Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

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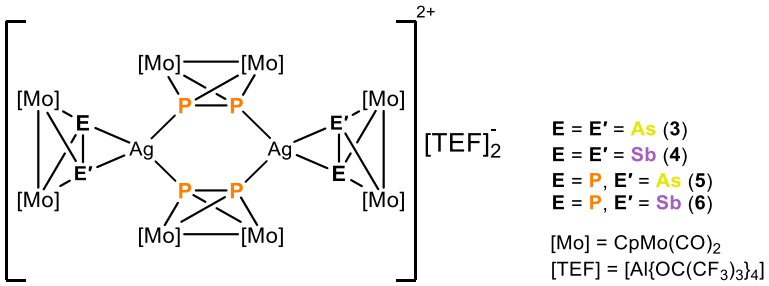
1. Materials and methods

All manipulations were carried out under an inert atmosphere of dry nitrogen using standard glovebox and Schlenk techniques. All solvents were taken from the solvent purification machine MB SPS-800 of the company MBRAUN. The ligand complexes $[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}E_2)]$[1] (E = P (**A**), As (**B**), Sb (**C**), Cp = C_5H_5), $[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}PE)]$[1] (E = As (**D**), E = Sb (**E**), Cp = C_5H_5)) and Ag salts $[Ag(CH_2Cl_2)][Al\{OC(CF_3)_3\}_4]$[2] (Ag[TEF]) and $[Cu(CH_3CN)_4][Al\{OC(CF_3)_3\}_4]$[3] (Cu[TEF]) were prepared according to literature procedures. Solid state IR spectra were recorded using a ThermoFisher Nicolet iS5 FT-IR spectrometer with an ATR-Ge disc. The NMR spectra were recorded on a Bruker Avance III HD 400 spectrometer (^{1}H: 400 MHz, ^{13}C: 100 MHz, ^{19}F: 376 MHz, ^{31}P: 162 MHz) with dichloromethane-d_2 or acetonitirile-d_3 as solvent at room temperature. The chemical shifts (δ) are presented in parts per million ppm and coupling constants (J) in Hz. The following samples were used as external reference: TMS (^{1}H, ^{13}C), $CFCl_3$ (^{19}F), 85% H_3PO_4 (^{31}P). ^{13}C, ^{19}F, ^{31}P and spectra were decoupled from the protons. The ESI-MS (ESI = Electrospray ionization) spectra were recorded on a Finnigan Thermoquest TSQ 7000 mass spectrometer with dichloromethane as solvent. Due to the experimental setup of the ESI-MS experiments, traces of CH_3CN are present in the device causing species containing CH_3CN. Elemental analyses were performed on an Elementar Vario EL III apparatus by the microanalytical laboratory of the University of Regensburg.

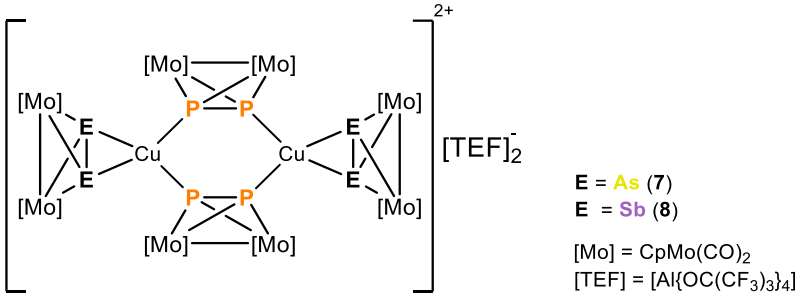
2. Experimental details and characterization

