Supporting Information

Synthesis of Heteropnictogen Ligands via P^I Transfer

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1. Author Contributions

L. Zimmermann: conceptualization, synthesis and characterization of **1-As**, **1-Sb**, **2-As** and **2-Sb**, writing of original draft

M. A. Land: synthesis of [(BZIMPY)P][OTf], performance and interpretation of DFT computations

C. Riesinger: refinement of crystallographic data

C. L. B. Macdonald: project administration, funding acquisition

M. Scheer: project administration, funding acquisition

All authors contributed in preparing the final manuscript.

2. General considerations

All manipulations were carried out using standard Schlenk techniques at a Stock apparatus under N_2 as an inert gas or in a glovebox with Ar atmosphere. The nitrogen inert gas was passed over a BASF R 3-1 ($CuO/MgSiO_3$) catalyst to remove traces of oxygen. Trace moisture was removed by passing the nitrogen inert gas through concentrated sulfuric acid, orange gel and sica-pent. All glassware was dried with a heatgun (600 °C) for at least 30 min prior to use. *o*-DFB and CD_2Cl_2 were distilled from CaH_2 and other solvents were directly taken from an MBraun SPS-800 solvent purification system, and degassed at room temperature prior to use. Solution ^{1}H (400.130 MHz), ^{11}B (128.379 MHz), ^{13}C (100.627 MHz), ^{19}F (376.498 MHz) and ^{31}P (161.976 MHz) NMR spectra were recorded on a Bruker Avance400 spectrometer using $(H_3C)_4Si$ (^{1}H, ^{13}C), $BF_3{\cdot}Et_2O$ (^{11}B), $CFCl_3$ (^{19}F) or 85% phosphoric acid (^{31}P), respectively, as external standards. Chemical shifts (δ) are provided in parts per million (ppm) and coupling constants (*J*) are reported in Hertz (Hz). The following abbreviations are used: s = singlet, d = doublet, dd = doublet of doublets, t = triplet, br = broad and m = multiplet. Elemental analysis of the products was conducted by the elemental analysis department at the University of Regensburg using an Elementar Vario EL. ESI mass spectra were either recorded at the internal mass spectrometry department using a ThermoQuest Finnigan TSQ 7000 mass spectrometer. FD-MS was performed on a ThermoQuest Finnigan MAT 95 mass spectrometer. The peak assignment was performed using the molecular weight calculator 6.50.[1] IR spectra were recorded as solids using a ThermoFisher Nicolet iS5 FT-IR spectrometer with an iD7 ATR module and an ITX Germanium or ITX Diamond crystal. The starting materials $[\{CpMo(CO)_2\}_2(\mu,\eta^{2:2}\text{-}P_2)]$[2] (**A**), $[\{CpMo(CO)_2\}_2(\mu,\eta^{2:2}\text{-}PAs)]$[2b] (**B**), $[\{CpMo(CO)_2\}_2(\mu,\eta^{2:2}\text{-}PSb)]$[2b] (**C**), [(BZIMPY)P][OTf],[4] $K[BArF_{20}]$,[5] $CpMo(CO)_3H$[6] and $[CPh_3][BArF_{24}]$[7] were synthesized following literature procedures. All other chemicals were purchased from commercial vendors.

3. Compound synthesis

Reaction of [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] with [(BZIMPY)P][OTf] and K[B(C$_6$F$_5$)$_4$]

[{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] (275 mg, 0.5 mmol, 1 equiv.), [(BZIMPY)P][OTf] (335 mg, 0.5 mmol, 1 equiv.) and K[B(C$_6$F$_5$)$_4$] (350 mg, 0.5 mmol, 1 equiv.) were dissolved in 15 mL *o*-DFB and the reaction mixture was stirred for 48 h, at ambient temperature. The color of the reaction mixture was purple for the first 24 h and then gradually changed to red. The solvent of the reaction mixture was removed under reduced pressure (10^{-3} mbar) and the red residue was extracted with toluene (3 x 30 mL). The solvent of the toluene extract was removed *in vacuo*. The red residue was pre-adsorbed onto dried silica gel using CH_2Cl_2 (10 mL) and purified by column chromatography (15 x 3 cm). Elution with *n*-hexane yielded a yellow fraction containing [CpMo(CO)$_2$(η^3-P$_2$As)] (**1-As**). Changing the eluent to a mixture of *n*-hexane/toluene (3:1) led to a red fraction of unreacted starting material, [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] (**B**). Elution with a mixture of toluene/CH_2Cl_2 (1:1) led to a dark red fraction of [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][B(C$_6$F$_5$)$_4$] (**2-As**). The solvent of all fractions was removed under reduced pressure (10^{-3} mbar) and the resulting powders were dried *in vacuo*.

Fraction 1: **1-As**

Yellow crystals of **1-As** were obtained by storing a concentrated solution in *n*-hexane at -30 °C overnight.

Yield:	33 mg (0.093 mmol, 18%).
Elemental analysis:	calc. (%) for $C_7H_5O_2MoP_2As\cdot(C_6H_{14})_{0.5}$: C: 30.25, H: 3.04.
	found (%): C: 30.56, H: 2.31.
FD-MS (*n*-hexane):	*m/z* (%) = 355.82 (100%) [(**1-As**)]$^+$ (M^+).
NMR (CD_2Cl_2, r.t.):	^{1}**H**: *δ*/ppm = 5.32 (s, 5 H, Cp).
	^{31}**P{^{1}H}**: *δ*/ppm = -313.0 (s, 2 P, P$_2$As).
	^{31}**P**: *δ*/ppm = -313.0 (s, 2 P, P$_2$As).
IR:	$\tilde{\nu}$(CO)/cm^{-1} = 1972 (m), 1925 (s).

Fraction 2: **B**

Yield:	111 mg (0.4 mmol, 40%).
NMR (CD_2Cl_2, r.t.):	^{1}**H**: *δ*/ppm = 5.32 (s, 10 H, Cp).
	^{31}**P{^{1}H}**: *δ*/ppm = 30.4 (s, 1 P, PAs).
	^{31}**P**: *δ*/ppm = 30.4 (s, 1 P, PAs).

Since **B** is known to literature,[2b,3] no further analytical characterization was carried out.

Fraction 3: **2-As**

Yield: 159 mg (0.08 mmol, 32%).

ESI-MS (*o*-DFB): *m/z* (%) = 1296.47 (100%) [(**2-As**)]$^+$ (M^+), 1268.47 (50%) [(**2-As**)-CO]$^+$, 784.69 (40%) [(**2-As**)-**B**+CO]$^+$, 756.70 (50%) [(**2-As**)-**B**]$^+$ + other unidentified fragments.

NMR (CD_2Cl_2, r.t.): **^{1}H**: *δ*/ppm = 5.32 (s, 20 H, Cp), 5.34 (s, 5 H, Cp).

^{31}P{^{1}H}: *δ*/ppm = 33.1 (s, 2 P, PAs).

^{31}P: *δ*/ppm = 33.2 (s, 2 P, PAs).

^{19}F{^{1}H}: -167.24 (t, $^3J_{F-F}$ = 17 Hz, 8 F, *m*-C_6F_5), -163.42 (t, $^3J_{F-F}$ = 20 Hz, 4 F, *p*-C_6F_5), -132.82 (s(*br*), 8 F, *o*-C_6F_5).

^{11}B{^{1}H}: -16.90 (s, 1 B, $[B(C_6F_5)_4]^-$).

Unfortunately, no crystals of **2-As** were obtained. To nevertheless get a solid-state structure, we developed another synthesis for **2-As**[$BArF_{24}$]. The complete analytical characterization of the compound is listed below.

Reaction of [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-PSb)] with [(BZIMPY)P][OTf] and K[B(C$_6$F$_5$)$_4$]

[{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-PSb)] (295 mg, 0.5 mmol, 1 equiv.), [(BZIMPY)P][OTf] (335 mg, 0.5 mmol, 1 equiv.) and K[B(C_6F_5)$_4$] (350 mg, 0.5 mmol, 1 equiv.) were dissolved in 15 mL *o*-DFB and the reaction mixture was stirred for 72 h. The color of the reaction mixture was purple for the first 48 h and then gradually changed to dark red. The solvent of the reaction mixture was removed under reduced pressure (10^{-3} mbar) and the red residue was extracted with toluene (3 x 30 mL). The solvent of the toluene extract was removed *in vacuo*. The dark red residue was pre-adsorbed onto dried silica gel using CH_2Cl_2 (10 mL) and purified by column chromatography (15 x 3 cm). Elution with *n*-hexane yields a yellow fraction containing [CpMo(CO)$_2$(η^3-P_2Sb)] (**1-Sb**) and [CpMo(CO)$_2$(η^3-P_3)] (**1-P**) in a ratio of 1:1. Changing the eluent to a mixture of *n*-hexane/toluene (3:1) led to a red fraction of unconsumed [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-PSb)] (**C**) and minor traces of [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-P_2)] (**A**). Elution with a mixture of toluene/CH_2Cl_2 (1:1) led to a dark red fraction of [{CpMo(CO)$_2$}$_5$(μ$_3$,η$^{2:2:1}$-PSb)$_2$][B(C_6F_5)$_4$] (**2-Sb**). The solvent of all fractions was removed under reduced pressure (10^{-3} mbar) and the resulting powders were dried *in vacuo*.

Fraction 1: **1-Sb**

Orange crystals of **1-Sb** were obtained by storing a concentrated solution in *n*-hexane at −30 °C overnight. **1-Sb** and **1-P** co-crystallize and cannot be separated.

Yield: 86 mg (0.12 mmol, 24%).

Elemental analysis: calc. (%) for ($C_7H_5O_2MoP_2As$)($C_7H_5O_2MoP_3$)·(C_6H_{14})$_{0.5}$: C: 27.73, H: 2.43.

found (%): C: 27.92, H: 2.00.

FD-MS (*n*-hexane): *m/z* (%) = 401.79 (100%) [(**1-Sb**)]$^+$ (M^+).

NMR (CD_2Cl_2, r.t.): ^{1}**H**: *δ*/ppm = 5.30 (s. 5 H, Cp), 5.32 (s, 5 H, Cp).

^{31}**P{^{1}H}**: *δ*/ppm = -351.3 (s, 3 P, P_3), -288.2 (s, 2 P, $\underline{P}_2$Sb).

^{31}**P**: *δ*/ppm = -351.3 (s, 3 P, P_3), -288.2 (s, 2 P, $\underline{P}_2$Sb).

IR: $\tilde{\nu}$(CO)/cm^{-1} = 1984 (m), 1901 (s).

Fraction 2: **C** plus traces of **A**

Yield: 65 mg (0.11 mmol, 22%).

NMR (CD_2Cl_2, r.t.): ^{1}**H**: *δ*/ppm = 5.32 (s, 10 H, Cp).

^{31}**P{^{1}H}**: *δ*/ppm = -43.2 (s, 2 P, $\underline{P}_2$), 90.6 (s, 1 P, $\underline{P}$Sb).

^{31}**P**: *δ*/ppm = -43.2 (s, 2 P, $\underline{P}_2$), 90.6 (s, 1 P, $\underline{P}$Sb).

Since **C** and **A** are known to literature,[2b,3] no further analytical characterization was carried out.

Fraction 3: **2-Sb**

Yield: 187 mg (0.09 mmol, 36%).

ESI-MS (*o*-DFB): *m/z* (%) = 1390.31 (5%) [(**2-Sb**)]$^+$ (M^+), 804.61 (20%) [(**2-Sb**)-**C**]$^+$ + other unidentified fragments.

NMR (CD_2Cl_2, r.t.): ^{1}**H**: *δ*/ppm = 5.32 (s, 20 H, Cp), 5.34 (s, 5 H, Cp).

^{31}**P{^{1}H}**: *δ*/ppm = 81.4 (s, 2 P, $\underline{P}$Sb).

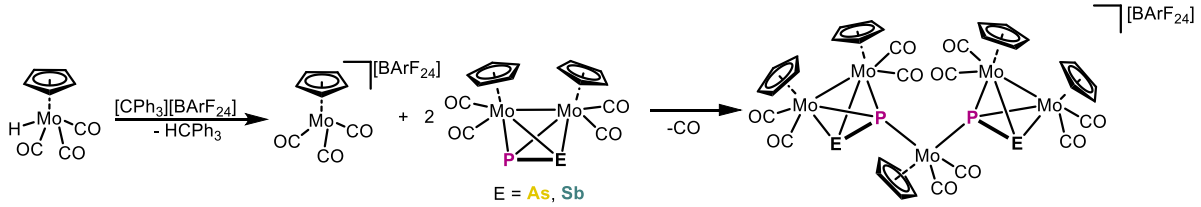
^{31}**P**: *δ*/ppm = 81.4 (s, 2 P, $\underline{P}$Sb).

^{19}**F{^{1}H}**: -167.18 (t, $^{3}J_{F\text{-}F}$ = 17 Hz, 8 F, *m*-C_6F_5), -163.37 (t, $^{3}J_{F\text{-}F}$ = 20 Hz, 4 F, *p*-C_6F_5), -132.81 (s(*br*), 8 F, *o*-C_6F_5).

^{11}**B{^{1}H}**: -16.91 (s, 1 B, $[B(C_6F_5)_4]^-$).

Unfortunately, no crystals of **2-Sb** were obtained. To nevertheless get a solid-state structure, we developed another synthesis for **2-Sb**[$BArF_{24}$]. The complete analytical characterization of the compound is listed below.

Alternative Synthesis Pathway for **2-As** and **2-Sb**



Scheme S 1: Alternative Synthesis Pathway for **2-As** and **2-Sb**.

Synthesis of [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][BArF$_{24}$] (**2-As**[BArF$_{24}$])

[CPh$_3$][BArF$_{24}$] (220 mg, 0.2 mmol, 1 equiv.) in *o*-DFB (3 mL) was added to a colorless solution of CpMo(CO)$_3$H (50 mg, 0.2 mmol, 1 eq.) in *o*-DFB (3 mL) at -30 °C. An immediate color change to purple was observed. After stirring for 15 min at -30 °C, [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] (216 mg, 0.4 mmol, 2 equiv.) in *o*-DFB (5 mL) was added slowly. The reaction mixture was allowed to reach room temperature and was subsequently stirred for 40 h at 80 °C until complete conversion was observed in the ^{31}P NMR spectrum. *n*-hexane (30 mL) was added to the dark red reaction mixture to precipitate a dark red powder which was washed twice with *n*-hexane (10 mL each) and then dried under reduced pressure (10^{-3} mbar). The powder was dissolved in *o*-DFB (5 mL) and the solution was then filtered through a glass fiber filter paper. Adding *n*-hexane (30 mL) precipitated a dark red powder which was dried *in vacuo*. Dark red crystals of [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][BArF$_{24}$] (**2-As**[BarF$_{24}$]) were obtained by layering a concentrated solution of **2-As** in *o*-DFB with *n*-hexane (30 mL) and storage for a few days at room temperature.

Yield:	238 mg (0.11 mmol, 55%).
Elemental analysis:	calc. (%) for $C_{67}H_{37}O_{10}Mo_5P_2As_2BF_{24}$: C: 37.25, H: 1.73.
	found (%): C: 37.60, H: 2.06.
ESI-MS (*o*-DFB):	*m/z* (%) = 1296.47 (100%) [(**2-As**)]$^+$ (M^+), 756.70 (80%) [(**2-As**)-**B**]$^+$, 784.96 (10%) [(**2-As**)-**B**+CO]$^+$, 539.76 (5%) [**B**]$^+$.
NMR (CD_2Cl_2, r.t.):	**^{1}H**: δ/ppm = 5.38 (s, 20 H, Cp), 5.41 (s, 5 H, Cp), 7.60 (s(*br*), 4 H, [BArF$_{24}$]$^-$), 7.76 (s(*br*), 8 H, [BArF$_{24}$]$^-$).
	^{31}P{^{1}H}: δ/ppm = 32.2 (s, 2 P, PAs).
	^{31}P: δ/ppm = 32.2 (s, 2 P, PAs).
	^{19}F: -62.84 (s, 24 F, [BArF$_{24}$]$^-$).
	^{11}B{^{1}H}: -6.60 (s, 1 B, [BArF$_{24}$]$^-$).
IR:	$\tilde{\nu}$(CO)/cm^{-1} = 1972 (s), 1929 (s), 1891 (s).

Synthesis of [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PSb)$_2$][BArF$_{24}$] (**2-Sb**[BArF$_{24}$])

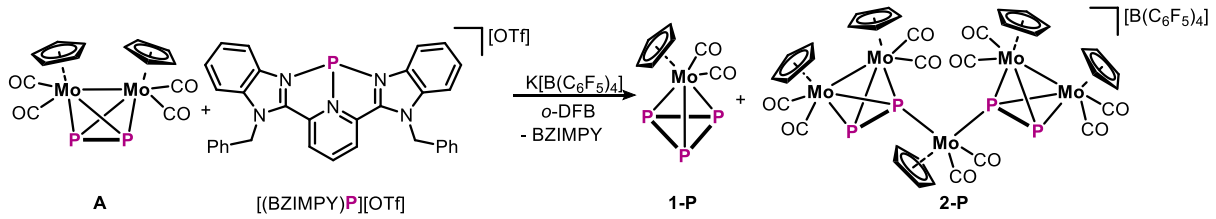
[CPh$_3$][BArF$_{24}$] (220 mg, 0.2 mmol, 1 equiv.) in *o*-DFB (3 mL) was added to a colorless solution of CpMo(CO)$_3$H (50 mg, 0.2 mmol, 1 equiv.) in *o*-DFB (3 mL) at -30 °C. An immediate color change to purple was observed. After stirring for 15 min at -30 °C, [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PSb)] (236 mg, 0.4 mmol, 2 equiv.) in *o*-DFB (5 mL) was added slowly. The reaction mixture was allowed to reach room temperature and was subsequently stirred for 40 h at 80 °C until complete conversion was observed in the ^{31}P NMR spectrum. *n*-hexane (30 mL) was added to the dark red reaction mixture to precipitate a dark red powder which was washed twice with *n*-hexane (10 mL each) and then dried under reduced pressure (10^{-3} mbar). The powder was dissolved in *o*-DFB (5 mL) and the solution was then filtered through a glass fiber filter paper. Adding *n*-hexane (30 mL) precipitated a dark red powder which was dried *in vacuo*. Dark red crystals of [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][BArF$_{24}$] (**2-Sb**) were obtained by layering a concentrated solution of **2-Sb** in *o*-DFB with *n*-hexane (30 mL) and storage for a few days at room temperature.

Yield:	228 mg (0.10 mmol, 50%).
Elemental analysis:	calc. (%) for $C_{67}H_{37}O_{10}Mo_5P_2As_2BF_{24}$: C: 35.70, H: 1.65.
	found (%): C: 36.06, H: 2.11.
ESI-MS (*o*-DFB):	*m/z* (%) = 1390.43 (20%) [(**2-Sb**)]$^+$ (M^+), 804.68 (100%) [(**2-Sb**)-**C**]$^+$, 832.68 (5%) [(**2-Sb**)-**C**+CO]$^+$, 1089.08 (10%) [2x**C**-3CO)]$^+$, 587.74 (5%) [**C**]$^+$.
NMR (CD_2Cl_2, r.t.):	**^{1}H**: *δ*/ppm = 5.35-5.37 (s(*br*), 25 H, Cp), 7.60 (s(*br*), 4 H, [BArF$_{24}$]$^-$), 7.76 (s(*br*), 8 H, [BArF$_{24}$]$^-$).
	^{31}P{^{1}H}: *δ*/ppm = 80.7 (s, 2 P, PSb).
	^{31}P: *δ*/ppm = 32.2 (s, 2 P, PSb).
	^{19}F: -62.84 (s, 24 F, [BArF$_{24}$]$^-$).
	^{11}B{^{1}H}: -6.60 (s, 1 B, [BArF$_{24}$]$^-$).
IR:	$\tilde{\nu}$(CO)/cm^{-1} = 1963 (s), 1912 (s), 1889 (s).

4. NMR Spectra

Initial Screening Reaction

We started our investigations with an initial screening and performed the reaction of [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] (**A**) with [(BZIMPY)P][OTf]. We chose to use **A** as screening substance since it has two NMR active phosphorus centers which allowed us to monitor the reaction more precisely by ^{31}P NMR spectroscopy. Since we did not observe a reaction, or color change within the course of 24 hours, we added one equivalent of K[B(C$_6$F$_5$)$_4$] to increase the solubility of [(BZIMPY)P]$^+$ After an additional 24 hours, the crude ^{31}P NMR spectrum revealed signals for unconsumed starting material **A**, the known compound [CpMo(CO)$_2$(η^3-P$_3$)] (**1-P**), and two doublets in an AX spin system with a coupling constant of $^1J_{P\text{-}P}$ = 487 Hz (**2-P**) (see Figure S2). With these results, we were able to reconstruct the reaction sequence: Formally one {CpMo(CO)$_2$}$^+$ fragment and the P atom of [(BZIMPY)P]$^+$ were exchanged. The released {CpMo(CO)$_2$}$^+$ fragment was then saturated by coordination with two units **A** (Scheme S2). Since our interest was to synthesize new heteroatomic complexes with *cyclo*-P$_2$E ligands, we did not workup this reaction and directly pursued the heavier congeners **B** and **C**.



