR were subjected to a pressure of 4 atm for 24 h at room temperature for 1a and 80 °C for 1b. $^{31}\text{P}\{^1\text{H}\}$ NMR studies (in C_6D_6) showed complete conversion into **3a** in the first case. For **1b**, the $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum is shown below, only 10% of 3b was observed.

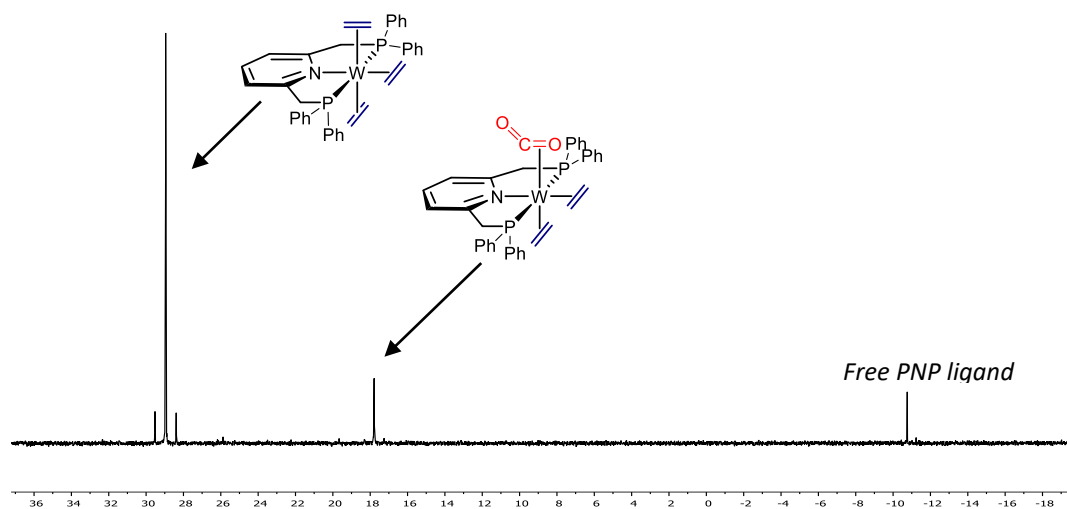


Figure S27: $^{31}\text{P}\{^1\text{H}\}$ NMR in C_6D_6 . Reaction **1b** with 4 atm CO_2 for 24 h at 80 °C.

Computational Method

Computational details

The electronic structure and geometries of compounds were computed using density functional theory (DFT). Becke's three parameter functional,⁴ as in B3LYP, with the nonlocal correlation provided by Perdew's 86 expression⁵ (B3P86) was used. The Mo and W atoms were described with the LANL2DZ basis set,⁶ while the 6-311G* basis set was used for all other atoms. Geometry optimizations were carried out with the actual complexes, without symmetry constraints. The selected combination of method and basis sets provide a good structural description of these complexes because the comparison of the structural parameters of the optimized structures with those experimentally determined by X-ray diffraction methods is good (Table S1). Other functionals were tested (B3LYP and M06), but they afforded poorer description of the structural parameters of complex **1a**. Frequency calculations were carried out at the same level of theory to identify all of the stationary points as transition states (one imaginary frequency) or as minima (zero imaginary frequencies) and to provide the thermal correction to free energies at 298.15 K and 1 atm. Solution-phase SCF energies of intermediates and transition states shown in Schemes S1 and S2 were calculated by a single point calculation on the *in vacuo* optimized structure using the CPCM solvation model.⁷ Gibbs free energies in solution were estimated from the equation $G_{\text{solv}} = E_{\text{solv}} + (G_{\text{gas}} - E_{\text{gas}})$. The energy profiles are presented in terms of relative free energies, derived from thermochemical analysis (Figures S27-S34). The DFT calculations were performed using the Gaussian 09 suite of programs.⁸ Coordinates of all optimized compounds are reported in Table S2.

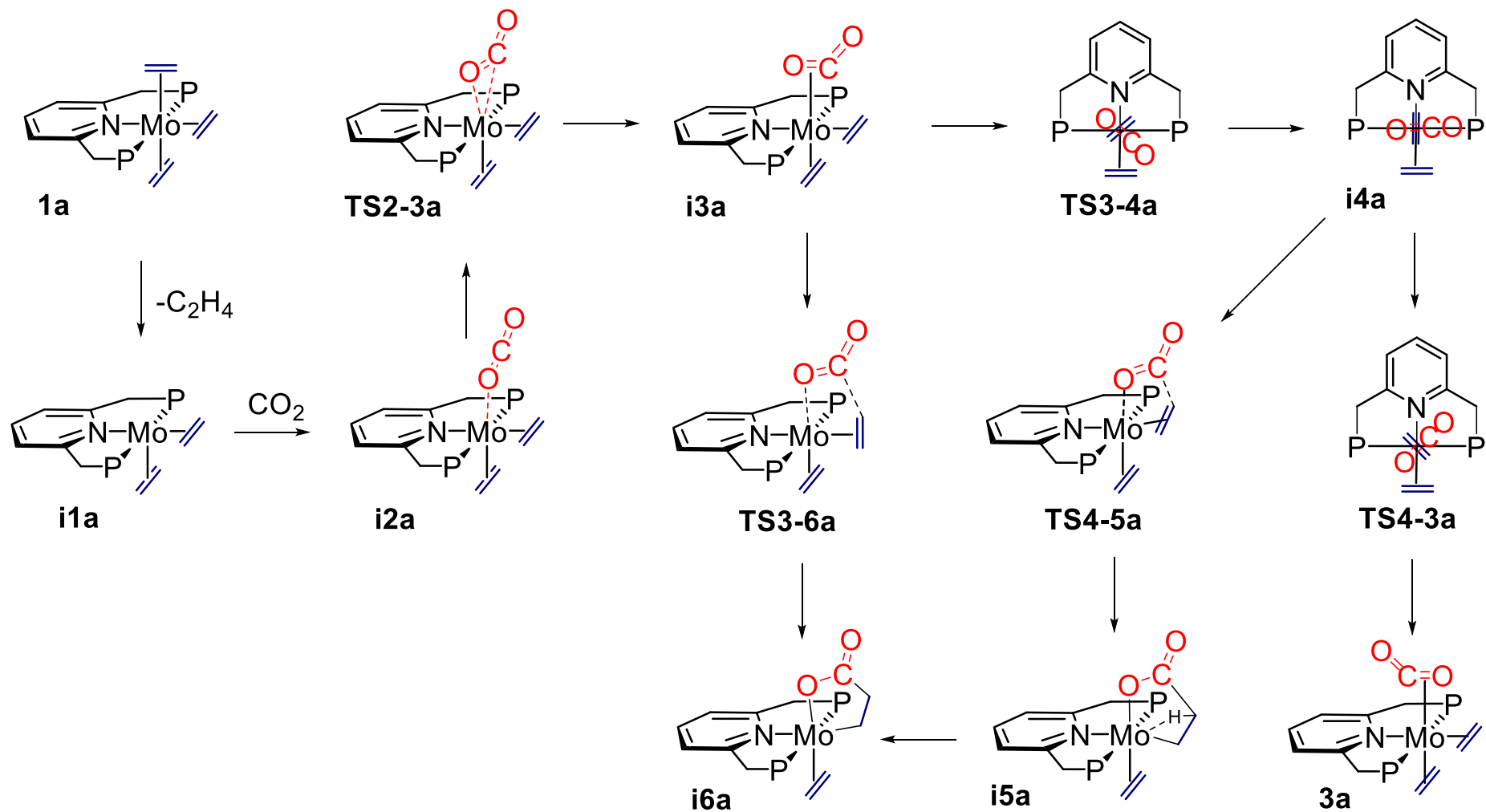
4 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.

5 (a) J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822; (b) J. P. Perdew, *Phys. Rev. B*, 1987, **34**, 7046.

6 (a) T. H. Dunning Jr., P. J. Hay, *Modern Theoretical Chemistry*, Plenum, New York, 1976, p. 1; (b) P. J. Hay, W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299.

7 Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* 2003, **24**, 669-681.

8 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision B.01, Gaussian, Inc., Wallingford CT, **2009**.



Scheme S1. Mechanism of formation of *cis*-Mo(CO)₂(C₂H₄)₂(PNP), **3a**, and lactone complex, **i6a**.

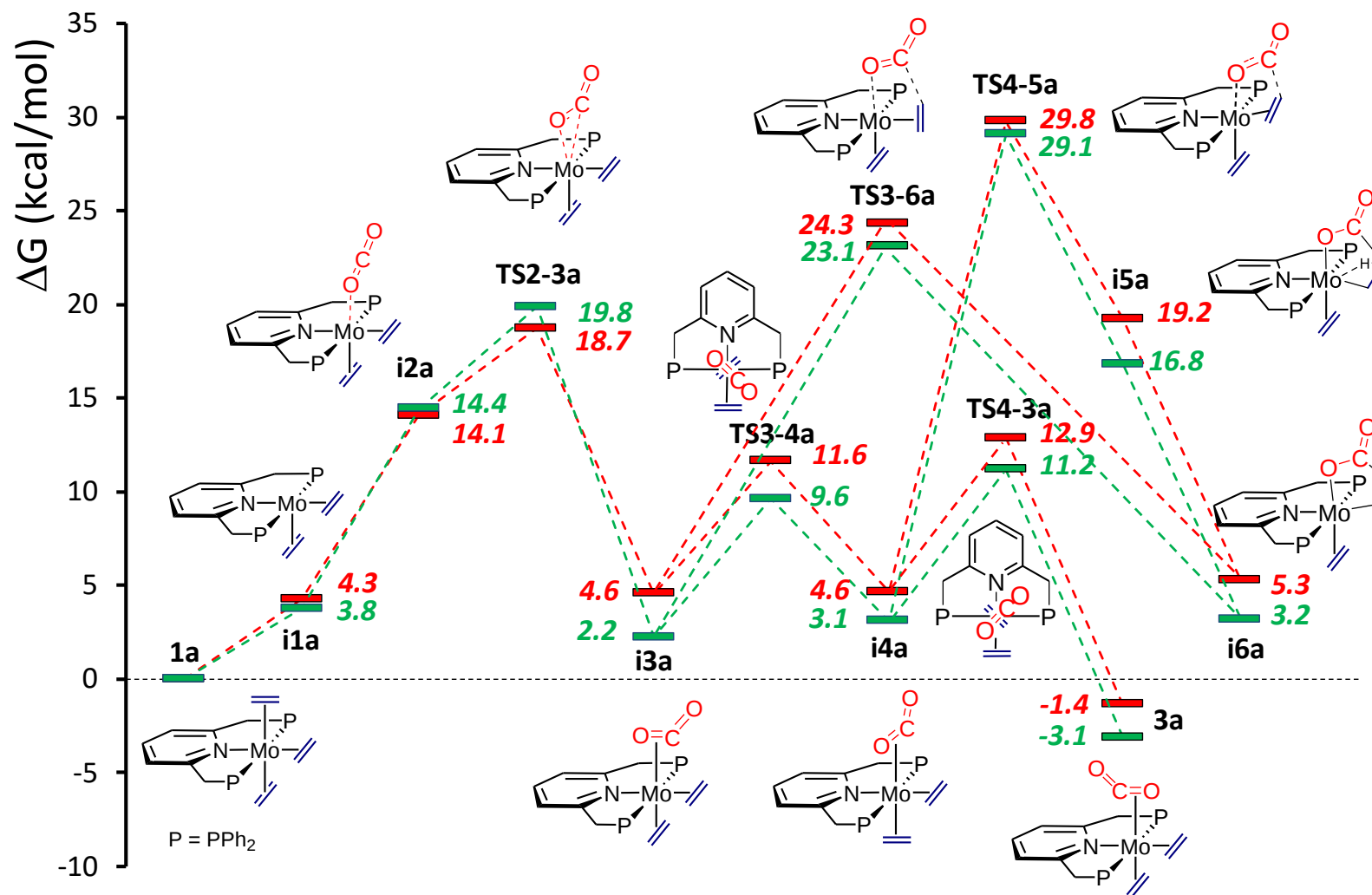
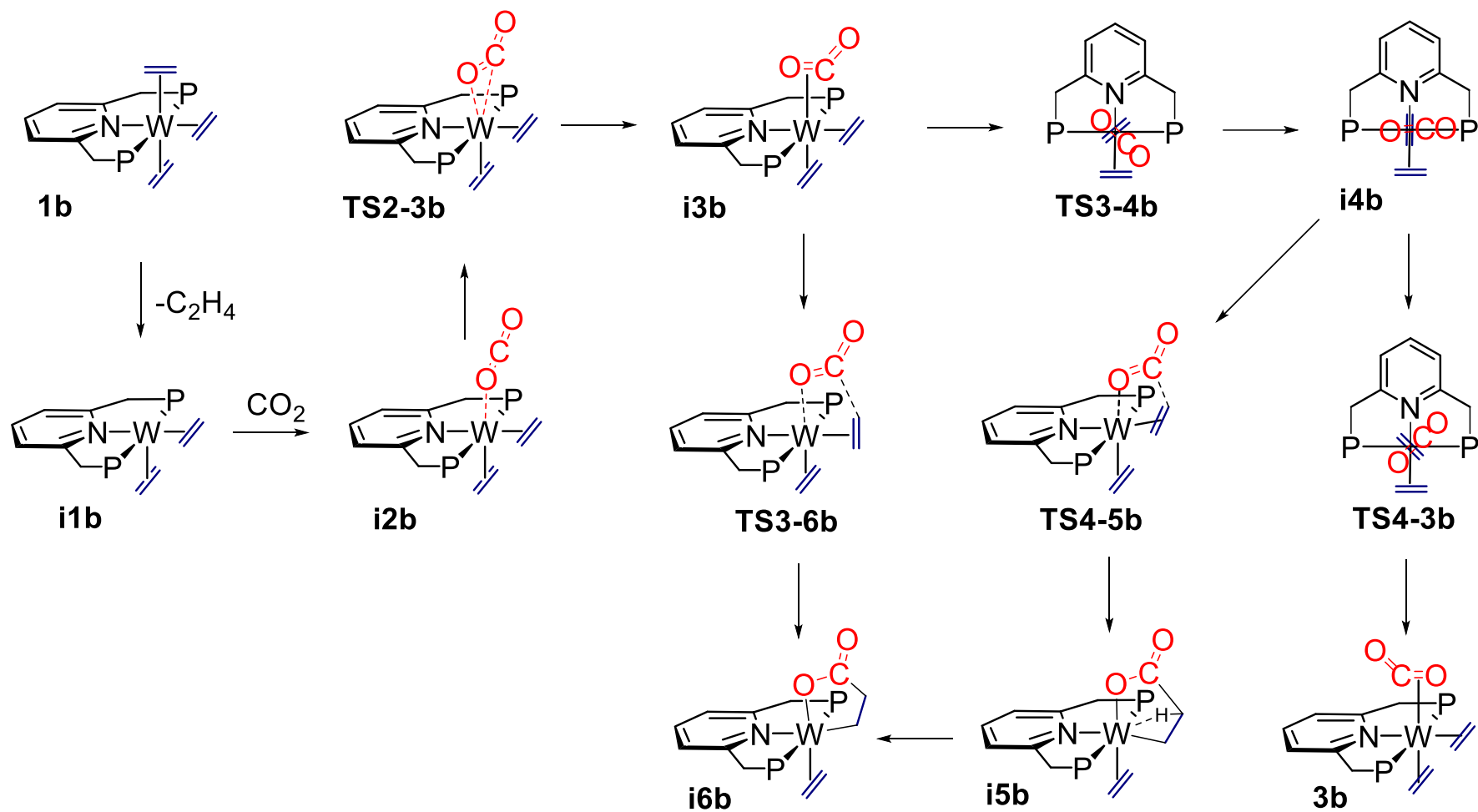


Figure S27. Comparative ΔG profiles for the formation of CO₂-complex **3a** and lactone-complex **i6a** (red, gas-phase; green, toluene).



Scheme S2. Mechanism of formation of *cis*-W(CO₂)(C₂H₄)₂(PNP), **3b**, and lactone complex, **i6b**.

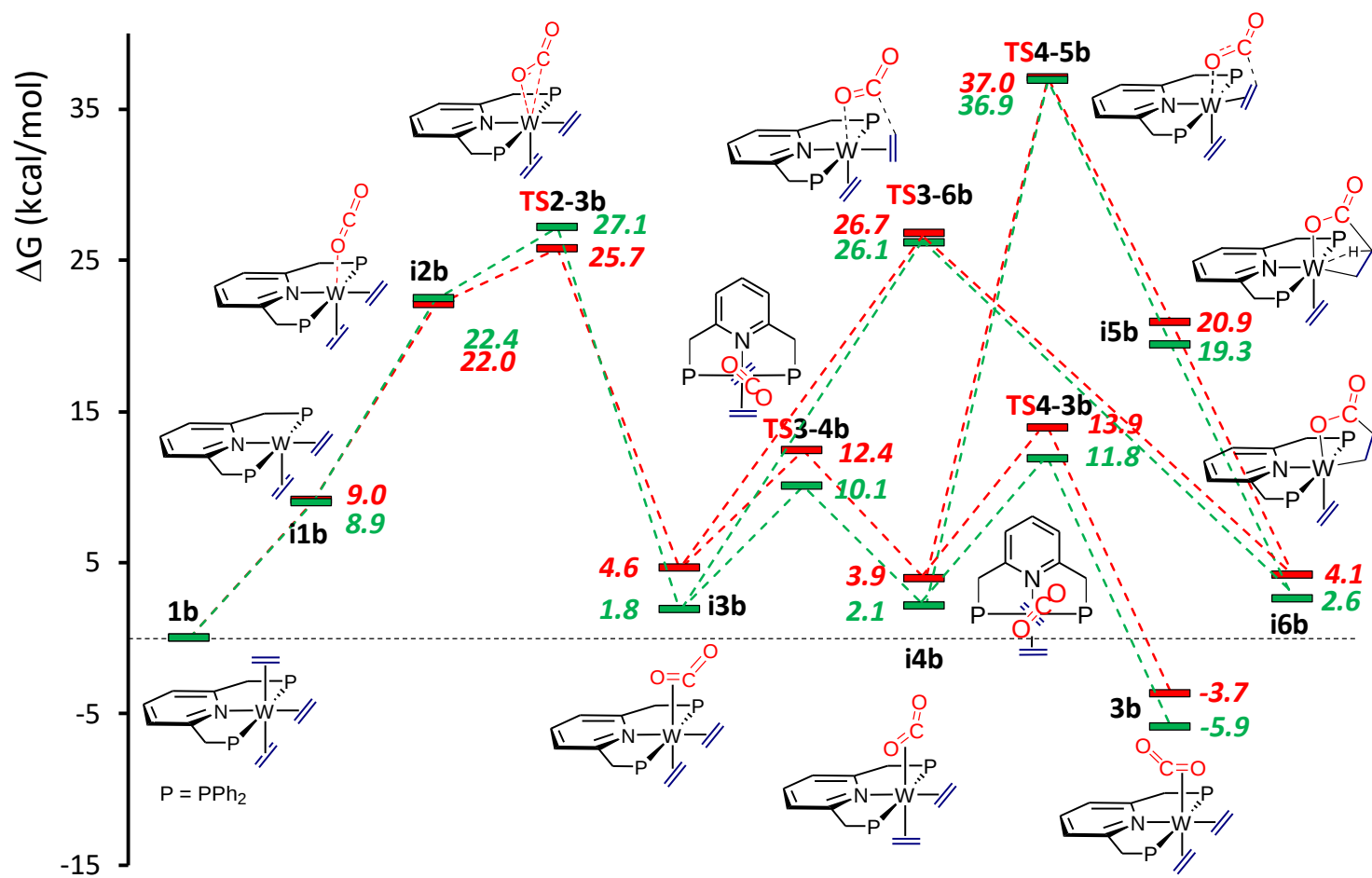


Figure S28. Comparative ΔG profiles for the formation of CO₂-complex **3b** and lactone-complex **i6b** (red, gas-phase; green, toluene).