2.1. General synthetic protocol for compounds 3-6:



A solution of Ag[TEF] (35 mg, 0.03 mmol, 2 eq.) in 4 mL of CH_2Cl_2 was slowly added to a vigorously stirred solution of $[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}P_2)]$ (**A**) (30 mg, 0.06 mmol, 4 eq.) in 4 mL of CH_2Cl_2. The orange solution was stirred for 30 minutes at room temperature, after which, a solution of a homo- ($[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}E_2)]$[1] (E = As (**B**), Sb (**C**)) or- hetero- ($[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}PE)]$ (E = As (**D**), E = Sb (**E**)) dipnictogen ligand complex (**B-E**) (0.03 mmol, 2 eq.) in 4mL of CH_2Cl_2 was slowly added to the reaction mixture. The red solution was stirred for 30 minutes at room temperature, after which, it was carefully layered with 45 mL of *n*-pentane. Within four to ten days, red crystals of products were obtained, washed with *n*-pentane and dried *in vacuo*. Yield (**3** (47 mg, 72%), **4** (45 mg, 67%), **5** (22 mg, 35%), **6** (25 mg, 38%)). Noteworthy, in the crystal structures of compounds **5**-**6** a partial disorder of the complexes **D** or **E** with the complex **A** indicates the presence of the all-phosphorus complex $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2][TEF]$ (**1**). For additional information see the crystallographic details section.

2.2. General synthetic protocol for compounds 7-8:

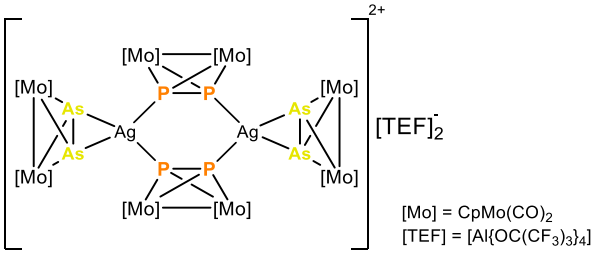


A solution of Cu[TEF] (36 mg, 0.03 mmol, 2 eq.) in 4 mL of CH_2Cl_2 was slowly added to a vigorously stirred solution of $[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}P_2)]$ (**A**) (30 mg, 0.06 mmol, 4 eq.) in 4 mL of CH_2Cl_2. The orange solution was stirred for 30 minutes at room temperature, after which, a solution of $[Cp_2Mo_2(CO)_4(\mu,\eta^2\text{-}E_2)]$[1] (E = As (**B**), Sb (**C**)) (0.03 mmol, 2 eq.) in 4mL of CH_2Cl_2 was slowly added to the reaction mixture. The red solution was stirred for 30 minutes at room temperature, after which, it was carefully layered with 45 mL of toluene*. Within four to ten days, red crystals of were obtained, washed with *n*-pentane and dried *in vacuo*. Yield (**7** (36 mg, 48%), **8** (33 mg, 38%). Noteworthy, in the crystal structures of compounds **7**-**8** a partial disorder of the complexes **B** or **C** with the complex **A** indicates the presence of the all-phosphorus complex $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2][TEF]$ (**1**). For additional information see the crystallographic details section.

* Reaction also yields the mixed dimer if pentane is used (different cell) but the crystal quality is not sufficient for the full experiment.

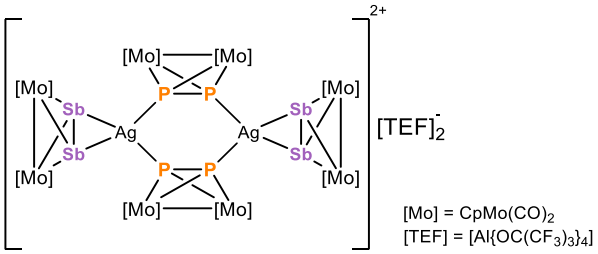
2.3. Characterization data for compounds 3-8:

2.3.1. $[\{\{CpMo(CO)_2\}_2\{\mu,\eta^2\text{-}As_2\}\}_2\{\{CpMo(CO)_2\}_2\{\mu,\eta^1\text{:}\eta^1\text{-}P_2\}\}_2Ag_2][Al\{OC(CF_3)_3\}_4]_2$ (3)