Scheme S2: Initial reaction screening of **A** with [(BZIMPY)P][OTf].

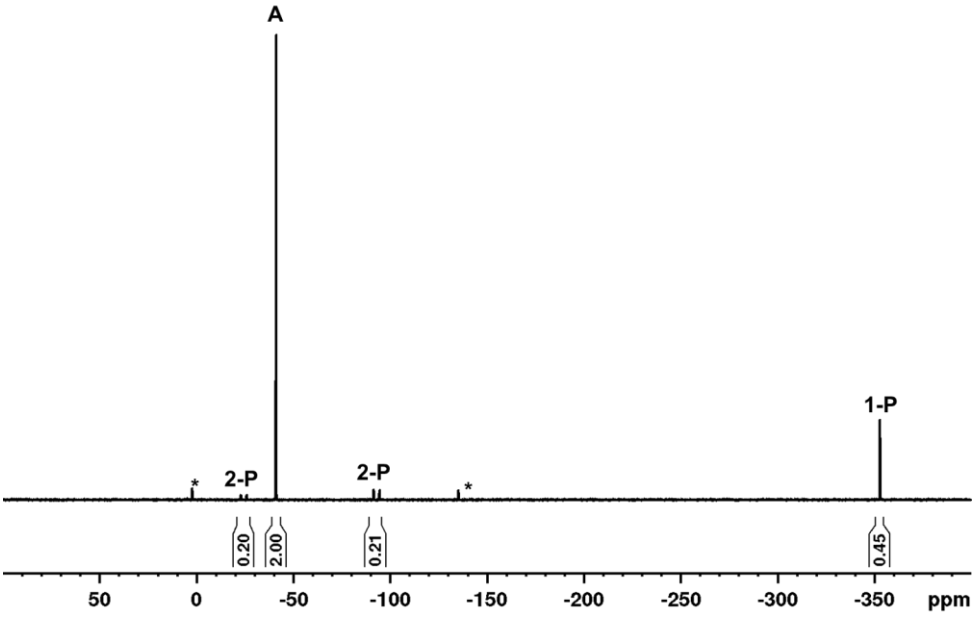


Figure S 1: Crude ^{31}P NMR spectrum from the reaction of **A** with [(BZIMPY)P][OTf] and K[B(C$_6$F$_5$)$_4$].

Reaction of [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] with [(BZIMPY)P][OTf] and K[B(C$_6$F$_5$)$_4$]

Fraction 1: [CpMo(CO)$_2$(η^3-P$_2$As)] (**1-As**)

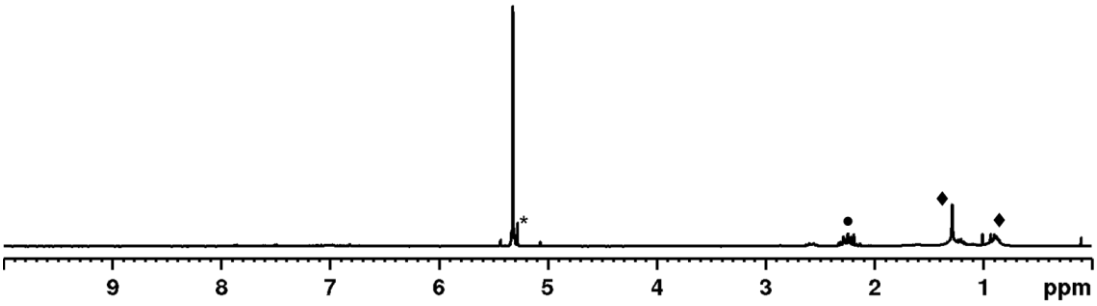


Figure S 2: ^{1}H NMR spectrum of **1-As** in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2, ♦ marks traces of *n*-hexane, • marks unidentified trace umpurity.

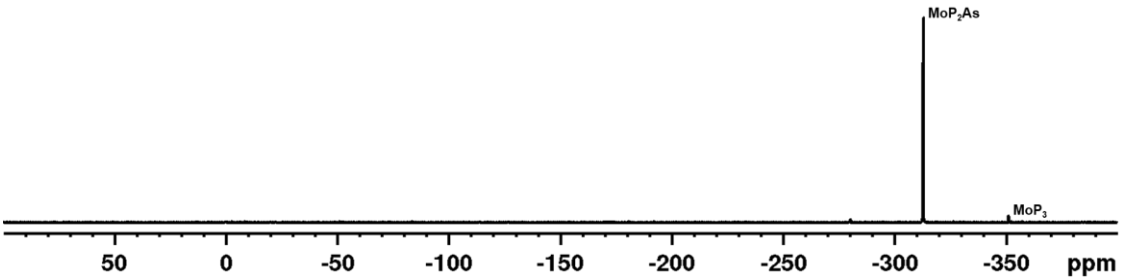


Figure S 3: ^{31}P{^{1}H} NMR spectrum of **1-As** in CD_2Cl_2 at room temperature. MoP_3 marks minor traces of **1-P** (<1%).

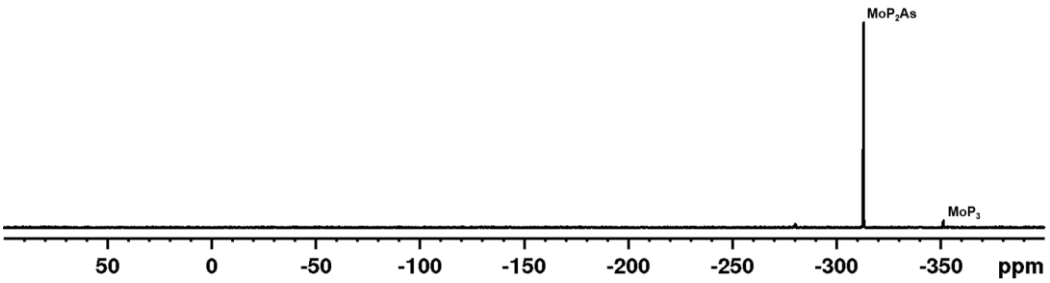


Figure S 4: ^{31}P NMR spectrum of **1-As** in CD_2Cl_2 at room temperature. MoP_3 marks minor traces of **1-P** (<1%).

Fraction 2: [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PAs)] (**B**)

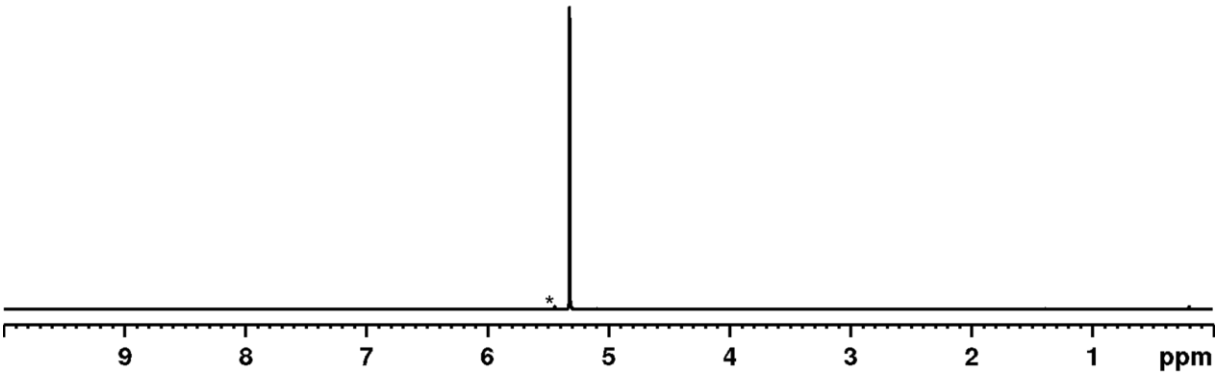


Figure S 5: ^{1}H NMR spectrum of **B** in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2.

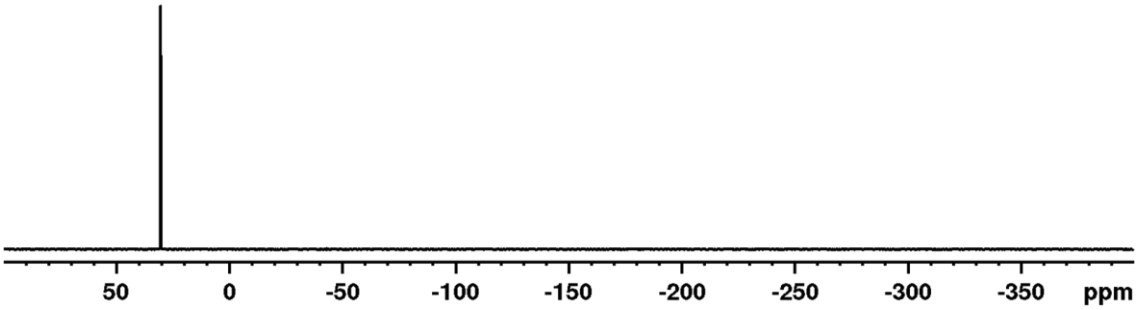


Figure S 6: $^{31}P\{^{1}H\}$ NMR spectrum of **B** in CD_2Cl_2 at room temperature.

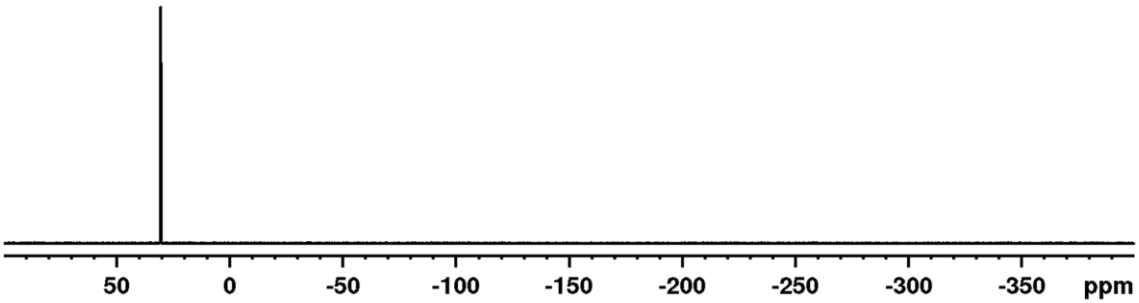


Figure S 7: ^{31}P NMR spectrum of **B** in CD_2Cl_2 at room temperature.

Fraction 3: $[\{CpMo(CO)_2\}_5(\mu_3,\eta^{2:2:1}\text{-}PAs)_2][B(C_6F_5)_4]$ (**2-As**)

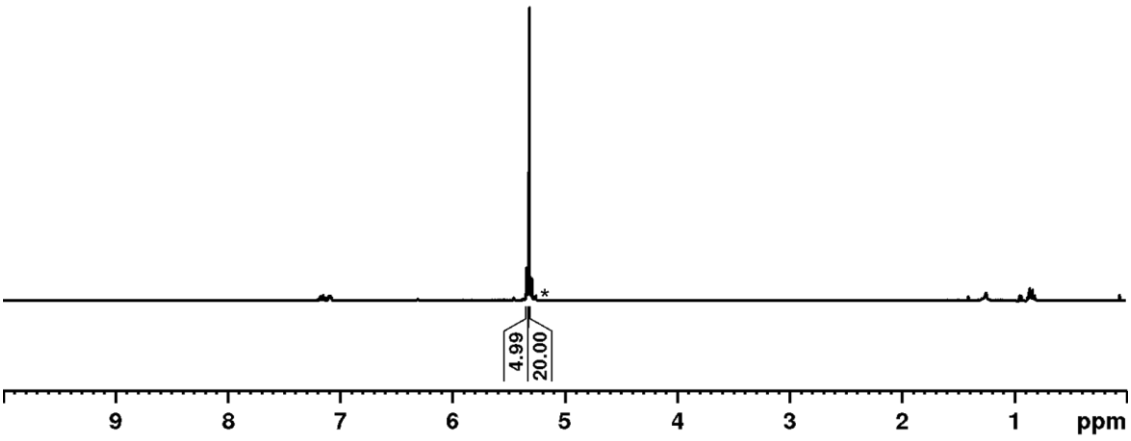


Figure S 8: ^{1}H NMR spectrum of **2-As** in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2.

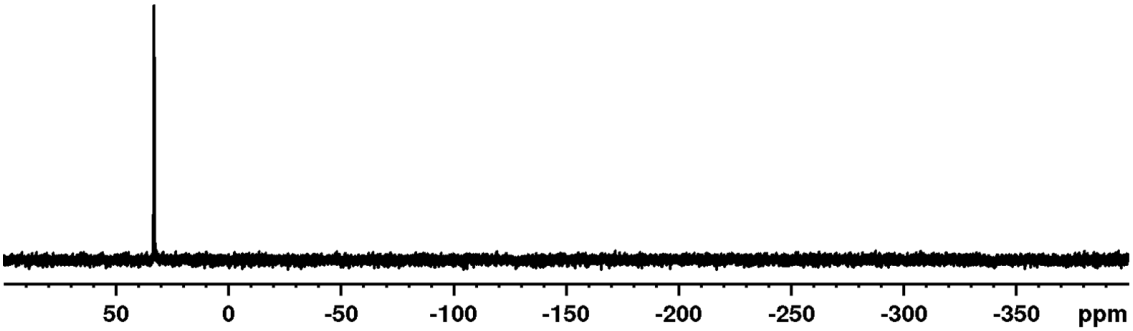


Figure S 9: $^{31}P\{^{1}H\}$ NMR spectrum of **2-As** in CD_2Cl_2 at room temperature.

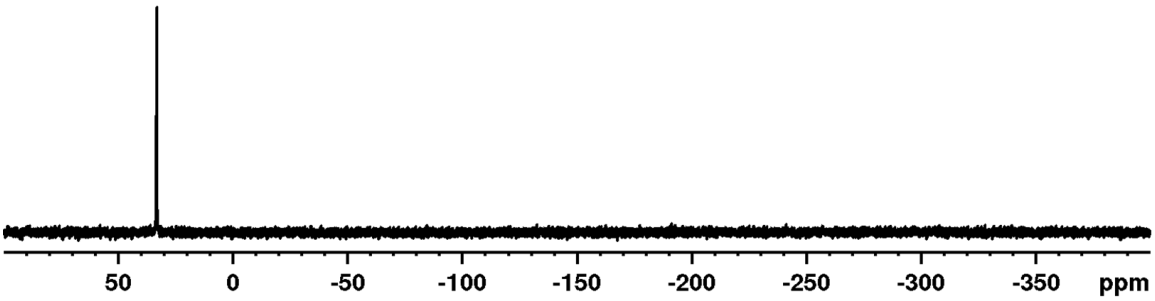


Figure S 10: ^{31}P NMR spectrum of **2-As** in CD_2Cl_2 at room temperature.

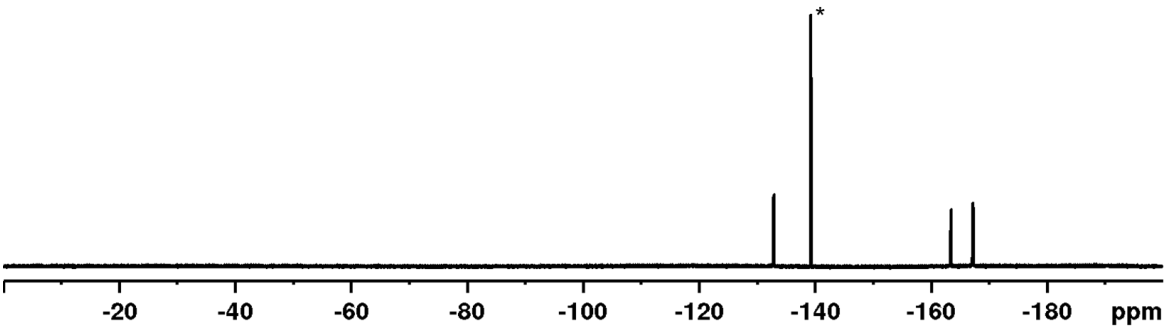


Figure S 11: $^{19}F\{^1H\}$ NMR spectrum of **2-As** in CD_2Cl_2 at room temperature. * marks traces of *o*-DFB.

Reaction of [{CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-PSb)] with [(BZIMPY)P][OTf] and K[B(C$_6$F$_5$)$_4$]

Fraction 1: [CpMo(CO)$_2$(η^3-P$_2$Sb)] (**1-Sb**) + [CpMo(CO)$_2$(η^3-P$_3$)] (**1-P**) in 1:1 ratio

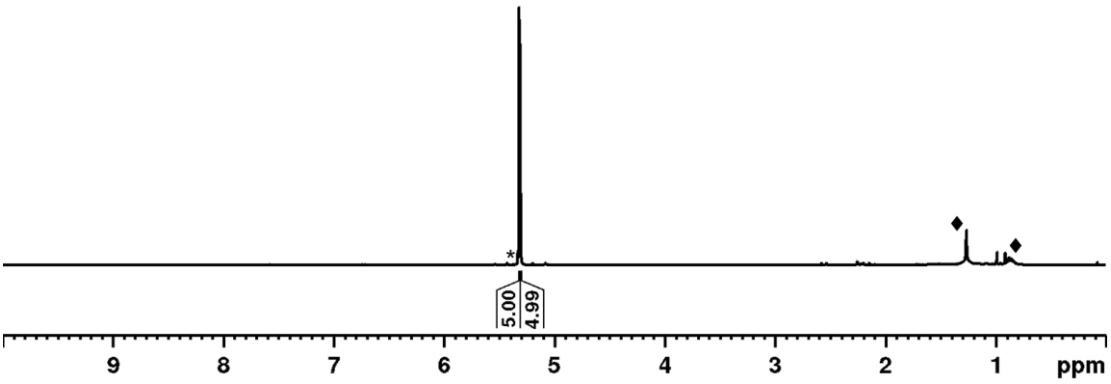


Figure S 12: ^1H NMR spectrum of **1-Sb** and **1-P** in a 1:1 ratio in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2, ♦ marks traces of *n*-hexane.

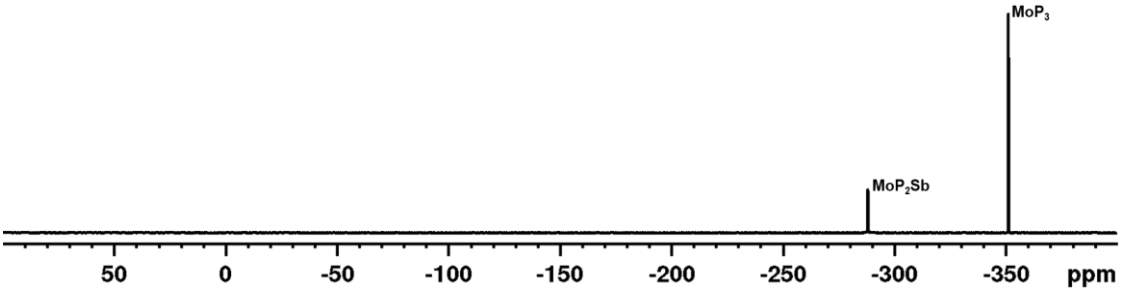


Figure S 13: $^{31}P\{^1H\}$ NMR spectrum of **1-Sb** and **1-P** in CD_2Cl_2 at room temperature.

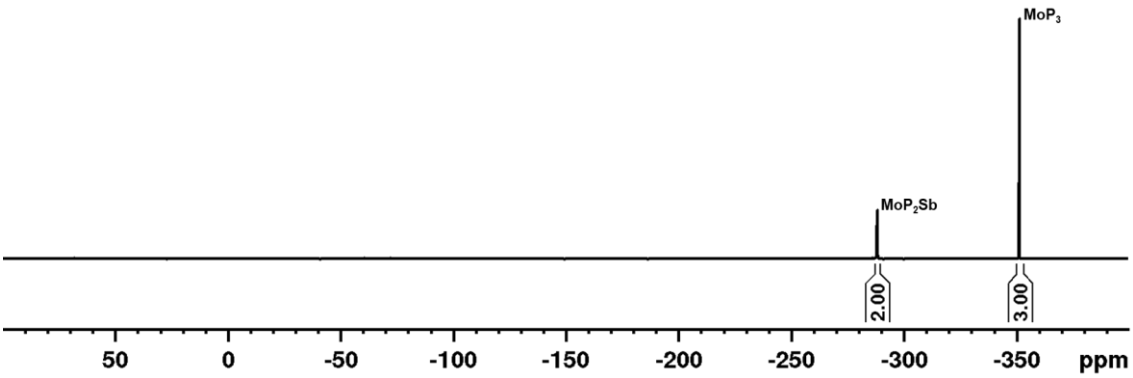


Figure S 14: ^{31}P NMR spectrum of **1-Sb** and **1-P** in CD_2Cl_2 at room temperature.