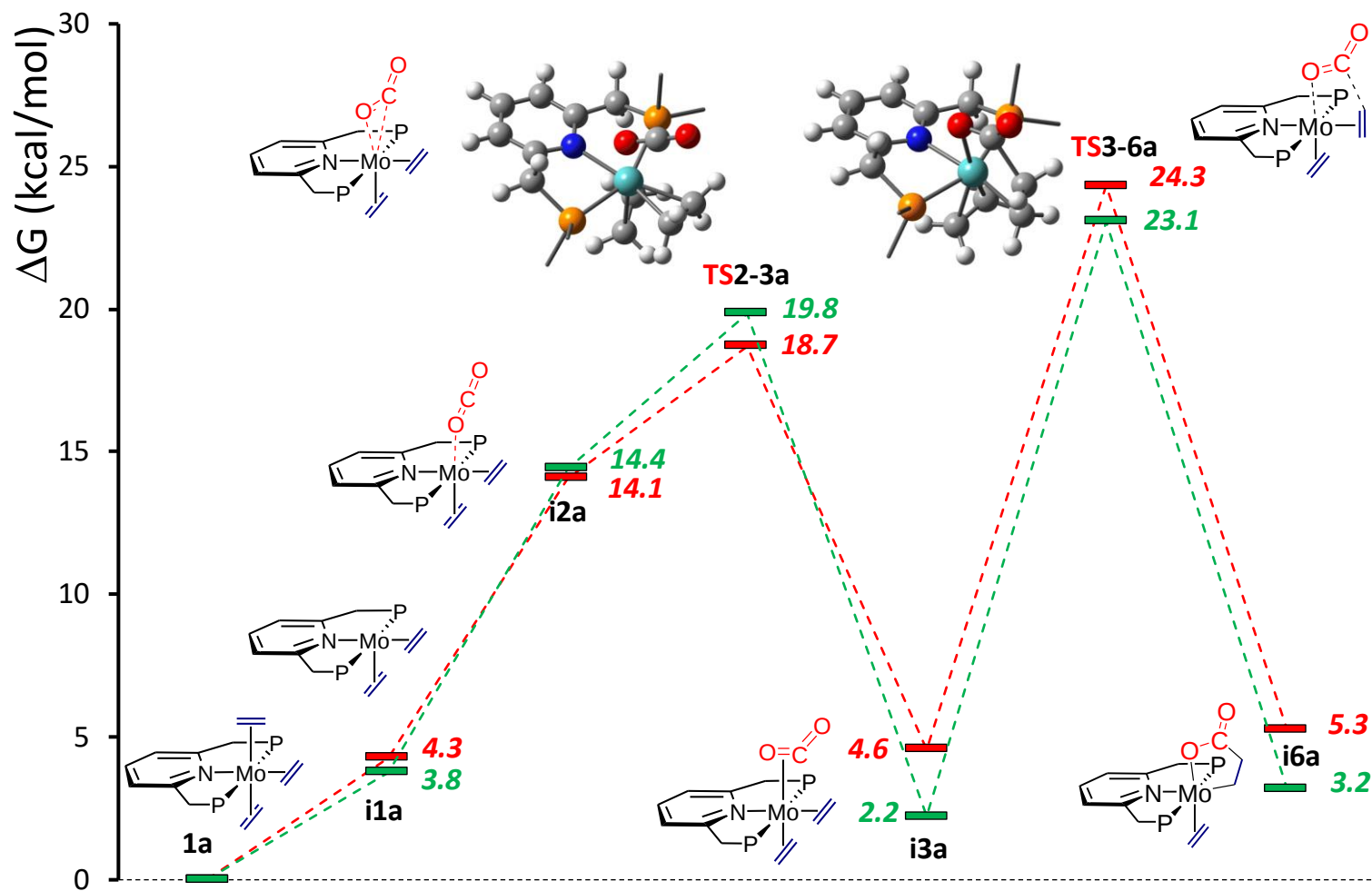


Figure S29. ΔG profile for the formation of lactone-complex **i6a** from **i3a** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

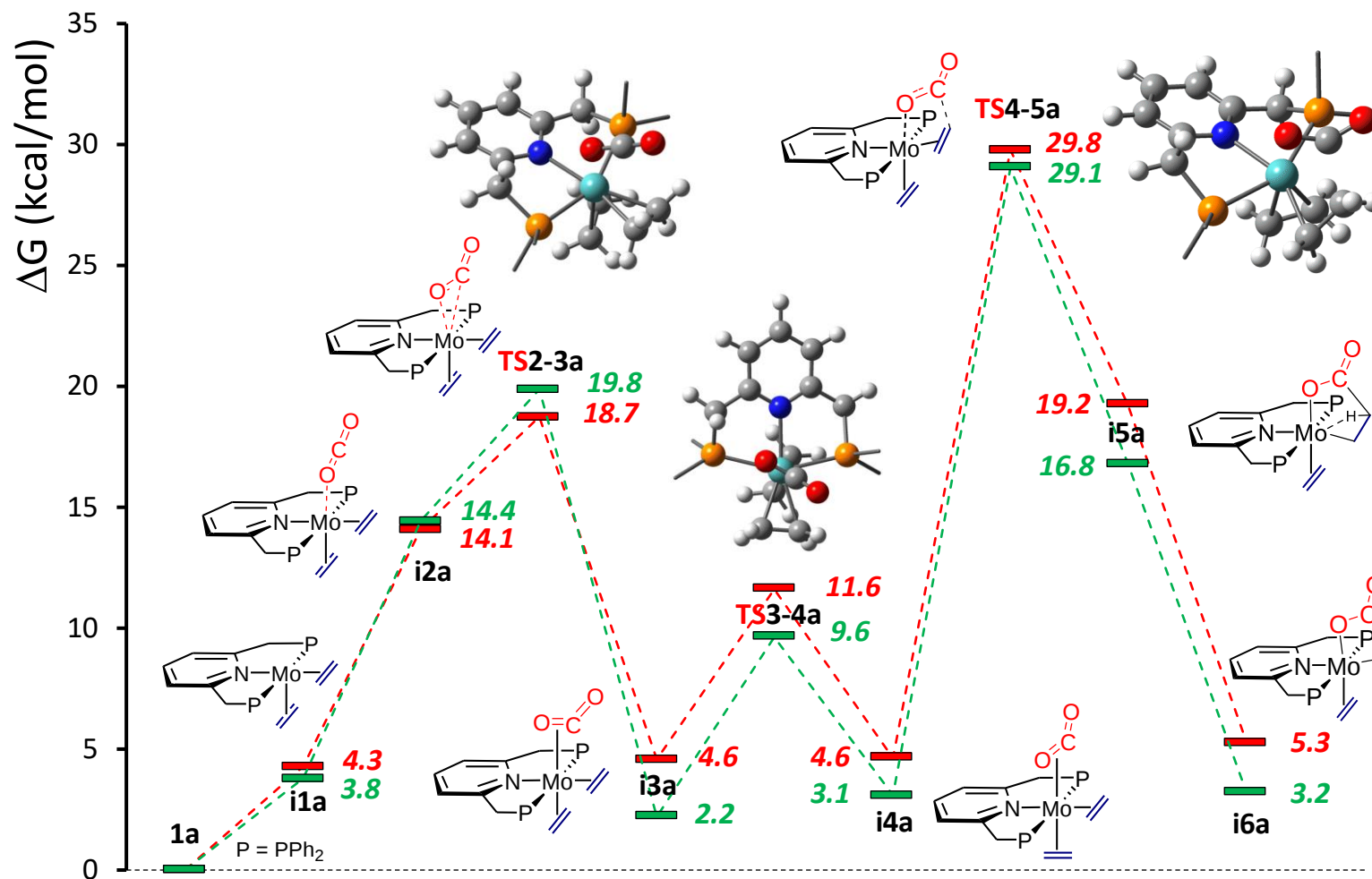


Figure S30. ΔG profile for the formation of lactone-complex **i6a** from **i4a** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

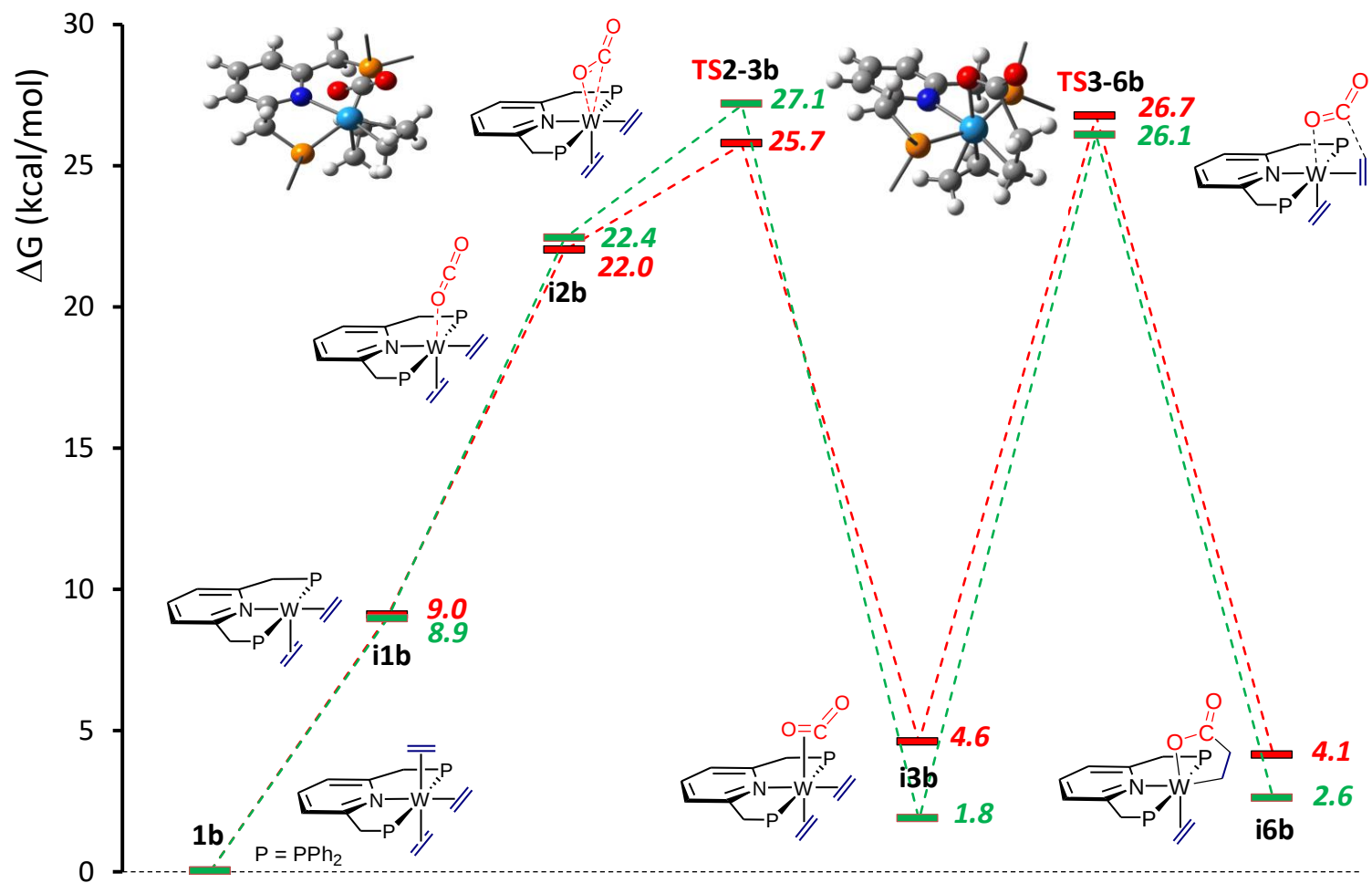


Figure S31. ΔG profile for the formation of lactone-complex **i6b** from **i3b** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

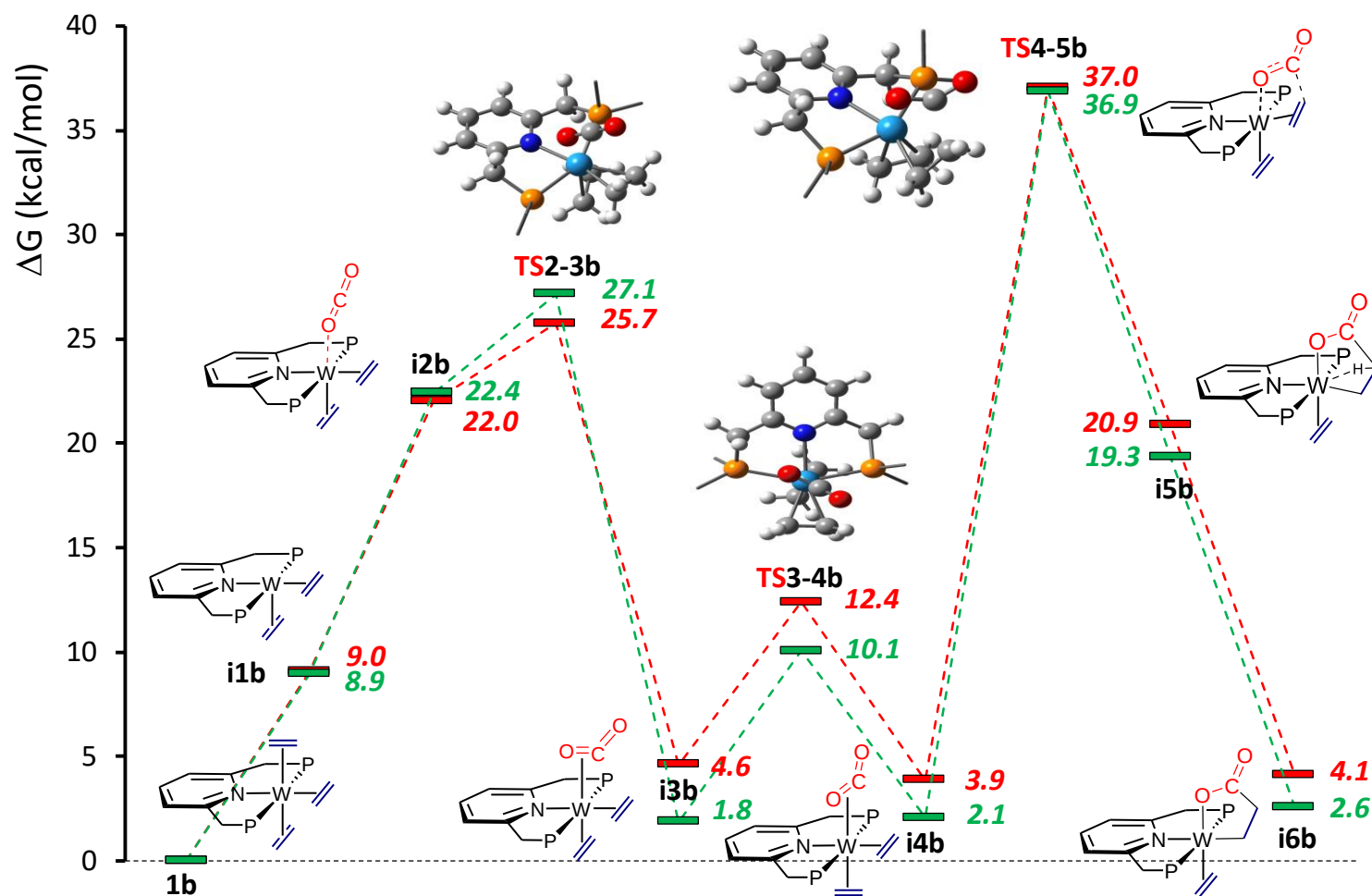


Figure S32. ΔG profile for the formation of lactone-complex **i6b** from **i4b** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

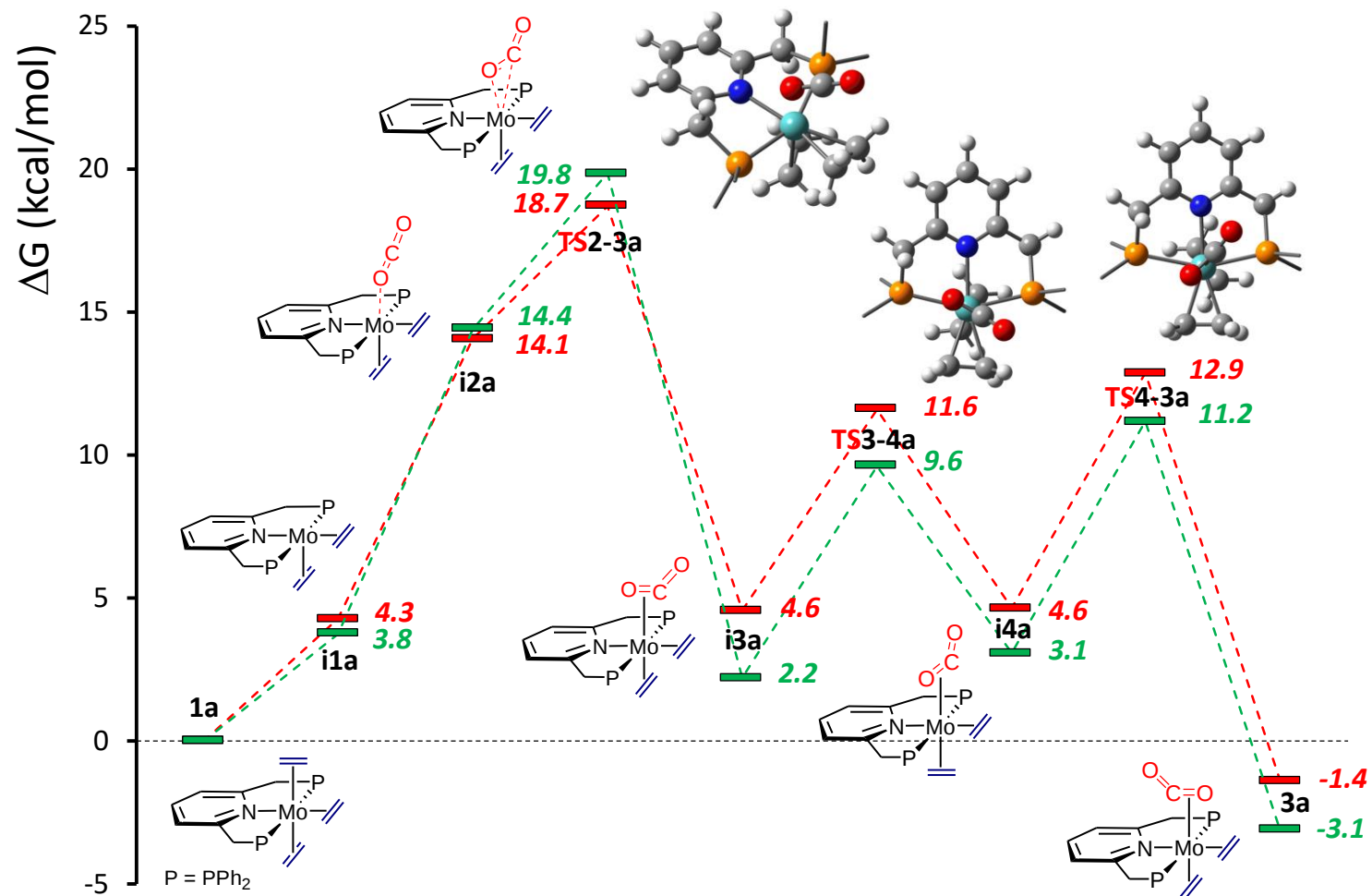


Figure S33. ΔG profile for the formation of CO_2 -complex **3a** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

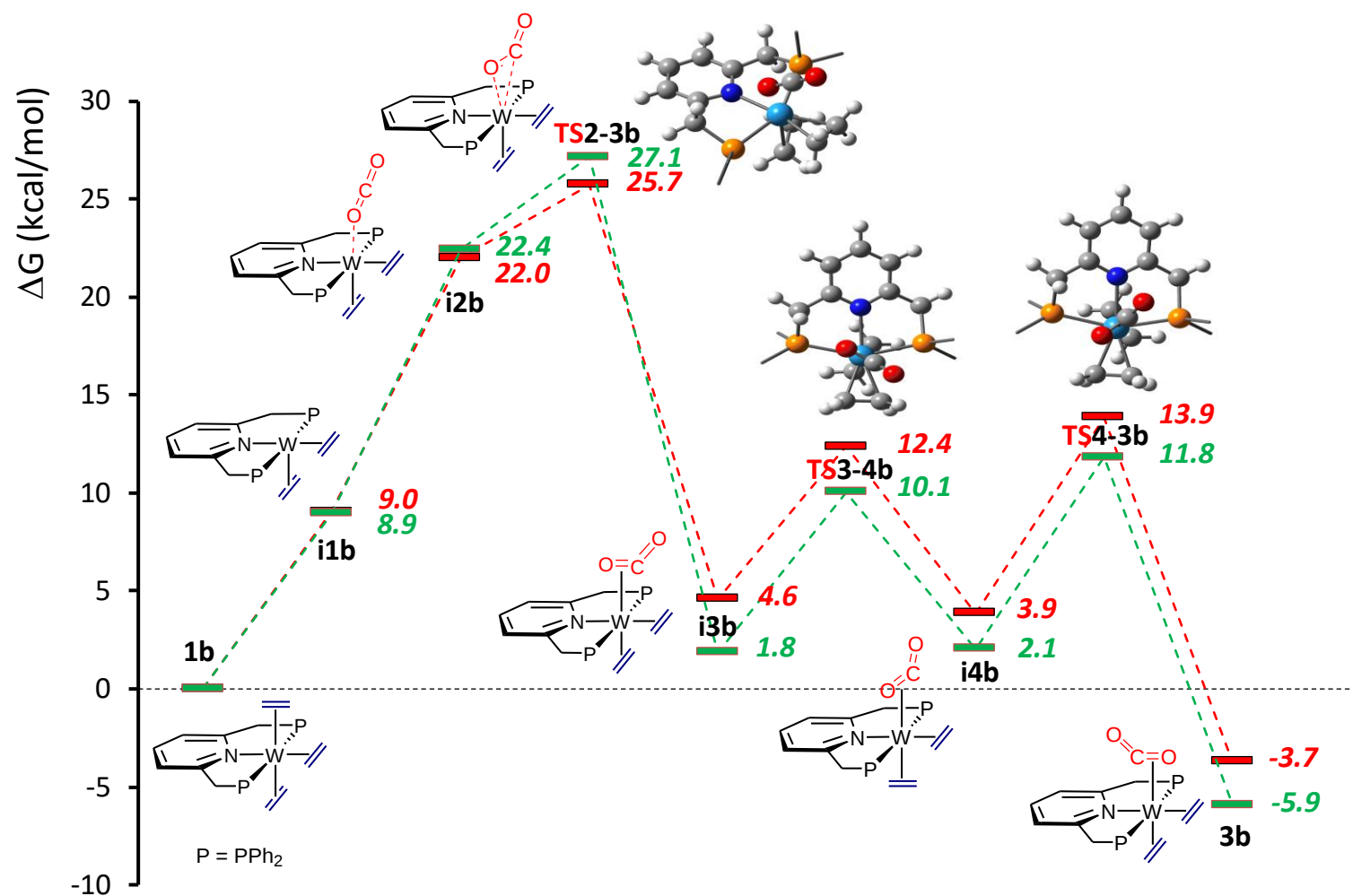
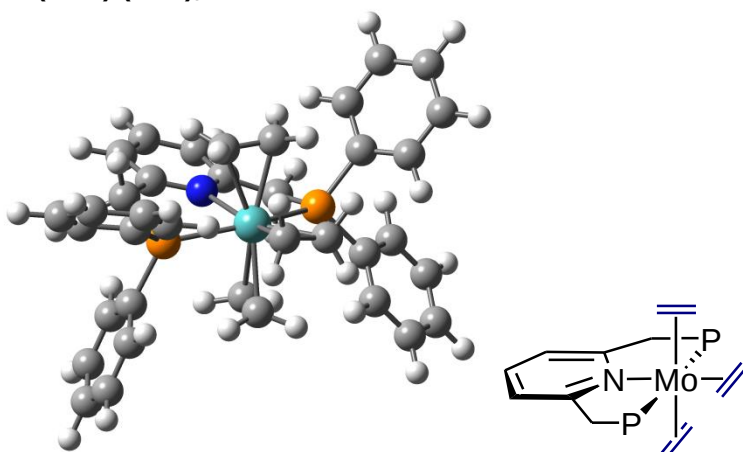


Figure S34. ΔG profile for the formation of CO_2 -complex **3b** (red, gas-phase; green, toluene). Ph substituents have been omitted for clarity in the optimized structures of depicted transition states.

Table S1. Comparison of selected experimental and calculated structural parameters of complexes **1a,b** and **3a,b**.