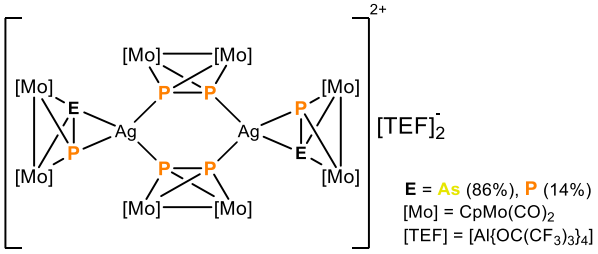
^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.29 (s, 10H, H_{Cp}), 5.34 (s, 10H, H_{Cp}).
^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 85.7 (s, C_{Cp}), 87.5 (s, C_{Cp}), 121.3 (q, $J_{(C,F)}$ = 292 Hz; C_{CF3}), 222.7 (broad s, C_{CO}), 222.8 (broad s, C_{CO}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -90.0 (broad s, $\omega_{1/2}$ = 470 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, $[Al\{OC(CF_3)_3\}_4]^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1188.4 (100%, $[\{Cp_2(CO)_4Mo_2P_2\}\{Cp_2(CO)_4Mo_2As_2\}Ag]^+$), 1275.3 (68%, $[\{Cp_2(CO)_4Mo_2As_2\}_2Ag]^+$), 1099.5 (34%, $[\{Cp_2(CO)_4Mo_2P_2\}_2Ag]^+$), 731.6 (25%, $[\{Cp_2(CO)_4Mo_2As_2\}\{CH_3CN\}Ag]^+$), 645.7 (17%, $[\{Cp_2(CO)_4Mo_2P_2\}\{CH_3CN\}Ag]^+$), 690.6 (5%, $[\{Cp_2(CO)_4Mo_2As_2\}Ag]^+$), 602.7 (3%, $[\{Cp_2(CO)_4Mo_2P_2\}Ag]^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, $[Al\{OC(CF_3)_3\}_4]^-$).
Elemental analysis (%) calculated for ($C_{88}H_{40}Ag_2Al_2F_{72}Mo_8O_{24}P_4As_4$) (4310.04 g·mol^{-1}): C, 24.52; H, 0.94; found: C, 24.35; H, 0.60.
IR (ATR-Ge): $\tilde{\nu}$ = 2356 (w), 2066 (m), 2040 (m), 2008 (s), 1997 (s), 1969 (s), 1945 (s), 1351 (m), 1298 (m), 1276 (s), 1241 (s), 1216 (s), 1168 (m), 1067 (w), 973 (s), 824 (m), 763 (s), 727 (s).

2.3.2. [{{CpMo(CO)$_2$}$_2${μ,η^2-Sb$_2$}}$_2${{CpMo(CO)$_2$}$_2${μ,η^1:η^1-P$_2$}}$_2$Ag$_2$][Al{OC(CF$_3$)$_3$}$_4$]$_2$ (4)



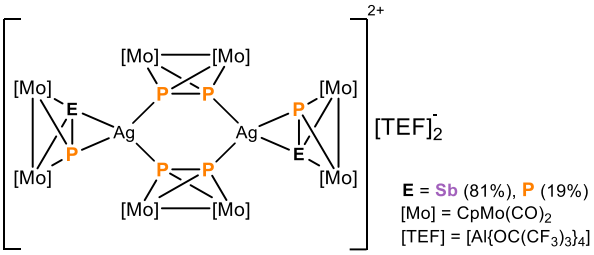
^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.25 (s, 10H, H_{Cp}), 5.36 (s, 10H, H_{Cp}).
^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 83.7 (s, C_{Cp}), 87.6 (s, C_{Cp}), 121.2 (q, $J_{(C,F)}$ = 291 Hz; C_{CF3}), 221.7 (s, C_{CO}), 222.5 (s, C_{CO}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -95.7 (broad s, $\omega_{1/2}$ = 163 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, [Al{OC(CF$_3$)$_3$}$_4$]$^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1282.4 (100%, [{Cp$_2$(CO)$_4$Mo$_2$P$_2$}{Cp$_2$(CO)$_4$Mo$_2$Sb$_2$}Ag]$^+$), 1100.5 (60%, [{Cp$_2$(CO)$_4$Mo$_2$P$_2$}$_2$Ag]$^+$), 645.7 (28%, [{Cp$_2$(CO)$_4$Mo$_2$P$_2$}{CH$_3$CN}Ag]$^+$), 825.6 (24%, [{Cp$_2$(CO)$_4$Mo$_2$Sb$_2$}{CH$_3$CN}Ag]$^+$), 784.6 (20%, [{Cp$_2$(CO)$_4$Mo$_2$Sb$_2$}Ag]$^+$), 1464.3 (19%, [{Cp$_2$(CO)$_4$Mo$_2$Sb$_2$}$_2$Ag]$^+$), 602.7 (3%, [{Cp$_2$(CO)$_4$Mo$_2$P$_2$}Ag]$^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, [Al{OC(CF$_3$)$_3$}$_4$]$^-$).
Elemental analysis (%) calculated for ($C_{88}H_{40}Ag_2Al_2F_{72}Mo_8O_{24}P_4Sb_4$) (4497.39 g·mol^{-1}): C, 23.50; H, 0.90; found: C, 23.84; H, 0.59.
IR (ATR-Ge): $\tilde{\nu}$ = 2356 (w), 2066 (m), 2041 (m), 2016 (s), 1990 (s), 1963 (s), 1944 (s), 1921 (s), 1905 (s), 1352 (m), 1297 (m), 1274 (s), 1238 (s), 1218 (s), 1168 (m),972 (s), 827 (s), 748 (m), 726 (s).