Fraction 2: [{CpMo(CO)$_2$}$_2$(μ,$\eta^{2:2}$-PSb)] (**C**)

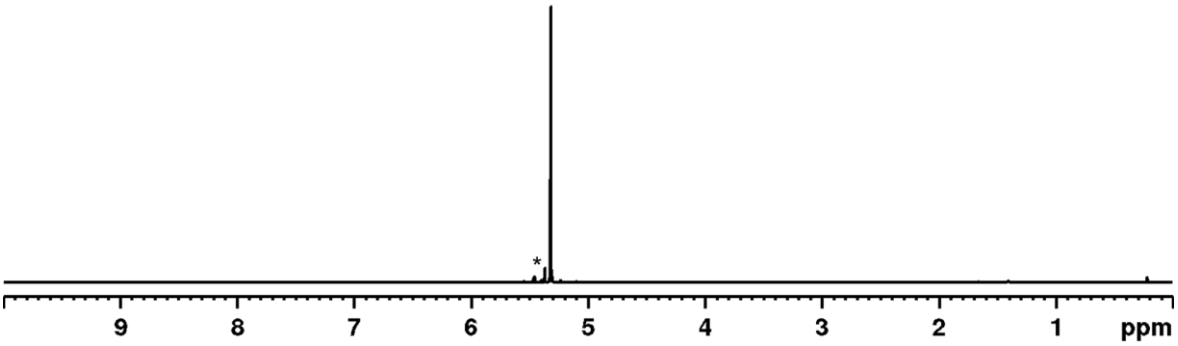


Figure S 15: ^{1}H NMR spectrum of **C** in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2.

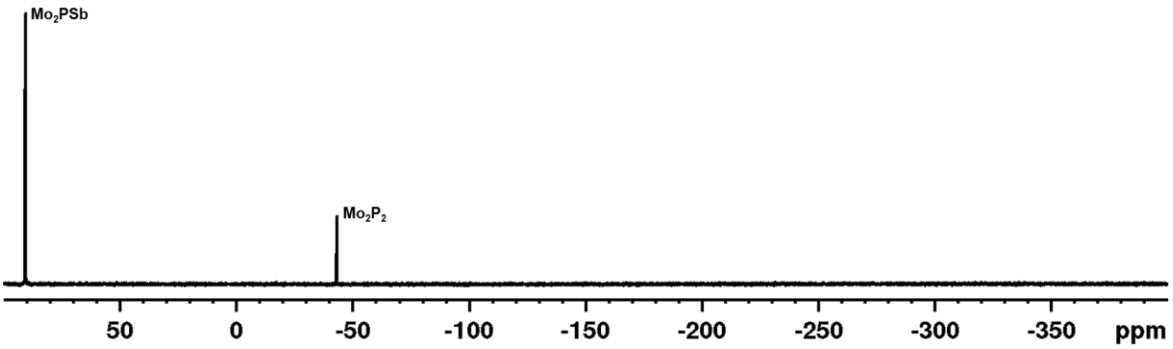


Figure S 16: $^{31}P\{^{1}H\}$ NMR spectrum of **C** and **A** in a 1:0.05 ratio in CD_2Cl_2 at room temperature.

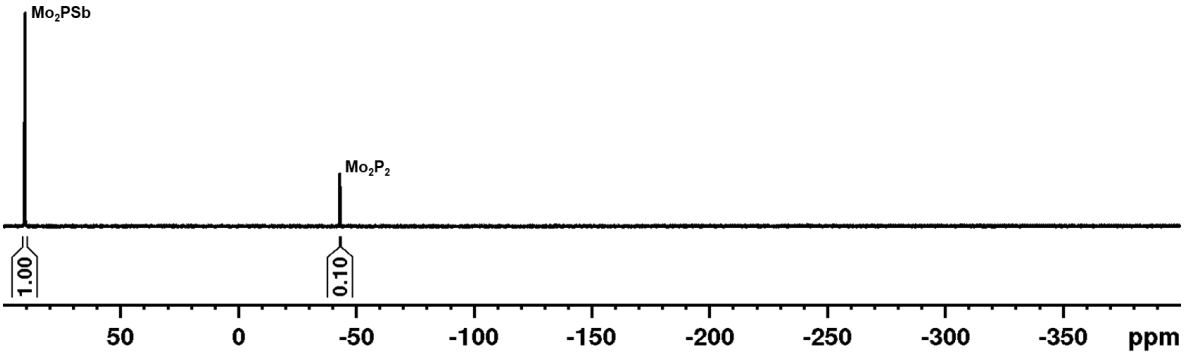


Figure S 17: ^{31}P NMR spectrum of **C** and **A** in a 1:0.05 ratio in CD_2Cl_2 at room temperature.

Fraction 3: [({CpMo(CO)$_2$}$_2$(μ,η$^{2:2}$-PSb))$_2$CpMo(CO)$_2$}][B(C$_6$F$_5$)$_4$] (**2-Sb**)

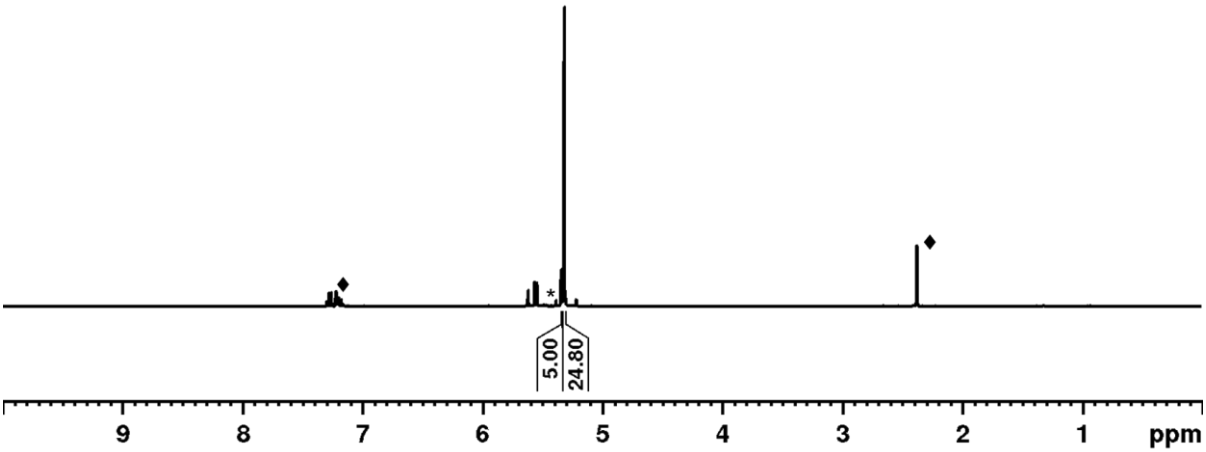


Figure S 18: ^{1}H NMR spectrum of **2-Sb** in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2, ♦ marks traces of toluene.

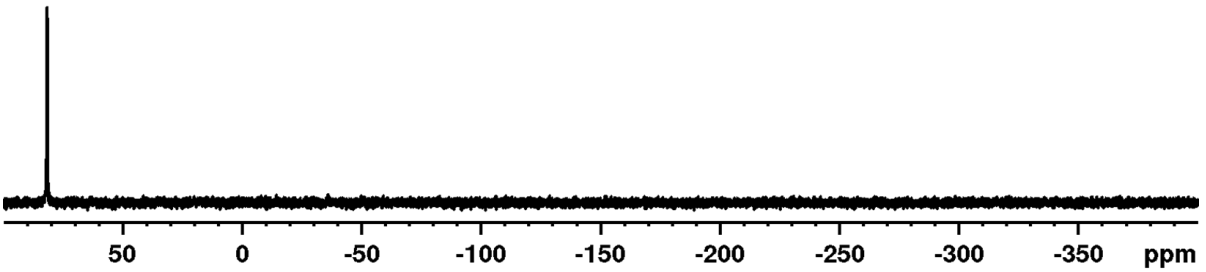


Figure S 19: ^{31}P{^{1}H} NMR spectrum of **2-Sb** in CD_2Cl_2 at room temperature.

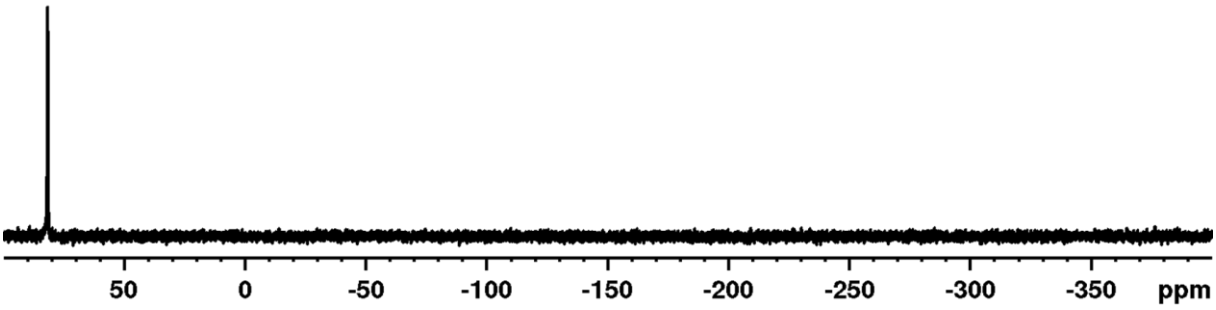


Figure S 20: ^{31}P NMR spectrum of **2-Sb** in CD_2Cl_2 at room temperature.

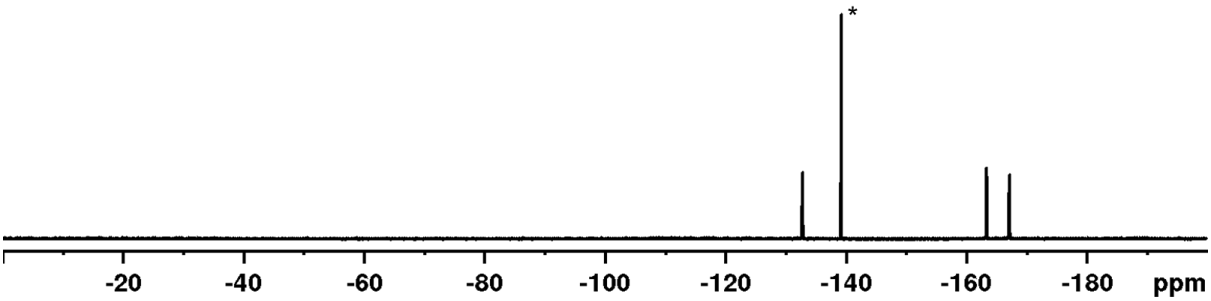


Figure S 21: ^{19}F{^{1}H} NMR spectrum of **2-Sb** in CD_2Cl_2 at room temperature. * marks traces of *o*-DFB.

Alternative Pathway for [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][BArF$_{24}$] (**2-As**[BArF$_{24}$])

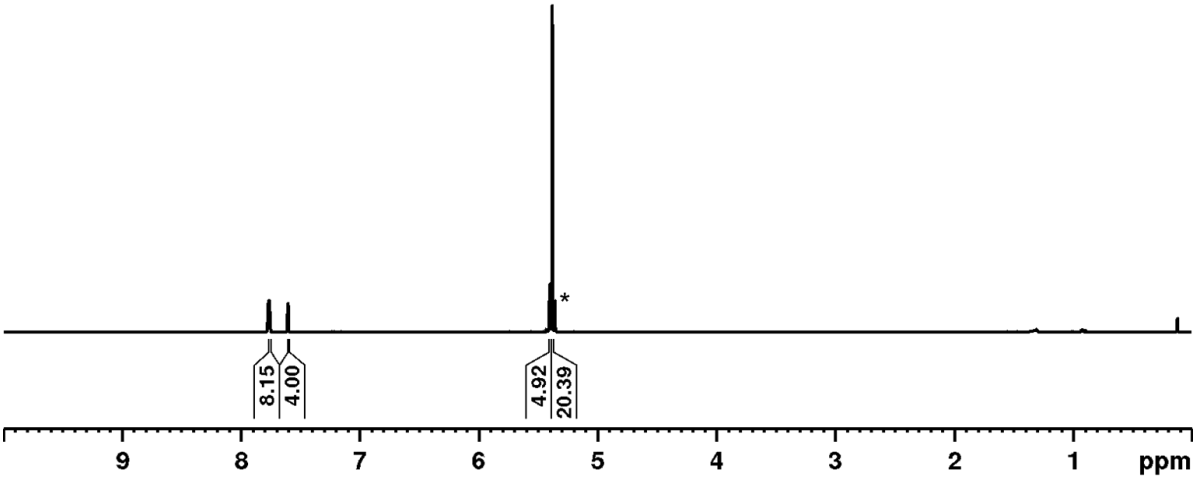


Figure S 22: ^{1}H NMR spectrum of **2-As**[BArF$_{24}$] in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2.

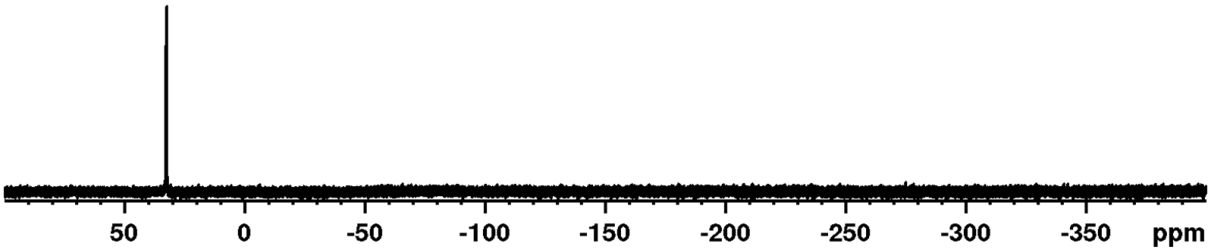


Figure S 23: $^{31}P\{^1H\}$ NMR spectrum of **2-As**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

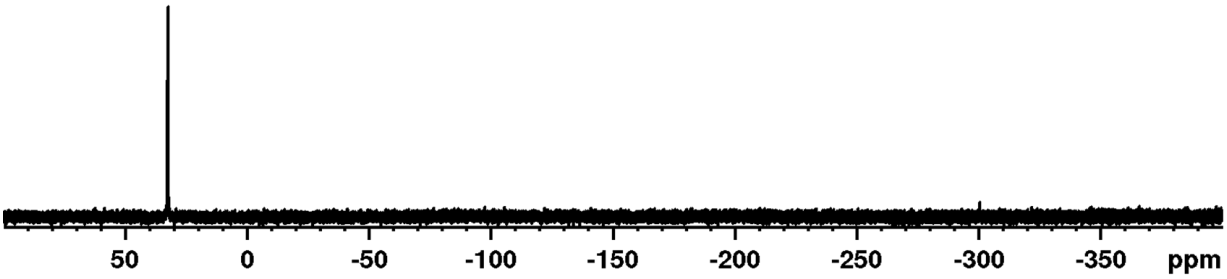


Figure S 24: ^{31}P NMR spectrum of **2-As**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

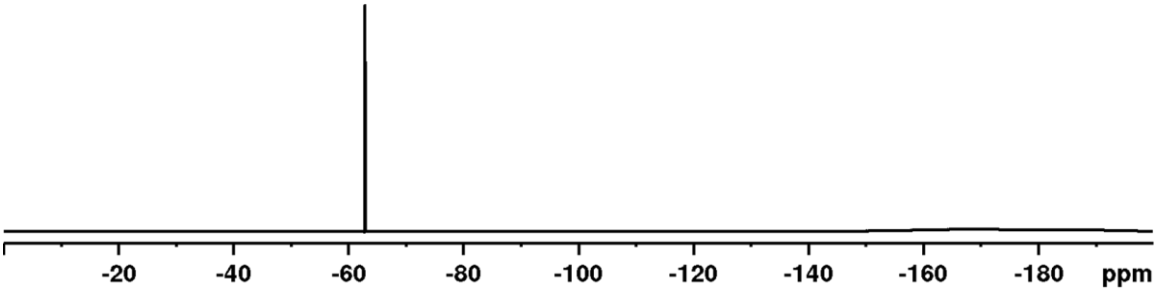


Figure S 25: ^{19}F NMR spectrum of **2-As**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

Alternative Pathway for [{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PSb)$_2$][BArF$_{24}$] (**2-Sb**[BArF$_{24}$])

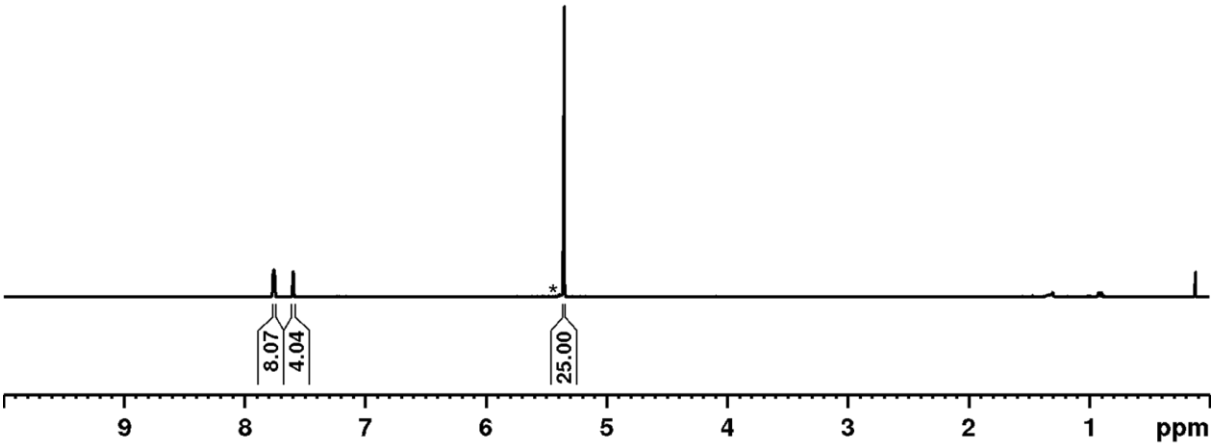


Figure S 26: ^{1}H NMR spectrum of **2-Sb**[BArF$_{24}$] in CD_2Cl_2 at room temperature. * marks residual solvent signal of CD_2Cl_2.

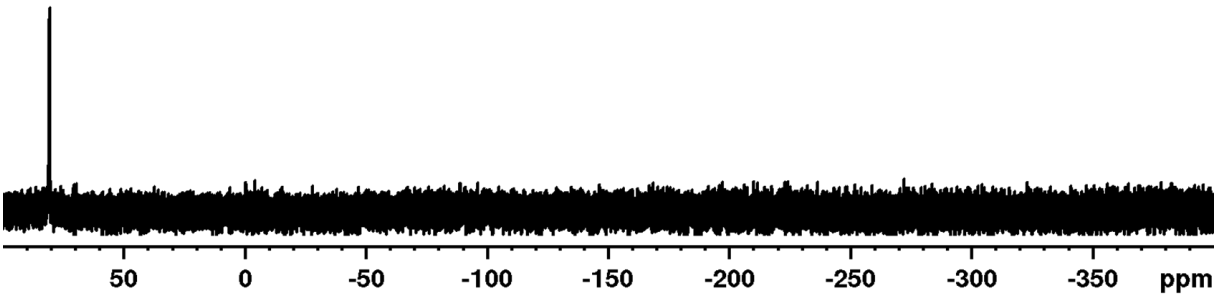


Figure S 27: $^{31}P\{^1H\}$ NMR spectrum of **2-Sb**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

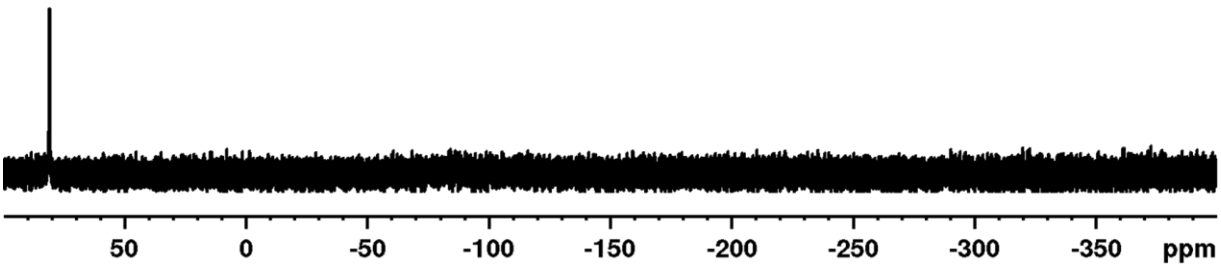


Figure S 28: ^{31}P NMR spectrum of **2-Sb**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

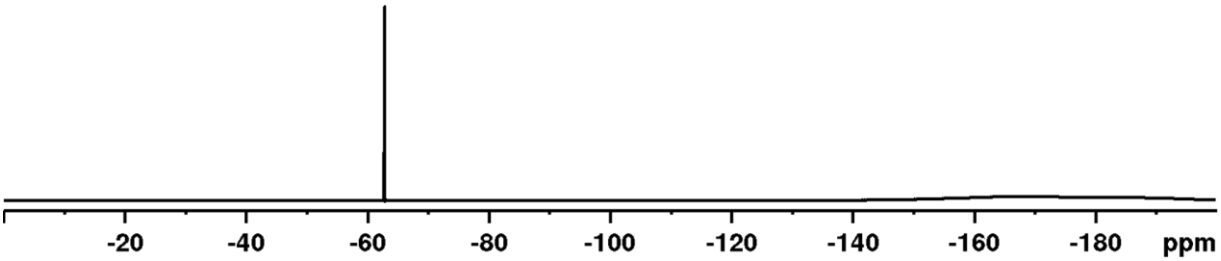


Figure S 29: ^{19}F NMR spectrum of **2-Sb**[BArF$_{24}$] in CD_2Cl_2 at room temperature.