Structural parameters (Å and °)	Mo(C ₂ H ₄) ₃ (PNP), 1a		Mo(CO ₂)(C ₂ H ₄) ₂ (PNP), 3a		W(C ₂ H ₄) ₃ (PNP), 1b		W(CO ₂)(C ₂ H ₄) ₂ (PNP), 3b	
	Calculated	Experimental	Calculated	Experimental	Calculated	Experimental	Calculated	Experimental
Mo-N	2.303	2.277	2.304	2.290, 2.305	2.287	2.276	2.287	2.275
Mo-P	2.434 2.472	2.423 2.443	2.449, 2.468	2.445, 2.449 2.442, 2.455	2.433 2.467	2.435	2.433 2.467	2.434, 2.445
Mo-C (C ₂ H ₄)	2.295, 2.272 2.295, 2.269 2.284, 2.303	2.272, 2.274 2.262, 2.268 2.261, 2.269	2.258, 2.266 2.256, 2.268	2.257, 2.262 2.252, 2.255 2.245, 2.247 2.255, 2.262	2.279, 2.260 2.242, 2.269 2.271, 2.245	2.258, 2.269 2.246, 2.251 2.224, 2.243	2.279, 2.260 2.242, 2.269 2.271, 2.245	2.219, 2.238 2.241, 2.232
Mo-C (CO ₂)	-	-	2.136	2.100, 2.107	-	-	-	2.077
Mo-O (CO ₂)	-	-	2.252	2.215, 2.233	-	-	-	2.212
P-Mo-P	154.6	155.8	154.8	155.4, 156.6	153.6	154.4	154.4	157.2

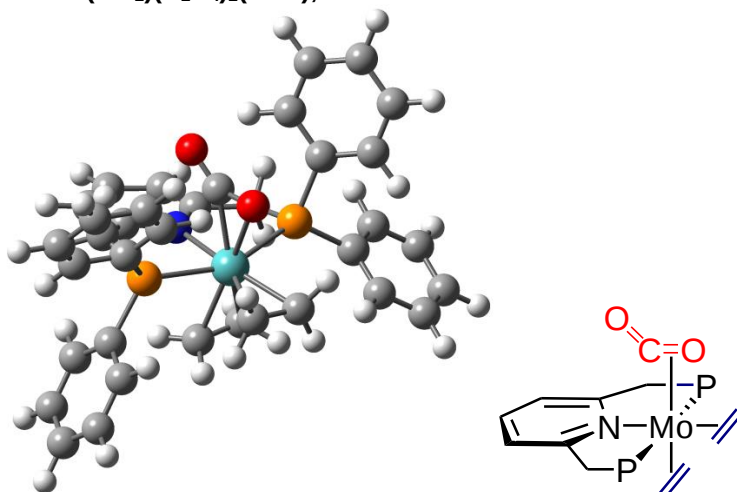
Table S2. Structures and coordinates of optimized compounds
Mo(C₂H₄)₃(PNP), 1a



Mo	-0.00164300	-0.21521400	-0.45503700
C	1.16152700	-0.24358200	3.93342300
C	1.10014200	-0.04959100	2.55819200
C	-1.16002400	-0.56396100	2.54180300
C	-1.15731800	-0.73284500	3.92353900
C	0.02113100	-0.59782600	4.63403300
H	2.10360800	-0.08708100	4.44683200
H	-2.08549300	-0.98554700	4.42429100
H	0.04792600	-0.74763400	5.70807100
N	-0.03883800	-0.25137100	1.84752600
C	-2.45959300	-0.74891100	1.81430200
H	-2.69547600	-1.81498400	1.75674400
H	-3.27120900	-0.28797200	2.38376100
C	2.30293900	0.49932800	1.85751700
H	3.22098000	0.23230700	2.38597700
H	2.23357700	1.59224600	1.89746800
P	-2.41967800	-0.15495600	0.05356300
P	2.35776000	0.12288800	0.03641400
C	-0.44168300	1.82179100	-1.36077300
H	0.19365200	2.08784300	-2.19979400
H	-1.49399500	1.95015000	-1.59345000
C	-0.00053700	2.04221000	-0.03922400
H	-0.71813400	2.32172700	0.72699900
H	0.97113600	2.50255100	0.11868800
C	0.92511800	-0.42854000	-2.54339000
H	1.24753300	0.49543600	-3.01239200
H	1.67740200	-1.21107400	-2.58047300
C	-0.43590800	-0.80214000	-2.60300400
H	-0.65583800	-1.86384100	-2.70268500
H	-1.13559000	-0.15235600	-3.12056700
C	0.76068500	-2.36313600	-0.31252300
H	1.16598700	-2.70871700	-1.25874100
H	1.41521300	-2.56640800	0.52847800
C	-0.62719100	-2.39968800	-0.07751700
H	-0.95480000	-2.62784100	0.93289200
H	-1.29266600	-2.78662700	-0.84065500
C	-3.34550200	1.44266200	0.18444700
C	-4.11058300	1.89774200	-0.89337200
C	-3.23684400	2.25895400	1.31299700

C	-4.75803300	3.12497500	-0.83848500
H	-4.21571800	1.27887500	-1.77934300
C	-3.88798700	3.48645600	1.37034400
H	-2.64185900	1.94122200	2.16421400
C	-4.65065600	3.92299200	0.29492300
H	-5.35241900	3.45696400	-1.68395700
H	-3.79498900	4.10318200	2.25887200
H	-5.15887900	4.88091700	0.33877600
C	-3.77454100	-1.18538500	-0.66518000
C	-4.98582100	-1.34219600	0.01696100
C	-3.62534200	-1.79065200	-1.91093600
C	-6.01186600	-2.10292800	-0.52601500
H	-5.13935800	-0.85145300	0.97312300
C	-4.65748700	-2.54540900	-2.46116900
H	-2.69672500	-1.66591100	-2.45046100
C	-5.84916000	-2.70813800	-1.76862500
H	-6.94451000	-2.21720500	0.01768900
H	-4.52378300	-3.00860200	-3.43362500
H	-6.65273600	-3.30001200	-2.19534000
C	3.62518100	-1.21037200	-0.08756500
C	4.30654100	-1.38551600	-1.29527300
C	3.89549500	-2.08849200	0.96346100
C	5.23445700	-2.40778500	-1.44494000
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C	4.82864900	-3.10894300	0.81578200
H	3.37242300	-1.98809300	1.90960600
C	5.50041500	-3.27212000	-0.38881200
H	5.75582900	-2.52560300	-2.38967100
H	5.02664400	-3.78030200	1.64559100
H	6.22759000	-4.06936100	-0.50473900
C	3.44156000	1.52889900	-0.51077300
C	4.67767700	1.73744800	0.11158600
C	3.06273200	2.38746700	-1.54046600
C	5.50085100	2.78598100	-0.27377400
H	5.01129100	1.06093400	0.89261300
C	3.89029700	3.43536100	-1.93402300
H	2.11301500	2.24190000	-2.03668800
C	5.10771100	3.63966400	-1.30004100
H	6.45572900	2.93228200	0.22163300
H	3.57629400	4.09329600	-2.73806300
H	5.75252300	4.45762200	-1.60558300

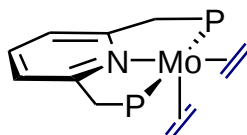
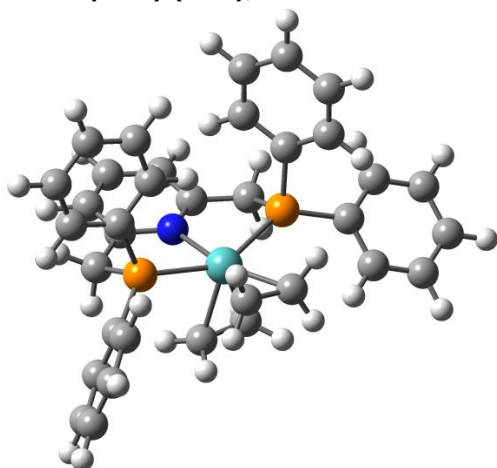
cis-Mo(CO₂)(C₂H₄)₂(PNP), 3a



Mo	0.00119900	-0.30823100	-0.44730300
C	-1.15936700	-0.73854200	3.93157300
C	-1.15733600	-0.59180600	2.54707200
C	1.12057900	-0.15561300	2.55187400
C	1.17866300	-0.32989600	3.93034700
C	0.02789900	-0.64075900	4.63282700
H	-2.09553600	-0.93607100	4.44158700
H	2.12206600	-0.18337400	4.44366300
H	0.05173500	-0.77429500	5.70922700
N	-0.02335600	-0.35510900	1.85620100
C	2.31916700	0.39656100	1.84574200
H	2.20677800	1.48646900	1.88770700
H	3.24694200	0.15065400	2.36715100
C	-2.46906300	-0.69966400	1.82459700
H	-3.22667500	-0.13190800	2.37165400
H	-2.80355500	-1.74103000	1.83237500
P	2.37556500	0.05987600	0.02604100
P	-2.41618700	-0.18643900	0.03490800
C	0.78875500	-2.39690000	-0.12407300
H	1.31903100	-2.73703500	-1.00799700
H	1.33823400	-2.56789100	0.79600400
C	-0.62058400	-2.45826500	-0.07972500
H	-1.09192000	-2.68476500	0.87181600
H	-1.16688900	-2.85305900	-0.92931900
C	-0.51476800	-0.63977600	-2.62059700
H	-0.84911800	-1.65529500	-2.81163600
H	-1.16230200	0.14362500	-2.99985400
C	0.87116500	-0.41671100	-2.53752400
H	1.27521200	0.54344700	-2.83934800
H	1.55024100	-1.25521400	-2.65779900
C	-0.04765200	1.75399500	0.10638300
C	3.61901300	-1.27935500	-0.17302100
C	4.21613400	-1.46333100	-1.42389700
C	3.95194000	-2.15372000	0.86193300
C	5.12213800	-2.49479600	-1.63109100
H	3.98491900	-0.78324700	-2.23744900
C	4.86272200	-3.18445500	0.65529000
H	3.49893300	-2.04039100	1.84177400
C	5.44908300	-3.35868800	-0.59134900

H	5.57840800	-2.62046700	-2.60783800
H	5.11133100	-3.85382400	1.47283000
H	6.15892900	-4.16348300	-0.75282300
C	3.39334900	1.49496800	-0.53762600
C	4.73512300	1.59050300	-0.15022400
C	2.84191700	2.51057700	-1.31970300
C	5.50590000	2.67947500	-0.53154100
H	5.18660200	0.80021000	0.44156400
C	3.62045300	3.59799300	-1.70551900
H	1.79988900	2.46396400	-1.61215000
C	4.94911200	3.68606800	-1.31432700
H	6.54464600	2.73975400	-0.22185200
H	3.17740800	4.38078000	-2.31274000
H	5.55223400	4.53646700	-1.61686100
C	-3.29003600	1.43517300	0.04703100
C	-4.13426100	1.78513200	-1.00960800
C	-3.06612400	2.36259500	1.06691300
C	-4.75242000	3.02810600	-1.03765400
H	-4.32143400	1.07911200	-1.81215100
C	-3.69096400	3.60348900	1.03937800
H	-2.37818400	2.13869700	1.87433100
C	-4.53643500	3.93908800	-0.01029500
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C	-3.77198200	-1.24977000	-0.63201900
C	-4.95884200	-1.41123100	0.09158400
C	-3.66062700	-1.86758400	-1.87544700
C	-5.99392400	-2.18978200	-0.40688500
H	-5.08759600	-0.91033000	1.04589900
C	-4.70128600	-2.64154700	-2.38088100
H	-2.75760800	-1.73633000	-2.45476400
C	-5.86641100	-2.80971800	-1.64607600
H	-6.90653400	-2.30591000	0.16923900
H	-4.59569500	-3.11419700	-3.35217000
H	-6.67681700	-3.41613000	-2.03774700
O	-0.20813800	1.82640900	-1.13399300
O	0.08073800	2.50748700	1.04348600

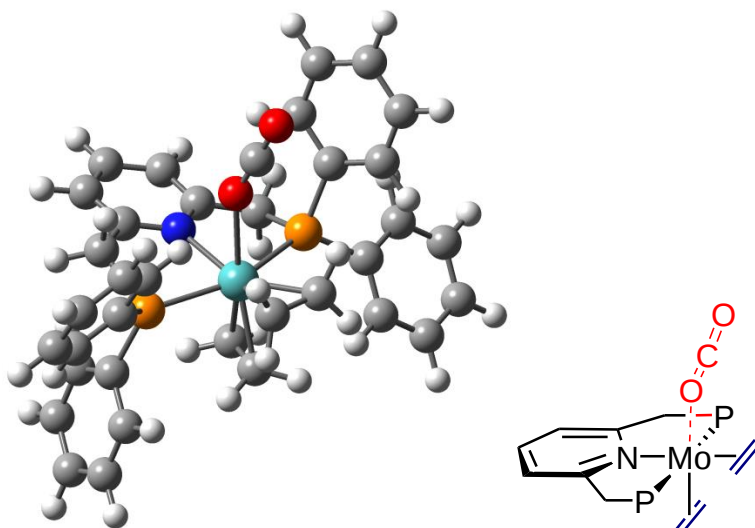
cis-Mo(C₂H₄)₂(PNP), i1a



Mo	-0.01505300	-0.81427200	-0.12860500
C	1.11985500	1.13404800	3.79485400
C	1.11430900	0.43444400	2.59963400
C	-1.20387000	0.41189700	2.58183800
C	-1.24256400	1.10542500	3.78118000
C	-0.06995000	1.49539100	4.41020500
H	2.07460400	1.38717900	4.24352800
H	-2.20917300	1.33503600	4.21716700
H	-0.08212800	2.04729200	5.34294700
N	-0.03697900	0.09617300	1.93099400
C	-2.49442100	-0.00134900	1.94652500
H	-2.76888000	-1.00619600	2.28531700
H	-3.31123500	0.66582000	2.23271600
C	2.42972100	0.02141700	2.00759700
H	2.70113100	-0.96048100	2.40335300
H	3.22569200	0.71232900	2.29392200
P	-2.31660900	-0.19602400	0.11916700
P	2.27904000	-0.16191500	0.18095900
C	0.78218800	-1.35718300	-2.13690700
H	1.15550400	-0.50186800	-2.70426000
H	1.49195700	-2.17855800	-2.08706400
C	-0.61109900	-1.61635000	-2.14216400
H	-0.95565000	-2.64724800	-2.09026200
H	-1.26210600	-0.97579700	-2.73573200
C	0.75760200	-2.63576400	0.83952700
H	1.30855200	-3.26178000	0.13959400
H	1.25564600	-2.53099900	1.80319900
C	-0.66794400	-2.68439500	0.83606200
H	-1.18519100	-2.60459500	1.79163900
H	-1.15930700	-3.36539300	0.14520000
C	-2.60407900	1.47846400	-0.58314600
C	-3.25187900	1.65212900	-1.80935700
C	-2.04786600	2.59598600	0.04955300
C	-3.35146500	2.91399800	-2.38403400
H	-3.68876400	0.79664600	-2.31441500
C	-2.16006000	3.85844700	-0.52101400
H	-1.52381200	2.48159500	0.99346800
C	-2.81029100	4.02057100	-1.73986900
H	-3.85741600	3.03197700	-3.33715000
H	-1.73515100	4.71730500	-0.01090300
H	-2.89459800	5.00637700	-2.18619000

C	-3.89148400	-1.05464200	-0.29040800
C	-5.12844200	-0.46001100	-0.02014200
C	-3.86300800	-2.33224300	-0.84587400
C	-6.31003800	-1.13549100	-0.29287100
H	-5.16906900	0.54380900	0.39207400
C	-5.04744200	-3.00861500	-1.12122700
H	-2.90635600	-2.79151000	-1.06125200
C	-6.27076200	-2.41285700	-0.84409700
H	-7.26398300	-0.66371800	-0.07867900
H	-5.01126000	-4.00308700	-1.55447200
H	-7.19475000	-2.94026700	-1.05932300
C	3.71956000	-1.19124100	-0.30213400
C	4.26719400	-1.03396900	-1.58028700
C	4.20907300	-2.21980100	0.50683300
C	5.28565600	-1.86601200	-2.02564900
H	3.89759900	-0.24962700	-2.23234000
C	5.23096700	-3.05028300	0.06137800
H	3.79302700	-2.39260600	1.49255900
C	5.77466500	-2.87554500	-1.20461600
H	5.69728900	-1.72418500	-3.01992400
H	5.59965900	-3.83949200	0.70899000
H	6.57170400	-3.52511800	-1.55175300
C	2.76984600	1.50379900	-0.44127000
C	4.07579400	1.99312100	-0.34000700
C	1.78159800	2.33123300	-0.97404500
C	4.38244700	3.27854800	-0.76617900
H	4.86037900	1.35995300	0.06344800
C	2.08802400	3.61693500	-1.40668000
H	0.75702200	1.97300700	-1.03762100
C	3.38910000	4.09214200	-1.30326200
H	5.40034200	3.64652000	-0.68200600
H	1.30655600	4.24399600	-1.82349900
H	3.63114600	5.09549100	-1.63939300

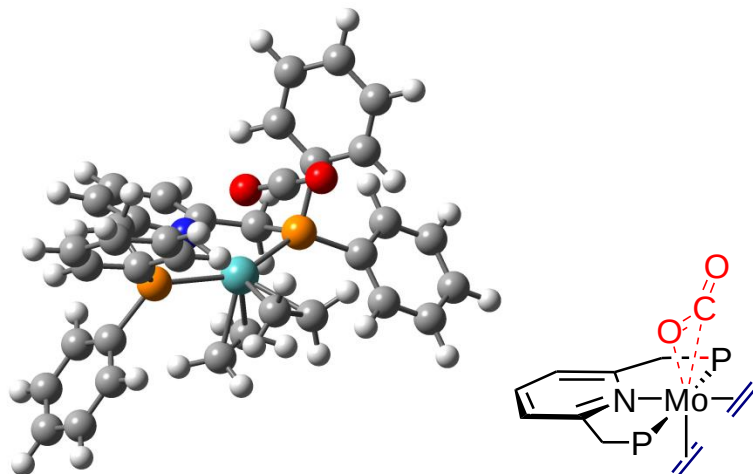
i2a



Mo	0.03865100	-0.12080500	-0.47765500
C	-1.03133500	-0.63339100	3.90398500
C	-1.01180600	-0.61543200	2.51283000
C	1.17508000	0.16410500	2.51498000
C	1.21455200	0.13352200	3.90479000
C	0.09535500	-0.26309400	4.61756700
H	-1.93067800	-0.96108700	4.41342400
H	2.12018200	0.44365900	4.41399400
H	0.10154800	-0.28328700	5.70221800
N	0.07881200	-0.21079500	1.80965200
C	2.36114200	0.67388300	1.76216700
H	2.26627300	1.76040000	1.65272700
H	3.29075700	0.50051600	2.31234100
C	-2.20932400	-1.10617700	1.76218100
H	-3.12746300	-0.93955400	2.33229000
H	-2.11503300	-2.18949200	1.62844100
P	2.40929500	0.06954400	0.00404000
P	-2.27076600	-0.43260900	0.03161400
C	0.46497900	-1.99668800	-1.54472600
H	-0.23491000	-2.23070000	-2.34587800
H	1.49661100	-2.08134100	-1.87855500
C	0.15400400	-2.35175500	-0.20535000
H	0.95444100	-2.67954600	0.45559300
H	-0.77990700	-2.87712100	-0.00812500
C	-0.85877500	0.46756000	-2.46720900
H	-1.28319300	-0.34643600	-3.04701100
H	-1.52980000	1.32403000	-2.39039200
C	0.53816600	0.71440200	-2.50078700
H	0.87797700	1.74709400	-2.46105700
H	1.18420700	0.07925100	-3.09760500
C	-0.84347800	3.30331000	-0.26298600
C	3.44093500	-1.45373600	0.08814000
C	3.96766500	-1.98623400	-1.09467200
C	3.58566700	-2.18814100	1.26739000
C	4.64555300	-3.19786300	-1.09044800
H	3.85991300	-1.43920200	-2.02698000
C	4.26144200	-3.40376500	1.27125200
H	3.16518600	-1.81886100	2.19725300

C	4.79687900	-3.91055100	0.09421200
H	5.05266900	-3.58917300	-2.01752600
H	4.36675700	-3.95663600	2.19964800
H	5.32324400	-4.85961300	0.09749700
C	3.63117600	1.30163700	-0.64550700
C	5.00962100	1.07647700	-0.67041500
C	3.15437700	2.54660800	-1.06329100
C	5.88223100	2.06467400	-1.11311300
H	5.40813800	0.12251200	-0.34399300
C	4.02556500	3.53776200	-1.49733300
H	2.08735300	2.73657600	-1.05035100
C	5.39411300	3.29703300	-1.52905900
H	6.94989400	1.86828900	-1.12930900
H	3.63310600	4.49645700	-1.82198000
H	6.07639200	4.06619200	-1.87686400
C	-3.30363700	1.08454400	0.21911000
C	-4.01747000	1.57757900	-0.87916700
C	-3.29406300	1.83949900	1.39677800
C	-4.71047800	2.77912400	-0.79677300
H	-4.04540400	1.00608800	-1.80161100
C	-3.99153500	3.04022200	1.47966100
H	-2.73861800	1.49218700	2.26314100
C	-4.70222000	3.51423000	0.38326000
H	-5.26140300	3.14127900	-1.65914100
H	-3.97878700	3.60627100	2.40611700
H	-5.24256100	4.45301700	0.44657500
C	-3.52114800	-1.58002900	-0.70257700
C	-4.83818600	-1.61106600	-0.23267100
C	-3.14460200	-2.46745000	-1.70945900
C	-5.75491200	-2.51225700	-0.75659500
H	-5.15325600	-0.91418800	0.53834300
C	-4.06374400	-3.37005400	-2.23607500
H	-2.12695300	-2.45308500	-2.07904600
C	-5.36833300	-3.39429400	-1.76126200
H	-6.77464300	-2.52394000	-0.38402000
H	-3.75626500	-4.05422200	-3.02052600
H	-6.08569500	-4.09699200	-2.17353000
O	-0.33557400	2.28314900	-0.03191600
O	-1.30240100	4.34195800	-0.48057500

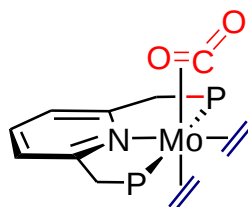
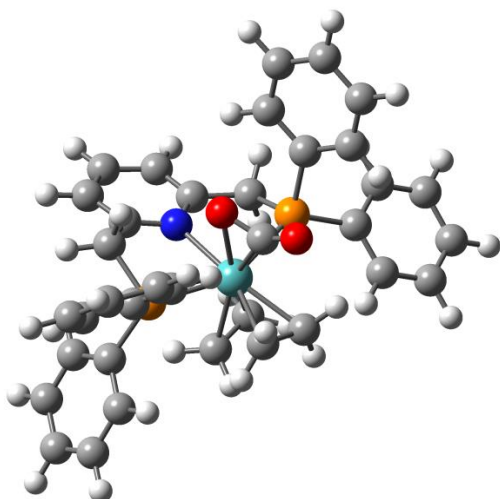
TS2-3a



Mo	-0.01282600	-0.27787600	-0.56075000
C	-0.98964900	-1.84188200	3.55763000
C	-1.03702800	-1.40233800	2.24108700
C	1.12443200	-0.57628400	2.41021800
C	1.21994700	-1.01696600	3.71780500
C	0.15744300	-1.68437400	4.31666800
H	-1.87162200	-2.31558300	3.97611500
H	2.12948000	-0.81053500	4.27207000
H	0.21532600	-2.04058400	5.33874200
N	0.03106100	-0.80664400	1.61357900
C	2.21958400	0.25597300	1.83400200
H	1.94886600	1.31295000	1.94744800
H	3.16255600	0.11029900	2.36642900
C	-2.32017700	-1.54729400	1.48365200
H	-3.17935700	-1.43048900	2.15026000
H	-2.40159800	-2.53840200	1.02998800
P	2.37564300	0.05011100	-0.00061700
P	-2.36715300	-0.39316100	0.03323900
C	0.78795900	-2.18702300	-1.36486500
H	0.91227100	-2.14397700	-2.44706900
H	1.65746500	-2.59547100	-0.86224300
C	-0.48766600	-2.46019900	-0.82267000
H	-0.52644600	-3.01485900	0.11345800
H	-1.31525000	-2.68122800	-1.49122200
C	-0.72991000	-0.09525400	-2.67628500
H	-0.76518100	-1.04982100	-3.20277000
H	-1.62132500	0.50853400	-2.83400800
C	0.51285900	0.57785500	-2.55959300
H	0.50618300	1.66658500	-2.65042700
H	1.40196500	0.13427200	-3.00065900
C	-0.66716100	2.91906000	-0.66193400
C	3.63728700	-1.27567300	-0.18534800
C	4.42918400	-1.32435000	-1.33511900
C	3.76779300	-2.28994600	0.76530800
C	5.34003600	-2.35519300	-1.52295800
H	4.34130600	-0.54491500	-2.08592600
C	4.68254200	-3.32048000	0.57691900
H	3.14553700	-2.28850500	1.65492700
C	5.47149400	-3.35557200	-0.56587100
H	5.94999500	-2.37669000	-2.42061300