2.3.3. [{{CpMo(CO)$_2$}$_2${μ,η^2-PAs}}$_2${{CpMo(CO)$_2$}$_2${μ,η^1:η^1-P$_2$}}$_2$Ag$_2$]$_{0.86}$[Al{OC(CF$_3$)$_3$}$_4$]$_2$ (5)



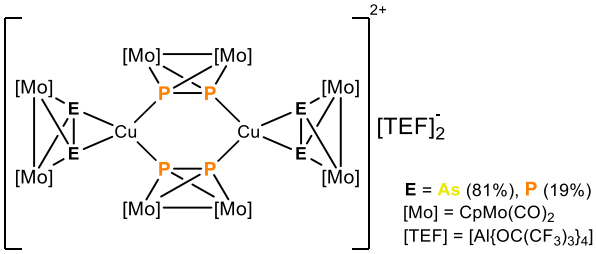
^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.30 (s, 10H, H_{Cp}), 5.32 (s, 11.6H, H_{Cp}).
^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 86.5 (s, C_{Cp}), 87.5 (s, C_{Cp}), 121.2 (q, $J_{(C,F)}$ = 291 Hz; C_{CF3}), 222.1 (s, C_{CO}), 222.5 (s, C_{CO}), 223.0 (s, C_{CO}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -91.1 (broad s, $\omega_{1/2}$ = 123 Hz), 30.9 (broad s, $\omega_{1/2}$ = 24 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, [Al{OC(CF$_3$)$_3$}$_4$]$^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1144.45(100%, [{Cp$_2$(CO)$_4$Mo$_2$PAs}{Cp$_2$(CO)$_4$Mo$_2$P$_2$}Ag]$^+$), 1100.5 (88%, [{Cp$_2$(CO)$_4$Mo$_2$P$_2$}$_2$Ag]$^+$), 1188.4 (58%, [{Cp$_2$(CO)$_4$Mo$_2$PAs}$_2$Ag]$^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, [Al{OC(CF$_3$)$_3$}$_4$]$^-$).
Elemental analysis (%) calculated for $C_{88}H_{40}Ag_2Al_2As_{1.72}F_{72}Mo_8O_{24}P_{6.28}$ (4209.84 g·mol^{-1}): C, 25.11; H 0.96; found: C, 25.51; H, 1.01.
IR (ATR-Ge): $\tilde{\nu}$ = 1972 (bs), 1945 (s), 1351 (w), 1298 (m), 1276 (s), 1241 (s), 1216 (s), 1170 (w), 973 (s), 828 (w), 727 (s), 560 (w).

2.3.4. $[\{\{CpMo(CO)_2\}_2\{\mu,\eta^2\text{-}PSb\}\}_2\{\{CpMo(CO)_2\}_2\{\mu,\eta^1\text{:}\eta^1\text{-}P_2\}\}_2Ag_2]_{0.81}[Al\{OC(CF_3)_3\}_4]_2$ (6)