5. X-ray single crystal structure analysis

The crystallographic data for all synthesized compounds were collected on a XtaLAB Synergy R, DW system with HyPix-Arc 150 detector applying Cu-Kα radiation (**2-Sb**) or Mo-Kα radiation (**1-As**, **1-Sb**, **2-As**) from a rotating anode X-ray source. All measurements were performed at 123 K. Data collection, data reduction and absorption correction were performed with the CrysAlisPro[8] software package. Structure solution and refinement was conducted in Olex2[9] using ShelXT[10] and ShelXL[11] (full-matric least-squares method against F^2). All non-hydrogen atoms were refined with anisotropic displacement parameters and hydrogen atoms were treated as riding models with isotropic displacement parameters and fixed C-H bond lengths (sp^3: 0.96 (CH_3), 0.97 (CH_2), sp^2: 0.93 (CH)). Visualization of the crystal structures was performed with Olex2.[9]

CIF files with comprehensive information on the details of the diffraction experiments and full tables of bond lengths and angles for **1** – **4** are deposited in Cambridge Crystallographic Data Centre under the deposition codes CCDC-2428359 (**1-As**), CCDC-2428360 (**1-Sb**), CCDC-2428361 (**2-As**), and CCDC-2428362 (**2-Sb**), respectively.

[$CpMo(CO)_2(\eta^3\text{-}P_2As)$] (**1-As**)

Compound **1-As** crystallizes from a concentrated solution in *n*-hexane stored at -30 °C overnight in the orthorhombic space group *Pbca* as yellow blocks. The asymmetric unit contains one molecule **1**-**As**. The *cyclo*-P_2As ring is disordered over all three positions. Disorder within the P_2As ligand was treated with adequate restraints.

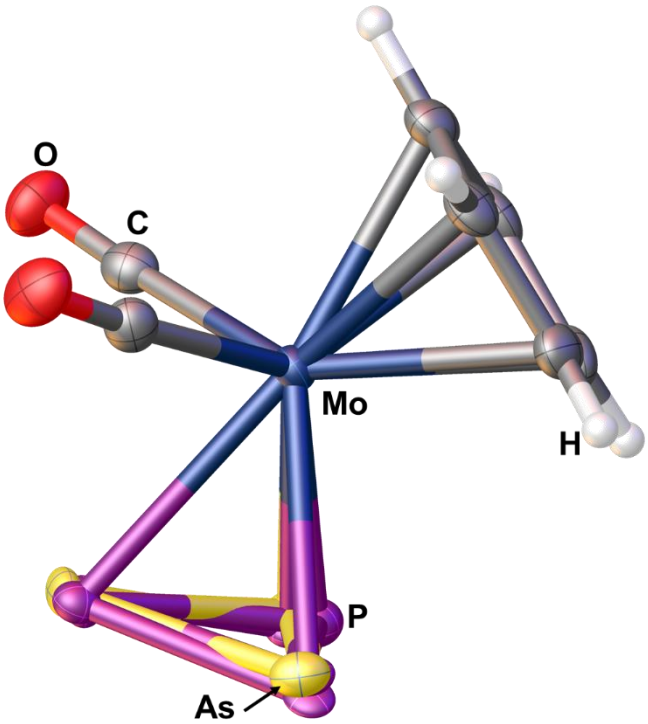


Figure S 30: Solid state structure of **1-As**. Depicted is the asymmetric unit and ADPs (anisotropic displacement parameters) are drawn at 50 % probability.

[$CpMo(CO)_2(\eta^3\text{-}P_2Sb)$] (**1-Sb**) + [$CpMo(CO)_2(\eta^3\text{-}P_3)$] (**1-P**)

Compound **1-Sb** and **1-P** crystallize together from a concentrated solution in *n*-hexane stored at -30 °C overnight in the monoclinic space group $P2_1/n$ as orange blocks. The asymmetric unit contains **1-Sb** and **1-P** in the ratio of 58 % **1-Sb** and 42 % **1-P**. The mixed occupancy was refined with adequate restraints.

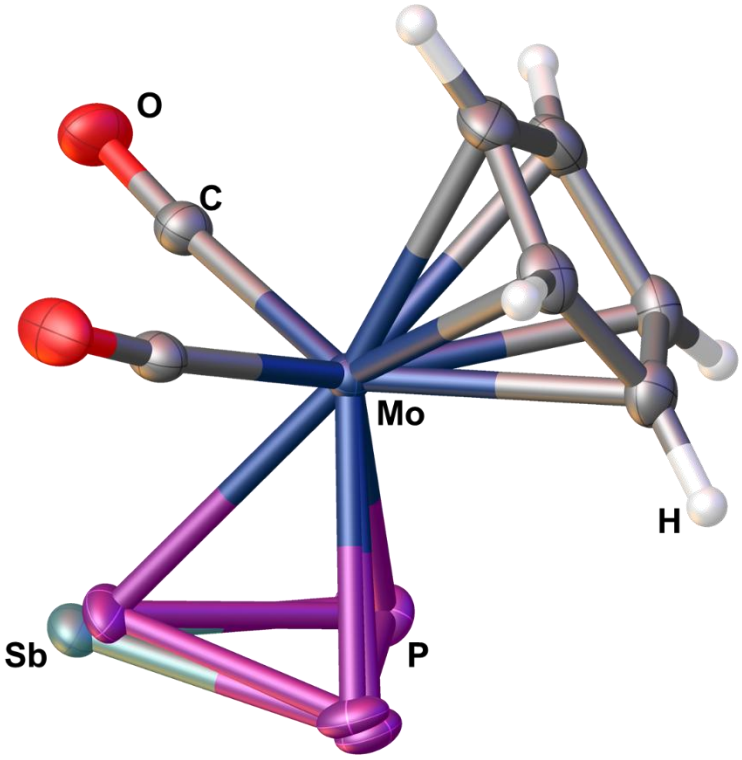


Figure S 31: Solid state structure of **1-Sb** and **1-P**. Depicted is the asymmetric unit and ADPs (anisotropic displacement parameters) are drawn at 50 % probability.

[{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PAs)$_2$][BArF$_{24}$] (**2-As**[BArF$_{24}$])

Compound **2-As**[BArF$_{24}$] crystallizes from a concentrated solution in *o*-DFB layered with *n*-hexane stored at room temperature in the monoclinic space group $P2_1/c$ as dark red blocks. The asymmetric unit contains one cation and one anion. One complete tetrahedrane unit, one {CpMo(CO)$_2$} fragment as well as the CF_3 groups within the anion are disorderd . Moreover, the bridging {CpMo(CO)$_2$}$^+$ unit shows a disorder with an occupancy of 4%. Therefore, only the disorder of the Mo atom was resolved since the residual electron density did not allow for solving the disorder of the respective Cp and CO ligands. Disorder within the residual structure was treated with adequate restraints

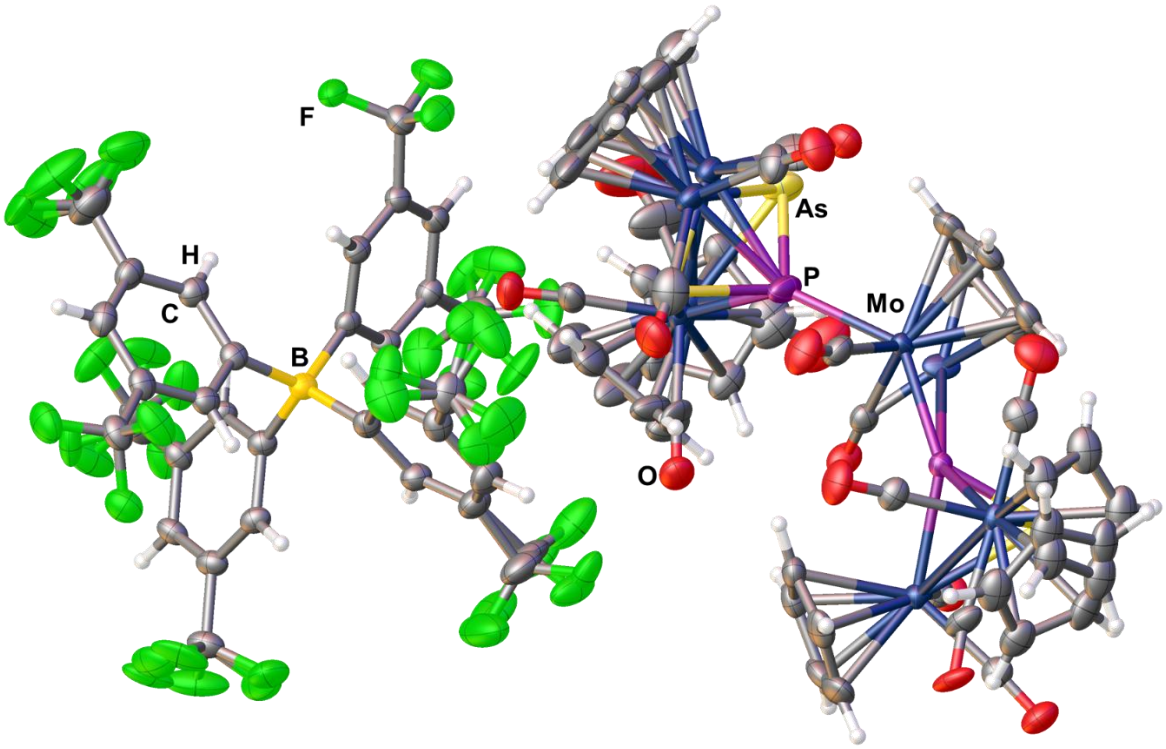


Figure S 32: Solid state structure of **2-As**[BArF$_{24}$]. Depicted is the asymmetric unit and ADPs (anisotropic displacement parameters) are drawn at 50 % probability.

[{CpMo(CO)$_2$}$_5$(μ_3,$\eta^{2:2:1}$-PSb)$_2$][BArF$_{24}$] (**2-Sb**[BArF$_{24}$])

Compound **2-Sb**[BArF$_{24}$] crystallizes from a concentrated solution in *o*-DFB layered with *n*-hexane stored at room temperature in the monoclinic space group $P2_1/c$ as dark red blocks. The asymmetric unit contains one cation and one anion. One complete tetrahedrane unit, one {CpMo(CO)$_2$} fragment as well as the CF_3 groups within the anion are disorderd. This disorder was treated with adequate restraints

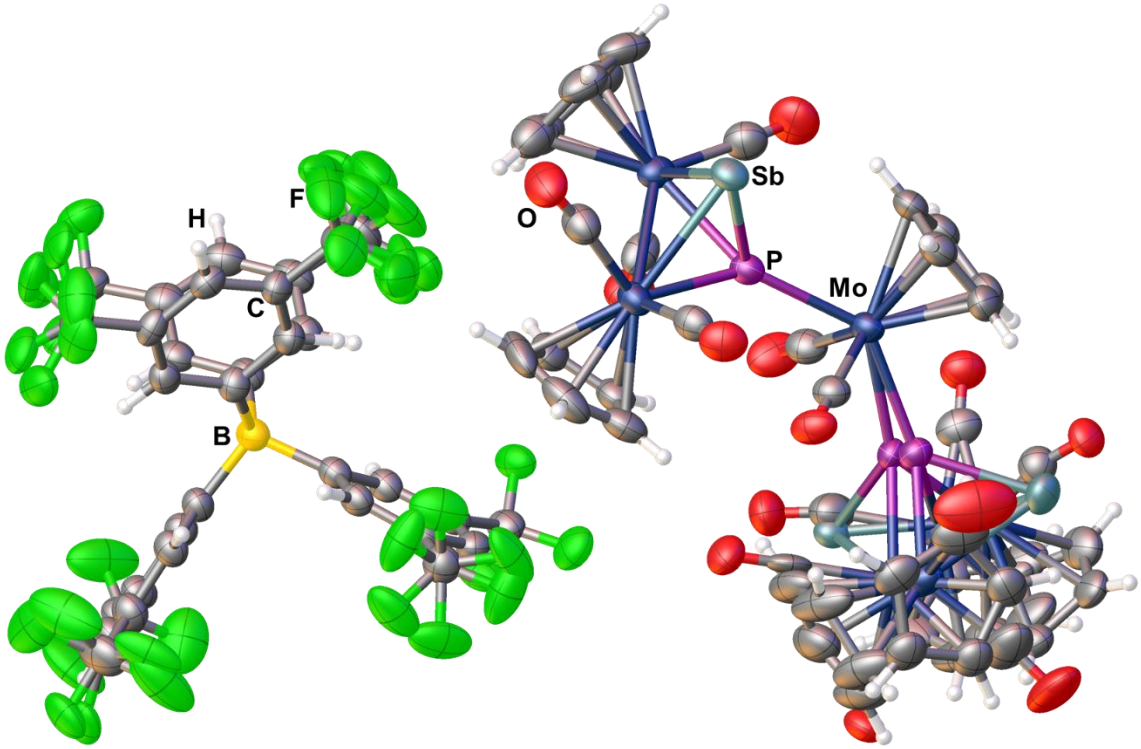


Figure S 33: Solid state structure of **2-Sb**[BArF$_{24}$]. Depicted is the asymmetric unit and ADPs (anisotropic displacement parameters) are drawn at 50 % probability.

Table S 1: X-ray crystallographic data of compounds **1-As** and **1-Sb** + **1-P**.

Compound	**1-As**	**1-Sb** + **1-P**
CCDC Entry	2428359	2428360
Formula	$C_7H_5AsMoO_2P_2$	$C_7H_5MoO_2P_{2.42}Sb_{0.58}$
ρ_{calc}	2.357	2.367
μ/mm^{-1}	4.888	3.137
Formula Weight	353.91	362.61
Colour	clear intense yellow	clear dark orange
Shape	block-shaped	block-shaped
Size/mm^3	0.10×0.08×0.06	0.25×0.17×0.16
***T*/K**	123.00(10)	123.00(10)
Crystal System	orthorhombic	monoclinic
Space Group	*Pbca*	$P2_1/n$
***a*/Å**	10.8696(3)	6.12950(10)
***b*/Å**	7.5409(2)	11.38350(10)
***c*/Å**	24.3360(5)	14.6754(2)
α/°	90	90
β/°	90	96.4590(10)
γ/°	90	90
V/Å^3	1994.74(9)	1017.48(2)
Z	8	4
Z'	1	1
Wavelength/Å	0.71073	0.71073
Radiation type	Mo K_α	Mo K_α
Θ_{min}/°	2.513	2.270
Θ_{max}/°	30.499	40.790
Measured Refl's.	39262	46908
Indep't Refl's	3047	6515
Refl's I≥2 *s*(I)	2562	5845
R_{int}	0.0678	0.0334
Parameters	172	146
Restraints	226	90
Largest Peak	1.395	0.967
Deepest Hole	-1.018	-0.700
GooF	1.086	1.141
ωR_2 **(all data)**	0.0834	0.0479
ωR_2	0.0796	0.0469
R_1 **(all data)**	0.0457	0.0279
R_1	0.0344	0.0229

Table S 2: X-ray crystallographic data of compounds **2-As**[$BArF_{24}$] and **2-Sb**[$BArF_{24}$].

Compound	**2-As**[$BArF_{24}$]	**2-Sb**[$BArF_{24}$]
CCDC Entry	2428361	2428362
Formula	$C_{67}H_{37}As_2BF_{24}Mo_5O_{10}P_2$	$C_{67}H_{37}BF_{24}Mo_5O_{10}P_2Sb_2$
ρ_{calc}	2.009	2.067
μ/mm^{-1}	1.939	14.185
Formula Weight	2160.25	2253.91
Colour	dark red	dark red
Shape	block-shaped	block-shaped
Size/mm^3	0.25×0.17×0.10	0.16×0.11×0.06
***T*/K**	123.01(10)	123.00(10)
Crystal System	monoclinic	monoclinic
Space Group	$P2_1/c$	$P2_1/c$
***a*/Å**	18.8305(5)	18.9232(2)
***b*/Å**	20.6156(5)	20.7180(2)
***c*/Å**	20.0687(6)	20.1171(2)
α/°	90	90
β/°	113.556(4)	113.3230(10)
γ/°	90	90
V/Å^3	7141.5(4)	7242.46(14)
Z	4	4
Z'	1	1
Wavelength/Å	0.71073	1.54184
Radiation type	Mo K_α	Cu K_α
Θ_{min}/°	2.153	2.543
Θ_{max}/°	30.508	75.163
Measured Refl's.	64302	112565
Indep't Refl's	21767	14709
Refl's I≥2 *s*(I)	14946	12354
R_{int}	0.0591	0.0439
Parameters	1411	1303
Restraints	951	592
Largest Peak	1.045	1.182
Deepest Hole	-0.904	-1.091
GooF	1.042	1.060
ωR_2 **(all data)**	0.1192	0.1181
ωR_2	0.1078	0.1129
R_1 **(all data)**	0.0814	0.0508
R_1	0.0471	0.0419

6. DFT Calculations

All calculations were performed using ORCA 6.0.0,[12] using default settings, and were carried out using the Cedar cluster, located at Simon Fraser University and maintained by the Digital Research Alliance of Canada. Initial geometries were either extracted from single-crystal X-ray structures or drawn by hand in Avogadro 1.2.0.[13] Global minimums were first located using the Global Optimizer Algorithm (GOAT) using the GFN2-xTB method.[14] The global minima were then used as initial structures for geometry optimizations which were performed using the density functional theory (DFT) composite method r^{2}SCAN-3c,[15] which combines the r^{2}SCAN meta-generalized gradient approximation density functional,[16] D4 London dispersion correction,[16,17] a geometrical counterpoise correction,[16,18] and the def2-mTZVPP basis set. Transition states were found using the climbing image nudged elastic band method (NEB-CI) with 12 images between the previously optimized intermediates,[19] followed by transition state optimizations to find the true saddle point. The minimum energy path (MEP) for **INT1** → **INT2** was also generated using the NEB-CI method. All stationary points were confirmed to have only real frequencies, and all saddle points have exactly one imaginary frequency. Saddle points were confirmed to connect the reactants to the products by intrinsic reaction coordinate (IRC). Single-point energy calculations were performed on the optimized structures using Kozuch and Martin's dispersion-corrected, spin-component-scaled Double-hybrid functional (DSD-PBEP86),[20] Grimme's dispersion correction with Becke-Johnson damping (D3BJ),[21] and the Karlsruhe basis set of quadruple-zeta quality with polarization (def2-QZVPP) on all atoms,[22] with a 28-electron effective core potential (ECP-28) on Mo,[23] and Sb.[24] All atomic coordinates are provided as a separate supplementary file.

Table S 3: Energy values (in Ha) obtained from r^{2}SCAN-3c optimizations. "DSD" energies were obtained from single-point energy calculations at the DSD-PBEP86-D3BJ/def2-QZVPP level of theory. {Mo} = (CpMo(CO)$_2$.