H	4.77385100	-4.10068900	1.32613800
H	6.18337900	-4.16143400	-0.71291100
C	3.44187400	1.52272300	-0.35271200
C	4.70108300	1.64562400	0.24593800
C	2.99737200	2.54814800	-1.18474400
C	5.48352100	2.77095200	0.02835200
H	5.08098200	0.84615000	0.87470200
C	3.78317400	3.67500600	-1.40920200
H	2.03758500	2.45208500	-1.67517700
C	5.02503000	3.79082600	-0.80025800
H	6.45734300	2.85010400	0.50159200
H	3.42339000	4.45956400	-2.06751400
H	5.63920500	4.66861300	-0.97460000
C	-3.09420800	1.14754100	0.74403600
C	-3.88358600	1.99186100	-0.04319100
C	-2.77654800	1.54990000	2.04496400
C	-4.35056700	3.20049300	0.45999800
H	-4.14717300	1.69638100	-1.05410000
C	-3.25021300	2.75536200	2.54955000
H	-2.15279000	0.92024100	2.67143600
C	-4.03750600	3.58484500	1.75884500
H	-4.96249500	3.84221800	-0.16591600
H	-3.00045500	3.04752500	3.56485600
H	-4.40500300	4.52695900	2.15287800
C	-3.83068700	-1.06013500	-0.86762200
C	-5.07717400	-1.10905400	-0.23291200
C	-3.72006800	-1.55561700	-2.16587200
C	-6.18081900	-1.64803700	-0.87913200
H	-5.19074500	-0.70833300	0.76979300
C	-4.82797600	-2.09219100	-2.81534000
H	-2.76426800	-1.51950900	-2.67088900
C	-6.05806900	-2.14181300	-2.17438100
H	-7.14026500	-1.67921800	-0.37225800
H	-4.72428100	-2.47102200	-3.82710300
H	-6.92157300	-2.56071100	-2.68138200
O	-0.15613500	2.21001900	0.10815100
O	-1.15193400	3.64918100	-1.41274100

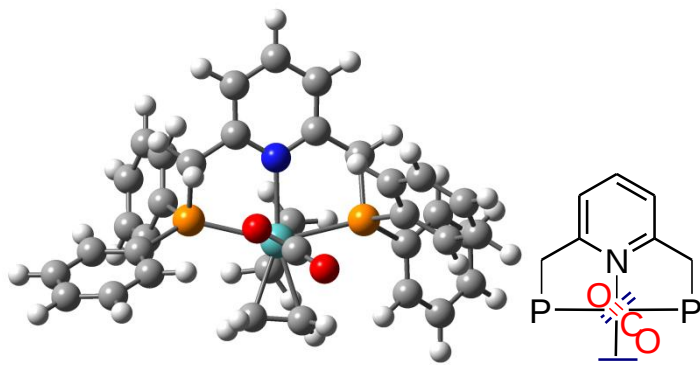
i3a



Mo	0.00223600	-0.28026900	-0.51515500
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C	-1.09831400	-1.15558400	2.38160100
C	1.09529800	-0.38623900	2.48494400
C	1.18660600	-0.74569600	3.82563300
C	0.10058300	-1.33320700	4.45258400
H	-1.95400000	-1.92212000	4.19024300
H	2.09830000	-0.53416400	4.37243600
H	0.15250700	-1.62061200	5.49753900
N	-0.01276600	-0.65176900	1.75210000
C	2.19272800	0.40904000	1.85198600
H	1.88187200	1.45955500	1.87942300
H	3.12762700	0.32961800	2.41140400
C	-2.38036200	-1.30270600	1.61759700
H	-3.22769800	-1.06885500	2.26812100
H	-2.51469500	-2.33817900	1.29389800
P	2.38202700	0.10967700	0.02907900
P	-2.39115200	-0.28988100	0.05394600
C	0.79484600	-2.34084400	-0.97669000
H	1.12054800	-2.45477100	-2.00622300
H	1.53385800	-2.67879400	-0.25740100
C	-0.56621200	-2.48549700	-0.63626000
H	-0.78844900	-2.92529700	0.33258200
H	-1.29862000	-2.73115600	-1.39628200
C	-0.49094400	-0.40206900	-2.73934100
H	-0.65271300	-1.43100400	-3.04940000
H	-1.26563300	0.29937300	-3.02787000
C	0.82873000	0.07304800	-2.65546900
H	1.02653300	1.11069100	-2.89391000
H	1.65059600	-0.60322700	-2.86791100
C	-0.41051300	1.75593300	-0.96694500
C	3.64216600	-1.21444000	-0.08938100
C	4.30828200	-1.40018300	-1.30457000
C	3.89974800	-2.09743300	0.96002800
C	5.21742800	-2.43714800	-1.45997600
H	4.12300500	-0.72140200	-2.13124400
C	4.81097200	-3.13672800	0.80269400
H	3.38428100	-1.98659200	1.90898800

C	5.47242600	-3.30856800	-0.40606900
H	5.72918400	-2.56520100	-2.40843300
H	5.00147000	-3.81427500	1.62904200
H	6.18258000	-4.11986100	-0.52868800
C	3.38178700	1.59003500	-0.42396100
C	4.71740200	1.68208000	-0.01677900
C	2.81171700	2.65694200	-1.11999900
C	5.46580700	2.81663800	-0.29895100
H	5.18078600	0.85587400	0.51321800
C	3.56549100	3.79153900	-1.40209600
H	1.77937500	2.61721300	-1.44134900
C	4.89003100	3.87481800	-0.99401100
H	6.50152900	2.87227100	0.02142300
H	3.10733000	4.61194000	-1.94455800
H	5.47491100	4.76153000	-1.21753700
C	-3.14713200	1.29131800	0.61717300
C	-3.83777800	2.08371900	-0.30242700
C	-2.97274700	1.76740100	1.91744700
C	-4.36561800	3.30970800	0.07847500
H	-3.96295600	1.74284400	-1.32486900
C	-3.50345900	2.99377700	2.29858200
H	-2.40796000	1.19166100	2.64348300
C	-4.20492000	3.76605400	1.38149300
H	-4.89807000	3.91356700	-0.64914200
H	-3.35952100	3.34952000	3.31407000
H	-4.61602700	4.72573900	1.67809400
C	-3.82146600	-1.04800600	-0.81998500
C	-5.06982200	-1.11919100	-0.19240600
C	-3.68731000	-1.55368700	-2.11138300
C	-6.15197000	-1.70122800	-0.83722900
H	-5.20373300	-0.69583700	0.79839400
C	-4.77477500	-2.13025500	-2.76079500
H	-2.73090000	-1.48668500	-2.61210900
C	-6.00570600	-2.20993000	-2.12436300
H	-7.11478400	-1.74925800	-0.33829400
H	-4.65575800	-2.51400400	-3.76892500
H	-6.85379400	-2.65943100	-2.63106200
O	-0.05464100	1.81274100	0.24194600
O	-0.74405600	2.53166300	-1.82727800

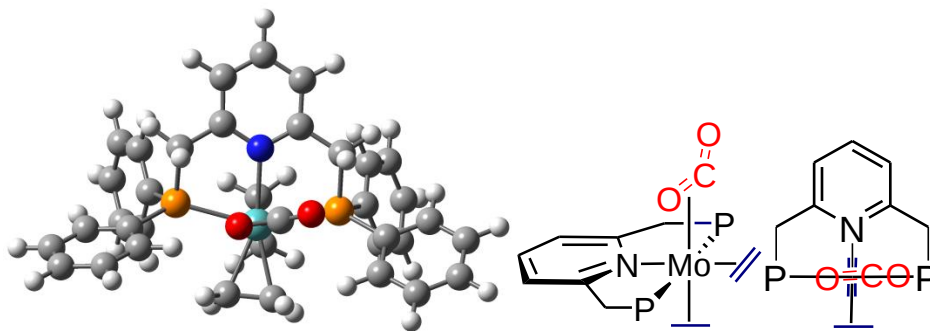
TS3-4a



Mo	-0.04736100	-0.10021800	-0.54413600
C	1.04222800	0.15502200	3.87359900
C	1.00072700	0.26838100	2.48870400
C	-1.17010800	-0.55130500	2.43863300
C	-1.19084300	-0.65497800	3.82716500
C	-0.06842100	-0.31036500	4.55758400
H	1.94325700	0.44353100	4.40230200
H	-2.08436000	-1.02511000	4.31705700
H	-0.05828900	-0.40091200	5.63865600
N	-0.08562600	-0.09606000	1.77004100
C	-2.37303600	-0.98006400	1.65943300
H	-2.24291600	-2.02804100	1.37494000
H	-3.28614300	-0.90883300	2.25566300
C	2.17133200	0.84933600	1.76523600
H	3.08665700	0.69227100	2.33942700
H	2.01352900	1.92855100	1.67947900
P	-2.51388800	-0.12619000	0.02494800
P	2.32717300	0.21548800	0.01853500
C	-0.43651800	1.91644400	-1.47319500
H	0.14512300	2.13836100	-2.36155000
H	-1.50200400	2.06602400	-1.61261900
C	0.13927400	2.15258200	-0.21116700
H	-0.49650200	2.42422400	0.63012700
H	1.12179500	2.61465400	-0.17809900
C	0.64641400	-0.38283400	-2.73980200
H	0.92667600	0.53863500	-3.23687600
H	1.37225900	-1.18425000	-2.82146600
C	-0.71781500	-0.70357600	-2.63015000
H	-1.00598100	-1.75142600	-2.64414300
H	-1.46571200	-0.03398800	-3.04285100
C	0.63247500	-2.13883700	-0.66102000
C	-3.35193600	1.45915100	0.38825900
C	-3.87956900	2.21359200	-0.66640900
C	-3.39710100	1.99089200	1.67854300
C	-4.45326800	3.45547900	-0.43128200
H	-3.85463400	1.82174500	-1.67882100
C	-3.96625300	3.23823100	1.91136900
H	-2.98373400	1.43700900	2.51453900
C	-4.49725600	3.97215400	0.85903800
H	-4.86226600	4.02358700	-1.26044900
H	-3.99354000	3.63533600	2.92108500
H	-4.94109400	4.94534200	1.04165800
C	-3.81789200	-1.15401900	-0.76279200

C	-5.16250800	-0.78032500	-0.81113100
C	-3.43686100	-2.39568200	-1.28316100
C	-6.10606900	-1.62528700	-1.38475900
H	-5.48043200	0.17030400	-0.39820900
C	-4.38560000	-3.23873300	-1.84677000
H	-2.39861800	-2.70413600	-1.22650400
C	-5.72039800	-2.85379900	-1.90567700
H	-7.14754800	-1.32107000	-1.41828900
H	-4.07652000	-4.19945100	-2.24573300
H	-6.45848800	-3.51161200	-2.35350900
C	3.56107000	-1.13284500	0.27551200
C	3.27760700	-2.12394200	1.21905000
C	4.76217800	-1.19933800	-0.42795500
C	4.18174900	-3.14588400	1.46511400
H	2.33085700	-2.11491500	1.75125600
C	5.66323900	-2.23201400	-0.18964000
H	5.00425900	-0.44255000	-1.16567900
C	5.37905800	-3.20373000	0.75954400
H	3.94272100	-3.91006200	2.19786800
H	6.59135100	-2.27310700	-0.75119100
H	6.08275300	-4.00908600	0.94485900
C	3.40208100	1.50917000	-0.73926900
C	4.22844600	2.34449500	0.01777500
C	3.42957100	1.62628700	-2.13011500
C	5.04371000	3.28501700	-0.59982300
H	4.25249700	2.26212000	1.09886800
C	4.25279800	2.56027700	-2.74882300
H	2.80624200	0.97560900	-2.73002900
C	5.05721600	3.39658500	-1.98525700
H	5.67509000	3.92871400	0.00466700
H	4.26023000	2.63523400	-3.83151800
H	5.69519800	4.13066000	-2.46687300
O	-0.45861000	-2.23999400	-0.04271000
O	1.46351300	-2.88056700	-1.10916900

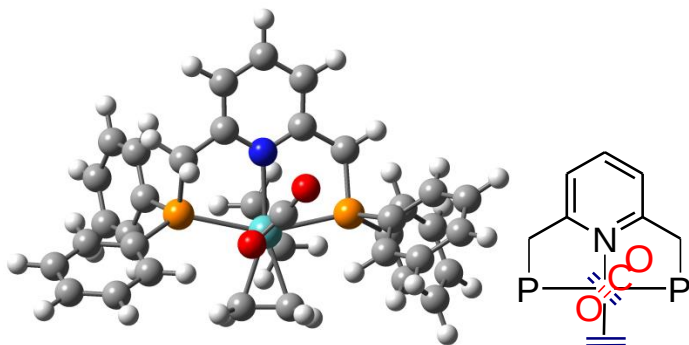
i4a



Mo	-0.06015000	-0.49191200	-0.32240900
C	1.09862000	1.32934600	3.66409900
C	1.08873400	0.61583800	2.46947900
C	-1.23141800	0.51593800	2.50077800
C	-1.27749100	1.22070300	3.69866900
C	-0.09815700	1.65914700	4.27695600
H	2.04734300	1.60051800	4.11295200
H	-2.23406900	1.40452000	4.17448900
H	-0.11022900	2.22117400	5.20483600
N	-0.06810900	0.27529700	1.85730300
C	-2.47978500	-0.08263300	1.93128600
H	-2.46747500	-1.15210200	2.17252200
H	-3.38243800	0.33333700	2.38407400
C	2.37538200	0.11475100	1.89243000
H	2.49329300	-0.92382900	2.22434400
H	3.23254800	0.67784500	2.26649500
P	-2.51510600	-0.09933500	0.08223900
P	2.37503000	-0.07252500	0.04844300
C	-0.00804800	1.74011300	-0.58755800
H	-0.95988200	2.21670700	-0.37657500
H	0.81259600	2.25227900	-0.09600200
C	0.19764000	1.12643300	-1.84636900
H	1.16643500	1.18718900	-2.33209300
H	-0.62780800	1.11397700	-2.55311800
C	0.51034000	-1.79507200	-2.10485100
H	1.17548800	-1.30588300	-2.80801000
H	0.83530700	-2.78288900	-1.79181400
C	-0.87463500	-1.55838200	-2.14803600
H	-1.54312800	-2.35469200	-1.83829000
H	-1.29417000	-0.88938200	-2.89178300
C	0.58859100	-2.21991800	0.78706600
C	-3.27459300	1.48424400	-0.43095800
C	-3.46483500	1.70145400	-1.79967200
C	-3.62561900	2.49342300	0.46578100
C	-4.00754000	2.89414200	-2.25654300
H	-3.19138600	0.92839800	-2.51129600
C	-4.16338500	3.69090000	0.00599400
H	-3.47258800	2.35992500	1.53121200
C	-4.35777900	3.89294900	-1.35408600
H	-4.15033500	3.04685300	-3.32132700
H	-4.42921700	4.46794100	0.71556100
H	-4.77631200	4.82800200	-1.71180200
C	-3.87721500	-1.30262900	-0.21492400
C	-5.17838900	-0.89028600	-0.51389400

C	-3.60775500	-2.67155500	-0.10250100
C	-6.18872200	-1.82656800	-0.70209600
H	-5.40939000	0.16491000	-0.60427500
C	-4.62401400	-3.60095600	-0.28592500
H	-2.60379200	-3.00546300	0.13225400
C	-5.91470400	-3.18341100	-0.58936400
H	-7.19371300	-1.48995800	-0.93666400
H	-4.39997500	-4.65918500	-0.19705200
H	-6.70408500	-3.91344400	-0.73804700
C	3.80923400	-1.20986600	-0.17582100
C	3.65753400	-2.47599700	-0.73397100
C	5.08409000	-0.79505100	0.22380300
C	4.75735400	-3.31131400	-0.89482100
H	2.67366600	-2.81402300	-1.02244200
C	6.17965100	-1.63382100	0.07458100
H	5.22819700	0.19711800	0.64013100
C	6.01831300	-2.89478300	-0.48977500
H	4.62195800	-4.29590800	-1.33064600
H	7.16193900	-1.29907700	0.39313000
H	6.87504100	-3.55006200	-0.61223900
C	3.17833800	1.47680700	-0.54727000
C	3.24782600	2.63883700	0.22263300
C	3.72236400	1.49560400	-1.83518200
C	3.85200000	3.78790400	-0.27703000
H	2.82614600	2.65942900	1.22277300
C	4.32253600	2.64262100	-2.33571300
H	3.69375900	0.59721500	-2.44459100
C	4.38999800	3.79294600	-1.55694400
H	3.89905700	4.68119800	0.33785200
H	4.74199400	2.63674800	-3.33665300
H	4.86116800	4.68926800	-1.94726600
O	-0.64234800	-2.41359500	0.63052000
O	1.48753200	-2.79749200	1.35544200

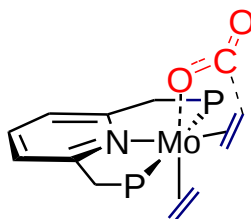
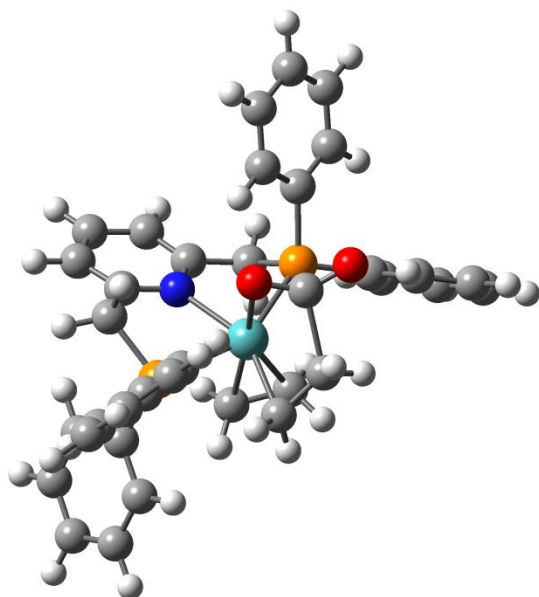
TS4-3a



Mo	-0.03591000	-0.05639000	-0.48278200
C	0.93937700	0.66484200	3.88335900
C	0.93931700	0.58169500	2.49502000
C	-1.27287500	-0.11905500	2.49835400
C	-1.33766600	-0.01625100	3.88223900
C	-0.21526900	0.37996700	4.58966800
H	1.84628500	0.96083900	4.39781900
H	-2.25413400	-0.28736200	4.39402300
H	-0.23561900	0.44831000	5.67207800
N	-0.16126700	0.21227500	1.80532900
C	-2.41880900	-0.71717400	1.74341000
H	-2.22147900	-1.79120400	1.63735400
H	-3.36254000	-0.62451400	2.28642700
C	2.17396900	0.98424400	1.74296900
H	3.05627400	0.85871700	2.37326000
H	2.08379700	2.05660900	1.53885400
P	-2.52733100	-0.14974000	-0.01365500
P	2.35187700	0.19227200	0.07016100
C	-0.39028100	2.18584200	-0.27982100
H	-1.43001500	2.46583500	-0.39260500
H	0.06002300	2.60193800	0.61874800
C	0.40107700	1.95668800	-1.41737100
H	1.43465400	2.27643000	-1.45257400
H	-0.07688400	1.97708700	-2.39378100
C	0.74628100	-0.69840800	-2.51727800
H	1.37681300	0.03856600	-3.00240600
H	1.16515500	-1.70026500	-2.47439300
C	-0.65645100	-0.57987200	-2.57852200
H	-1.26246000	-1.47818500	-2.59104000
H	-1.10698900	0.26377300	-3.09391600
C	0.50991700	-1.91247100	0.51747200
C	-3.53344200	1.38005500	0.03541000
C	-3.95372400	1.93542500	-1.17832100
C	-3.82686400	2.05506600	1.21965700
C	-4.66547600	3.12628000	-1.20215500
H	-3.72439700	1.42923300	-2.11147500
C	-4.53611600	3.25202900	1.19423400
H	-3.49401100	1.66070100	2.17377600
C	-4.95946200	3.78849300	-0.01420600
H	-4.98718300	3.54157100	-2.15176100
H	-4.75569000	3.76561300	2.12487500
H	-5.51246700	4.72194000	-0.03296800
C	-3.74152300	-1.37341700	-0.67343000
C	-5.11429700	-1.10898100	-0.70254100

C	-3.28552100	-2.62017600	-1.11484500
C	-6.00817600	-2.06361800	-1.17321700
H	-5.49367100	-0.15287600	-0.36050800
C	-4.18500400	-3.57230200	-1.57944300
H	-2.22801000	-2.84846100	-1.07518600
C	-5.54633200	-3.29682500	-1.61574700
H	-7.07022800	-1.83964600	-1.19144000
H	-3.81379500	-4.53423100	-1.91847000
H	-6.24509300	-4.04070900	-1.98537600
C	3.60683200	-1.14607800	0.29616600
C	3.47747100	-2.35503000	-0.38333100
C	4.76295800	-0.91464600	1.04312200
C	4.47615800	-3.31862200	-0.30782800
H	2.58467600	-2.55281300	-0.96428900
C	5.75466300	-1.88197900	1.13243400
H	4.90989400	0.03614700	1.54675000
C	5.61300400	-3.08820500	0.45557300
H	4.35650300	-4.25733900	-0.83906400
H	6.64322900	-1.68986300	1.72569400
H	6.38908400	-3.84418400	0.52102100
C	3.49094200	1.36463700	-0.80179400
C	3.84985900	2.63412700	-0.34793300
C	4.00880200	0.92921700	-2.02714700
C	4.69989300	3.44490300	-1.09510600
H	3.47737400	3.01671900	0.59573600
C	4.84980400	1.73920100	-2.77519600
H	3.75927200	-0.06081100	-2.39476600
C	5.19971200	3.00312200	-2.31134900
H	4.96760700	4.42756800	-0.71948700
H	5.23734700	1.37970000	-3.72310000
H	5.85963400	3.63729400	-2.89438500
O	-0.36405000	-2.29573000	-0.28881100
O	1.14148300	-2.37352100	1.43299800

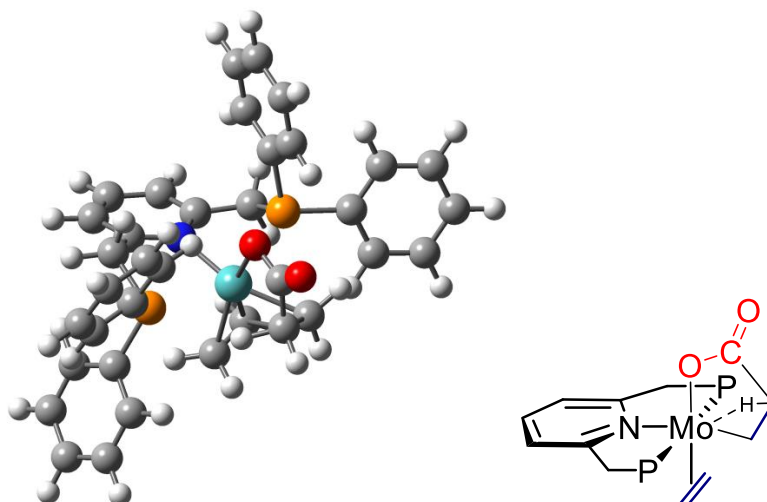
TS4-5a



Mo	0.06534800	0.02661200	-0.57570200
C	-1.05336100	-2.19338100	3.21627000
C	-1.01807200	-1.61409100	1.95756800
C	1.06051300	-0.67969800	2.39356200
C	1.08581000	-1.26157800	3.65605800
C	0.01661100	-2.02802200	4.08398000
H	-1.91585300	-2.78467800	3.50086600
H	1.93934200	-1.08452200	4.30090300
H	0.01190100	-2.48107500	5.06927900
N	0.02700200	-0.85650600	1.52923400
C	2.17443800	0.21890300	1.96182300
H	1.87361300	1.26167700	2.12247500
H	3.08532000	0.05260400	2.54196400
C	-2.15045700	-1.82760900	1.00208600
H	-3.06459700	-2.08611900	1.54240800
H	-1.90100400	-2.65749300	0.33184100
P	2.42167500	0.12787500	0.13320300
P	-2.32929200	-0.30459800	-0.02488100
C	0.62501200	-2.07986400	-1.14340100
H	1.57010800	-2.14850500	-1.67466100
H	0.54851900	-2.78738700	-0.31881000
C	-0.53378900	-1.71491900	-1.86209600
H	-1.47447900	-2.21289900	-1.64545400
H	-0.45192700	-1.48169200	-2.92386600
C	-0.11781100	1.29245300	-2.55279100
C	1.10116500	0.51804400	-2.46044700
H	2.01128800	1.11484600	-2.45066400
H	1.20014400	-0.36127900	-3.09668700
C	-0.91748700	2.16370700	-0.97758900
C	3.55767000	-1.28033000	-0.13472200
C	4.18973700	-1.40611900	-1.37665500
C	3.74221400	-2.28157800	0.81842800
C	5.00150200	-2.49843300	-1.64817000
H	4.04982200	-0.64109700	-2.13420100
C	4.55490700	-3.37677100	0.54376400
H	3.24582200	-2.22040500	1.78123100
C	5.18813500	-3.48689500	-0.68714600