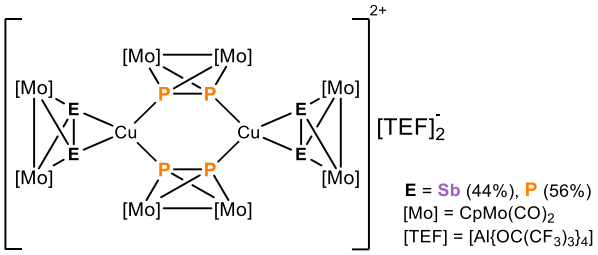
^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.30 (s, 10H, H_{Cp}), 5.32 (s, 12H, H_{Cp}).
^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 85.9 (s, C_{Cp}), 87.4 (s, C_{Cp}), 121.2 (q, $J_{(C,F)}$ = 291 Hz; C_{CF3}), 221.3 (s, C_{CO}), 222.8 (s, C_{CO}), 222.9 (s, C_{CO}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -85.3 (broad s, $\omega_{1/2}$ = 103 Hz), -36.3 (broad s, $\omega_{1/2}$ = 24 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, $[Al\{OC(CF_3)_3\}_4]^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1190.7 (99%, $[\{Cp_2(CO)_4Mo_2P_2\}\{Cp_2(CO)_4Mo_2PSb\}Ag]^+$), 1100.5 (100%, $[\{Cp_2(CO)_4Mo_2P_2\}_2Ag]^+$), 1282.4 (25%, $[\{Cp_2(CO)_4Mo_2PSb\}_2Ag]^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, $[Al\{OC(CF_3)_3\}_4]^-$).
Elemental analysis (%) calculated for $C_{88}H_{40}Ag_2Al_2F_{72}Mo_8O_{24}P_{6.38}Sb_{1.62}$ (4281.32 g·mol^{-1}): C, 24.69; H 0.94; found: C, 25.17; H, 0.92.
IR (ATR-Ge): $\tilde{\nu}$ = 1970 (bs), 1945 (s), 1351 (w), 1298 (w), 1276 (m), 1240 (s), 1216 (s), 1164 (w), 973 (s), 836 (w), 828 (w), 817 (w), 727 (s), 558 (w).

2.3.5. $[\{\{CpMo(CO)_2\}_2\{\mu,\eta^2\text{-}As_2\}\}_2\{\{CpMo(CO)_2\}_2\{\mu,\eta^1\text{:}\eta^1\text{-}P_2\}\}_2Cu_2]_{0.81}[Al\{OC(CF_3)_3\}_4]_2$ (7)



^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.37 (s, 10H, H_{Cp}), 5.20 (s, 16.7H, H_{Cp}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -82.1 (broad s, $\omega_{1/2}$ = 385 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, $[Al\{OC(CF_3)_3\}_4]^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1144.4 (27%, $[\{Cp_2(CO)_4Mo_2P_2\}\{Cp_2(CO)_4Mo_2As_2\}Cu]^+$), 1056.6 (100%, $[\{Cp_2(CO)_4Mo_2P_2\}_2Cu]^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, $[Al\{OC(CF_3)_3\}_4]^-$).
IR (ATR-Ge): $\tilde{\nu}$ = 1979 (bs), 1946 (bs), 1351 (w), 1298 (w), 1276 (s), 1240 (s), 1216 (s), 1169 (w), 973 (s), 828 (w), 727 (s), 561 (m).

2.3.6. $[\{\{CpMo(CO)_2\}_2\{\mu,\eta^2\text{-}Sb_2\}\}_2\{\{CpMo(CO)_2\}_2\{\mu,\eta^1\text{:}\eta^1\text{-}P_2\}\}_2Cu_2]_{0.46}[Al\{OC(CF_3)_3\}_4]_2$ (8)



^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ [ppm] = 5.37 (s, 10H, H_{Cp}), 5.31 (s, 40.0H, H_{Cp}).
^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -87.5 (broad s, $\omega_{1/2}$ = 360 Hz).
^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2, 25 °C): δ [ppm] = -75.6 (s, $[Al\{OC(CF_3)_3\}_4]^-$).
ESI-MS (CH_2Cl_2) positive mode: m/z = 1238.4 (100%, $[\{Cp_2(CO)_4Mo_2P_2\}\{Cp_2(CO)_4Mo_2Sb_2\}Cu]^+$), 1056.6 (36%, $[\{Cp_2(CO)_4Mo_2P_2\}_2Cu]^+$), 1418.8 (50%, $[\{Cp_2(CO)_4Mo_2Sb_2\}_2Cu]^+$).
ESI-MS (CH_2Cl_2) negative mode: m/z = 966.9 (100%, $[Al\{OC(CF_3)_3\}_4]^-$).
IR (ATR-Ge): $\tilde{\nu}$ = 1943 (s), 1930 (s), 1906 (m), 1876 (s), 1351 (w), 1299 (w), 1276 (s), 1250 (s), 1217 (s), 1162 (w), 974 (s), 828 (m), 805 (w), 728 (s), 569 (m).