	E(r^{2}SCAN-3c)	Gcorr	Hcorr	E(DSD)	E(DSD) +Gcorr	E(DSD) +Hcorr
{Mo}$_2$P$_2$ (**A**)	-1659.716853	0.15803946	0.230646	-1658.188971	-1658.030931	-1657.958325
{Mo}$_2$PAs (**B**)	-3554.261372	0.15654594	0.230261	-3552.326936	-3552.17039	-3552.096675
{Mo}$_2$PSb (**C**)	-1558.745333	0.15564001	0.229999	-1557.123871	-1556.968231	-1556.893872
{Mo}P$_3$ (**1-P**)	-1512.561821	0.06698701	0.121212	-1511.302438	-1511.235451	-1511.181226
{Mo}P$_2$As (**1-As**)	-3407.105306	0.06535985	0.120825	-3405.43814	-3405.37278	-3405.317315
{Mo}P$_2$Sb (**1-Sb**)	-1411.591957	0.0643442	0.120587	-1410.232251	-1410.167906	-1410.111664
[({Mo}$_2$P$_2$)$_2${Mo}]$^+$ (**[2-P]$^+$**)	-3807.774566	0.43582681	0.577375	-3804.216015	-3803.780188	-3803.638639
[({Mo}$_2$AsP)$_2${Mo}]$^+$ (**[2-As]$^+$**)	-7596.865377	0.43314853	0.576632	-7592.493939	-7592.06079	-7591.917306
[({Mo}$_2$SbP)$_2${Mo}]$^+$ (**[2-Sb]$^+$**)	-3605.834684	0.43137386	0.576098	-3602.082561	-3601.651187	-3601.506463
[P(BZIMPY)]$^+$	-1425.165198	0.29539976	0.365488	-1423.759258	-1423.463859	-1423.393771
BZIMPY	-1084.027311	0.29207893	0.360839	-1082.865322	-1082.573243	-1082.504482
[P(dppe)]$^+$	-2028.808123	0.3722581	0.452205	-2026.945734	-2026.573475	-2026.493529
dppe	-1687.639658	0.36651249	0.446772	-1686.019137	-1685.652624	-1685.572365
[{Mo}BZIMPY]$^+$	-1572.34121	0.38821138	0.475487	-1570.65057	-1570.262358	-1570.175083
A + [P(BZIMPY)]$^+$ (**TS1-P**)	-3084.871402	0.47977149	0.593226	-3081.939639	-3081.459867	-3081.346412
B + [P(BZIMPY)]$^+$ (**TS1-As**)	-4979.413899	0.47905815	0.592415	-4976.076868	-4975.59781	-4975.484453
C + [P(BZIMPY)]$^+$ (**TS1-Sb**)	-2983.89497	0.47751786	0.593706	-2980.871297	-2980.393779	-2980.277591
[{Mo}$_2$P$_3$(BZIMPY)]$^+$ (**INT1-P**)	-3084.888955	0.48034005	0.598105	-3081.96593	-3081.48559	-3081.367825
[{Mo}$_2$P$_2$As(BZIMPY)]$^+$ (**INT1-As**)	-4979.437013	0.47911206	0.597736	-4976.107353	-4975.628241	-4975.509617
[{Mo}$_2$P$_2$Sb(BZIMPY)]$^+$ (**INT1-Sb**)	-2983.926856	0.47810496	0.597397	-2980.906464	-2980.428359	-2980.309067
INT1 → **INT2** climbing image	-3084.868992	0.48361989	0.590734	-3081.947891	-3081.464271	-3081.357157
[{Mo}$_2$P$_3$]$^+$ (**INT2**)	-2000.823084	0.15975931	0.234887	-1999.057475	-1998.897716	-1998.822588
A + **INT2** (**TS2**)	-3660.530261	0.34173912	0.463316	-3657.235957	-3656.894218	-3656.772641
[({Mo}$_2$P$_2$){Mo}({Mo}P$_3$)]$^+$ (**INT3**)	-3660.602534	0.34305561	0.467738	-3657.309549	-3656.966493	-3656.841811

Atomic coordinates:

{Mo}2P2 - Compound A

Mo1	-0.6880039290	-0.2922052719	5.4770973866
Mo2	-1.1904694465	-0.0261819783	2.4424420664
P3	-1.0265961670	1.8577862010	4.1176436284
P4	0.7808532783	0.8402410932	3.8091205437
O5	-3.6414359319	0.6337132229	5.8885904459
O6	-1.6549644044	-3.0227905630	4.3371050271
O7	0.4545007690	1.6351732577	0.3595706649
O8	0.9207752508	-2.3148605967	2.0260433495
C9	-2.5467725280	0.3064441664	5.6769836247

C10	-1.3131555978	-1.9455169866	4.6298226162
C11	0.7129285231	0.5029680199	7.2333008014
C12	-0.4789432626	-0.0335272976	7.7862051938
C13	-0.5109113125	-1.4302263193	7.4902056001
C14	0.6809285131	-1.7492799732	6.7653482780
C15	1.4301884997	-0.5622291659	6.6098865716
C16	-0.1145085627	1.0383136965	1.1669306388
C17	0.1741282087	-1.4558826491	2.2090006204
C18	-2.9366859188	0.6752288548	1.0655201508
C19	-2.4996912558	-0.6222817487	0.6404432739
C20	-2.7991556792	-1.5393741120	1.6902229382
C21	-3.4345139635	-0.8160549866	2.7371723751
C22	-3.5161734413	0.5484971580	2.3564648322
H23	1.0223300346	1.5387830262	7.2699707275
H24	-1.2252256746	0.5155994507	8.3438055874
H25	-1.2783237189	-2.1289966468	7.7926725944
H26	0.9586582199	-2.7287558550	6.4008264729
H27	2.3817383571	-0.4733097563	6.1053945303
H28	-2.8592165091	1.5896333216	0.4932638054
H29	-2.0515306288	-0.8644760387	-0.3129010403
H30	-2.5952488190	-2.6011940003	1.6915055514

H31	-3.7860124482	-1.2331068804	3.6695913619
H32	-3.9460724735	1.3461573558	2.9451297803

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{Mo}2PAs - Compound B

Mo1	-0.0425366182	-0.0840097674	5.0107782758
Mo2	-1.9303854643	-0.5010450743	2.5890940381
As3	-0.5676300516	1.6949626829	3.0923219430
P4	0.5979962199	-0.1199631572	2.5956580194
O5	-2.1904316456	1.8815349662	6.1441113462
O6	-1.9189852336	-2.5081548677	5.5506343187
O7	-1.2782624798	-0.1272094218	-0.4498702836
O8	-0.7889022577	-3.4141205673	2.3237545756
C9	-1.4211580757	1.1580706959	5.6568859646
C10	-1.2906336305	-1.5803625216	5.2227268211
C11	2.2765732992	-0.7150622435	5.2312781616
C12	2.1374039631	0.6459719900	5.6348346195
C13	1.2819505457	0.6840802013	6.7679986674
C14	0.8766575836	-0.6532796299	7.0582717191
C15	1.5012288471	-1.5152360411	6.1011308373
C16	-1.4637384690	-0.2579466488	0.6814191719

C17	-1.1636078657	-2.3288697935	2.4283572298
C18	-4.0441430371	-1.0769611729	1.8729507138
C19	-3.9374872503	-1.5006001719	3.2307161670
C20	-3.8263984572	-0.3411228173	4.0461525783
C21	-3.8420176953	0.8031756280	3.2068726335
C22	-3.9710253935	0.3540355557	1.8637952928
H23	2.8720085036	-1.0708845966	4.4027132722
H24	2.5982055355	1.4987718512	5.1550936415
H25	0.9978216489	1.5689920528	7.3207616918
H26	0.2400595189	-0.9634116630	7.8750468058
H27	1.4019721269	-2.5910587013	6.0561691670
H28	-4.1841603430	-1.7147198572	1.0116243333
H29	-3.9511497421	-2.5214358550	3.5866930957
H30	-3.7356986383	-0.3323720071	5.1224759202
H31	-3.7797223792	1.8304350625	3.5357239757
H32	-4.0303850571	0.9860838828	0.9882052797

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{Mo}2PSb - Compound C

Mo1	-0.8668965824	-0.0147049153	5.6778204881
Mo2	-1.5737188106	0.4218245122	2.7222516124

Sb3	-2.6425198739	2.0316405591	4.7257843141
P4	-0.2509840591	1.9949578222	4.3296659367
O5	-1.3223875806	1.7158624785	8.2431063019
O6	-3.7266656255	-1.2512154171	5.9788274352
O7	-1.6004119031	3.0237276408	0.9847555188
O8	1.4742409999	0.0909144610	2.1094458854
C9	-1.2002938871	1.1255819870	7.2552118135
C10	-2.7021024892	-0.7182254323	5.8399062147
C11	0.1607868187	-1.5155109626	7.1131071058
C12	-0.1628400387	-2.2416435616	5.9311391970
C13	0.6142115996	-1.7209751996	4.8621991278
C14	1.4147671977	-0.6609516289	5.3733594863
C15	1.1386940779	-0.5323422876	6.7592112981
C16	-1.5633933761	2.0970437832	1.6734384337
C17	0.3600019640	0.2630207708	2.3865276795
C18	-2.5925942217	-1.7471876609	2.8460781853
C19	-3.6308795979	-0.7875538112	2.6715822981
C20	-3.4253270744	-0.1436452707	1.4217361430
C21	-2.2542621172	-0.7007411226	0.8181203063
C22	-1.7433216942	-1.6880486193	1.7109664231
H23	-0.2404825755	-1.6922484740	8.1010463812

H24	-0.8660441609	-3.0612251822	5.8683213788
H25	0.6130129000	-2.0752061022	3.8420781209
H26	2.1128196092	-0.0643995083	4.8040528679
H27	1.5973618961	0.1777114169	7.4336522586
H28	-2.4838713319	-2.4135858238	3.6886497498
H29	-4.4418509124	-0.6044598831	3.3613360270
H30	-4.0551852268	0.6236443764	0.9927494712
H31	-1.8485747601	-0.4441085123	-0.1501872089
H32	-0.8678711665	-2.2996624345	1.5384397471

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{Mo}P3 - Compound 1P

Mo1	-1.8611417363	-1.2510847257	2.8604437604
P2	-2.8438278880	0.3357763215	1.1203546739
P3	-0.7310420693	0.6401911507	1.4708722113
P4	-1.3859684631	-1.0950391165	0.3577533172
O5	-1.7849348148	1.1075271927	4.9329040247
O6	1.1850560736	-1.8126196586	3.3805380582
C7	-3.6549231374	-2.0058929577	4.1396055161
C8	-3.9926736124	-2.3019633830	2.7924498084
C9	-3.0406846923	-3.2362906511	2.2936420000

C10	-2.1141021001	-3.5186249807	3.3321065838
C11	-2.4915106806	-2.7621069451	4.4855542386
C12	-1.7847914720	0.2695294010	4.1406898444
C13	0.0799645043	-1.5627199046	3.1660771275
H14	-4.1947730674	-1.3363801851	4.7951336263
H15	-4.8276962039	-1.8925577873	2.2422755840
H16	-3.0281958765	-3.6587021557	1.2991875009
H17	-1.2771769795	-4.2001485655	3.2656326914
H18	-2.0079187755	-2.7851810558	5.4517964416

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{Mo}P2As - Compound 1As

Mo1	-1.7518080785	-1.3272382352	2.9242332245
As2	0.7999763478	-2.0622023347	3.1250102491
P3	0.3783612560	-0.1090674433	2.0239575915
P4	-0.1476282833	-1.9566701095	1.0366390830
O5	-1.1912093713	0.6816598350	5.2713383951
O6	-2.9457283051	1.0153186435	1.2095920532
C7	-1.3606791238	-0.0320034852	4.3816648508
C8	-2.4577794987	0.1736961993	1.8300386041
C9	-2.9122374918	-2.5220973439	4.5466471326

C10	-2.2431778555	-3.4982311190	3.7594584941
C11	-2.7596683470	-3.4256158030	2.4344395322
C12	-3.7480178884	-2.4065758686	2.4015337240
C13	-3.8539648156	-1.8437104727	3.7126701738
H14	-2.7496266440	-2.3384382009	5.5998233195
H15	-1.4827985310	-4.1824289845	4.1073361211
H16	-2.4548791760	-4.0417001267	1.6008323777
H17	-4.3312467742	-2.1183085357	1.5377950439
H18	-4.5442284196	-1.0726746147	4.0240070297

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{Mo}P2Sb - Compound 1Sb

Mo1	-1.8657353671	-1.2089324951	2.9773637204
Sb2	-0.5442786454	1.3657247186	2.8364677826
P3	-1.4847241428	0.4231678336	4.9304632934
P4	-2.9347067547	1.0860130712	3.4429102808
O5	-1.8260155535	-0.6521477140	-0.1103585166
O6	1.1668315970	-2.0141786391	2.9487995470
C7	-1.8015103318	-0.7926668968	1.0371070441
C8	0.0710513352	-1.6448670596	2.9508119758
C9	-2.4693716637	-3.4008800543	2.5937349656

C10	-3.6410831120	-2.6034260096	2.4043763305
C11	-3.9938302672	-2.0287054224	3.6540075394
C12	-3.0433732586	-2.4601421393	4.6229070081
C13	-2.1026118199	-3.3017640205	3.9723212456
H14	-1.9723347144	-3.9958416923	1.8408156242
H15	-4.1759812108	-2.4716507656	1.4738421637
H16	-4.8370427000	-1.3787102113	3.8385314378
H17	-3.0396585565	-2.1942724522	5.6701692255
H18	-1.2619658407	-3.7930080579	4.4427463356

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[({Mo}2P2)2{Mo}]+ - Compound [2P]+

Mo1	1.9834658866	12.4870025641	5.2834385993
Mo2	-0.0573113124	15.4577951759	2.3313999952
Mo3	2.7032422224	16.5695162209	3.0846793997
Mo4	1.5587800923	12.3127195527	9.9492661933
Mo5	-1.0858578540	11.3233781773	8.6411569898
P6	1.6419806686	14.3561498666	3.6827173502
P7	2.2895770025	14.5377608036	1.6851289011
P8	1.0649034304	11.9642003215	7.5558000597
P9	1.1401261853	10.1523815989	8.6281596934

O10	-0.8359510697	12.6094197157	1.2828437453
O11	-1.1249694951	12.5110882181	4.8870278455
O12	1.4214085461	17.1510564061	5.8894248833
O13	3.1161044294	14.8592621256	6.9947258653
O14	0.5336282132	16.4122456061	-0.6025896023
O15	-1.5051996410	14.3051515549	7.7784622087
O16	5.1231642364	15.0999628324	4.4202582766
O17	-1.5940236939	11.9597564495	11.6552622064
O18	1.4012618539	10.0403260877	12.1259361774
C19	-0.5112222903	13.6538869802	1.6422236821
C20	0.3548224223	16.0355590579	0.4739594987
C21	1.8930279482	16.8942391862	4.8657413335
C22	0.0213700656	12.5532348421	5.0555595127
C23	2.6195271811	14.0226372142	6.3699964981
O24	4.4912661128	11.4190240458	9.2928631239
C25	-2.1152661544	15.2564279464	3.4009256140
H26	-2.5383902298	14.2843177671	3.6100123987
C27	3.6773087936	11.8338415278	3.7771419902
H28	4.0890054684	12.5257121511	3.0555993827
C29	3.3624552565	10.6181081585	5.6882317733
H30	3.4915750149	10.2152719220	6.6831537898

C31	4.2091581546	15.6201151616	3.9449511252
C32	-0.9795549216	17.2429310199	3.6399860116
H33	-0.4046621773	18.0510574366	4.0666956771
C34	-1.3227633690	13.2210856568	8.1425378426
C35	2.3344106046	10.2474922328	4.7653186113
H36	1.5691787115	9.5033891321	4.9379493634
C37	2.6743613313	18.9048137807	2.8554098303
H38	2.1182672280	19.5386242976	3.5331592830
C39	2.6634956898	14.3553151611	10.1313248959
H40	3.5914200860	14.5461078469	9.6108085472
C41	4.1971133513	11.5814865349	5.0696989020
H42	5.0614946033	12.0579851117	5.5122931108
C43	-1.2975898821	16.0117765927	4.2830559918
H44	-0.9923648978	15.7137834030	5.2769893342
C45	2.5292393699	11.0036820833	3.5766186330
H46	1.9381823086	10.9481296578	2.6723932263
C47	4.0198447428	18.4704290654	3.0384405711
H48	4.6656584466	18.7244552056	3.8671661715
C49	2.2085429608	18.4009784199	1.6117358123
H50	1.2389199062	18.5868228892	1.1737951375
C51	-1.2790197236	11.7680479334	10.5536998037

C52	-2.2973051440	16.0129716834	2.2010400242
H53	-2.8985873293	15.7270970983	1.3493213070
C54	3.2582662887	17.6406583201	1.0229570373
H55	3.2168412847	17.1389499434	0.0665101414
C56	1.4489015619	10.8409636741	11.3043282509
C57	-1.8040786725	9.0953794204	8.0883485855
H58	-1.1686291334	8.2233706806	8.1531546001
C59	-1.9740595705	9.9228349807	6.9400216306
H60	-1.4798480393	9.8007681051	5.9858639368
C61	2.5290256042	13.7817596408	11.4377817849
H62	3.3370961626	13.4741507386	12.0868422266
C63	-1.5856299633	17.2402672917	2.3570724920
H64	-1.5451662041	18.0419894328	1.6319358387
C65	3.4030655206	11.7070291752	9.5326931601
C66	4.3759216597	17.6834527963	1.8970446467
H67	5.3386194351	17.2243030867	1.7181030360
C68	-2.9183931425	10.9337406098	7.2619814979
H69	-3.2777652949	11.6992823491	6.5887626743
C70	0.4277725874	14.3066326624	10.6533880838
H71	-0.6435810105	14.4331335954	10.5957696496
C72	-2.6259708767	9.5999185578	9.1242629334

H73	-2.7260979899	9.1824437988	10.1167982518
C74	1.1367219560	13.7448978422	11.7486676371
H75	0.6938905109	13.3746225429	12.6634678093
C76	1.3638727734	14.6762511151	9.6524251690
H77	1.1312322245	15.1431969644	8.7064426825
C78	-3.3217918419	10.7438764921	8.6187514894
H79	-4.0556231710	11.3298287019	9.1545661558

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[({Mo}2AsP)2{Mo}]+ - Compound [2As]+

Mo1	2.0133580180	12.3962223109	5.2464662116
Mo2	-0.0352645819	15.4008011263	2.3223725306
Mo3	2.7007968586	16.5447935404	3.1506499390
Mo4	1.5787138643	12.3742739081	9.9144841131
Mo5	-1.0869066275	11.3624374766	8.6226310406
P6	1.6791887312	14.2786671685	3.6535995801
As7	2.4009810913	14.4998787969	1.5600774094
P8	1.0883774901	11.9035196105	7.5282472247
As9	1.1688330404	10.0221128793	8.7124042030
O10	-0.8060828981	12.5809766454	1.1952222072
O11	-1.0964998818	12.4719419401	4.8706736205

O12	1.4080877298	16.9196500954	5.9824016705
O13	3.2535379955	14.7235368748	6.9383984201
O14	0.5131254596	16.4991917754	-0.5673111368
O15	-1.4471835463	14.3340816797	7.7058504835
O16	5.1770625300	15.0619153252	4.3651693066
O17	-1.5695771936	12.0610383152	11.6262903273
O18	1.4597349923	10.2477203478	12.2314644715
C19	-0.4784874613	13.6152193087	1.5825681144
C20	0.3615993569	16.0582802526	0.4903053220
C21	1.8900847363	16.7350623405	4.9472320160
C22	0.0516855728	12.4955435636	5.0320863210
C23	2.7102529993	13.9086317707	6.3238520687
O24	4.5144763399	11.4917404452	9.2610089449
C25	-2.0964658870	15.1600226440	3.3764913029
H26	-2.5175150463	14.1805226690	3.5517362282
C27	3.6970582142	11.7157924483	3.7400692892
H28	4.1230815745	12.4036236813	3.0231780579
C29	3.3581860786	10.4995317204	5.6465946612
H30	3.4779331061	10.0956492587	6.6421964975
C31	4.2439267931	15.5861020559	3.9340192448
C32	-0.9667364531	17.1400885619	3.6841981110

H33	-0.3933103196	17.9341404892	4.1381372078
C34	-1.2836509290	13.2543244652	8.0910365039
C35	2.3242013631	10.1513219497	4.7226031298
H36	1.5448477016	9.4209900691	4.8909925486
C37	2.5483259317	18.8812937341	3.0768766698
H38	1.9590070817	19.4392612541	3.7921493030
C39	2.6854423097	14.4208449647	10.0214737581
H40	3.6190796588	14.5867937933	9.5031691463
C41	4.2106888333	11.4496802398	5.0321038156
H42	5.0833232361	11.9083997574	5.4774683069
C43	-1.2841904630	15.8884126528	4.2859829819
H44	-0.9818804979	15.5597542002	5.2709070377
C45	2.5338229398	10.9085021028	3.5360461045
H46	1.9425596223	10.8653505235	2.6312393127
C47	3.9153645706	18.5078057734	3.2389313465
H48	4.5446051157	18.7393602181	4.0866551821
C49	2.1120306570	18.4375986228	1.7999594974
H50	1.1353648763	18.6003115131	1.3689790432
C51	-1.2603216967	11.8410518082	10.5283189621
C52	-2.2755511844	15.9541324925	2.2012174744
H53	-2.8713791322	15.6940186533	1.3375091562

C54	3.2017858183	17.7749409859	1.1680974704
H55	3.1904743943	17.3421778775	0.1777720797
C56	1.4886386870	10.9837663336	11.3486801226
C57	-1.8850646294	9.1565035351	8.1018691867
H58	-1.2964283601	8.2533896278	8.1813060222
C59	-2.0176939266	9.9695495609	6.9384908370
H60	-1.5242411468	9.8122404912	5.9892595027
C61	2.5371428858	13.9018495858	11.3487384874
H62	3.3381999938	13.6185633479	12.0172813878
C63	-1.5676055989	17.1774294763	2.3993971258
H64	-1.5268253071	18.0018293989	1.7001886582
C65	3.4239899996	11.7709821318	9.5029170851
C66	4.3141625368	17.8179434531	2.0509731573
H67	5.3003331512	17.4232204597	1.8475495008
C68	-2.9229745089	11.0214844743	7.2386912754
H69	-3.2494495877	11.7882243774	6.5504265251
C70	0.4454040620	14.3979116669	10.5232958310
H71	-0.6250457874	14.5239568120	10.4517210967
C72	-2.6923577825	9.7118484161	9.1254907114
H73	-2.8127714838	9.3157667363	10.1245154135
C74	1.1417848204	13.8817576885	11.6478319304

H75	0.6892043454	13.5505450872	12.5727558301
C76	1.3917658158	14.7222613897	9.5153343003
H77	1.1699262836	15.1495071626	8.5479603316
C78	-3.3417485264	10.8709831969	8.5967817401
H79	-4.0565068192	11.4931609119	9.1171281003

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[({Mo}2SbP)2{Mo}]+ - Compound [2Sb]+

Mo1	2.0410872238	12.3064086106	5.2152107244
Mo2	-0.0431814080	15.3703455982	2.3436976149
Mo3	2.7096628723	16.5144188320	3.1914964924
Mo4	1.5955911954	12.4436866757	9.8790509403
Mo5	-1.0877772144	11.3668001997	8.6004229181
P6	1.7055402720	14.2035926314	3.6218910158
Sb7	2.4982263550	14.4314177536	1.3296583847
P8	1.1156408633	11.7980941849	7.5061583915
Sb9	1.2330709310	9.7853789360	8.8805049720
O10	-0.8752082526	12.6039898629	1.1359055008
O11	-1.0673833061	12.4313217166	4.8543888236
O12	1.4435327999	16.7328796350	6.0473565270
O13	3.3499637678	14.5950254614	6.9002188646