H	5.48779300	-2.57922300	-2.61507100
H	4.69131100	-4.14634100	1.29705400
H	5.82212600	-4.34150800	-0.89993100
C	3.52735300	1.57401300	-0.13522000
C	4.91087900	1.48753800	0.04544200
C	2.95831700	2.80873300	-0.45761900
C	5.71032000	2.61430700	-0.10167000
H	5.36829900	0.53581100	0.29368200
C	3.76281100	3.93370600	-0.60003400
H	1.88303500	2.88422100	-0.57447700
C	5.13828900	3.83897000	-0.42696700
H	6.78392300	2.53344200	0.03700300
H	3.30895900	4.88720400	-0.85054100
H	5.76453000	4.71776900	-0.54451100
C	-3.26397400	0.75970900	1.16081000
C	-4.62862900	0.56402600	1.39028700
C	-2.58031600	1.72272700	1.90369800
C	-5.29482600	1.31109600	2.35269200
H	-5.17889100	-0.16408200	0.80214400
C	-3.25079500	2.46889900	2.86690900
H	-1.53215800	1.91318300	1.70175400
C	-4.60518500	2.26346300	3.09564600
H	-6.35658200	1.15502500	2.51698400
H	-2.71187600	3.22374700	3.43081500
H	-5.12699000	2.85165600	3.84416600
C	-3.60960600	-0.70380200	-1.26750600
C	-4.25258200	-1.94089200	-1.33481700
C	-3.94196100	0.29049200	-2.19401900
C	-5.21227300	-2.18347300	-2.31259400
H	-4.01426200	-2.72733200	-0.62635700
C	-4.90358500	0.04321100	-3.16459600
H	-3.44701000	1.25630000	-2.14780000
C	-5.53966400	-1.19234000	-3.22823600
H	-5.70327300	-3.15060400	-2.35561500
H	-5.15473200	0.82195800	-3.87759600
H	-6.28837200	-1.38203900	-3.99080600
O	-1.93877400	2.69091600	-1.32500900
O	-0.10278500	2.27874500	-0.04120000
H	0.05717900	2.34553800	-2.77704500
H	-0.95577100	0.90950800	-3.12716700

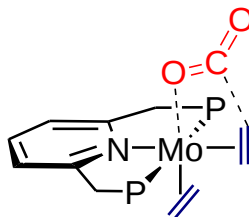
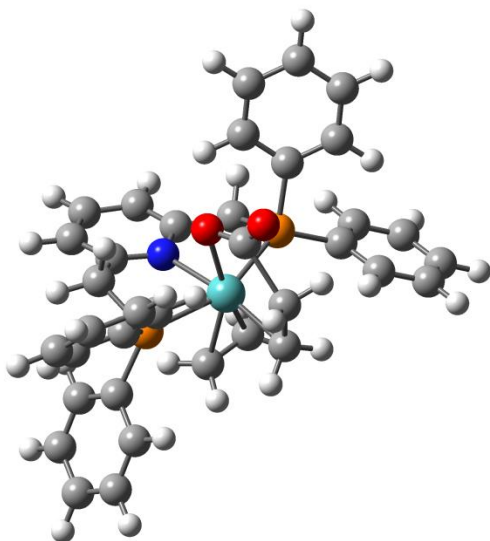
i5a



Mo	-0.02686700	-0.42244000	-0.62258700
C	-1.06104000	-2.51874200	3.20594500
C	-1.14182600	-1.85395600	1.99236300
C	0.98049900	-0.96576500	2.29835800
C	1.10647400	-1.62325600	3.50922500
C	0.08997300	-2.44799600	3.97317800
H	-1.92047500	-3.09012900	3.54039000
H	1.99996900	-1.45629100	4.10106100
H	0.17646200	-2.97698100	4.91505700
N	-0.09791100	-1.13216800	1.46986700
C	1.98689000	0.05552700	1.90000900
H	1.54947200	1.04628000	2.07850700
H	2.90004600	-0.00294700	2.49636300
C	-2.42966600	-1.84109900	1.23062000
H	-3.29269400	-1.87074600	1.90070800
H	-2.51898100	-2.70031800	0.56081900
P	2.33833100	0.10775800	0.09337300
P	-2.39999000	-0.38581900	0.11122200
C	0.97729900	-2.32476000	-1.22858500
H	1.29888100	-2.26563800	-2.26872000
H	1.75302500	-2.70016500	-0.56804600
C	-0.36776900	-2.63527700	-0.93714600
H	-0.55436200	-3.21554300	-0.03650600
H	-1.04607400	-2.87318700	-1.75091600
C	-0.89931300	-0.31971000	-2.59689300
C	0.20238700	0.67715600	-2.75717000
C	-0.16135800	2.00236000	-2.09202500
C	3.70213500	-1.06727100	-0.22683700
C	4.25969100	-1.10771100	-1.50858800
C	4.16528300	-1.96190100	0.73767700
C	5.27025000	-2.00886900	-1.81080600
H	3.90808100	-0.42295400	-2.27501400
C	5.17369200	-2.87027000	0.43087000
H	3.73438400	-1.96914200	1.73300500
C	5.73041200	-2.89372600	-0.84059700
H	5.69694800	-2.02387300	-2.80847900
H	5.52143200	-3.56259500	1.19086100
H	6.51707800	-3.60217000	-1.07857400
C	3.17168900	1.74121100	-0.02777000

C	4.56397800	1.86877100	-0.01845900
C	2.37639000	2.89149700	-0.06755400
C	5.15110600	3.12741400	-0.05080800
H	5.19355600	0.98669500	0.01393400
C	2.97353400	4.14628000	-0.10121000
H	1.29402200	2.80219400	-0.09581200
C	4.35747000	4.26804300	-0.09380100
H	6.23310000	3.21486200	-0.04327000
H	2.34579100	5.02974200	-0.14990500
H	4.81868300	5.25014300	-0.12665000
C	-2.82483700	1.04612300	1.16989200
C	-3.10468400	0.90496700	2.53159900
C	-2.85202700	2.32686500	0.60491600
C	-3.41078700	2.01521000	3.31102400
H	-3.07830500	-0.07005900	3.00397500
C	-3.16795200	3.43062800	1.38492400
H	-2.59160700	2.46731900	-0.43546500
C	-3.44795700	3.27971900	2.73862600
H	-3.62150000	1.88679700	4.36810700
H	-3.17995200	4.41608600	0.93094100
H	-3.68854600	4.14637600	3.34634000
C	-3.90934800	-0.64656500	-0.89875000
C	-3.88486200	-1.61207700	-1.90942900
C	-5.08927400	0.06552900	-0.67334600
C	-5.01888200	-1.86996600	-2.66755000
H	-2.96884900	-2.15656500	-2.10854600
C	-6.22087200	-0.18920600	-1.43994600
H	-5.12514200	0.82314200	0.10111400
C	-6.19000800	-1.15715300	-2.43569600
H	-4.98356700	-2.62209400	-3.44915000
H	-7.12995700	0.37431300	-1.25569500
H	-7.07404200	-1.35194400	-3.03432500
O	-0.38201000	1.77903700	-0.82644400
O	-0.22124300	3.06707000	-2.67040900
H	1.12225600	0.30574000	-2.16982300
H	0.63317800	0.72886800	-3.76051600
H	-0.80996100	-1.19483700	-3.24502800
H	-1.88776600	0.12724100	-2.67282600

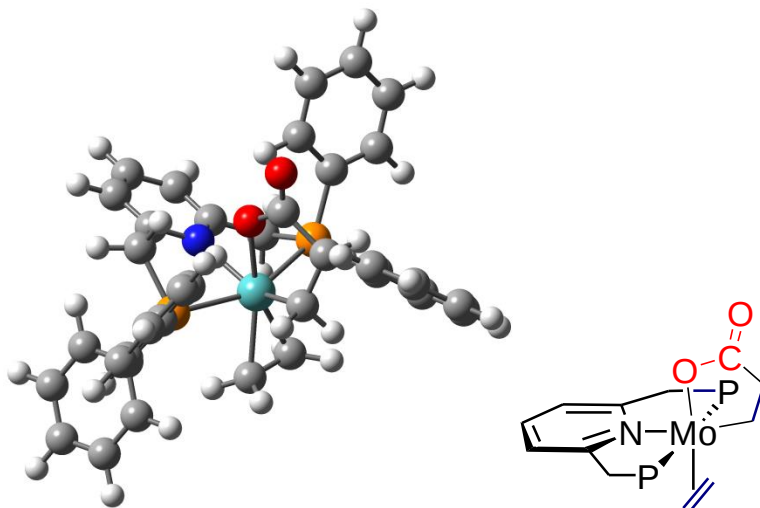
TS3-6a



Mo	-0.05649200	-0.20962100	-0.45845100
C	-1.03648700	-1.43938300	3.78863000
C	-1.09310200	-1.10717300	2.43776000
C	1.13089100	-0.40324000	2.47817400
C	1.24213000	-0.74107000	3.82280400
C	0.15127400	-1.28403200	4.48200400
H	-1.92604400	-1.81267200	4.28299800
H	2.17160600	-0.55063100	4.34711700
H	0.21800400	-1.55308400	5.53110200
N	-0.00530200	-0.64387800	1.78091900
C	2.23533300	0.34509000	1.80162300
H	1.97422600	1.40892900	1.84280600
H	3.18391700	0.23183400	2.33244000
C	-2.40027000	-1.22793000	1.70830300
H	-3.20756900	-0.89171000	2.36438700
H	-2.60098200	-2.27633000	1.47428300
P	2.37007300	0.06792200	-0.03985600
P	-2.40117600	-0.28146700	0.08734500
C	0.75010100	-2.31255400	-0.58914000
H	1.31470900	-2.48017400	-1.49857500
H	1.27074600	-2.64044600	0.30624000
C	-0.66081600	-2.40827100	-0.58779400
H	-1.11904400	-2.84844300	0.29150600
H	-1.19524300	-2.62958000	-1.50396200
C	-0.21198400	1.03536200	-2.45028100
C	-0.06595900	-0.44025000	-2.56603000
H	0.87181600	-0.76165300	-3.02126100
H	-0.91205800	-0.94603100	-3.03163800
C	-0.26289800	2.22504700	-0.97514300
C	3.57798500	-1.30767200	-0.19703900
C	4.16391700	-1.52974300	-1.44652900
C	3.89185700	-2.17018100	0.85265800
C	5.05104800	-2.57982300	-1.63625000
H	3.93136800	-0.86785700	-2.27575000
C	4.78124700	-3.22345100	0.66271700
H	3.43794700	-2.03254900	1.82916000
C	5.36432100	-3.42984900	-0.58026700

H	5.49941500	-2.73554200	-2.61233000
H	5.01569000	-3.88515300	1.49074100
H	6.05724400	-4.25177300	-0.72831600
C	3.50534700	1.48236100	-0.42981300
C	4.82752400	1.48276700	0.02974500
C	3.05363500	2.57798900	-1.16441700
C	5.66983800	2.55368300	-0.23468100
H	5.20851200	0.63039600	0.58371300
C	3.89825600	3.65144700	-1.43055400
H	2.03681000	2.61096200	-1.53172000
C	5.20638300	3.64213300	-0.96719900
H	6.69333400	2.53600900	0.12700100
H	3.52450700	4.49448600	-2.00233300
H	5.86597000	4.47820900	-1.17722300
C	-3.29421700	1.25080000	0.60871300
C	-4.49496700	1.66531100	0.02880800
C	-2.72280200	2.04450100	1.60950900
C	-5.11434300	2.83853900	0.44576600
H	-4.95731700	1.06898700	-0.75020200
C	-3.34730700	3.21109600	2.02889900
H	-1.76922000	1.76633800	2.04355000
C	-4.54545100	3.61222800	1.44867700
H	-6.04679800	3.14592400	-0.01746200
H	-2.88710600	3.81736700	2.80280000
H	-5.02825500	4.52905700	1.77181000
C	-3.71503000	-1.14778900	-0.86309000
C	-4.73383200	-1.89905200	-0.27273800
C	-3.70060200	-1.01407500	-2.25316900
C	-5.70524300	-2.51281400	-1.05449100
H	-4.78707200	-1.99880700	0.80638400
C	-4.67780400	-1.61846900	-3.03535700
H	-2.91690500	-0.43030100	-2.72436600
C	-5.67922400	-2.37417800	-2.43751200
H	-6.48894500	-3.09578200	-0.58073100
H	-4.65172400	-1.50344700	-4.11418800
H	-6.43895600	-2.85289500	-3.04700400
O	-0.07444400	1.84769100	0.20566600
O	-0.44456500	3.29797900	-1.47841600
H	-1.15944000	1.41257800	-2.82662700
H	0.61277500	1.57869100	-2.90594300

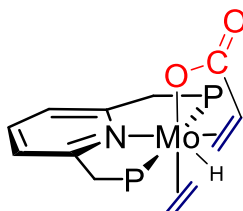
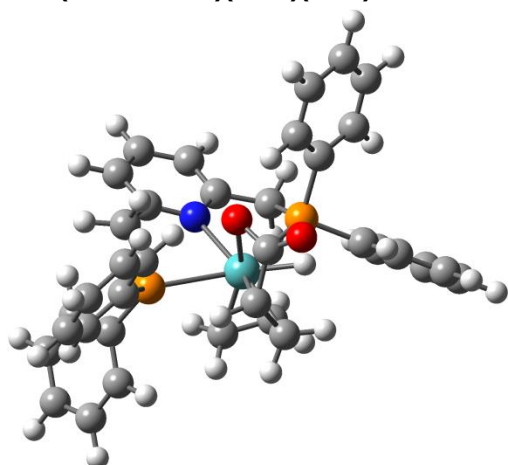
i6a



Mo	0.03612700	-0.27506100	-0.54736000
C	-1.07112200	-1.00640000	3.69676700
C	-1.02007600	-0.93500700	2.31009400
C	1.06187600	0.13135400	2.40738600
C	1.05312400	0.06982400	3.79285100
C	-0.02436500	-0.50513200	4.45101000
H	-1.93876100	-1.44904400	4.17185500
H	1.88548700	0.48961700	4.34615700
H	-0.05133300	-0.55021800	5.53441900
N	0.04358800	-0.37993300	1.66722700
C	2.17929900	0.78687800	1.67223000
H	1.85684400	1.80281600	1.42174500
H	3.09206200	0.84853700	2.26825800
C	-2.14563400	-1.45872300	1.47974800
H	-3.05490500	-1.54028900	2.07961000
H	-1.90365700	-2.45581300	1.09755000
P	2.42871100	0.02568900	-0.00553400
P	-2.35576600	-0.36599300	-0.03645900
C	0.82675700	-2.11674700	-1.53223000
H	1.30943600	-1.86246600	-2.47243500
H	1.42642600	-2.74658300	-0.88412300
C	-0.58400300	-2.20535400	-1.47851100
H	-1.04236300	-2.91819200	-0.79592000
H	-1.18251400	-2.03251700	-2.36831500
C	0.19250300	0.97167700	-2.29843000
C	-0.56291000	2.26219700	-2.10774400
C	-0.29006100	2.76926000	-0.69360100
C	3.46907100	-1.45218100	0.30343100
C	3.98651400	-2.16005900	-0.78835300
C	3.71034500	-1.94294600	1.58747300
C	4.74010800	-3.30998000	-0.59824100
H	3.79891600	-1.80698500	-1.79753900
C	4.45607500	-3.10208600	1.77745900
H	3.31240700	-1.42819800	2.45470700
C	4.97706400	-3.78564800	0.68726200
H	5.13698300	-3.84043000	-1.45786000
H	4.63132300	-3.46777300	2.78430800
H	5.56194500	-4.68749300	0.83623400

C	3.61965000	1.23684300	-0.72580000
C	4.96077400	0.94504400	-0.98570000
C	3.13853500	2.51573000	-1.02916700
C	5.79695700	1.90517300	-1.54464700
H	5.36450300	-0.03097500	-0.74289800
C	3.97906200	3.47398200	-1.58011900
H	2.10822700	2.77646400	-0.82029600
C	5.30932500	3.17024700	-1.84610000
H	6.83707600	1.66119700	-1.73782500
H	3.58568800	4.46058800	-1.80196500
H	5.96376100	3.91816100	-2.28246100
C	-3.37577600	0.99770000	0.66988300
C	-4.76816500	1.01807300	0.53498100
C	-2.74822100	2.02060600	1.38948700
C	-5.51655600	2.03693100	1.11068300
H	-5.27404300	0.24036200	-0.02630200
C	-3.50459900	3.03672000	1.96180400
H	-1.66688600	2.04761000	1.46081100
C	-4.88690800	3.04822500	1.82692000
H	-6.59582000	2.04155700	0.99278400
H	-2.99956700	3.83435100	2.49646400
H	-5.47218900	3.84905200	2.26805600
C	-3.57978900	-1.28527100	-1.04670000
C	-4.29669100	-2.39474500	-0.59667700
C	-3.77980600	-0.84287700	-2.35770400
C	-5.19270000	-3.04681200	-1.43807900
H	-4.16852700	-2.75985600	0.41692500
C	-4.68289600	-1.48567200	-3.19327100
H	-3.21794900	0.01082400	-2.72630400
C	-5.38975400	-2.59287400	-2.73571100
H	-5.73967000	-3.91105300	-1.07459900
H	-4.82857600	-1.12670500	-4.20699000
H	-6.08967200	-3.10156300	-3.39063000
O	-0.02382600	1.78935900	0.13361100
O	-0.31775200	3.94220900	-0.37650400
H	-1.64615000	2.09446600	-2.16298300
H	-0.32343300	3.05373700	-2.82501600
H	1.21434600	1.15321900	-2.64565800
H	-0.29544800	0.29001500	-3.01428900

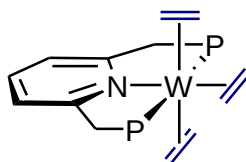
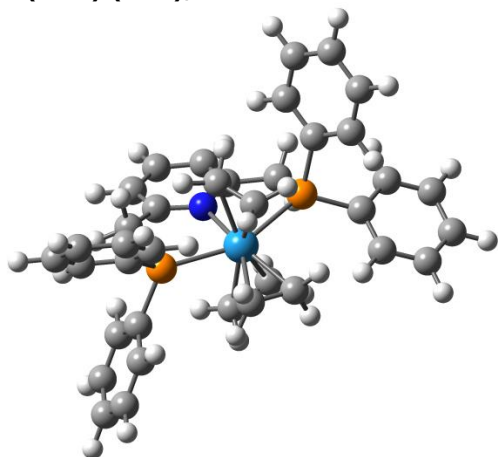
MoH(OOCCHCH₂)(C₂H₄)(PNP)



Mo	-0.07072300	-0.05152400	-0.61068800
C	-1.02507200	-2.05472100	3.41769500
C	-1.03769300	-1.56695300	2.11682100
C	1.06847300	-0.64870200	2.39002100
C	1.14419400	-1.13814400	3.68839000
C	0.08868700	-1.86149700	4.21504600
H	-1.89312200	-2.58656300	3.78920500
H	2.02094400	-0.91617400	4.28613900
H	0.12382200	-2.24397700	5.22934400
N	0.00868300	-0.88969200	1.57960800
C	2.14307700	0.25870900	1.89093800
H	1.77961100	1.28901000	1.97826600
H	3.05469100	0.18274500	2.48754500
C	-2.24806200	-1.76454400	1.26812600
H	-3.14486000	-1.84981100	1.88551800
H	-2.14662200	-2.68962400	0.69723500
P	2.44400400	0.08310100	0.08798000
P	-2.34101600	-0.35306600	0.06160400
C	0.67672400	-2.02369300	-1.32870200
H	1.37643000	-1.90873400	-2.15177000
H	1.05475000	-2.66834800	-0.53677600
C	-0.71176800	-2.01471000	-1.58729100
H	-1.32749600	-2.70980700	-1.02361700
H	-1.08009000	-1.86241500	-2.59575500
C	0.02892000	0.56526800	-2.90400400
C	0.55586200	1.52648000	-2.04531300
C	-0.18897100	2.51619600	-1.18472600
C	3.54177000	-1.36936400	-0.08729500
C	3.98377400	-1.71082900	-1.37041500
C	3.91085900	-2.18068000	0.98561100
C	4.79202000	-2.82101800	-1.56985300
H	3.69805600	-1.09894600	-2.22096200
C	4.71157900	-3.30015700	0.78357400
H	3.57035300	-1.95336200	1.98974400
C	5.15689400	-3.62067300	-0.49179400
H	5.13002100	-3.06745400	-2.57109500
H	4.98752800	-3.92232100	1.62901400
H	5.78217600	-4.49366200	-0.64776100
C	3.57608100	1.50667700	-0.18987100
C	4.92306100	1.34930600	-0.52483200

C	3.05964800	2.79919000	-0.03245400
C	5.73611700	2.46247200	-0.70576400
H	5.34748400	0.35864200	-0.63825600
C	3.87985600	3.90540300	-0.21233900
H	2.01155800	2.93108300	0.21920900
C	5.21782600	3.74182300	-0.55222400
H	6.78087400	2.32426900	-0.96574400
H	3.46322000	4.90024800	-0.09361600
H	5.85432500	4.60889100	-0.69717200
C	-3.27087400	0.90576400	1.03298800
C	-4.59758300	0.64927900	1.40009300
C	-2.66133500	2.09163700	1.44148100
C	-5.29887800	1.55863100	2.17756800
H	-5.09567100	-0.25355500	1.05858000
C	-3.37644500	3.00378700	2.21387600
H	-1.64363700	2.30783900	1.12495000
C	-4.68655000	2.74008800	2.58727300
H	-6.32851800	1.35252200	2.45330900
H	-2.90105300	3.93270800	2.51230700
H	-5.23863000	3.45729000	3.18703600
C	-3.63183500	-0.87444200	-1.13445600
C	-4.27464800	-2.11104800	-1.09576700
C	-3.99711700	0.04486000	-2.12252300
C	-5.25487000	-2.42770400	-2.03202600
H	-4.02424300	-2.84437200	-0.33676500
C	-4.97730600	-0.27041700	-3.05222900
H	-3.51435000	1.01734700	-2.16137400
C	-5.60745800	-1.51023400	-3.01177900
H	-5.74185400	-3.39692300	-1.99173900
H	-5.24877400	0.45583100	-3.81135500
H	-6.37183800	-1.75802200	-3.74114600
O	0.00471200	2.13887700	0.06481500
O	-0.87593600	3.43934900	-1.56836300
H	1.63649200	1.62733800	-2.00252800
H	0.71399200	-0.03474700	-3.49857100
H	-0.96874600	0.65329100	-3.31797300
H	-1.47600200	0.53903600	-1.39023200