Note: For complexes **5**-**8**, we have realized a slight impact of the homoleptic complex **1** as impurity on the recorded elemental analysis results. For complexes **5** and **6**, this impact is very small and the found %C and %H values fits within the tolerated 0.5% error. For **7** and **8**, although this impact is also small, however, we did not add the elemental analysis data because we realized that variable samples of **7** and **8** includes variable found %C and %H values.

2.4. NMR Spectra:

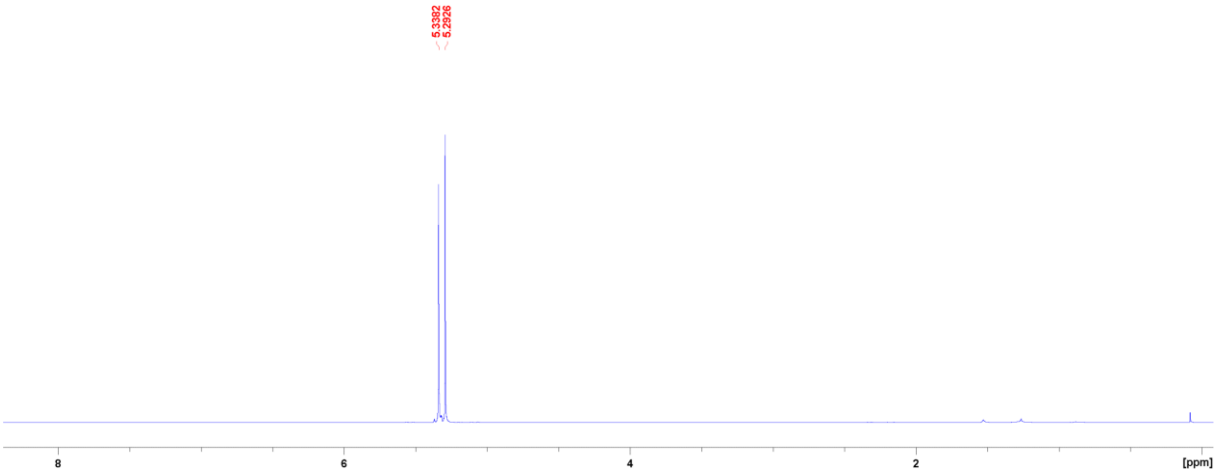


Fig. S1: ^{1}H NMR spectrum of complex **3** in CD_2Cl_2 at 400 MHz.

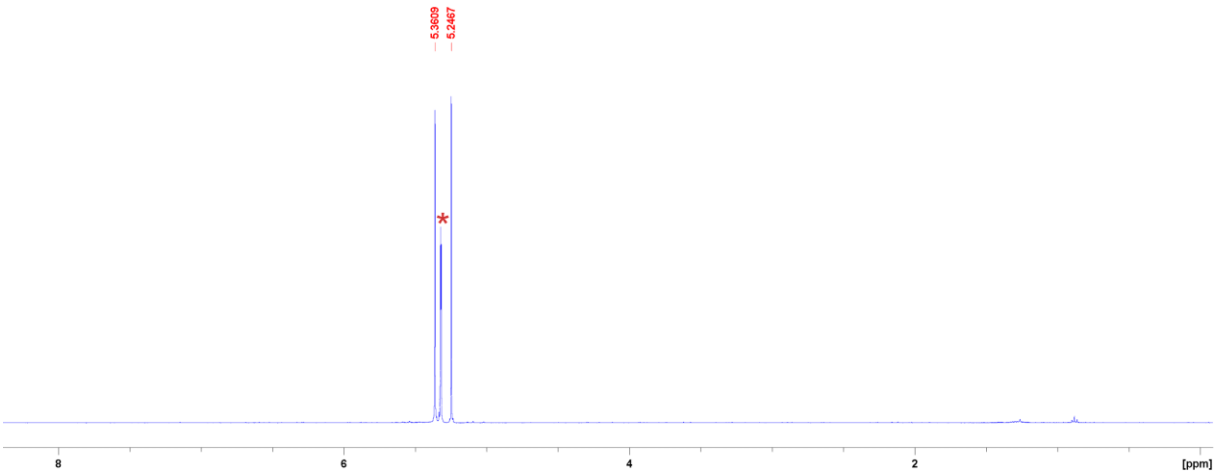


Fig. S2: ^{1}H NMR spectrum of complex **4** in CD_2Cl_2 at 400 MHz. *solvent signal