O14	0.3856142450	16.6526888307	-0.4866334201
O15	-1.4137547082	14.3359530185	7.6729305560
O16	5.2196879154	14.9974187995	4.2883605862
O17	-1.5371530779	12.0657992184	11.6115519784
O18	1.6238661416	10.5399000280	12.3737781241
C19	-0.5130124082	13.6179845451	1.5497676056
C20	0.2997536563	16.1275606451	0.5427108156
C21	1.9189430303	16.5962676242	5.0008557601
C22	0.0818805704	12.4361038166	5.0141297965
C23	2.7742303463	13.7970079365	6.2926882423
O24	4.5386225502	11.6519398308	9.1562750205
C25	-2.0851219357	15.0992103945	3.4257268777
H26	-2.5043683357	14.1145914457	3.5733951394
C27	3.7243279386	11.6206745141	3.7083152693
H28	4.1594769221	12.3154074891	3.0042263915
C29	3.3683039223	10.3877155799	5.5986176258
H30	3.4798912389	9.9775097217	6.5922572076
C31	4.2740427580	15.5308211816	3.8957378444
C32	-0.9458969966	17.0652137025	3.7826206255
H33	-0.3626066847	17.8418446551	4.2536411672
C34	-1.2559967156	13.2584122677	8.0667988267

C35	2.3326425815	10.0608611784	4.6697301917
H36	1.5436895675	9.3386879930	4.8286158837
C37	2.4896607563	18.8430222203	3.2640723342
H38	1.8922457498	19.3399177091	4.0167796154
C39	2.6649095650	14.5131977203	9.9226872171
H40	3.6012392496	14.6744137490	9.4084662916
C41	4.2322794979	11.3348698859	4.9976151074
H42	5.1081381691	11.7796808496	5.4507156682
C43	-1.2552311703	15.7942141888	4.3455453471
H44	-0.9357519819	15.4308431113	5.3123227969
C45	2.5525150293	10.8294724558	3.4921452312
H46	1.9616541118	10.8036472454	2.5864164061
C47	3.8684126309	18.4982909787	3.3942207787
H48	4.4973558734	18.6933043238	4.2512224056
C49	2.0548533541	18.4705125311	1.9645539618
H50	1.0714858960	18.6345355880	1.5497491597
C51	-1.2430009875	11.8446423905	10.5101720416
C52	-2.2829190192	15.9337122105	2.2823774775
H53	-2.8927369625	15.7045152579	1.4196964365
C54	3.1570836439	17.8801686562	1.2847742640
H55	3.1533233057	17.5288070628	0.2629066500

C56	1.5895083036	11.1656629129	11.4052626284
C57	-1.9505980186	9.1874788034	8.0679459742
H58	-1.4253619101	8.2468672002	8.1550649240
C59	-2.0273069632	9.9982781342	6.8983286926
H60	-1.5218509757	9.8168766174	5.9599610358
C61	2.5119444858	14.0396412289	11.2649637005
H62	3.3106501435	13.7905219676	11.9497397116
C63	-1.5686379959	17.1479362050	2.5103714046
H64	-1.5379405666	17.9956868915	1.8391122518
C65	3.4431853422	11.8866472426	9.4277119212
C66	4.2757370137	17.8959634922	2.1639602547
H67	5.2709087679	17.5431563023	1.9297687932
C68	-2.8978301110	11.0849165687	7.1741672295
H69	-3.1818885700	11.8577963707	6.4743487522
C70	0.4211683993	14.4711645475	10.4041000928
H71	-0.6503807691	14.5785208550	10.3213970354
C72	-2.7587989346	9.7832534115	9.0728900063
H73	-2.9159565647	9.3980085378	10.0710742971
C74	1.1139326192	14.0102391193	11.5531622127
H75	0.6580106549	13.7057108787	12.4855920207
C76	1.3725403806	14.7717349580	9.3917414639

H77	1.1556581997	15.1574761157	8.4058871568
C78	-3.3556310579	10.9578110769	8.5233005048
H79	-4.0605652057	11.6076619122	9.0224874590

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[P(BZIMPY)]+

P1	-0.8289468384	-1.6181955567	2.7151109090
N2	0.1262642889	-2.1919789549	-1.1938115462
N3	-0.8515587004	-1.6240143907	0.7340171640
N4	1.2505928022	-2.7526542806	6.0165653628
N5	-0.2512143502	-1.9246315527	4.5834830755
N6	0.6944735067	-2.4756944110	2.4102122222
C7	2.4380431568	-3.4138271739	6.5393867999
C8	1.0840033125	-2.7389885009	-2.1445161058
C9	-2.8533197033	-0.5416371345	-2.6894673759
C10	-3.4652453827	-0.1866108366	-1.4755058818
C11	-2.8857911473	-0.4969055259	-0.2559931732
C12	-1.6424743047	-1.2184624804	-2.7320367353
C13	-1.6702719295	-1.1763867503	-0.2866810919
C14	-1.0582341475	-1.5318835687	-1.5087693455
C15	0.2029692279	-2.2207903323	0.1692786107

C16	-2.0360872646	-0.8905984876	7.6693810165
C17	-1.0940614834	-1.4095963712	8.5734819338
C18	0.0552875998	-2.0592873773	8.1457572709
C19	-1.8615245872	-1.0032880553	6.2997029077
C20	0.2334202245	-2.1739651206	6.7706329965
C21	-0.7112276467	-1.6533942991	5.8591106997
C22	0.9103702780	-2.5751765351	4.7060105155
C23	3.1123399575	-3.8375911676	1.9264395628
C24	2.6910306872	-3.5891614954	3.2253460842
C25	2.3238276493	-3.4042738140	0.8696035135
C26	1.5011921335	-2.9186063041	3.4667416967
C27	1.1328841703	-2.7336250421	1.1048026458
H28	2.4023760124	-3.3841590195	7.6285629924
H29	2.4681741356	-4.4628159537	6.2261487025
H30	3.3464490340	-2.8970010972	6.2120618971
H31	1.1855753320	-3.8216603085	-2.0143169363
H32	0.7191160295	-2.5500817469	-3.1543127804
H33	2.0598014412	-2.2535797047	-2.0363711933
H34	-4.4122947463	0.3421668169	-1.4969241757
H35	-3.3550475994	-0.2245632249	0.6831236876
H36	-1.1886605460	-1.4823136862	-3.6811556725

H37	-3.3411195844	-0.2792100631	-3.6225828112
H38	-1.2692527912	-1.2996860730	9.6387245574
H39	0.7685567249	-2.4517406378	8.8623678598
H40	-2.9184950532	-0.3912553255	8.0553794251
H41	-2.5860807917	-0.6043026111	5.5982348964
H42	3.2898605966	-3.9181951347	4.0648425596
H43	4.0422678296	-4.3615368709	1.7404962930
H44	2.6322353565	-3.5864480256	-0.1517986455

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BZIMPY

N1	-5.8254625833	1.8043247519	-0.1221835827
N2	-6.5264039673	-0.0855989929	-1.1354109658
N3	-0.6340984176	2.0274480051	0.1317393663
N4	0.2275159612	0.1999228174	1.1355525308
N5	-3.1713240866	0.5394806794	0.0032042743
C6	-5.0794904560	2.7445515399	0.7021875904
C7	-1.4596388621	2.9040675733	-0.6869612458
C8	-7.9052536870	3.1894037979	-0.5168066521
C9	-9.1602686042	3.0951144709	-1.1047763960
C10	-9.5912236526	1.9161669581	-1.7397737089

C11	-8.7828724016	0.7918364030	-1.8076785819
C12	-7.5170814747	0.8633409918	-1.2201497864
C13	-7.0973971570	2.0573613390	-0.5908096769
C14	-5.5346754796	0.4988324543	-0.4852397073
C15	1.3230887416	3.5811616652	0.5226663178
C16	2.5841892029	3.5912802484	1.1052819965
C17	3.1153736290	2.4510407341	1.7351284573
C18	2.4046460604	1.2625222703	1.8028691021
C19	0.6138106334	2.3850490362	0.5965656052
C20	1.1348712110	1.2287982336	1.2204658333
C21	-0.8122762659	0.7007365128	0.4903320441
C22	-1.9063582013	-1.4939571761	0.2320934054
C23	-3.0506520305	-2.2411023821	-0.0034030666
C24	-4.2554662940	-1.5949433438	-0.2356462662
C25	-2.0115831556	-0.0981212065	0.2230111569
C26	-4.2714778196	-0.1952324746	-0.2199312892
H27	0.9179577529	4.4682251668	0.0448992751
H28	3.1734835313	4.5028288460	1.0763096077
H29	4.1054969410	2.5082978385	2.1772425533
H30	2.8110967572	0.3798675405	2.2866396708
H31	-4.6302703485	3.5311586998	0.0840504807

H32	-5.7653414456	3.2059460798	1.4209560182
H33	-4.2851833890	2.2242940001	1.2334637112
H34	-1.9558960229	3.6595169318	-0.0657744411
H35	-0.8211061282	3.4101068636	-1.4192190413
H36	-2.2219020408	2.3221170018	-1.2008120169
H37	-3.0035016884	-3.3262268415	-0.0059576840
H38	-0.9431932440	-1.9526112824	0.4228327926
H39	-5.1752420120	-2.1344810327	-0.4287702390
H40	-10.5808907370	1.8915172603	-2.1859257359
H41	-9.1117041059	-0.1203587990	-2.2956191583
H42	-7.5781657839	4.1062654788	-0.0355284216
H43	-9.8242021024	3.9538259032	-1.0761388549

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[P(dppe)]+

C1	9.0955411287	3.4233838998	7.9771008721
H2	8.5558214708	4.3586091473	8.1070530162
C3	11.4957001079	3.1527658557	2.2929137948
C4	11.1733717194	1.8822428545	2.7863950220
H5	10.7789345677	1.7636181590	3.7929930491
C6	11.3806679289	0.7621132703	1.9945775961

H7	11.1223480380	-0.2215648932	2.3740062185
C8	11.9285302958	0.8991571357	0.7202848458
H9	12.0951780273	0.0197208905	0.1057618387
C10	12.2720250799	2.1575732246	0.2393100442
H11	12.7112802756	2.2637190498	-0.7476211215
C12	12.0576040246	3.2887496584	1.0207983576
H13	12.3302262770	4.2679614899	0.6400419249
C14	9.4610188713	5.4088645981	5.2762264773
H15	8.5106433498	5.2820869173	5.8068039663
H16	9.5905939611	6.4728414493	5.0476602578
C17	9.5172579674	4.5558632805	4.0116323455
H18	8.8423956653	4.9358891309	3.2365058335
H19	9.2471832209	3.5150394415	4.2235017694
C20	10.2694800052	3.3731293031	7.2124110633
C21	8.6248982069	2.2714448672	8.5932147525
H22	7.7146415215	2.3099759176	9.1836388092
C23	9.3218813124	1.0718170095	8.4577711667
H24	8.9514542236	0.1743571998	8.9440207794
C25	10.4904408910	1.0231335459	7.7056765583
H26	11.0370169539	0.0904240213	7.6063964904
C27	10.9653581694	2.1709751050	7.0773138831

H28	11.8741648638	2.1384408105	6.4813593915
C29	11.1440984936	6.1421763654	7.6263740547
C30	11.2021953368	5.8154867635	8.9836953022
H31	11.0482264885	4.7923176090	9.3118994598
C32	11.4650154105	6.8112789856	9.9191914770
H33	11.5141871061	6.5568813431	10.9732838103
C34	11.6671261829	8.1233847927	9.5063555499
H35	11.8700020615	8.8973367488	10.2403214557
C36	11.6215585266	8.4466854308	8.1512098079
H37	11.7906225819	9.4692780028	7.8286973634
C38	11.3719269967	7.4595825719	7.2089015001
H39	11.3746086804	7.7103598530	6.1506882602
C40	11.3880603499	6.0801575983	2.3424942003
C41	12.3077148433	7.0801709193	2.6608255026
H42	12.9593377676	6.9574119636	3.5222692959
C43	12.3797761425	8.2273348689	1.8758104093
H44	13.1008998494	9.0012811533	2.1196767251
C45	11.5315315048	8.3806276756	0.7847414688
H46	11.5876788420	9.2780442640	0.1759982402
C47	10.6093931746	7.3842981828	0.4675959653
H48	9.9490341506	7.5038948229	-0.3857598710

C49	10.5364448200	6.2325242860	1.2392815620
H50	9.8285607550	5.4513521793	0.9718834698
P51	12.5533849119	4.5821133818	5.0867729455
P52	10.8553334753	4.8742835046	6.3652062770
P53	11.2545524226	4.5875093936	3.3747377655

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dppe

C1	-0.3815106100	-0.8102011936	-0.6601111505
C2	-1.7278670338	-1.0888511403	-0.4544311460
C3	0.5966505187	-1.7049192121	-0.2324623892
C4	-2.0924700317	-2.2694758441	0.1894241471
C5	-1.1189373892	-3.1606266119	0.6216906263
C6	0.2410722246	-2.8969904264	0.4078012631
H7	-0.0853243016	0.1076289583	-1.1604815051
H8	-2.4892210482	-0.3915260253	-0.7915231203
H9	-3.1416046229	-2.4972297559	0.3562843719
H10	-1.4168384933	-4.0800983630	1.1203754829
H11	1.6410826232	-1.4637146388	-0.4071610129
C12	0.5654958579	-8.0482340646	0.7910469736
C13	0.0642231509	-8.1783009762	-0.4992166487

C14	0.9616433879	-6.7977171436	1.2616886785
C15	-0.0408539946	-7.0555047235	-1.3189419095
C16	0.3570390587	-5.8094237537	-0.8503531452
C17	0.8653506457	-5.6675594326	0.4459674949
H18	0.2637420088	-4.9359278328	-1.4912163337
H19	0.6445909098	-8.9189926282	1.4358029181
H20	-0.4340015180	-7.1532744766	-2.3270785778
H21	-0.2477290857	-9.1515750418	-0.8674087897
H22	1.3494338632	-6.6939969498	2.2724365903
C23	5.9306741102	-1.8919590927	-1.2594181129
C24	6.0275434741	-3.0202496484	-0.4411928648
C25	6.3260564662	-0.6401650136	-0.7915092671
C26	6.5355867189	-2.8752308620	0.8548754228
C27	6.9327694238	-1.6278916145	1.3207443302
C28	6.8271764297	-0.5069915628	0.4984987626
H29	7.3257088793	-1.5276912943	2.3287237970
H30	5.5430282394	-1.9981224310	-2.2699716756
H31	6.6290821586	-3.7472020114	1.4977619876
H32	7.1386013705	0.4672591142	0.8645533761
H33	6.2465020836	0.2291131660	-1.4381999576
C34	8.6228566019	-7.5970122378	0.4668132256

C35	7.2764916487	-7.8765713531	0.6713430982
C36	8.9871710200	-6.4163940991	-0.1771778793
C37	6.2980956389	-6.9827733672	0.2424375667
C38	6.6533652360	-5.7906912244	-0.3980697367
C39	8.0133952097	-5.5261309158	-0.6107445124
H40	9.3843714049	-8.2936274752	0.8050035318
H41	5.2536515067	-7.2245214163	0.4162160494
H42	8.3111374531	-4.6066425129	-1.1094859976
H43	6.9805846285	-8.7944147879	1.1718411430
H44	10.0362781695	-6.1878631469	-0.3431723970
P45	1.4922313275	-4.0567426808	1.1017548043
P46	5.4016648972	-4.6327149255	-1.0938606001
C47	2.9231285309	-3.7948791977	-0.0804514056
C48	3.9711265453	-4.8936519443	0.0892939130
H49	3.3712546714	-2.8210284668	0.1531486192
H50	2.5600729619	-3.7577546881	-1.1166614719
H51	3.5227509540	-5.8675925516	-0.1434299446
H52	4.3350532045	-4.9302152947	1.1251975157

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[{Mo}BZIMPY]+

Mo1	0.7162951540	4.9483843139	5.3144921917
O2	1.7085084587	3.8513921368	8.0644878819
O3	0.7171066830	1.8299716091	5.0423244424
N4	-0.6205995915	4.0164755828	1.9471775696
N5	0.4084795845	2.0094198313	1.9140285826
N6	2.4066913650	6.2663343943	5.5974354377
N7	1.9982354530	4.8441290554	3.4313767227
N8	4.1784000214	7.4243389422	4.8738896892
C9	1.4116041727	0.9717090044	2.1034060363
C10	5.1720586467	8.0340097875	3.9963247395
C11	-1.6005546705	0.6023313403	1.2895982834
C12	-2.9498047667	0.7391857699	0.9957615270
C13	-2.8955184025	3.1586803447	1.2939387768
C14	-3.5858534216	1.9949491184	0.9969714823
C15	-1.5319222628	4.9145103025	4.6840039746
C16	-1.0434703089	6.1441948588	4.1608090384
C17	-0.9110006653	1.7761349908	1.5815470405
C18	3.9632230808	9.0651325189	8.1952272088
C19	-0.6175245800	6.9460578751	5.2421284460
C20	-0.8413143638	6.2211145571	6.4520749955
C21	-1.5357911186	3.0431119277	1.5968934845

C22	-1.4280105627	4.9654552715	6.1053906050
C23	2.8665705107	8.3205935503	8.6633200706
C24	0.5079845433	3.3658027688	2.1428528757
C25	2.7569500461	3.8804231734	1.3545630420
C26	3.9621476470	4.5626750600	1.4275324869
C27	4.1533762725	5.4397938397	2.4765658715
C28	3.8903492959	7.8817610403	6.1494198086
C29	2.2606302897	7.3525942113	7.8806215686
C30	1.7970350444	4.0429152788	2.3490461244
C31	3.1562575038	5.5842744338	3.4441336787
C32	3.2716333737	6.4378250852	4.5921380048
C33	2.7784531372	7.1426577981	6.6018814796
C34	1.3730898162	4.2547751524	7.0361993831
C35	0.7341719366	2.9849122795	5.0968848475
C36	4.4986862703	8.8581244173	6.9336832995
H37	1.6794826164	0.5153723112	1.1434739499
H38	2.3050867844	1.4006817307	2.5598109588
H39	1.0210345009	0.1999956615	2.7736211774
H40	4.7793426649	8.1186453934	2.9805388685
H41	5.3751929038	9.0423942034	4.3610483164
H42	6.1102240381	7.4681891007	3.9940854951

H43	-1.1181577409	-0.3701119474	1.2825217210
H44	-3.5304172392	-0.1454986905	0.7545209893
H45	-3.3837787525	4.1284047092	1.2905459343
H46	-4.6430262940	2.0472916146	0.7568410412
H47	-1.9467408821	4.1051907643	4.1013782929
H48	-0.9695993080	6.3785600627	3.1078737580
H49	4.4118908729	9.8107167388	8.8434524505
H50	-0.1778884202	7.9326973722	5.1704320292
H51	-0.6813215563	6.5912924687	7.4544856374
H52	-1.7728318523	4.2104727727	6.7984673198
H53	2.4950825138	8.5025815722	9.6663223437
H54	2.5306290459	3.2301274531	0.5163833601
H55	4.7274834018	4.4265961030	0.6707905882
H56	5.0839000524	5.9825135195	2.5661594301
H57	1.4359217596	6.7612081993	8.2589577987
H58	5.3615430085	9.4216159834	6.5954154055

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{Mo}2P2 + [P(BZIMPY)]+ - Transition State (TS1-P)

Mo1	-0.5471906565	3.2015807159	-1.1823982193
Mo2	-1.0526311511	1.6690226288	1.5616582076

P3	-1.5605217447	0.9673682579	-0.7599547964
P4	0.5899982454	0.9064349086	-0.2114307658
P5	-0.2889808581	-1.1873598771	-0.5624787441
O6	-0.5308077351	4.7033381332	1.9623112445
O7	1.1459869117	2.0469770638	-3.5438439450
O8	1.7007817578	1.1180592162	2.9292778145
O9	2.2194057578	4.2245737315	-0.1146916661
C10	-2.4729068956	4.5934974917	-0.7379210988
C11	-2.7901260776	3.7857168346	-1.8581240159
C12	-0.6496425156	3.5936095214	1.6278773327
C13	-1.3426469775	5.3916213040	-1.0701636760
C14	-1.8612287475	4.0807909065	-2.8935399093
C15	-2.9919946526	2.2787360359	2.7701647712
C16	-3.3925795829	1.2450760215	1.8908965670
C17	-0.9700921387	5.0925750818	-2.4135665790
C18	-2.0221580746	1.7418657417	3.6683121682
C19	-2.6820075009	0.0566542349	2.2472346809
C20	0.5370035000	2.4525848778	-2.6470125122
C21	-1.8475327771	0.3589861132	3.3477909418
C22	0.7147606208	1.3430880439	2.3628522928
C23	1.2023377790	3.8262997022	-0.4825901890