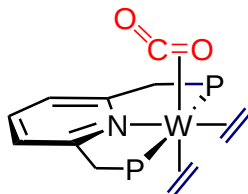
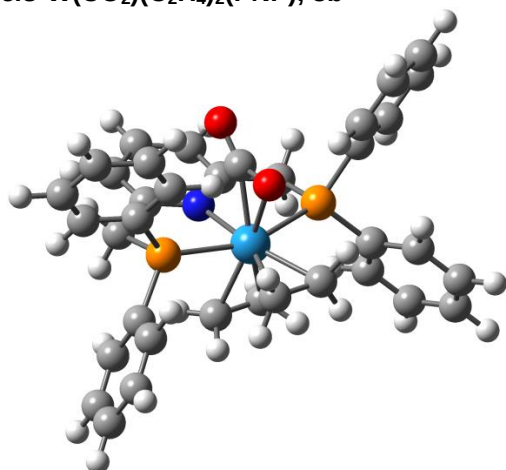
W(C₂H₄)₃(PNP), 1b



W	-0.00097000	-0.22078800	-0.39666100
C	1.14956700	-0.12924200	3.98415200
C	1.09815400	0.02185900	2.60360900
C	-1.16758400	-0.47291100	2.59292000
C	-1.17118600	-0.59549400	3.97863300
C	0.00444700	-0.45079400	4.69141200
H	2.09122000	0.03604600	4.49541000
H	-2.10486000	-0.82200000	4.48149800
H	0.02508800	-0.56697000	5.76963800
N	-0.03910700	-0.19465800	1.89017500
C	-2.46906200	-0.66763100	1.87299500
H	-2.71240000	-1.73311100	1.84451900
H	-3.27673400	-0.18449200	2.42910800
C	2.31054600	0.54517500	1.90144200
H	3.22267800	0.27261400	2.43666100
H	2.25367000	1.63932100	1.92794400
P	-2.41619300	-0.12603800	0.09942000
P	2.35460400	0.14716700	0.08782400
C	-0.43596400	1.74767700	-1.38543300
H	0.21000600	2.02386900	-2.21431800
H	-1.48068700	1.90230800	-1.64165700
C	-0.02523500	2.02243900	-0.04555400
H	-0.76577100	2.36817000	0.67201300
H	0.93179900	2.51668500	0.10774400
C	0.94993300	-0.51018800	-2.43715200
H	1.25764500	0.38431400	-2.97138300
H	1.70200600	-1.29434600	-2.46521300
C	-0.42068100	-0.91066300	-2.48811000
H	-0.60338500	-1.98217500	-2.57331400
H	-1.10979100	-0.30575600	-3.07169600
C	0.77954700	-2.32722900	-0.14505300
H	1.19143000	-2.74660700	-1.05925800
H	1.41181200	-2.52047800	0.71636100
C	-0.62698000	-2.36037800	0.07631700
H	-0.95407100	-2.57980800	1.08994500
H	-1.26692700	-2.81372300	-0.67259900
C	-3.34121500	1.47510500	0.16521200
C	-4.08244600	1.89782800	-0.94170300
C	-3.26132300	2.31986400	1.27461900
C	-4.73574400	3.12308400	-0.93379000

H	-4.16371800	1.25553600	-1.81331900
C	-3.91858700	3.54535700	1.28514800
H	-2.68325700	2.02624200	2.14579800
C	-4.65780700	3.95002900	0.18118200
H	-5.31098600	3.43100500	-1.80124700
H	-3.84864800	4.18563700	2.15897900
H	-5.17077100	4.90641800	0.18869700
C	-3.75432200	-1.18255200	-0.60731100
C	-4.98891900	-1.27270400	0.04483100
C	-3.57369900	-1.87634600	-1.80117000
C	-6.00998400	-2.05410600	-0.47748200
H	-5.16347500	-0.71351500	0.95898600
C	-4.60087700	-2.65257100	-2.33033400
H	-2.62519800	-1.80389100	-2.31432000
C	-5.81740900	-2.74713300	-1.66887300
H	-6.96139700	-2.11605100	0.04155200
H	-4.44386500	-3.18580200	-3.26254500
H	-6.61707800	-3.35495900	-2.08028700
C	3.62469600	-1.18072600	-0.04513900
C	4.29304400	-1.35828900	-1.25952900
C	3.91953000	-2.04386900	1.01145200
C	5.22942300	-2.37256900	-1.41168300
H	4.09219100	-0.68853000	-2.08934800
C	4.86168000	-3.05540800	0.86124100
H	3.40900700	-1.93941100	1.96383600
C	5.51827000	-3.22364300	-0.35105500
H	5.73930600	-2.49407400	-2.36215100
H	5.07835400	-3.71609400	1.69488600
H	6.25220800	-4.01436800	-0.46909000
C	3.41671700	1.55426700	-0.49080800
C	4.64619800	1.79242800	0.13378000
C	3.03489900	2.37903700	-1.54631300
C	5.46050000	2.83897600	-0.27467200
H	4.98198600	1.14143000	0.93535000
C	3.85400100	3.42473400	-1.96266200
H	2.08970500	2.20833300	-2.04271000
C	5.06470800	3.65984300	-1.32639600
H	6.41043800	3.00924200	0.22252100
H	3.53827100	4.05712100	-2.78626000
H	5.70253700	4.47631200	-1.65003700

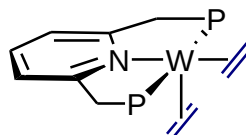
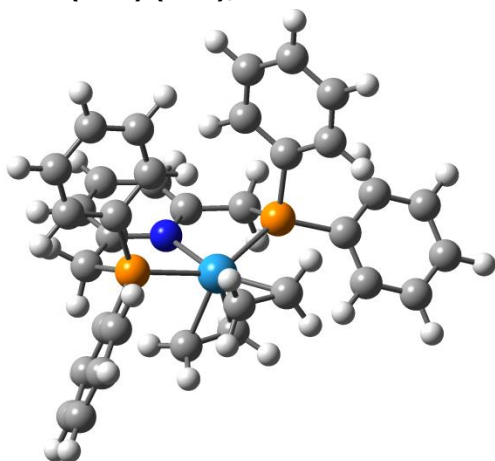
cis-W(CO₂)(C₂H₄)₂(PNP), 3b



W	0.00000500	0.35539400	-0.19052900
P	-2.39959000	0.01781000	0.16023900
P	2.39958400	0.01775700	0.16024100
O	-0.00000300	-2.78239900	0.40690000
O	-0.00002000	-1.46029700	-1.47274800
N	-0.00000700	-0.27474800	2.00393600
C	-0.00000700	-1.75608500	-0.22962500
C	0.71559600	2.23367600	0.78269500
H	1.21166100	2.16228000	1.74770200
H	1.23630800	2.88917500	0.09199000
C	-0.71553800	2.23369800	0.78269000
H	-1.23621800	2.88921400	0.09197600
H	-1.21161200	2.16233400	1.74769500
C	0.71079600	1.20076900	-2.13210900
H	1.24208700	2.14103000	-2.01480800
H	1.22823600	0.47043700	-2.74671100
C	-0.71071700	1.20078400	-2.13212500
H	-1.22815000	0.47045500	-2.74673600
H	-1.24199800	2.14105500	-2.01484800
C	2.48560000	-0.24655200	1.99563600
H	3.18668500	-1.05293700	2.21870600
H	2.89670000	0.64991800	2.46777800
C	1.16101400	-0.55904800	2.63694200
C	1.18489400	-1.12462800	3.90667300
H	2.14078200	-1.34252200	4.36901900
C	-0.00003800	-1.41342800	4.55582300
H	-0.00005000	-1.86448500	5.54234200
C	-1.18495400	-1.12455000	3.90667800
H	-2.14085400	-1.34237800	4.36903100
C	-1.16104300	-0.55897000	2.63694800
C	-2.48561000	-0.24637100	1.99565200
H	-2.89658300	0.65018700	2.46773500
H	-3.18678900	-1.05265100	2.21880000
C	-3.59761500	1.37956200	-0.17635300
C	-3.94787800	2.37060000	0.74144600
H	-3.53750700	2.37099400	1.74474300
C	-4.82403200	3.39186600	0.38878800
H	-5.08571200	4.14834000	1.12187500
C	-5.35640200	3.44675500	-0.89197000
H	-6.03841000	4.24475300	-1.16707900
C	-5.00798200	2.47097300	-1.81892000

H	-5.41636000	2.50213500	-2.82394500
C	-4.14107100	1.44702500	-1.46371700
H	-3.89329200	0.68321300	-2.19311500
C	-3.41736000	-1.38688200	-0.48132400
C	-4.69940700	-1.59104400	0.04267300
H	-5.08509900	-0.92739100	0.81171300
C	-5.50379000	-2.61714400	-0.42887600
H	-6.49487200	-2.76287400	-0.01055000
C	-5.04216300	-3.44998700	-1.44434100
H	-5.67009100	-4.25358900	-1.81624600
C	-3.77918500	-3.24541400	-1.98039000
H	-3.41234300	-3.89071900	-2.77212300
C	-2.96553400	-2.21991000	-1.50447200
H	-1.97367700	-2.08007800	-1.91734200
C	3.59763900	1.37950900	-0.17624900
C	4.14107000	1.44708700	-1.46361700
H	3.89325400	0.68335400	-2.19308700
C	5.00799800	2.47104900	-1.81873600
H	5.41635600	2.50230100	-2.82376700
C	5.35646500	3.44672800	-0.89169500
H	6.03848700	4.24473700	-1.16673900
C	4.82412300	3.39172400	0.38906900
H	5.08583900	4.14811700	1.12222700
C	3.94794900	2.37044500	0.74164200
H	3.53760000	2.37074900	1.74494900
C	3.41732800	-1.38690200	-0.48142700
C	4.69936500	-1.59114000	0.04256400
H	5.08506000	-0.92756900	0.81167400
C	5.50373100	-2.61721000	-0.42907800
H	6.49480600	-2.76300300	-0.01075700
C	5.04209700	-3.44994400	-1.44462900
H	5.67001200	-4.25352300	-1.81660600
C	3.77912600	-3.24529600	-1.98066800
H	3.41227800	-3.89051800	-2.77246700
C	2.96549200	-2.21982200	-1.50465800
H	1.97363600	-2.07993400	-1.91751400

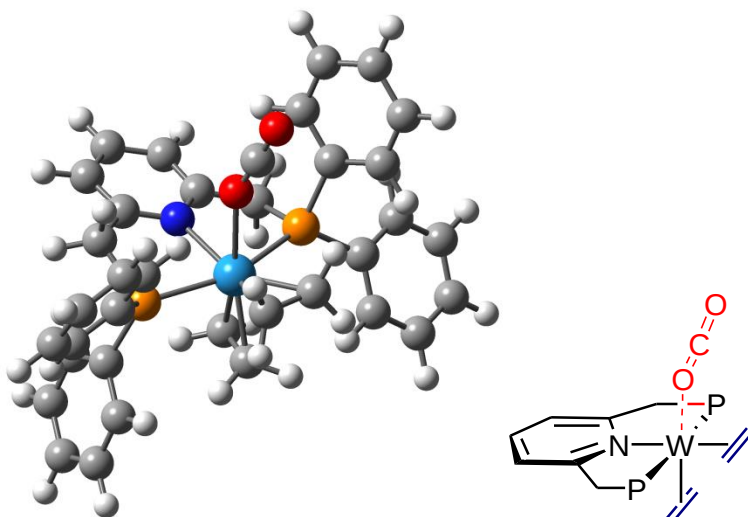
***cis*-W(C₂H₄)₂(PNP), i1b**



W	-0.00745900	-0.81135100	-0.11863400
C	1.11169000	0.97642700	3.88816000
C	1.11284600	0.35924600	2.64907900
C	-1.20498700	0.34956700	2.61745900
C	-1.24635600	0.96029700	3.85858300
C	-0.07733000	1.29517800	4.52623400
H	2.06647100	1.20245400	4.35118500
H	-2.21626700	1.17112100	4.29679000
H	-0.09261700	1.77900200	5.49570800
N	-0.03611800	0.05468400	1.95382400
C	-2.49442700	0.02295600	1.93559500
H	-2.81736200	-0.98633700	2.21231700
H	-3.29169400	0.70763500	2.23451600
C	2.43370900	0.03416400	2.02051800
H	2.76000900	-0.95366700	2.35340000
H	3.20146600	0.74666700	2.32937900
P	-2.27676400	-0.08433300	0.11247500
P	2.25511100	-0.05610200	0.19468700
C	0.78619100	-1.25510100	-2.11370100
H	1.22742900	-0.40894600	-2.64488400
H	1.42443800	-2.13572000	-2.12825100
C	-0.64197300	-1.39608800	-2.15237700
H	-1.07517400	-2.39230400	-2.20803200
H	-1.21041100	-0.66229400	-2.72493600
C	0.75920300	-2.57421100	0.91570600
H	1.31929300	-3.23202600	0.25151300
H	1.22474000	-2.47670400	1.89783300
C	-0.68389500	-2.63786100	0.86989300
H	-1.22645000	-2.58337800	1.81479300
H	-1.12810800	-3.35816500	0.18394300
C	-2.55689100	1.60988300	-0.54405900
C	-3.15538900	1.82918800	-1.78721400
C	-2.03534300	2.70269400	0.15684000
C	-3.23631000	3.11351700	-2.31478500
H	-3.56658600	0.99340900	-2.34422800
C	-2.13417800	3.98668200	-0.36324600
H	-1.53943800	2.54631600	1.11025200
C	-2.73243700	4.19520700	-1.60272100
H	-3.69980200	3.26810700	-3.28417400
H	-1.73746400	4.82616300	0.19910500

H	-2.80428900	5.19805400	-2.01168000
C	-3.84451900	-0.93170300	-0.35659500
C	-5.08043300	-0.30309700	-0.17212600
C	-3.81708000	-2.23598400	-0.84605200
C	-6.26179000	-0.96837500	-0.47112900
H	-5.11934600	0.71781500	0.19584400
C	-5.00073700	-2.90196900	-1.14757600
H	-2.86186400	-2.72627300	-0.98424400
C	-6.22327500	-2.26999500	-0.96149600
H	-7.21466400	-0.46940000	-0.32436200
H	-4.96479900	-3.91702200	-1.53023700
H	-7.14668200	-2.78897400	-1.19862600
C	3.68749200	-1.06276600	-0.36184500
C	4.24179300	-0.83028800	-1.62533700
C	4.15780300	-2.15190200	0.37694500
C	5.24690500	-1.64900900	-2.12393000
H	3.89033600	0.00326600	-2.22392900
C	5.16702800	-2.96754000	-0.12053000
H	3.73388100	-2.38606700	1.34640300
C	5.71706900	-2.71867200	-1.37154300
H	5.66331100	-1.44820100	-3.10599100
H	5.52059200	-3.80391300	0.47418700
H	6.50418300	-3.35699100	-1.75977000
C	2.71943400	1.63348700	-0.38183800
C	4.02866000	2.11782800	-0.29565300
C	1.71584500	2.48146800	-0.84813200
C	4.32433300	3.41986600	-0.67604600
H	4.82396300	1.46930500	0.05950000
C	2.01320100	3.78275400	-1.23893700
H	0.68964100	2.12182500	-0.88302000
C	3.31704800	4.25374100	-1.15328600
H	5.34427300	3.78471800	-0.60378200
H	1.22058200	4.42651200	-1.60654300
H	3.55062300	5.27019700	-1.45442800

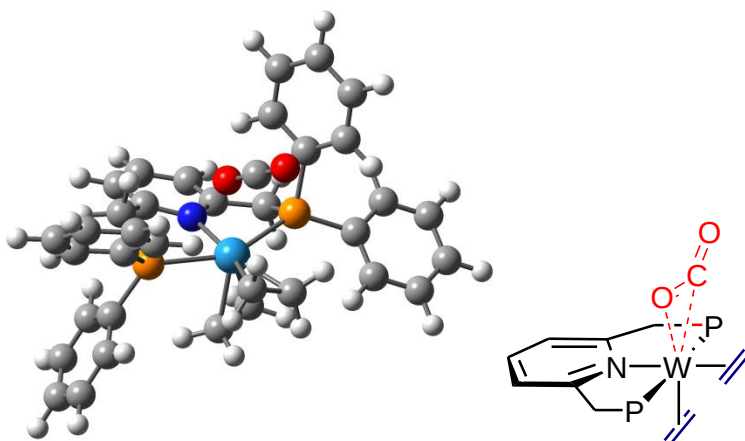
i2b



W	0.03959700	-0.11654500	-0.41890900
C	-1.05286400	-0.52672500	3.95048900
C	-1.02504500	-0.54494900	2.55964800
C	1.16604800	0.22885400	2.55892700
C	1.19257500	0.23336200	3.94858600
C	0.06698100	-0.13962700	4.66418300
H	-1.95649700	-0.84233500	4.45977000
H	2.09619300	0.55305900	4.45519500
H	0.06461500	-0.13130000	5.74890900
N	0.07128500	-0.15441600	1.85005000
C	2.36834100	0.70369700	1.81113200
H	2.30123600	1.79084100	1.68959800
H	3.28859600	0.51181500	2.37080200
C	-2.21579600	-1.06803100	1.82186500
H	-3.13630300	-0.89992300	2.38717000
H	-2.10590900	-2.15257100	1.70939500
P	2.39865500	0.07934200	0.06344100
P	-2.27068900	-0.42747900	0.08368700
C	0.46885700	-1.98042200	-1.46172800
H	-0.22464500	-2.26791800	-2.25334700
H	1.49843700	-2.10246200	-1.79571200
C	0.16423500	-2.32160400	-0.09974800
H	0.97197600	-2.67248500	0.54246200
H	-0.75838400	-2.87065700	0.09389100
C	-0.86225200	0.46548000	-2.38274500
H	-1.27061600	-0.33836200	-2.98912000
H	-1.53245800	1.32629500	-2.33705700
C	0.54686000	0.73267700	-2.40902000
H	0.85686500	1.77635900	-2.40364000
H	1.19236900	0.11635300	-3.02674700
C	-0.83193100	3.25969600	-0.23967800
C	3.43453800	-1.44293200	0.14547400
C	3.94646000	-1.98695600	-1.03867000
C	3.57804800	-2.17448000	1.32680900
C	4.61261400	-3.20515700	-1.03299800
H	3.83724700	-1.44366400	-1.97290800
C	4.24274800	-3.39600400	1.33232600
H	3.16519300	-1.79772300	2.25717100

C	4.76598000	-3.91316000	0.15411900
H	5.00885500	-3.60523000	-1.96107000
H	4.34872900	-3.94568500	2.26254300
H	5.28337000	-4.86714600	0.15842200
C	3.60210900	1.30563600	-0.62828100
C	4.97819700	1.07278500	-0.68630200
C	3.12320800	2.55413400	-1.03202700
C	5.84559300	2.05549600	-1.15115500
H	5.37938600	0.11754900	-0.36764800
C	3.98912900	3.53968900	-1.48837500
H	2.05866200	2.75121300	-0.99217000
C	5.35489100	3.29045300	-1.55549600
H	6.91123100	1.85232900	-1.19354000
H	3.59430300	4.50098000	-1.80219400
H	6.03281600	4.05537700	-1.92071100
C	-3.30641700	1.09199300	0.22868800
C	-3.99786100	1.57045200	-0.89007800
C	-3.31455900	1.86502600	1.39456000
C	-4.68591700	2.77679300	-0.83918400
H	-4.01189600	0.98440900	-1.80352100
C	-4.00784000	3.06972000	1.44618200
H	-2.77600800	1.52855700	2.27576300
C	-4.69551500	3.53011300	0.32916900
H	-5.21879600	3.12821300	-1.71716200
H	-4.00986800	3.64985900	2.36395000
H	-5.23201900	4.47242800	0.36799300
C	-3.50173700	-1.59005200	-0.65725100
C	-4.82755100	-1.60644100	-0.21236800
C	-3.10679000	-2.50110500	-1.63535900
C	-5.73656300	-2.51706700	-0.73343200
H	-5.15532500	-0.89103200	0.53609300
C	-4.01866900	-3.41274000	-2.15889900
H	-2.08208400	-2.49844300	-1.98445400
C	-5.33258600	-3.42264700	-1.70977700
H	-6.76348300	-2.51752100	-0.38098900
H	-3.69788200	-4.11575900	-2.92100300
H	-6.04370100	-4.13278800	-2.12012000
O	-0.36173000	2.22424800	0.00867700
O	-1.24177200	4.31687500	-0.46761700

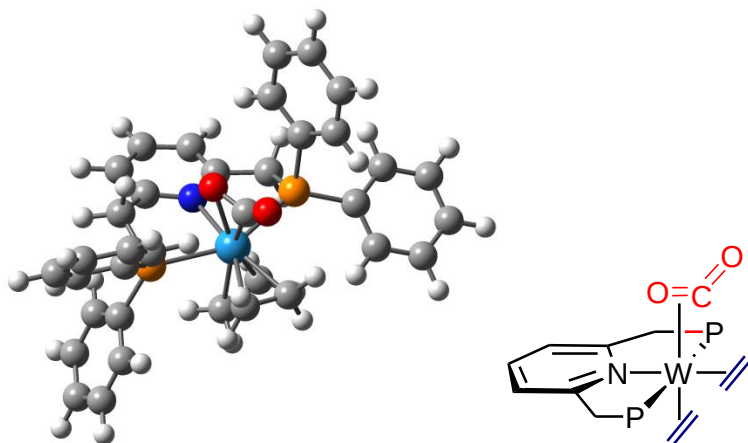
TS2-3b



W	-0.01318100	-0.29212600	-0.50093000
C	-0.98945000	-1.72806100	3.63148100
C	-1.03788900	-1.33244600	2.30315700
C	1.11895100	-0.47990600	2.46216200
C	1.20547300	-0.87968300	3.77971600
C	0.14929400	-1.54386300	4.39735300
H	-1.87378800	-2.19124500	4.05743500
H	2.10889200	-0.64085500	4.33152100
H	0.20426100	-1.86975800	5.42912000
N	0.03562600	-0.74980600	1.64603900
C	2.21076500	0.34705800	1.87625200
H	1.93140300	1.40536100	1.95094500
H	3.15110500	0.22473900	2.41829100
C	-2.32614900	-1.49383600	1.56078000
H	-3.18187100	-1.36721000	2.22986600
H	-2.41354900	-2.48570600	1.11036400
P	2.37025600	0.08303600	0.05525000
P	-2.36903400	-0.35979300	0.09780700
C	0.79329800	-2.19396900	-1.23835000
H	0.92025500	-2.20611800	-2.32273500
H	1.65074600	-2.61744300	-0.72580000
C	-0.50080600	-2.45532300	-0.69553100
H	-0.53368500	-3.00264100	0.24621700
H	-1.30816500	-2.72778900	-1.37121700
C	-0.73554900	-0.17893600	-2.59373800
H	-0.73474000	-1.12808500	-3.13492300
H	-1.63121700	0.40678600	-2.79598000
C	0.49883200	0.54407900	-2.48541100
H	0.44710900	1.62678800	-2.63583100
H	1.38963400	0.12348300	-2.94864100
C	-0.64748900	2.89828900	-0.65034000
C	3.62653600	-1.24737600	-0.10906900
C	4.41580400	-1.32343600	-1.25843800
C	3.76110400	-2.23319100	0.87060000
C	5.32921700	-2.35673700	-1.41933400
H	4.32395800	-0.56469800	-2.02952500
C	4.67924000	-3.26493700	0.70894900
H	3.13936900	-2.20802200	1.76019000
C	5.46547600	-3.32916000	-0.43470300
H	5.93746200	-2.40181600	-2.31722300
H	4.77501900	-4.02347800	1.47946500