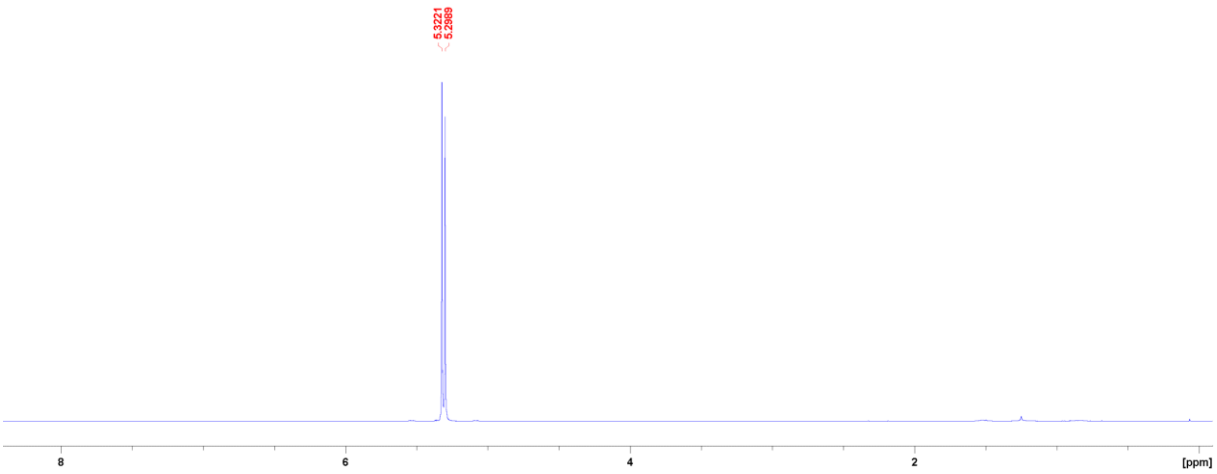


Fig. S3: ^{1}H NMR spectrum of complex **5** in CD_2Cl_2 at 400 MHz.

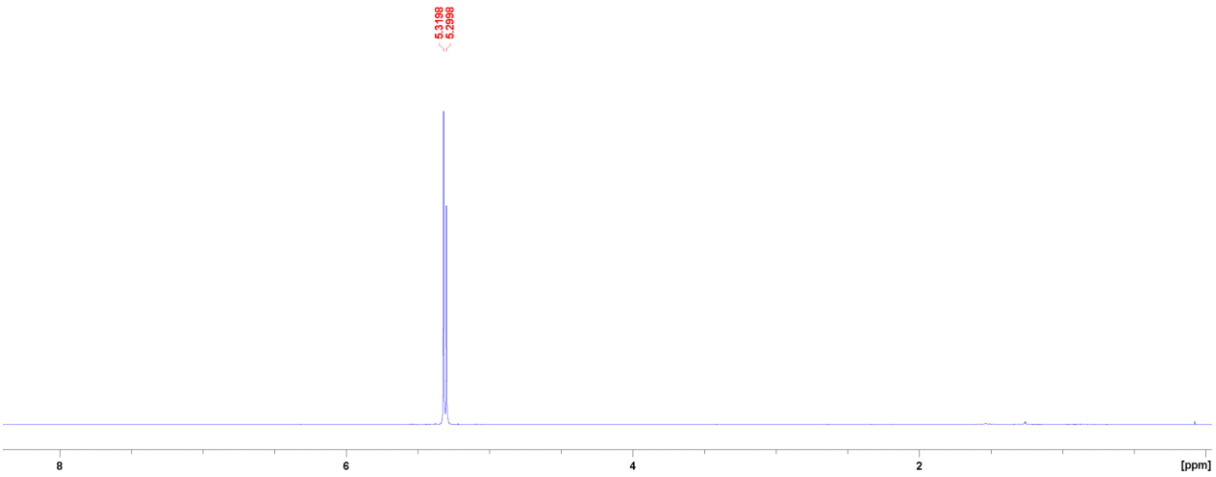


Fig. S4: ^{1}H NMR spectrum of complex **6** in CD_2Cl_2 at 400 MHz.