H24	-2.9911114010	4.5979372693	0.2106255561
H25	-3.5964807434	3.0679009656	-1.9167993464
H26	-3.3606113756	3.2955736757	2.7747163011
H27	-4.1218796661	1.3318166458	1.0973211273
H28	-0.8675094851	6.1146804104	-0.4214267584
H29	-1.8558615944	3.6462526204	-3.8840682256
H30	-1.5414860044	2.2758992880	4.4765121523
H31	-0.1794142654	5.5669051930	-2.9779106376
H32	-2.7638350596	-0.9066040794	1.7621454017
H33	-1.2047836092	-0.3385476019	3.8679183700
N34	1.5254662385	-2.3553405640	-0.3789858899
N35	-0.0297539305	-3.0365580241	1.8675094781
N36	1.5941077876	-2.3058693628	3.2592596307
N37	0.2464061946	-1.3567697547	-2.2939243890
N38	1.7055908650	-1.7623307743	-3.9273627144
C39	2.3039998845	-2.2176038561	-1.4913525406
C40	2.1229579287	-2.5915669869	0.8169004850
C41	3.6960489405	-2.3491488352	-1.4562232398
C42	3.4955736080	-2.8049380001	0.8918547169
C43	4.2881203305	-2.6802326966	-0.2523059811
C44	1.2315141310	-2.6527025096	1.9675234219

C45	-0.5326447760	-2.9571615715	3.1425477266
C46	0.4676829918	-2.4945509338	4.0307630313
C47	-1.8152810156	-3.2494383532	3.6181728702
C48	0.2226546496	-2.2870005995	5.3876347439
C49	-1.0613264186	-2.5686283464	5.8334976293
C50	-2.0630489242	-3.0449541348	4.9649078220
C51	1.4914825383	-1.8096375352	-2.5897882456
C52	0.5672013645	-1.2305330370	-4.5194259006
C53	-0.3669788560	-0.9968406708	-3.4925786115
C54	0.2770290780	-0.9687079220	-5.8530614027
C55	-1.6483184875	-0.5419420942	-3.7854869524
C56	-1.9384716291	-0.2799350206	-5.1169947599
C57	-0.9906320572	-0.4785124485	-6.1317535178
C58	2.8500221720	-2.3041479590	-4.6506361266
C59	2.8320406968	-1.7174901159	3.7567461665
H60	4.2965033057	-2.1773864423	-2.3413043533
H61	5.3610240639	-2.8259797785	-0.1900138704
H62	3.9432790603	-3.1068076195	1.8307564199
H63	-2.5798935195	-3.6259310998	2.9457736944
H64	-3.0472636188	-3.2611054552	5.3682649455
H65	0.9888583704	-1.9390275871	6.0732697264

H66	-1.2967956017	-2.4297961475	6.8840171141
H67	-1.2581327794	-0.2576977579	-7.1598518809
H68	1.0021946234	-1.1282139631	-6.6435877096
H69	-2.3914499349	-0.4123268252	-3.0085888043
H70	-2.9299178642	0.0731423267	-5.3817075370
H71	3.6404378913	-1.5534559566	-4.7584810460
H72	2.5185895976	-2.6197452255	-5.6420260141
H73	3.2348008482	-3.1801552117	-4.1237533679
H74	3.3244720027	-1.1524537724	2.9642935691
H75	3.5097636660	-2.4860342320	4.1470552115
H76	2.5878333015	-1.0173942225	4.5587526086

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{Mo}2PAs + [P(BZIMPY)]+ - Transition State (TS1-As)

Mo1	-0.7041184943	3.2507080241	-1.2616427486
Mo2	-0.9926837654	1.6959116464	1.4972444933
As3	-1.8063382558	0.9280889693	-0.8349512815
P4	0.5026869421	0.9316815170	-0.4099915523
P5	-0.2947236855	-1.2136613821	-0.6048763398
O6	-0.1279897958	4.6522184235	1.8701881335
O7	0.6122687583	2.0844112888	-3.8457897235

O8	1.7809748569	0.7838797053	2.5972945636
O9	2.2172892912	4.1556036549	-0.5823220389
C10	-2.4767748438	4.7225508572	-0.5329686191
C11	-2.9849616606	3.9491687551	-1.6082176023
C12	-0.3867860695	3.5655655949	1.5383166091
C13	-1.3683003786	5.4736743383	-1.0094514219
C14	-2.1958073846	4.2223048369	-2.7591985890
C15	-2.7599192403	2.4692912205	2.8569968134
C16	-3.3169084717	1.4578818581	2.0395908990
C17	-1.1976216818	5.1806334003	-2.3952281300
C18	-1.7595987094	1.8691512639	3.6797808633
C19	-2.6770279943	0.2196997292	2.3620724373
C20	0.1419277458	2.4889122237	-2.8690020233
C21	-1.7287068668	0.4721422908	3.3776635123
C22	0.7849985915	1.1468912281	2.1227678192
C23	1.1447985297	3.7939946044	-0.8033403033
H24	-2.8610739619	4.7396715936	0.4769540738
H25	-3.8313849070	3.2777290113	-1.5664574740
H26	-3.0461314017	3.5120451703	2.8740500380
H27	-4.1100526340	1.5895791852	1.3163530808
H28	-0.7733785226	6.1614555515	-0.4242351082

H29	-2.3502421630	3.8089171340	-3.7466565455
H30	-1.1699390484	2.3739360169	4.4325349210
H31	-0.4724945593	5.6312275890	-3.0582744083
H32	-2.8834134288	-0.7432919402	1.9156285445
H33	-1.0988706583	-0.2681892939	3.8528999920
N34	1.5634484965	-2.3472730080	-0.3407449201
N35	-0.0597061923	-2.9881362346	1.8372757234
N36	1.5425234307	-2.3836708187	3.3111543993
N37	0.2882045843	-1.4472831722	-2.3187186075
N38	1.8210374997	-1.7981173399	-3.8949090845
C39	2.3599501423	-2.2041178432	-1.4361325918
C40	2.1331756803	-2.5795409211	0.8681505148
C41	3.7530291327	-2.3074753771	-1.3699067322
C42	3.5079613525	-2.7778548978	0.9721583643
C43	4.3220361375	-2.6312010044	-0.1521100835
C44	1.2116327322	-2.6586923193	1.9934338467
C45	-0.6041896944	-2.9379084213	3.0953888567
C46	0.3824645384	-2.5557932552	4.0353300728
C47	-1.9154071438	-3.1894522660	3.5129578910
C48	0.0968291081	-2.3928617347	5.3906226937
C49	-1.2140467911	-2.6319580768	5.7789620318

C50	-2.2037408854	-3.0260704534	4.8570179369
C51	1.5618288698	-1.8436954923	-2.5648232363
C52	0.6823884424	-1.3222501913	-4.5320091452
C53	-0.2968126714	-1.1245797172	-3.5399346883
C54	0.4279281235	-1.0790418254	-5.8766696133
C55	-1.5869380683	-0.7301362819	-3.8798176595
C56	-1.8403350986	-0.4852125273	-5.2213488569
C57	-0.8487588597	-0.6446803669	-6.2009344536
C58	3.0195088856	-2.2797600054	-4.5721849995
C59	2.7803701570	-1.8628668571	3.8785037039
H60	4.3719471939	-2.1279092422	-2.2402594968
H61	5.3955556467	-2.7603985571	-0.0663151561
H62	3.9411284028	-3.0846972069	1.9157309828
H63	-2.6697501515	-3.5048152456	2.7986738431
H64	-3.2108719207	-3.2119332869	5.2165877751
H65	0.8514616403	-2.1090053474	6.1173765872
H66	-1.4817813579	-2.5240406516	6.8253643784
H67	-1.0888609903	-0.4375143913	-7.2385572707
H68	1.1860432819	-1.2090119327	-6.6412270250
H69	-2.3635784950	-0.6333905768	-3.1312246746
H70	-2.8357131557	-0.1756611015	-5.5226202109

H71	3.7868652322	-1.4994752848	-4.6183945843
H72	2.7502124669	-2.5762475585	-5.5876321860
H73	3.4085069540	-3.1577612701	-4.0514716857
H74	3.3165934440	-1.2735110026	3.1346439281
H75	3.4182529291	-2.6722287948	4.2534116239
H76	2.5299108386	-1.1965522067	4.7074689240

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{Mo}2PSb + [P(BZIMPY)]+ - Transition State (TS1-Sb)

Mo1	-0.2420729106	3.1364527502	-1.2035007179
Mo2	-1.0764442598	1.7604837225	1.6289437857
Sb3	-2.0668184270	1.0554955123	-0.8934119740
P4	0.3787489779	0.7097427237	-0.1507119216
P5	-0.5241727447	-1.3900801685	-0.5921268134
O6	-1.2734741026	4.8606581875	1.7842237053
O7	1.5604258066	1.5684605819	-3.2187729913
O8	1.8233259187	1.9777626588	2.7764418725
O9	2.4097755671	3.8870859273	0.2934228604
C10	-1.9672568894	4.8109924640	-1.2319994011
C11	-2.1047277807	4.0647290469	-2.4305394323
C12	-1.1543145679	3.7278581346	1.5440299396

C13	-0.6795672567	5.4167115781	-1.2293852127
C14	-0.8970087679	4.1966941007	-3.1712219968
C15	-2.9966758540	2.0025587719	2.9754343469
C16	-3.2125651458	0.8158859679	2.2313626632
C17	-0.0161759579	5.0514266163	-2.4408625967
C18	-1.8466266618	1.8093057633	3.7982600387
C19	-2.1905229824	-0.1186583870	2.5796685981
C20	0.8978207703	2.1069458343	-2.4332423298
C21	-1.3584933018	0.4853212055	3.5542983964
C22	0.7758655464	1.9476842947	2.2898088503
C23	1.4280836716	3.5643910738	-0.2149345430
H24	-2.7104259623	4.9034057770	-0.4532392175
H25	-2.9847039832	3.5236549923	-2.7478696607
H26	-3.6094047040	2.8931991027	2.9436582590
H27	-4.0409604280	0.6296623019	1.5632781883
H28	-0.2886300342	6.0636650207	-0.4562630859
H29	-0.6988249019	3.7594669813	-4.1404679964
H30	-1.4516925889	2.5155597035	4.5151862479
H31	0.9591440257	5.3875664602	-2.7639051286
H32	-2.0784980713	-1.1203389780	2.1859131875
H33	-0.5266310490	0.0092977160	4.0535432345

N34	1.3080449316	-2.3163225792	-0.4120934129
N35	-0.1380481095	-3.2111174752	1.8725215786
N36	1.3596441405	-2.2146648250	3.2418364152
N37	-0.0262330039	-1.4952034147	-2.3201947634
N38	1.4847905846	-1.6278037248	-3.9489757237
C39	2.1055416975	-2.0432718727	-1.5053250705
C40	1.9161239948	-2.4317942856	0.8076367312
C41	3.5001850469	-1.9762189241	-1.4272965105
C42	3.2986572926	-2.4363034875	0.9130048525
C43	4.1038601899	-2.2157234201	-0.2117589725
C44	1.0400983447	-2.6167765680	1.9529983674
C45	-0.6236375652	-3.2255546854	3.1588992560
C46	0.3005055942	-2.6072560211	4.0334793543
C47	-1.8339830282	-3.7223070032	3.6531472629
C48	0.0536190537	-2.4547146476	5.3965708290
C49	-1.1577502406	-2.9462206829	5.8626199257
C50	-2.0857191891	-3.5694120668	5.0061479786
C51	1.2782538168	-1.7410526186	-2.6154487684
C52	0.2805847632	-1.2561384188	-4.5348705606
C53	-0.6850256995	-1.2041738144	-3.5103615345
C54	-0.0448203809	-1.0012934193	-5.8611921152

C55	-2.0239037245	-0.9669505148	-3.8010429363
C56	-2.3491564195	-0.7099444131	-5.1272844437
C57	-1.3759451012	-0.7137892231	-6.1359060329
C58	2.7167501357	-1.9194944959	-4.6690149613
C59	2.4443930965	-1.3563080899	3.7034468549
H60	4.0871759532	-1.7155140790	-2.2997339154
H61	5.1837794459	-2.2048494275	-0.1175465286
H62	3.7566287285	-2.6611670917	1.8685233076
H63	-2.5419141509	-4.2095722530	2.9899303657
H64	-3.0145553501	-3.9446393133	5.4239401430
H65	0.7690093886	-1.9955607481	6.0723307935
H66	-1.3913328854	-2.8591604926	6.9190978397
H67	-1.6712842380	-0.5096630131	-7.1599005549
H68	0.6978384409	-1.0204376102	-6.6512849488
H69	-2.7831285790	-1.0094148185	-3.0297300919
H70	-3.3850895839	-0.5238628344	-5.3909939244
H71	3.3622909814	-1.0352932086	-4.7138193330
H72	2.4640066117	-2.2322468750	-5.6841528948
H73	3.2414933266	-2.7426838316	-4.1785775452
H74	2.8057721760	-0.7353103617	2.8819065750
H75	3.2737329459	-1.9409068243	4.1185814688

H76	2.0622456172	-0.6929539631	4.4848664891

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[{Mo}2P3(BZIMPY)]+ - INT1-P

Mo1	0.1464840673	2.8746329239	-0.5477240866
Mo2	-1.7908418302	1.5520649550	1.4593407646
P3	-1.9253230320	1.4956234281	-1.0581399218
P4	0.2166591995	0.4501992758	0.4358659759
P5	-1.2035405429	-0.6168833553	-0.8740473516
O6	-3.3274473364	4.2482581555	1.0019856703
O7	1.7533231905	1.2643946353	-2.6826472738
O8	0.2272178309	3.0569790069	3.3394110886
O9	2.6537750691	2.5861584947	1.3281743317
C10	-1.2397517646	4.6193586246	-1.3779724151
C11	-0.2329092801	4.3261196854	-2.3387815655
C12	-2.6863261082	3.2951175631	1.1217215505
C13	-0.6054518000	5.1344903905	-0.2129886230
C14	1.0339796318	4.6584674092	-1.7603726226
C15	-3.9274679363	0.9965422458	2.2325928035
C16	-3.4782184754	-0.1452219530	1.5196686669
C17	0.7931473628	5.1539798816	-0.4497010443

C18	-3.0624165269	1.1926948516	3.3538744415
C19	-2.3332811232	-0.6615970269	2.1899750528
C20	1.1381097678	1.7994754079	-1.8601610078
C21	-2.0739327495	0.1607456276	3.3197999270
C22	-0.4592201697	2.5271797631	2.5760242126
C23	1.7089401334	2.6818881037	0.6768132043
H24	-2.3035555786	4.4860033852	-1.5163636377
H25	-0.3992498826	3.9453513485	-3.3370666145
H26	-4.7921851031	1.5973941267	1.9848896217
H27	-3.9340080805	-0.5616634247	0.6324139245
H28	-1.0961685681	5.4674049352	0.6898852814
H29	1.9981445186	4.5814803920	-2.2435627787
H30	-3.1663090914	1.9554521418	4.1128537382
H31	1.5461239140	5.4979780334	0.2470359465
H32	-1.7748329327	-1.5434253694	1.9055138541
H33	-1.2852248496	0.0004615014	4.0437473867
N34	1.2244108324	-2.2301869915	-0.4876168960
N35	0.2299970518	-3.1528748466	2.0918489744
N36	1.7994485571	-1.8005816510	2.9977453818
N37	-0.3433460656	-1.0336447053	-2.5028234162
N38	0.9776817485	-1.9100047916	-4.0527802020

C39	1.7854808682	-1.9952262523	-1.6748671983
C40	2.0162329583	-2.3899630693	0.5779303116
C41	3.1690151340	-1.9314195615	-1.8708407908
C42	3.4119518318	-2.4261068123	0.4620854624
C43	3.9866576435	-2.1890754835	-0.7778712388
C44	1.3349198339	-2.4681419993	1.8751527453
C45	-0.0658136574	-2.9371436146	3.4213594169
C46	0.8951979196	-2.0774546526	4.0013475165
C47	-1.1406201241	-3.4018247131	4.1848099105
C48	0.8087299164	-1.6377809681	5.3208641473
C49	-0.2730915228	-2.1036432112	6.0573614209
C50	-1.2297687014	-2.9725473859	5.4995418999
C51	0.8226311983	-1.6706109051	-2.7261658781
C52	-0.1269863045	-1.4007783556	-4.7171509175
C53	-0.9686110976	-0.8572713352	-3.7343373268
C54	-0.4616038834	-1.3980546843	-6.0672041781
C55	-2.1981261429	-0.2954872951	-4.0760979760
C56	-2.5330360230	-0.2909042582	-5.4215048996
C57	-1.6809088402	-0.8277350130	-6.4005334830
C58	2.0100808541	-2.7138670895	-4.7026990060
C59	2.8195790682	-0.7638243732	3.0880192086

H60	3.5967610374	-1.6502326288	-2.8262930784
H61	5.0663771311	-2.1796548291	-0.8895199353
H62	4.0294722950	-2.6289621580	1.3310638858
H63	-1.8769297104	-4.0709118238	3.7503440730
H64	-2.0524232520	-3.3149442872	6.1195136054
H65	1.5495857590	-0.9803146387	5.7659142444
H66	-0.3773073289	-1.7985638545	7.0940233436
H67	-1.9848875437	-0.7985648965	-7.4417222437
H68	0.1934085471	-1.8108132478	-6.8269781258
H69	-2.8633092463	0.1215201258	-3.3287909404
H70	-3.4823789431	0.1369616838	-5.7266250433
H71	2.7733025274	-2.0757537068	-5.1604153925
H72	1.5356693291	-3.3197282938	-5.4787873101
H73	2.4723885071	-3.3810742464	-3.9744397868
H74	3.0763577115	-0.4081632117	2.0888004686
H75	3.7207423483	-1.1323985678	3.5917420323
H76	2.4184948541	0.0844134361	3.6524617143

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[{Mo}2P2As(BZIMPY)]+ - INT1-As

Mo1	0.1673529315	2.8879890424	-0.5527011562

Mo2	-1.8088007157	1.5829924710	1.4385362604
As3	-2.0465354204	1.5640983386	-1.1754541191
P4	0.1569965245	0.4453384160	0.3898334589
P5	-1.2505971116	-0.6446278010	-0.9298765958
O6	-3.3488516236	4.2771574629	0.9721104420
O7	1.5237500858	1.3204796302	-2.8854042899
O8	0.2963796451	3.0865063972	3.2163364896
O9	2.7659806416	2.3632492443	1.1341133186
C10	-1.1320030250	4.7439971114	-1.2778935682
C11	-0.0943421300	4.4935781564	-2.2191821726
C12	-2.7124748532	3.3213240911	1.0985871561
C13	-0.5286453614	5.1374384657	-0.0502577631
C14	1.1580501953	4.7249747658	-1.5670160548
C15	-3.9220421273	1.0352702062	2.2731015660
C16	-3.4923218415	-0.1119399828	1.5551841418
C17	0.8772253027	5.1179956777	-0.2259568905
C18	-3.0263164070	1.2386415040	3.3690594191
C19	-2.3309546938	-0.6248272408	2.1989926083
C20	0.9995570060	1.8411174621	-1.9941647797
C21	-2.0410210772	0.2049101467	3.3156797451
C22	-0.4267600136	2.5582538230	2.4836666259

C23	1.7868860415	2.5280002422	0.5484976285
H24	-2.1936464804	4.6760166444	-1.4711960686
H25	-0.2317906064	4.2103053524	-3.2537894522
H26	-4.7934255472	1.6344416244	2.0455498394
H27	-3.9738076586	-0.5368913991	0.6856864562
H28	-1.0442012025	5.4164527663	0.8568831350
H29	2.1378290839	4.6559692881	-2.0186442495
H30	-3.1083185025	2.0065765672	4.1253599732
H31	1.6101540579	5.3763872604	0.5269459581
H32	-1.7811557914	-1.5092268665	1.9056420705
H33	-1.2326398657	0.0495113267	4.0184301910
N34	1.2244207050	-2.2136902287	-0.4984432781
N35	0.2311429496	-3.1487793616	2.0672150607
N36	1.7697427766	-1.7759186961	2.9951861622
N37	-0.3794476476	-1.0987707601	-2.5338114037
N38	0.9884321049	-1.9381701808	-4.0633851616
C39	1.7846072086	-1.9554412381	-1.6810668957
C40	2.0142299401	-2.3428619309	0.5727569585
C41	3.1654104535	-1.8303663343	-1.8665721643
C42	3.4113324490	-2.3260451331	0.4659276616
C43	3.9849128377	-2.0588988972	-0.7684564961

C44	1.3262776285	-2.4440563211	1.8641934250
C45	-0.0798268021	-2.9462390431	3.3949475622
C46	0.8622499148	-2.0752285184	3.9891798854
C47	-1.1545270675	-3.4318212326	4.1455681728
C48	0.7579023005	-1.6466060040	5.3110511902
C49	-0.3233673192	-2.1335475136	6.0344968954
C50	-1.2621797855	-3.0123270414	5.4620055047
C51	0.8168627990	-1.6825598634	-2.7419419363
C52	-0.1373679607	-1.4962913789	-4.7402360914
C53	-1.0089544566	-0.9781183477	-3.7704579842
C54	-0.4662776010	-1.5345713749	-6.0910590061
C55	-2.2641171173	-0.4871130962	-4.1262199765
C56	-2.5938459539	-0.5230524732	-5.4724622704
C57	-1.7112259519	-1.0323018506	-6.4388533332
C58	2.0613223278	-2.7022849551	-4.6950013363
C59	2.7675551688	-0.7190781986	3.1006536779
H60	3.5871605927	-1.5291496315	-2.8187410888
H61	5.0641889943	-2.0049334774	-0.8714622815
H62	4.0310575479	-2.5102946784	1.3373602961
H63	-1.8765151306	-4.1090817047	3.6998990378
H64	-2.0854097544	-3.3708066769	6.0720396099