H	6.17974500	-4.13649800	-0.56060300
C	3.42268400	1.54733900	-0.35825300
C	4.67674200	1.69724700	0.24519800
C	2.98220800	2.53631100	-1.23479700
C	5.45762900	2.81541800	-0.01064100
H	5.05375700	0.92456500	0.90819000
C	3.76695900	3.65570400	-1.49742200
H	2.02846200	2.41658800	-1.73071600
C	5.00296000	3.80003200	-0.88287400
H	6.42718000	2.91638200	0.46707700
H	3.41071500	4.41172200	-2.19009600
H	5.61595400	4.67224400	-1.08672200
C	-3.07977700	1.20458000	0.76733000
C	-3.88248100	2.02875700	-0.02737500
C	-2.73406600	1.64004900	2.05053800
C	-4.33667200	3.25186000	0.45253500
H	-4.16542900	1.70719200	-1.02491100
C	-3.19531600	2.85983000	2.53143000
H	-2.09884500	1.02419100	2.67933900
C	-3.99689600	3.66949800	1.73422200
H	-4.95911700	3.87858100	-0.17815700
H	-2.92483700	3.17881200	3.53320900
H	-4.35450300	4.62279500	2.11004100
C	-3.81852000	-1.03613800	-0.81315600
C	-5.07374100	-1.04695600	-0.19352300
C	-3.69466600	-1.58592800	-2.08808600
C	-6.17468300	-1.59875700	-0.83352800
H	-5.19554900	-0.60896100	0.79242700
C	-4.80009900	-2.13586600	-2.73034500
H	-2.73158600	-1.58284500	-2.57948600
C	-6.03976700	-2.14504200	-2.10615200
H	-7.14087600	-1.60007200	-0.33877000
H	-4.68645200	-2.55766700	-3.72385100
H	-6.90089400	-2.57459600	-2.60825400
O	-0.15222200	2.17100200	0.11562100
O	-1.11616700	3.64569200	-1.39229400

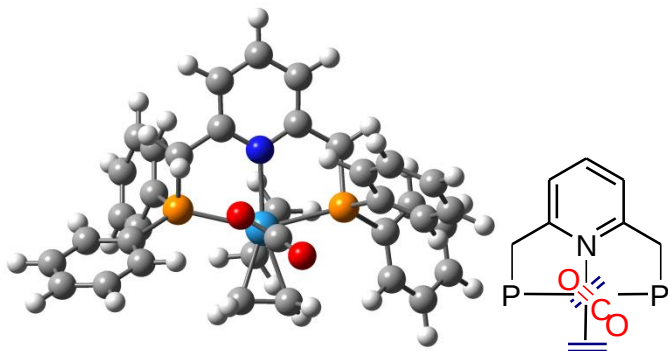
i3b



W	0.00116200	-0.29333600	-0.45070500
C	1.17280000	-0.65289100	3.89263900
C	1.08990500	-0.32429700	2.54391100
C	-1.11480500	-1.07066500	2.45522800
C	-1.08604700	-1.38967500	3.80914100
C	0.08004700	-1.21228100	4.53202200
H	2.08584000	-0.43727000	4.43529600
H	-1.98236300	-1.77673800	4.28004700
H	0.12699800	-1.47539800	5.58352300
N	-0.01909400	-0.59999900	1.81168300
C	-2.40147800	-1.21947600	1.70061000
H	-2.54890600	-2.26031200	1.40140800
H	-3.24316500	-0.95868600	2.34796000
C	2.19778800	0.45095300	1.90524000
H	3.13097800	0.36286500	2.46564700
H	1.89882700	1.50508800	1.92684600
P	-2.39417400	-0.25362800	0.11178300
P	2.37037500	0.13875500	0.08459400
C	-0.37981100	1.71646300	-0.95794100
C	0.85670200	-0.03124300	-2.56233000
H	1.05588700	0.98936300	-2.86804800
H	1.66696700	-0.72319500	-2.77214100
C	-0.47891900	-0.50828700	-2.63895800
H	-0.62689000	-1.54182300	-2.94507300
H	-1.23442700	0.18298400	-2.99790900
C	0.80598400	-2.34559800	-0.79800000
H	1.13976500	-2.53638100	-1.81469900
H	1.52192900	-2.69229100	-0.05789400
C	-0.57719800	-2.47589400	-0.46837200
H	-0.79994700	-2.90656800	0.50603700
H	-1.28383300	-2.78857600	-1.22911800
C	-3.14286900	1.35189600	0.60427300
C	-3.78082500	2.12717500	-0.36623800
C	-3.01667900	1.86032300	1.89744400
C	-4.30644000	3.37002100	-0.04175100
H	-3.86463400	1.76061900	-1.38398800
C	-3.54496300	3.10398600	2.22186000
H	-2.49089100	1.29725100	2.66174600
C	-4.19517300	3.85939500	1.25441800
H	-4.79695700	3.96143300	-0.80792700
H	-3.43924400	3.48632800	3.23233300

H	-4.60434700	4.83243000	1.50689900
C	-3.80718400	-1.03477100	-0.76459000
C	-5.06926100	-1.05533000	-0.16115000
C	-3.65058200	-1.61117800	-2.02304800
C	-6.14498500	-1.65818600	-0.79751300
H	-5.21790100	-0.57666700	0.80197200
C	-4.73184600	-2.20860400	-2.66361900
H	-2.68238900	-1.58231000	-2.50310000
C	-5.97727500	-2.23818500	-2.05138400
H	-7.11889900	-1.66706300	-0.31838900
H	-4.59636700	-2.64853000	-3.64637300
H	-6.82005100	-2.70453600	-2.55170200
C	3.63981700	-1.17291200	-0.04684500
C	4.31126800	-1.34257900	-1.26080500
C	3.90668100	-2.05588100	1.00001700
C	5.23429200	-2.36733400	-1.41814100
H	4.12002900	-0.66168700	-2.08398700
C	4.83315500	-3.08086700	0.84142200
H	3.38565000	-1.95615600	1.94721100
C	5.49928900	-3.23859200	-0.36695400
H	5.74989300	-2.48456400	-2.36587000
H	5.03159400	-3.75875400	1.66556300
H	6.22153200	-4.03895200	-0.49086100
C	3.34169400	1.62588100	-0.40215500
C	4.67069700	1.74378200	0.02068100
C	2.76936900	2.66539200	-1.13641400
C	5.41099800	2.87802700	-0.28228400
H	5.13623300	0.93722100	0.57845200
C	3.51648400	3.79921800	-1.43978700
H	1.74210400	2.60985900	-1.47139100
C	4.83375100	3.90938600	-1.01552900
H	6.44139700	2.95390500	0.05075500
H	3.05677500	4.59852200	-2.01159000
H	5.41204700	4.79601500	-1.25599300
O	-0.05447000	1.78323900	0.27959200
O	-0.66488400	2.53294400	-1.80227600

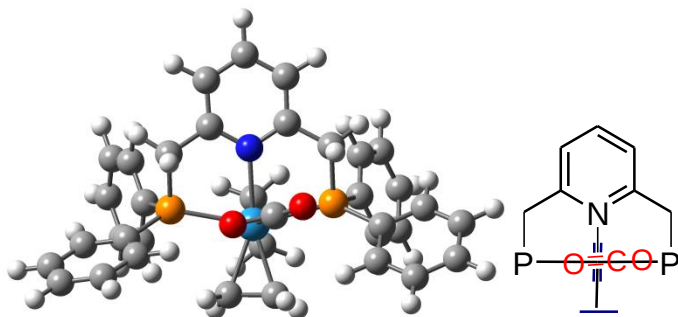
TS3-4b



W	-0.03734600	-0.06339900	-0.49983700
C	1.06160300	0.11095500	3.90903000
C	1.01326600	0.25604200	2.52858700
C	-1.14675700	-0.59784400	2.46846100
C	-1.15668800	-0.73343300	3.85392000
C	-0.03651300	-0.39057600	4.58757800
H	1.96062800	0.40257000	4.43909100
H	-2.04307800	-1.12673100	4.33851200
H	-0.01888700	-0.50797900	5.66587300
N	-0.07013400	-0.11390900	1.80232800
C	-2.35602800	-1.01435600	1.69302500
H	-2.22953300	-2.05629200	1.38669400
H	-3.26348800	-0.95009600	2.29804500
C	2.16981700	0.87632200	1.81655400
H	3.08892000	0.74438700	2.39062700
H	1.97229900	1.94863800	1.73195200
P	-2.50111500	-0.12537700	0.08012900
P	2.32787400	0.24004600	0.07639300
C	-0.48826000	1.94174800	-1.36955900
H	0.04952900	2.19807400	-2.27647100
H	-1.55295200	2.13826300	-1.45177300
C	0.15780100	2.16296900	-0.12179400
H	-0.44353900	2.45362400	0.74043600
H	1.12698200	2.65496800	-0.14179000
C	0.71184200	-0.23797200	-2.64271900
H	0.98270800	0.69779800	-3.11976500
H	1.44218000	-1.03166400	-2.76968400
C	-0.66263000	-0.60884500	-2.58264200
H	-0.89992900	-1.66427100	-2.70058700
H	-1.40864200	0.05009300	-3.01786900
C	0.61875600	-2.07925100	-0.68751400
C	-3.35451200	1.44333300	0.47459200
C	-3.91359000	2.20235500	-0.56001500
C	-3.38366400	1.95579100	1.77296100
C	-4.50197100	3.43159500	-0.29675500
H	-3.90072900	1.82435200	-1.57764900
C	-3.96847900	3.19030600	2.03368100
H	-2.94579900	1.39725100	2.59325900
C	-4.53015900	3.92960300	1.00133000
H	-4.93503100	4.00448400	-1.11018800
H	-3.98365900	3.57295200	3.04917400
H	-4.98634700	4.89270300	1.20567800
C	-3.77928200	-1.14309200	-0.75601700
C	-5.13353600	-0.80165500	-0.76512400

C	-3.37380800	-2.34436000	-1.34649500
C	-6.06345900	-1.63823700	-1.37197100
H	-5.46930400	0.11757900	-0.29864300
C	-4.30920600	-3.17861600	-1.94453500
H	-2.32844600	-2.62898300	-1.31619800
C	-5.65373200	-2.82549000	-1.96545200
H	-7.11259300	-1.35974000	-1.37550400
H	-3.98141000	-4.10747000	-2.39982600
H	-6.38120800	-3.47635300	-2.44000700
C	3.53591600	-1.12931100	0.35035300
C	3.16043300	-2.17564000	1.19782400
C	4.81282000	-1.14310000	-0.20854000
C	4.04614600	-3.20158200	1.48978400
H	2.15906700	-2.20693700	1.61603200
C	5.69547100	-2.18099400	0.07361700
H	5.12814700	-0.34332600	-0.86871000
C	5.31732300	-3.20903100	0.92537400
H	3.73455400	-4.00946800	2.14400000
H	6.68262700	-2.18159900	-0.37796800
H	6.00639400	-4.01868000	1.14402100
C	3.40043200	1.50936400	-0.71528600
C	4.08252700	2.49215000	0.00583400
C	3.56849000	1.46047600	-2.10208000
C	4.89481500	3.41448600	-0.64413900
H	3.99675500	2.54546500	1.08538300
C	4.38768100	2.37719500	-2.74962200
H	3.05937800	0.69646300	-2.67621900
C	5.04843500	3.36094600	-2.02365200
H	5.41202600	4.17449800	-0.06698200
H	4.50525700	2.32250000	-3.82710900
H	5.68283100	4.08101400	-2.53041800
O	-0.45719600	-2.18553800	-0.01049000
O	1.39714800	-2.86105100	-1.16865100

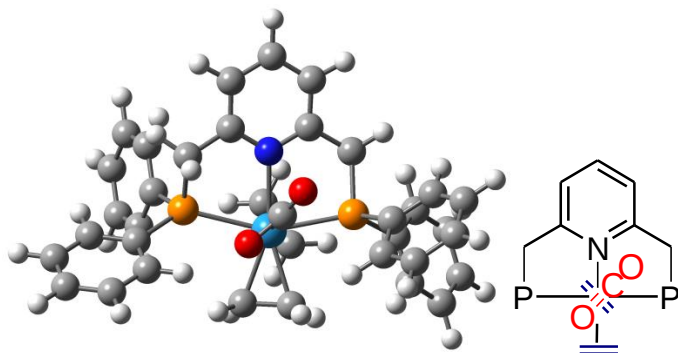
i4b



W	-0.05181000	-0.45084400	-0.28687900
C	1.12344300	1.33463500	3.70005200
C	1.10485400	0.63356200	2.49909400
C	-1.21711500	0.55735100	2.53599300
C	-1.25127700	1.25092200	3.74017600
C	-0.06708800	1.67156600	4.32039100
H	2.07662200	1.59055400	4.14818500
H	-2.20513000	1.43933200	4.21943000
H	-0.07067300	2.22429200	5.25381000
N	-0.05805800	0.30993200	1.88364700
C	-2.47698200	-0.01833700	1.97008600
H	-2.48575500	-1.08712700	2.21479100
H	-3.37078900	0.41760600	2.42088900
C	2.38731600	0.13186500	1.91603000
H	2.49385200	-0.91527300	2.22675700
H	3.24956500	0.67984600	2.30019200
P	-2.50260900	-0.04063700	0.12435800
P	2.37661500	-0.02264500	0.07210100
C	0.00328200	1.75971200	-0.54295200
H	-0.93893200	2.26785900	-0.35857600
H	0.82395900	2.30062300	-0.08048300
C	0.20792600	1.12922000	-1.81490400
H	1.16814200	1.22785600	-2.31381700
H	-0.61699900	1.15330500	-2.52423000
C	0.51045400	-1.77723200	-2.01963200
H	1.17160700	-1.32517800	-2.75156400
H	0.80383400	-2.78171300	-1.72620200
C	-0.88682400	-1.51901800	-2.06638000
H	-1.55482000	-2.32439200	-1.77715400
H	-1.29210000	-0.87744400	-2.84275200
C	0.58265800	-2.15627400	0.83391200
C	-3.24597900	1.53982600	-0.41439200
C	-3.41313800	1.74648200	-1.78756200
C	-3.61341600	2.55327700	0.47056200
C	-3.94845500	2.93614100	-2.26069900
H	-3.12625900	0.96956400	-2.48942200
C	-4.14471100	3.74692200	-0.00593300
H	-3.47819200	2.42655400	1.53921100
C	-4.31533500	3.93992500	-1.37055900
H	-4.07249900	3.08231200	-3.32869000
H	-4.42381300	4.52802800	0.69393700
H	-4.72871200	4.87216500	-1.74135500
C	-3.85691800	-1.24693000	-0.18863100
C	-5.15033600	-0.82915700	-0.51289100
C	-3.59791200	-2.61613900	-0.05686000

C	-6.16347200	-1.76088800	-0.70845000
H	-5.37389700	0.22619800	-0.61737400
C	-4.61720300	-3.54038300	-0.24863500
H	-2.59998300	-2.95357000	0.19730500
C	-5.89997100	-3.11805700	-0.57782900
H	-7.16209000	-1.42009600	-0.96310600
H	-4.40119500	-4.59897200	-0.14567200
H	-6.69135300	-3.84468100	-0.73242200
C	3.79019500	-1.17544000	-0.18316700
C	3.60771600	-2.45964600	-0.68819300
C	5.08134900	-0.75780800	0.15823300
C	4.69515000	-3.30942800	-0.85703100
H	2.61164300	-2.79815600	-0.92832500
C	6.16432900	-1.61108200	-0.00011500
H	5.24690200	0.24598000	0.53678400
C	5.97297800	-2.88970000	-0.51300000
H	4.53653000	-4.30784500	-1.25146700
H	7.15979000	-1.27412700	0.27168200
H	6.81977400	-3.55649200	-0.64239600
C	3.17685200	1.52869700	-0.51615200
C	3.26598100	2.67769300	0.27079700
C	3.69971400	1.56280500	-1.81220100
C	3.86967800	3.83030700	-0.22077800
H	2.85900400	2.68527400	1.27707800
C	4.29876500	2.71397700	-2.30472200
H	3.65467400	0.67431600	-2.43473400
C	4.38652200	3.85136600	-1.50934700
H	3.93243500	4.71386600	0.40658300
H	4.70087700	2.72145200	-3.31270000
H	4.85697900	4.75066800	-1.89365400
O	-0.66980300	-2.32366800	0.68887800
O	1.44219000	-2.78318200	1.41615000

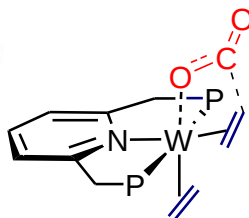
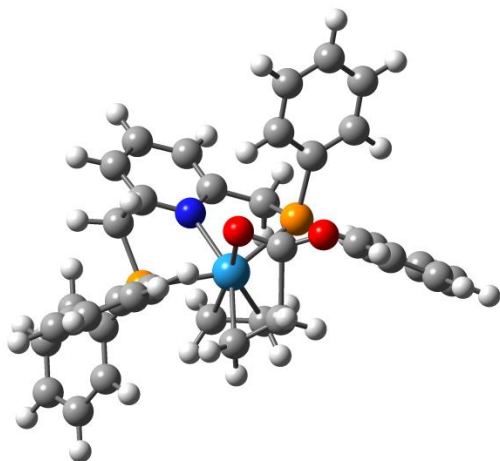
TS4-3b



W	-0.03565900	-0.04049700	-0.45495400
C	0.96617700	0.71780800	3.89392500
C	0.95195400	0.63348400	2.50670100
C	-1.24611300	-0.11241800	2.53674500
C	-1.29447600	-0.00893500	3.92087000
C	-0.17251400	0.40843800	4.61556600
H	1.87233400	1.03613100	4.39592300
H	-2.20030600	-0.29602600	4.44259500
H	-0.18110600	0.47685900	5.69801700
N	-0.14795000	0.23534800	1.82700600
C	-2.39745300	-0.72110100	1.79997000
H	-2.19539900	-1.79421300	1.69148900
H	-3.33491300	-0.63019200	2.35352600
C	2.16446500	1.06578700	1.73802800
H	3.05346900	1.01464100	2.36876000
H	2.01628100	2.12038900	1.47890100
P	-2.51855700	-0.15069200	0.04787100
P	2.35433200	0.21275900	0.10119900
C	-0.40919400	2.16672900	-0.26279200
H	-1.43258000	2.48199400	-0.42991400
H	0.01094600	2.61767600	0.63495000
C	0.43652400	1.93594900	-1.38283000
H	1.45518300	2.30542800	-1.38395500
H	-0.00925900	1.98720300	-2.37450800
C	0.73796800	-0.71615700	-2.44936700
H	1.37966400	-0.01580300	-2.97352200
H	1.11141700	-1.73752900	-2.43035400
C	-0.67751500	-0.55060000	-2.51477700
H	-1.30071700	-1.43638000	-2.56410900
H	-1.08656600	0.29305500	-3.06539600
C	0.48515800	-1.88914100	0.53287800
C	-3.51556200	1.38297000	0.09617300
C	-3.94006900	1.93590900	-1.11697500
C	-3.80128000	2.05974900	1.28082800
C	-4.64778600	3.12906200	-1.13935400
H	-3.71580500	1.42759500	-2.05010400
C	-4.50749100	3.25856300	1.25650400
H	-3.46512800	1.66578100	2.23394600
C	-4.93431100	3.79403500	0.04892200
H	-4.97210600	3.54402800	-2.08816300
H	-4.72160300	3.77439200	2.18713200
H	-5.48462400	4.72908300	0.03098500
C	-3.73276000	-1.36656900	-0.62325800
C	-5.10523300	-1.09644400	-0.61225100

C	-3.29287100	-2.60396400	-1.10514400
C	-6.01466500	-2.03541200	-1.08382300
H	-5.47251100	-0.14753700	-0.23867000
C	-4.20842800	-3.53948400	-1.57241900
H	-2.23672000	-2.83895100	-1.09296200
C	-5.56890400	-3.25847600	-1.56875300
H	-7.07570800	-1.80660900	-1.07035200
H	-3.84961600	-4.49402700	-1.94397100
H	-6.27955600	-3.99025700	-1.93986900
C	3.57929700	-1.14013900	0.37705100
C	3.46616800	-2.34273300	-0.31677100
C	4.70681100	-0.92267100	1.16978600
C	4.45357900	-3.31435200	-0.20907500
H	2.59458100	-2.52925400	-0.93234500
C	5.68632600	-1.89907500	1.29101200
H	4.84175200	0.02240100	1.68691000
C	5.56121300	-3.09907000	0.60052200
H	4.34699200	-4.24866900	-0.75067700
H	6.55203800	-1.71884600	1.92062800
H	6.32744900	-3.86242700	0.69145000
C	3.51106300	1.33948600	-0.80041200
C	3.93133900	2.58784600	-0.34088200
C	3.99482600	0.88737300	-2.03276500
C	4.80653500	3.36566900	-1.09356000
H	3.58760300	2.97754800	0.61113800
C	4.86172100	1.66534800	-2.78557800
H	3.69694700	-0.08778200	-2.40378900
C	5.27133200	2.90995500	-2.31866700
H	5.12190700	4.33318800	-0.71563500
H	5.22204500	1.29571000	-3.74026800
H	5.95121200	3.51836500	-2.90619500
O	-0.42382700	-2.24930700	-0.26818200
O	1.09572700	-2.41734200	1.42990100

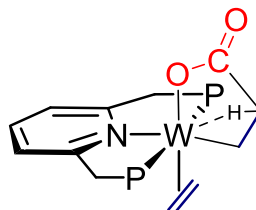
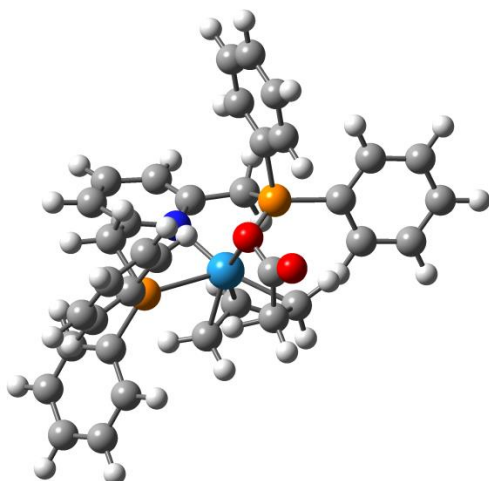
TS4-5b