H65	1.4851909553	-0.9816838333	5.7673576506
H66	-0.4413750170	-1.8374487419	7.0722827755
H67	-2.0119049753	-1.0368191727	-7.4813726077
H68	0.2117746372	-1.9277506741	-6.8409282936
H69	-2.9564383755	-0.0987678045	-3.3885397336
H70	-3.5629611433	-0.1505199172	-5.7876322903
H71	2.7923074826	-2.0357062392	-5.1646758299
H72	1.6206043296	-3.3477669851	-5.4589542071
H73	2.5551153086	-3.3297424005	-3.9522344609
H74	3.0240146193	-0.3497974090	2.1065952239
H75	3.6727899867	-1.0728089959	3.6077883828
H76	2.3454515808	0.1163791212	3.6688636702

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[{Mo}2P2Sb(BZIMPY)]+ - INT1-Sb

Mo1	0.1570284396	2.8216943012	-0.6328479584
Mo2	-1.8567082703	1.6295759474	1.4253540648
Sb3	-2.3171361768	1.5853711192	-1.3412062291
P4	0.0044733912	0.4047326837	0.3484344668
P5	-1.3598589284	-0.7682810051	-0.9802205434
O6	-3.2816742295	4.3935786927	0.9716682772

O7	0.8080683652	1.4847193513	-3.3781599626
O8	0.4926837366	2.9818750750	3.0040068845
O9	2.9365817694	1.7500930297	0.3290114948
C10	-0.8852371084	4.9291479934	-1.0438430646
C11	0.1358217040	4.7040316950	-2.0072439994
C12	-2.6995057051	3.4013155409	1.0866630409
C13	-0.2658216956	5.0316831645	0.2358459682
C14	1.3877471019	4.6464089519	-1.3209698984
C15	-3.9348679458	1.1648679824	2.3942602387
C16	-3.5872251438	-0.0034496597	1.6636689935
C17	1.1267764702	4.8520285830	0.0717072106
C18	-2.9676250442	1.3491781833	3.4303425575
C19	-2.4069617660	-0.5496717779	2.2447090759
C20	0.5184225037	1.9098254728	-2.3391136908
C21	-2.0236803394	0.2809589299	3.3307776153
C22	-0.3359828979	2.5243057475	2.3351291041
C23	1.8685178331	2.0765677390	0.0208525519
H24	-1.9405332498	5.0450759157	-1.2494717621
H25	-0.0082875263	4.6192113514	-3.0759368014
H26	-4.7972354859	1.7921647337	2.2125138233
H27	-4.1401247099	-0.4281327212	0.8376255196

H28	-0.7670333766	5.2281109196	1.1721605231
H29	2.3602893599	4.5241652632	-1.7768939139
H30	-2.9786687596	2.1260508545	4.1817741139
H31	1.8652972252	4.8823333599	0.8615348007
H32	-1.9031636447	-1.4549367542	1.9321241388
H33	-1.1790528951	0.1069946461	3.9848372762
N34	1.2501272639	-2.1323192545	-0.5081365092
N35	0.2792737446	-3.0849870238	2.0303966546
N36	1.7573892899	-1.6728099530	2.9973711361
N37	-0.4671448092	-1.2343888093	-2.5463324534
N38	0.9927360557	-1.9184624373	-4.0686430660
C39	1.7859888186	-1.8166120884	-1.6873914130
C40	2.0434592173	-2.1905690584	0.5669021410
C41	3.1484563211	-1.5514929372	-1.8661172699
C42	3.4336627073	-2.0485606237	0.4628990591
C43	3.9818030879	-1.7125997790	-0.7665738240
C44	1.3538732876	-2.3421430079	1.8514477088
C45	-0.0583977475	-2.9081576417	3.3540072221
C46	0.8467926537	-2.0156811466	3.9738990857
C47	-1.1280808419	-3.4374132749	4.0824790802
C48	0.7111574565	-1.6111451886	5.3006193824

C49	-0.3648005345	-2.1412377305	6.0011656793
C50	-1.2681168073	-3.0396696014	5.4025508295
C51	0.7965917544	-1.6604220872	-2.7509832356
C52	-0.1859362072	-1.6466468864	-4.7452703945
C53	-1.1144399972	-1.2303251678	-3.7805698625
C54	-0.5134656079	-1.7563741932	-6.0922646220
C55	-2.4258220520	-0.9219460897	-4.1356539755
C56	-2.7555583845	-1.0302185917	-5.4782240319
C57	-1.8166687334	-1.4345819855	-6.4406772152
C58	2.1543370228	-2.5478725518	-4.6917916906
C59	2.7099761166	-0.5775091433	3.1288777450
H60	3.5424477536	-1.2003397258	-2.8131728930
H61	5.0508554776	-1.5517211177	-0.8636493450
H62	4.0682816980	-2.1851099686	1.3320396310
H63	-1.8209965714	-4.1318669428	3.6174380985
H64	-2.0884753855	-3.4320537399	5.9953524086
H65	1.4121022480	-0.9326377160	5.7777971038
H66	-0.5062600915	-1.8645472060	7.0413666226
H67	-2.1190800095	-1.5015208608	-7.4805286967
H68	0.2075827710	-2.0697221333	-6.8395362885
H69	-3.1629085276	-0.6258453390	-3.3984812555

H70	-3.7683302408	-0.8011374760	-5.7929070197
H71	2.7989807322	-1.7985253584	-5.1630469078
H72	1.8005081269	-3.2477418374	-5.4528487864
H73	2.7189666246	-3.1047053319	-3.9431439355
H74	2.9260575229	-0.1515144063	2.1478843087
H75	3.6421153845	-0.9097863390	3.6007026098
H76	2.2634954109	0.2098464414	3.7447732686

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INT1 -> INT2 Minimum Energy Path (converged climbing image)

Mo1	-0.1625182043	2.9230147175	-0.4948610314
Mo2	-2.1511567464	1.4876810493	1.4341696105
P3	-2.5668247572	2.2571614218	-0.9988119103
P4	-0.3216437300	0.3666538142	0.0495948333
P5	-2.2757134398	0.1278933579	-0.7962912757
O6	-3.3401467356	4.3977492614	1.5383940109
O7	0.3461816325	1.9551842225	-3.4286945325
O8	0.4911641805	2.2925467812	2.9090963530
O9	2.6183898194	1.6542628837	0.2585592161
N10	1.3187735416	-2.0506889130	-0.6019202903
N11	0.2791082413	-2.8345481598	1.9989815990

N12	1.8586157234	-1.4925662169	2.8938738220
N13	-0.1008116802	-1.0057515432	-2.8354197468
N14	1.1287320165	-2.3116859968	-4.1928813502
C15	-1.1053625839	5.1162832937	-0.6286827366
C16	-0.2183232872	4.9066857423	-1.7199523281
C17	-2.8709178691	3.3511361558	1.4315189161
C18	-0.3493188539	5.0674818828	0.5736736806
C19	1.0972956553	4.7234263789	-1.1894573175
C20	-4.1479000233	1.0940962630	2.6141547395
C21	-3.9027871130	-0.0815276364	1.8688073089
C22	1.0052793525	4.8217377016	0.2349282325
C23	-3.0673107636	1.2610384152	3.5434875112
C24	-2.6805523192	-0.6601617548	2.3373403633
C25	0.1294035125	2.2038221460	-2.3317702824
C26	-2.1813309751	0.1519124082	3.3812720486
C27	-0.4223549897	2.0711214914	2.2313782712
C28	1.5758126257	2.0805454965	0.0151358497
C29	1.8945397736	-1.9875347560	-1.8084104905
C30	2.0981677337	-2.1537176164	0.4797896964
C31	3.2846626856	-2.0192766413	-1.9795722856
C32	3.4909037361	-2.2564707794	0.3961254737

C33	4.0847530902	-2.1767690213	-0.8566616682
C34	1.3937853459	-2.1659887152	1.7736650270
C35	-0.0091411064	-2.6154993400	3.3289620835
C36	0.9586828976	-1.7596133740	3.9036466880
C37	-1.0631523755	-3.0995611569	4.1095355230
C38	0.8898157297	-1.3314708229	5.2281977879
C39	-0.1780330010	-1.8096760079	5.9796431517
C40	-1.1341111659	-2.6842743260	5.4311824025
C41	0.9654893190	-1.7790383183	-2.9292161172
C42	0.0760998357	-1.8375465116	-4.9532991421
C43	-0.6782700595	-1.0200044402	-4.0849442468
C44	-0.2893730301	-2.0553051546	-6.2788373365
C45	-1.8273208012	-0.3759304959	-4.5507616321
C46	-2.1951515380	-0.5853021276	-5.8695280226
C47	-1.4391636369	-1.4129172406	-6.7188674346
C48	2.0666868806	-3.3314049623	-4.6398399512
C49	2.9561463916	-0.5436090714	3.0178734006
H50	-2.1685241454	5.2970970865	-0.7059446458
H51	-0.4882636105	4.9179016394	-2.7675067416
H52	-5.0085729870	1.7415544766	2.5116798250
H53	-4.5337329554	-0.4859572093	1.0897147900

H54	-0.7341583261	5.2017453179	1.5748015939
H55	2.0020310103	4.5826115406	-1.7648255350
H56	-2.9850863555	2.0399978205	4.2887486958
H57	1.8297941434	4.7497473561	0.9315520614
H58	-2.2113612265	-1.5611445542	1.9620434568
H59	-1.2814872395	-0.0412088447	3.9526254192
H60	3.7287949915	-1.8918558919	-2.9614316369
H61	5.1648043654	-2.2264858306	-0.9554285239
H62	4.0923883745	-2.4125076749	1.2858895135
H63	-1.7935632263	-3.7833885930	3.6870887728
H64	-1.9373836958	-3.0486584226	6.0641458375
H65	1.6370171343	-0.6781999499	5.6691800363
H66	-0.2649285326	-1.5167524062	7.0213587099
H67	-1.7629638280	-1.5512899188	-7.7454502135
H68	0.2892869812	-2.6857691862	-6.9463648670
H69	-2.4131929646	0.2620064543	-3.8954210601
H70	-3.0868536871	-0.1044098695	-6.2593664878
H71	2.8631225525	-2.8973636056	-5.2559247884
H72	1.5287127370	-4.0774758934	-5.2322557231
H73	2.5083326830	-3.8316468714	-3.7764733235
H74	3.2831648263	-0.2213246014	2.0291066485

H75	3.8042500479	-0.9863486729	3.5539315572
H76	2.6085739985	0.3355325205	3.5702201572

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[{Mo}2P3]+ - INT2

Mo1	-0.4437735040	-0.7595150357	5.3495064344
Mo2	-1.9521149428	0.6264532543	2.9619033751
P3	0.1989558298	2.0880570804	3.3822091339
P4	-1.0650618985	1.6760065502	5.1310785595
P5	0.5005814082	-0.0396307953	3.1548956951
O6	-3.0985294403	-1.3586847711	6.9569606524
O7	-1.2055944397	-3.3668620506	3.7401647422
O8	-4.3735878804	0.3732620990	4.9541499477
O9	-2.8275390813	3.6536386109	2.7835061986
C10	-2.2017724728	-1.0753360230	6.3018305468
C11	-0.9598480768	-2.3868189912	4.2899089958
C12	0.3248098316	-0.6392174827	7.5509811206
C13	0.4969515284	-1.9752643669	7.0660684033
C14	1.4497874999	-1.9269363223	6.0055874591
C15	1.8705657268	-0.5755269920	5.8471136091
C16	1.1740562140	0.2185047793	6.8012623806

C17	-3.4267100929	0.4290957616	4.3128226905
C18	-2.4695705767	2.5721884586	2.8804631429
C19	-3.6766841354	0.1287618843	1.4979711925
C20	-2.7261359465	0.8639342007	0.7261766336
C21	-1.5380207736	0.1049321294	0.6491787324
C22	-1.7502610206	-1.1224159193	1.3499884876
C23	-3.0685389293	-1.1144786128	1.8698416751
H24	-0.3173620770	-0.3372615979	8.3675077541
H25	0.0226070623	-2.8634218175	7.4600973306
H26	1.8154376779	-2.7736357949	5.4403496239
H27	2.6312383372	-0.2223328636	5.1647675035
H28	1.3027012233	1.2808039266	6.9574120359
H29	-4.6958858458	0.4278017391	1.7035424700
H30	-2.8879922080	1.8351269939	0.2768327453
H31	-0.6252971876	0.3956512642	0.1463979120
H32	-1.0362181590	-1.9292679750	1.4329979591
H33	-3.5404817153	-1.9153078279	2.4232134344

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{Mo}2P2 + [{Mo}2P3]+ - Transition State (TS2)

Mo1	1.8087391100	1.5122903533	0.9439328965

Mo2	1.4881441424	4.3464270582	-1.4650104952
P3	3.4749756076	4.9449834838	0.1008368040
P4	1.7455444404	4.0790967835	1.1176430618
P5	3.3388993899	2.8801668735	-0.5626136372
O6	-1.1283342491	2.0772393725	1.9038779067
O7	1.1753368518	0.4173586333	-1.9635132100
O8	-1.4381231781	3.4713564515	-0.7305135072
O9	0.8348275480	7.2702191461	-0.4911370510
C10	-0.0909723737	1.8845477218	1.4404426980
C11	1.3575955168	0.8194007863	-0.8955415733
C12	2.6051553315	1.5470608782	3.2245881379
C13	2.0957460571	0.2603607918	2.8828302854
C14	2.9434550690	-0.3007240520	1.8844399736
C15	3.9723266612	0.6344507716	1.6035383203
C16	3.7512738599	1.7713905426	2.4283476316
C17	-0.3346266481	3.7473046801	-0.9008217185
C18	1.0716207865	6.1909181936	-0.7920302698
C19	0.5068018371	4.7852196897	-3.5106179505
C20	1.7269752609	5.5285869869	-3.4726223918
C21	2.8043170343	4.6076730549	-3.4301334863
C22	2.2575502204	3.2880288862	-3.4566039017

C23	0.8458374539	3.3938107581	-3.5050997759
H24	2.1881961104	2.2240246538	3.9573394681
H25	1.2355776948	-0.2204519962	3.3278652284
H26	2.8275228489	-1.2735095323	1.4271179349
H27	4.7787386754	0.5014703346	0.8959314971
H28	4.3496890256	2.6729769063	2.4287712956
H29	-0.4894324992	5.2000613484	-3.5816234445
H30	1.8156670295	6.6066971540	-3.4897193275
H31	3.8556687286	4.8590539266	-3.3911883403
H32	2.8226748526	2.3669666816	-3.4587080707
H33	0.1513192670	2.5659273903	-3.5507964805
O34	-1.6552998749	-0.6229151029	4.3951713780
H35	-4.9657609899	-1.3461441734	2.9957687023
C36	-1.8735646761	-1.1381192859	3.3883525963
C37	-4.5241951677	-1.2933499058	2.0104020145
C38	-3.8274213482	-0.1749365784	1.4534688527
C39	-4.5723036067	-2.3094651793	1.0115256488
O40	-2.6618737817	-4.7203376036	3.0868208544
Mo41	-2.3348846889	-1.9547716478	1.6389375814
C42	-2.4941249993	-3.7070945929	2.5587782498
H43	-5.0499579623	-3.2744911187	1.1164280126

C44	-3.9246539035	-1.8208855567	-0.1533577339
P45	0.0685023983	-2.8353968770	2.0226715219
P46	-0.1837648716	-1.1546989173	0.7798858990
H47	-2.9735596978	-5.2299920646	0.2694093871
H48	-0.6806435091	-5.9294508193	1.4912590026
Mo49	-0.4874243314	-3.4225683264	-0.3325810022
C50	-1.9983179740	-5.2756491843	-0.1929024609
C51	-1.1513323692	-2.1142292615	-1.6692155017
C52	-0.7854223066	-5.6525522875	0.4518180845
C53	1.3732570822	-2.9546311347	-0.8247964033
C54	-1.7074078392	-5.0119388514	-1.5578067806
C55	0.2517887719	-5.6300537948	-0.5162932901
H56	-2.4224974602	-4.7215904132	-2.3159091288
O57	2.4663452401	-2.7296258286	-1.1182188390
C58	-0.3156528720	-5.2324016217	-1.7694637668
H59	1.2867771487	-5.8913604121	-0.3426299359
H60	0.2069999389	-5.1541738303	-2.7124127205
H61	-3.6352428115	0.7668585176	1.9486877190
C62	-3.4577319839	-0.5045112167	0.1214960712
H63	-2.9337100551	0.1382651672	-0.5716598936
O64	-1.5593494506	-1.4114835729	-2.4913254847

H65	-3.8262595118	-2.3466892377	-1.0915171420

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[({Mo}2P2){Mo}({Mo}P3)]+ - INT3

Mo1	1.6935958618	0.7570776067	1.2816867567
Mo2	1.2737712589	4.5216136090	-1.5524618151
P3	3.7077754059	3.8016273262	-1.0594860584
P4	2.7361664841	4.8601149346	0.5989224346
P5	2.1242788090	2.8694269027	0.0650105053
O6	-1.1141895496	2.1624369008	1.2816179302
O7	2.4311064745	-0.1514242088	-1.6322710860
O8	-0.9784708325	5.4151753190	0.4606844606
O9	2.1717853827	7.5410726424	-1.7506236699
C10	-0.0857351081	1.6332114221	1.2531446066
C11	2.1097654941	0.1800503075	-0.5734584116
C12	2.3483665031	1.4318636329	3.4472847562
C13	1.9783765729	0.0627340236	3.4779230138
C14	2.9143474362	-0.6651492000	2.6645994091
C15	3.8566585875	0.2553879061	2.1451887300
C16	3.4960629664	1.5482701281	2.6118599868
C17	-0.1271370077	5.0954337320	-0.2399227028

C18	1.8598745047	6.4420531231	-1.6474511693
C19	-0.0966905023	4.8532369447	-3.3689412868
C20	1.2255678197	4.6292535996	-3.8723358099
C21	1.5971717966	3.2939292835	-3.5583550496
C22	0.5192740265	2.6875765718	-2.8544542945
C23	-0.5233459424	3.6475589971	-2.7329609268
H24	1.8553762298	2.2424742672	3.9663324373
H25	1.1604331477	-0.3654282776	4.0412265419
H26	2.9168662287	-1.7345617992	2.5050654373
H27	4.6914672716	0.0209212416	1.4986797553
H28	4.0204381182	2.4672662327	2.3855924029
H29	-0.6811531109	5.7553943940	-3.4844905250
H30	1.8251459556	5.3416557860	-4.4223755584
H31	2.5303249311	2.8152455750	-3.8202091516
H32	0.4897114580	1.6680217611	-2.4950850491
H33	-1.4842569922	3.4854062569	-2.2637087635
O34	-1.8714320370	-0.5048833270	4.2789981469
H35	-5.0120806590	-1.1452783457	2.3318563078
C36	-1.9685829611	-1.0148683008	3.2515143552
C37	-4.3919307379	-1.0573432987	1.4507393540
C38	-3.5675621481	0.0585283737	1.1039781176

C39	-4.2904418859	-2.0112954101	0.3937423913
O40	-2.9415269268	-4.5593751330	2.7442702945
Mo41	-2.2012017780	-1.7975873004	1.4426252587
C42	-2.6251556167	-3.5500850658	2.2827741659
H43	-4.8161978497	-2.9555948738	0.3458210476
C44	-3.4191843953	-1.4877324295	-0.5961289978
P45	0.0227610713	-2.9224629066	2.1905865616
P46	0.1110269934	-1.1519726502	1.0454214189
H47	-2.8770740367	-4.8145327468	-0.2296868078
H48	-0.9051403469	-5.8780209816	1.2603420456
Mo49	-0.1393319051	-3.2850083811	-0.2777591927
C50	-1.8501008491	-4.9432157654	-0.5381942129
C51	-0.3693962153	-1.8152565725	-1.5860500671
C52	-0.8084774264	-5.5142584035	0.2470494226
C53	1.8298681308	-3.0664844656	-0.3314935489
C54	-1.3124996065	-4.6162358364	-1.8120087602
C55	0.3692160603	-5.5485914329	-0.5439676933
H56	-1.8575868052	-4.1891630613	-2.6431835849
O57	2.9800314524	-3.0068803165	-0.3613540527
C58	0.0627026492	-4.9923809637	-1.8267983521
H59	1.3258485431	-5.9512537585	-0.2395522158

H60	0.7381130973	-4.9107229179	-2.6668219933
H61	-3.4403256942	0.9606853630	1.6854516712
C62	-2.9638617799	-0.2128728313	-0.1527229522
H63	-2.2926664326	0.4419746221	-0.6896718003
O64	-0.5415248642	-0.9880488561	-2.3776373860
H65	-3.1638387195	-1.9614659686	-1.5325017775

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