W	0.04954900	-0.01478200	-0.50770600
C	-1.03191400	-2.02620800	3.36479700
C	-1.01216300	-1.50853500	2.08484900
C	1.06733900	-0.54496400	2.46028500
C	1.10178200	-1.07339300	3.74436900
C	0.04351500	-1.82250600	4.22350900
H	-1.88978400	-2.61078900	3.67669500
H	1.96193800	-0.86156000	4.37028800
H	0.04880700	-2.23139600	5.22728100
N	0.02508500	-0.75687100	1.59607100
C	2.17656600	0.34274700	1.99898700
H	1.87318300	1.39253900	2.10398200
H	3.08556900	0.20757100	2.58948300
C	-2.15160800	-1.78565500	1.15391700
H	-3.06024000	-2.01667700	1.71502200
H	-1.89713400	-2.64770900	0.52780500
P	2.42078200	0.14822300	0.18532100
P	-2.33199200	-0.32969300	0.05351800
C	0.62908800	-2.11142000	-0.97153000
H	1.57176700	-2.22509500	-1.50294000
H	0.53315500	-2.82532400	-0.15267400
C	-0.52290200	-1.76560900	-1.74132500
H	-1.45985500	-2.28081900	-1.54365400
H	-0.39819800	-1.60594000	-2.81488200
C	-0.18970200	1.15743200	-2.53673200
C	1.07240700	0.45299400	-2.39767900
H	1.94346100	1.10496200	-2.42684100
H	1.22207300	-0.44249900	-3.00373100
C	-0.97313100	2.08615100	-0.96865800
C	3.54754700	-1.27367500	-0.02324000
C	4.14362700	-1.48077000	-1.27161900
C	3.76913600	-2.20190900	0.99346600
C	4.95970500	-2.58208400	-1.48828200
H	3.97183400	-0.77350000	-2.07704900
C	4.58624000	-3.30592600	0.77322400
H	3.29675600	-2.07767700	1.96205100
C	5.18543000	-3.49687500	-0.46486100
H	5.41794900	-2.72823100	-2.46109700
H	4.75241800	-4.01885400	1.57456700
H	5.82285800	-4.35848100	-0.63491600
C	3.50922000	1.58008100	-0.19561600

C	4.89794100	1.49736400	-0.05849500
C	2.93137000	2.80240200	-0.54932400
C	5.69361700	2.61453000	-0.28072800
H	5.36270600	0.55602400	0.21374700
C	3.73249400	3.91752900	-0.76655600
H	1.85357200	2.87691500	-0.63742800
C	5.11303100	3.82613700	-0.63721900
H	6.77115600	2.53572000	-0.17608100
H	3.27168900	4.86089900	-1.04140400
H	5.73620200	4.69728600	-0.81314600
C	-3.26673700	0.81127000	1.16449800
C	-4.65397500	0.72464500	1.30163200
C	-2.55942500	1.71729700	1.95545200
C	-5.32120700	1.52733200	2.21806600
H	-5.21858300	0.03781800	0.67913000
C	-3.22994700	2.51835700	2.87230100
H	-1.48681900	1.81563800	1.83034800
C	-4.60945600	2.42407200	3.00707900
H	-6.40064400	1.45725500	2.31031800
H	-2.67131100	3.22758900	3.47484600
H	-5.13155600	3.05489600	3.71976300
C	-3.59058300	-0.78460500	-1.18912600
C	-4.21176900	-2.03424900	-1.21577500
C	-3.93317900	0.16953600	-2.15294900
C	-5.15661300	-2.32984400	-2.19318700
H	-3.96902500	-2.78893700	-0.47509900
C	-4.87914000	-0.13102900	-3.12406600
H	-3.46184600	1.14767100	-2.13281700
C	-5.49121000	-1.37989800	-3.14906600
H	-5.63054400	-3.30627700	-2.20419300
H	-5.13781900	0.61699100	-3.86663100
H	-6.22803500	-1.61147300	-3.91159500
O	-1.99944400	2.61314400	-1.29400500
O	-0.10124500	2.24045900	-0.08510200
H	-0.06874300	2.20883900	-2.79827600
H	-1.00786300	0.71343800	-3.09521300

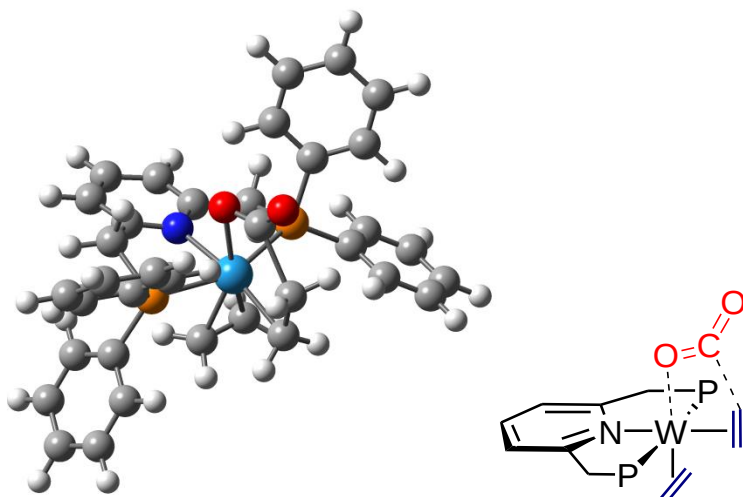
i5b



W	-0.02284600	-0.41235200	-0.54301000
C	-1.04846000	-2.44174600	3.28224500
C	-1.12990900	-1.80939200	2.05429200
C	0.97912000	-0.87821500	2.36877100
C	1.09490400	-1.50587900	3.59227800
C	0.09103900	-2.34388200	4.06518200
H	-1.90810100	-3.01167500	3.61990200
H	1.97636900	-1.30299300	4.19164600
H	0.17431700	-2.85140600	5.01846200
N	-0.08183700	-1.08624400	1.50956900
C	1.96901800	0.15198800	1.96383000
H	1.51240600	1.14124000	2.10402000
H	2.87753100	0.12509900	2.56905300
C	-2.42027200	-1.80827600	1.29857300
H	-3.28155100	-1.83985900	1.97073400
H	-2.51014100	-2.66227900	0.62176700
P	2.33006200	0.15812200	0.16031100
P	-2.39591700	-0.35609800	0.17980000
C	0.98663000	-2.28144700	-1.13830100
H	1.27578000	-2.27711800	-2.19151700
H	1.77393200	-2.67476100	-0.50093700
C	-0.36641900	-2.60073700	-0.80764300
H	-0.51420600	-3.18833500	0.09681100
H	-1.04095400	-2.89117200	-1.60928300
C	-0.82732300	-0.36882000	-2.53821900
C	0.25035100	0.66925100	-2.72969200
C	-0.16814700	1.97871000	-2.07537300
C	3.69419800	-1.01617900	-0.15051000
C	4.24757700	-1.08547000	-1.43256200
C	4.16048300	-1.88618000	0.83476600
C	5.25825000	-1.99275800	-1.71561900
H	3.89322500	-0.42012300	-2.21452500
C	5.16940900	-2.79997100	0.54688700
H	3.72977500	-1.87072500	1.82988900
C	5.72223900	-2.85309300	-0.72539900
H	5.68198600	-2.03182300	-2.71388600
H	5.51986100	-3.47370200	1.32209500
H	6.50909800	-3.56611100	-0.94865200
C	3.13914500	1.79662600	-0.01766600
C	4.52957900	1.93805500	-0.05703200

C	2.33173200	2.93868200	-0.05521800
C	5.10214600	3.20138100	-0.13458300
H	5.16901600	1.06318800	-0.02556500
C	2.91400400	4.19816500	-0.13465300
H	1.25052400	2.83996800	-0.04808200
C	4.29612700	4.33325100	-0.17530000
H	6.18284200	3.29919900	-0.16336600
H	2.27610400	5.07439800	-0.18103200
H	4.74587800	5.31877600	-0.24348000
C	-2.81317100	1.08959400	1.21889900
C	-3.07439400	0.96010700	2.58542900
C	-2.85135700	2.36434100	0.64100700
C	-3.37189400	2.07776100	3.35771300
H	-3.03746600	-0.01068900	3.06553300
C	-3.15861900	3.47505000	1.41432600
H	-2.61045200	2.49389100	-0.40569400
C	-3.41934400	3.33637500	2.77343500
H	-3.56745700	1.95954700	4.41882300
H	-3.18081700	4.45600400	0.95101200
H	-3.65373200	4.20843500	3.37580300
C	-3.88707600	-0.61607400	-0.85312100
C	-3.85332400	-1.59080500	-1.85463400
C	-5.06387500	0.10908000	-0.65407700
C	-4.97635700	-1.84380600	-2.63063100
H	-2.93984000	-2.14698100	-2.03114800
C	-6.18415100	-0.14186100	-1.43808100
H	-5.10647600	0.87266500	0.11414300
C	-6.14454200	-1.11819000	-2.42545600
H	-4.93465300	-2.60317100	-3.40486800
H	-7.09133400	0.43081500	-1.27387400
H	-7.01972600	-1.30991800	-3.03790200
O	-0.39534700	1.73392700	-0.80757800
O	-0.26561000	3.04676200	-2.63640100
H	1.18008800	0.34730600	-2.14129400
H	0.65826200	0.72503700	-3.74187400
H	-0.69277600	-1.24677000	-3.17534900
H	-1.82231100	0.05210400	-2.67457900

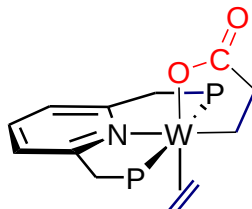
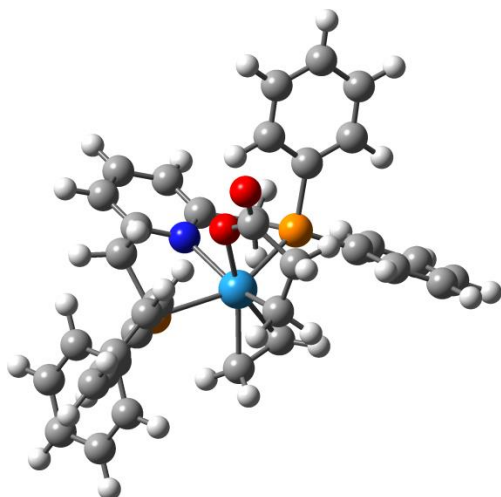
TS3-6b



W	-0.04829300	-0.23437200	-0.39497300
C	-1.04552000	-1.30150400	3.86628000
C	-1.09904300	-1.01576800	2.50650000
C	1.12649800	-0.30271100	2.53471700
C	1.22834000	-0.59613700	3.88980900
C	0.13767100	-1.12100300	4.56248500
H	-1.93769400	-1.65863500	4.36773400
H	2.15573000	-0.38702900	4.41059000
H	0.19984800	-1.35624200	5.61981500
N	-0.00667400	-0.57015400	1.83237200
C	2.24132900	0.41436300	1.84607000
H	1.99649700	1.48249600	1.85659600
H	3.18691900	0.30143000	2.38200300
C	-2.40689300	-1.15993500	1.78437100
H	-3.21538500	-0.81006700	2.43171000
H	-2.60324600	-2.21327000	1.57149000
P	2.35283700	0.08802400	0.00695500
P	-2.38731900	-0.25941600	0.13893000
C	0.77874400	-2.30554400	-0.42582400
H	1.32632900	-2.54972800	-1.32936800
H	1.30019200	-2.61725600	0.47586900
C	-0.64696700	-2.40922800	-0.40079900
H	-1.07573300	-2.83787900	0.49931300
H	-1.17909700	-2.70837300	-1.29728600
C	-0.17771300	0.87735700	-2.47878400
C	-0.06734600	-0.58185000	-2.51599200
H	0.86567100	-0.95947200	-2.93591500
H	-0.92528500	-1.10408200	-2.93922600
C	-0.25707700	2.15542200	-0.92118000
C	3.57785700	-1.27090500	-0.14656200
C	4.15884700	-1.49631000	-1.39728800
C	3.91444000	-2.11351200	0.91189500
C	5.06213500	-2.53376700	-1.58085100
H	3.90930200	-0.84791400	-2.23206900
C	4.82097500	-3.15291200	0.72826600
H	3.46400900	-1.97165700	1.88942000
C	5.39770700	-3.36488400	-0.51687400
H	5.50584300	-2.69395600	-2.55832000
H	5.07319700	-3.80012900	1.56246300

H	6.10351100	-4.17665400	-0.66013800
C	3.46227000	1.50939700	-0.43557800
C	4.77346400	1.55509700	0.05285000
C	3.01311900	2.55668500	-1.23860200
C	5.60588800	2.62422700	-0.24664000
H	5.15491500	0.73734800	0.65667700
C	3.84819600	3.62854600	-1.54049000
H	2.00626000	2.55415600	-1.63424700
C	5.14396400	3.66576100	-1.04549700
H	6.62064500	2.64149100	0.13885600
H	3.47654300	4.43412100	-2.16524400
H	5.79557000	4.50074400	-1.28292600
C	-3.26544100	1.29990800	0.60105000
C	-4.42700400	1.73290900	-0.04125700
C	-2.72488600	2.09430700	1.61809000
C	-5.03719600	2.92653100	0.32818100
H	-4.86612100	1.13428300	-0.83181700
C	-3.33955900	3.28241200	1.98941800
H	-1.80384400	1.79663900	2.10657900
C	-4.49792700	3.70259800	1.34561000
H	-5.93924200	3.24807600	-0.18307100
H	-2.90391600	3.88868800	2.77744400
H	-4.97369200	4.63511100	1.63223800
C	-3.69765200	-1.13869600	-0.80479600
C	-4.71918400	-1.87853400	-0.20517000
C	-3.67948600	-1.02585700	-2.19662900
C	-5.69050100	-2.50154400	-0.97965100
H	-4.77447400	-1.96265000	0.87514800
C	-4.65619000	-1.64035400	-2.97155700
H	-2.89412600	-0.45049200	-2.67483900
C	-5.66091000	-2.38427200	-2.36456000
H	-6.47681800	-3.07511400	-0.49881000
H	-4.62715100	-1.54210500	-4.05197500
H	-6.42037400	-2.87045900	-2.96846200
O	-0.05806300	1.81649100	0.26855700
O	-0.45518900	3.18872400	-1.48663200
H	-1.11654000	1.29643600	-2.82772000
H	0.66569500	1.42412300	-2.89084300

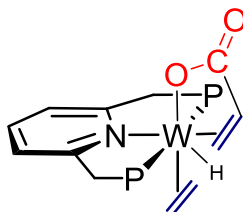
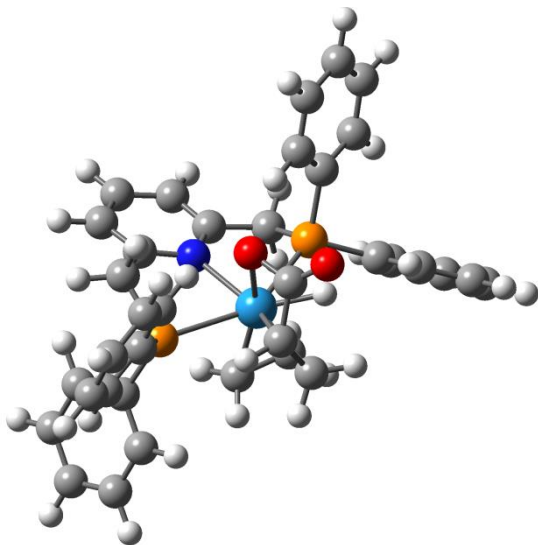
i6b



W	0.03012400	-0.26099300	-0.50115300
C	-1.05279100	-1.14534900	3.71024300
C	-1.01714300	-1.02079000	2.32759000
C	1.04079900	0.10355700	2.45653600
C	1.03475700	-0.00502600	3.83603100
C	-0.02007000	-0.64007200	4.47992300
H	-1.90539500	-1.62959000	4.17202100
H	1.85659000	0.42060300	4.40065900
H	-0.03980300	-0.72530500	5.56082700
N	0.03401800	-0.41539200	1.69212000
C	2.14720000	0.79828600	1.74228400
H	1.81418500	1.81342500	1.50383800
H	3.05611900	0.86402300	2.34336800
C	-2.14483400	-1.51793800	1.48968700
H	-3.04902000	-1.62996000	2.09249100
H	-1.90676400	-2.49200900	1.05078700
P	2.40869700	0.06480400	0.05315500
P	-2.34530100	-0.35235200	0.01829600
C	0.81959000	-2.02541600	-1.54649200
H	1.27783000	-1.77540200	-2.50078400
H	1.41752900	-2.70613800	-0.94818800
C	-0.60803800	-2.12452400	-1.47358000
H	-1.04003300	-2.89066600	-0.83058300
H	-1.20986100	-1.95318600	-2.36175000
C	0.15711100	0.96314300	-2.28848100
C	-0.58414900	2.26606400	-2.07279300
C	-0.29532500	2.75982500	-0.66225700
C	3.44961100	-1.41692100	0.33111300
C	3.94622600	-2.11903600	-0.77381000
C	3.72349500	-1.90727600	1.60874000
C	4.70909300	-3.26592100	-0.60272600
H	3.73518900	-1.76399800	-1.77741000
C	4.47864700	-3.06324700	1.77939600
H	3.34435700	-1.39541300	2.48585100
C	4.97720600	-3.74262000	0.67620700
H	5.08927300	-3.79273700	-1.47205000
H	4.67880800	-3.42970100	2.78127300
H	5.56957900	-4.64194500	0.81019300
C	3.59168100	1.29232600	-0.65216500

C	4.92347100	0.99439200	-0.95075900
C	3.11513900	2.58181200	-0.91473800
C	5.75546000	1.95977000	-1.50677800
H	5.32344500	0.00942900	-0.74016000
C	3.95172900	3.54458700	-1.46375600
H	2.09297200	2.84963200	-0.67668000
C	5.27267800	3.23560800	-1.76768100
H	6.78839400	1.71105800	-1.73012600
H	3.56208100	4.53911000	-1.65475000
H	5.92348000	3.98750900	-2.20262300
C	-3.32656300	1.00625100	0.78014900
C	-4.71491500	1.08221900	0.62643000
C	-2.67664500	1.96781800	1.56212800
C	-5.43755400	2.09479600	1.24452000
H	-5.23760100	0.35269200	0.01793300
C	-3.40714000	2.97759200	2.17712900
H	-1.59652700	1.95654700	1.64726700
C	-4.78594400	3.04404500	2.02309800
H	-6.51392400	2.14309100	1.11138800
H	-2.88512600	3.72784500	2.76176400
H	-5.35085100	3.83996400	2.49825900
C	-3.58253700	-1.20459300	-1.03075200
C	-4.33703600	-2.30074000	-0.61134900
C	-3.76457100	-0.71860200	-2.32877200
C	-5.25313600	-2.89879100	-1.47069400
H	-4.22156200	-2.69589800	0.39226400
C	-4.68711400	-1.30827400	-3.18224400
H	-3.17500000	0.12633600	-2.67363200
C	-5.43190900	-2.40287200	-2.75565500
H	-5.82985300	-3.75346400	-1.13144700
H	-4.81863600	-0.91728800	-4.18597600
H	-6.14749100	-2.86941600	-3.42489300
O	-0.03989000	1.76460600	0.16127700
O	-0.28976300	3.92611100	-0.32730100
H	-1.66962100	2.10509200	-2.11536300
H	-0.35098700	3.06346500	-2.78509900
H	1.17509200	1.15661200	-2.64641900
H	-0.33672500	0.33988800	-3.04970600

WH(OOCCHCH₂)(C₂H₄)(PNP)



W	-0.05214400	-0.09285800	-0.54785100
C	-1.02551000	-1.95888400	3.53412400
C	-1.04500800	-1.49340900	2.22536900
C	1.07749800	-0.60323600	2.46769000
C	1.15576400	-1.07302200	3.77182800
C	0.09647000	-1.77383300	4.32030500
H	-1.90004900	-2.46929000	3.92009600
H	2.03996000	-0.85061600	4.35820200
H	0.13465700	-2.14138100	5.33984800
N	0.00940300	-0.84335700	1.66129200
C	2.15919600	0.29161100	1.96202800
H	1.80596400	1.32568300	2.04853600
H	3.07081200	0.21071200	2.55746900
C	-2.27757200	-1.68769400	1.40851000
H	-3.16146200	-1.71969700	2.04881100
H	-2.21608500	-2.63840000	0.87593800
P	2.44537500	0.10473400	0.16277000
P	-2.34785000	-0.33148700	0.14586000
C	0.71804500	-2.08192700	-1.09276500
H	1.41321300	-2.07140900	-1.92891400
H	1.07950600	-2.69875600	-0.26902100
C	-0.68766000	-2.09083400	-1.36435900
H	-1.28958000	-2.77170400	-0.76685100
H	-1.03358900	-2.05071700	-2.39216000
C	0.14252000	0.33967600	-2.82859000
C	0.60287100	1.39863900	-2.01881400
C	-0.19613600	2.42257100	-1.25392400
C	3.56999700	-1.32473500	-0.01599900
C	4.00337300	-1.66906900	-1.30098800
C	3.97239400	-2.11311900	1.06154100
C	4.83673200	-2.76112100	-1.49752700
H	3.69020200	-1.07569200	-2.15491000
C	4.79918700	-3.21387900	0.86241900
H	3.63732000	-1.88391000	2.06706300
C	5.23602000	-3.53786000	-0.41494700
H	5.16748600	-3.01149900	-2.50015300
H	5.10137100	-3.81883100	1.71132600

H	5.88138300	-4.39645200	-0.56893100
C	3.53627500	1.55143200	-0.15008400
C	4.88512700	1.42024800	-0.48818300
C	2.98784500	2.83327600	-0.01578500
C	5.66928100	2.54951100	-0.69534700
H	5.33283400	0.43821500	-0.58539400
C	3.77917800	3.95555900	-0.22257400
H	1.93649900	2.94352900	0.23254700
C	5.11947700	3.81816200	-0.56528400
H	6.71576900	2.43231600	-0.95844500
H	3.33801300	4.94198500	-0.12431300
H	5.73308900	4.69773200	-0.73192100
C	-3.29589700	0.97011200	1.04058400
C	-4.63109300	0.73021100	1.38790200
C	-2.69493500	2.17256200	1.41129200
C	-5.34891300	1.67269800	2.10870900
H	-5.12204000	-0.18670900	1.07495100
C	-3.42602500	3.11754100	2.12708700
H	-1.67206900	2.37258000	1.10332900
C	-4.74471300	2.87058900	2.48108500
H	-6.38498400	1.47918800	2.36901500
H	-2.95689700	4.05866200	2.39579900
H	-5.30975200	3.61336500	3.03595600
C	-3.60823800	-0.90233400	-1.05928200
C	-4.27753600	-2.12133000	-0.95892500
C	-3.92547000	-0.04306500	-2.11537300
C	-5.23454600	-2.48229200	-1.90288000
H	-4.06643500	-2.80659100	-0.14532300
C	-4.88310700	-0.40239100	-3.05273500
H	-3.42030300	0.91444700	-2.20376500
C	-5.53811400	-1.62571200	-2.95165600
H	-5.74129900	-3.43810300	-1.81451600
H	-5.11654200	0.27638700	-3.86645400
H	-6.28384900	-1.90798800	-3.68781100
O	-0.04314600	2.10009200	0.02862800
O	-0.88655200	3.31599100	-1.69110800
H	1.67486900	1.56372000	-1.96851000
H	0.88968000	-0.24822400	-3.36026100
H	-0.81729900	0.38026600	-3.33138400
H	-1.42349500	0.45690400	-1.42428500