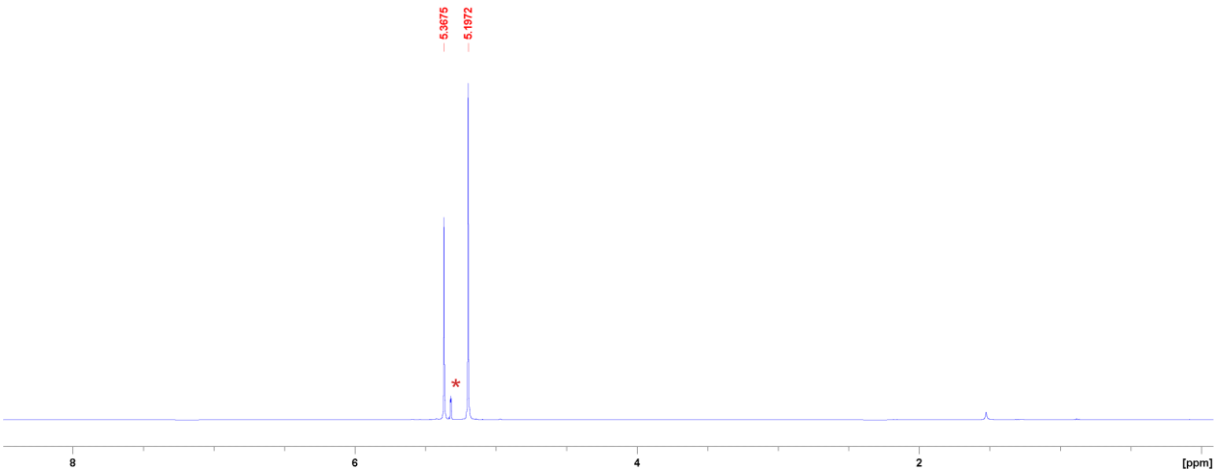


Fig. S5: ^{1}H NMR spectrum of complex **7** in CD_2Cl_2 at 400 MHz. *solvent signal

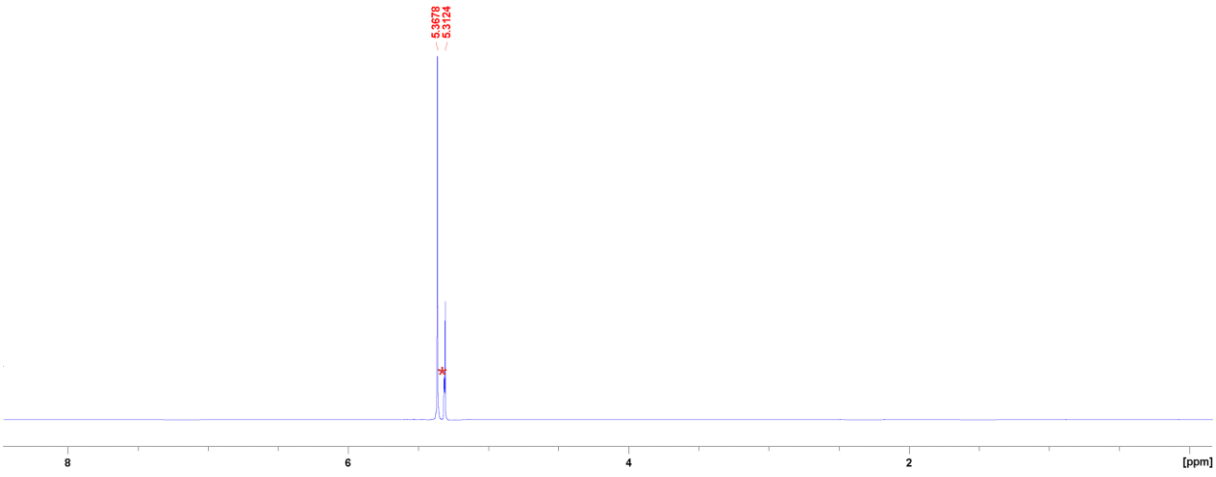


Fig. S6: ^{1}H NMR spectrum of complex **8** in CD_2Cl_2 at 400 MHz. *solvent signal

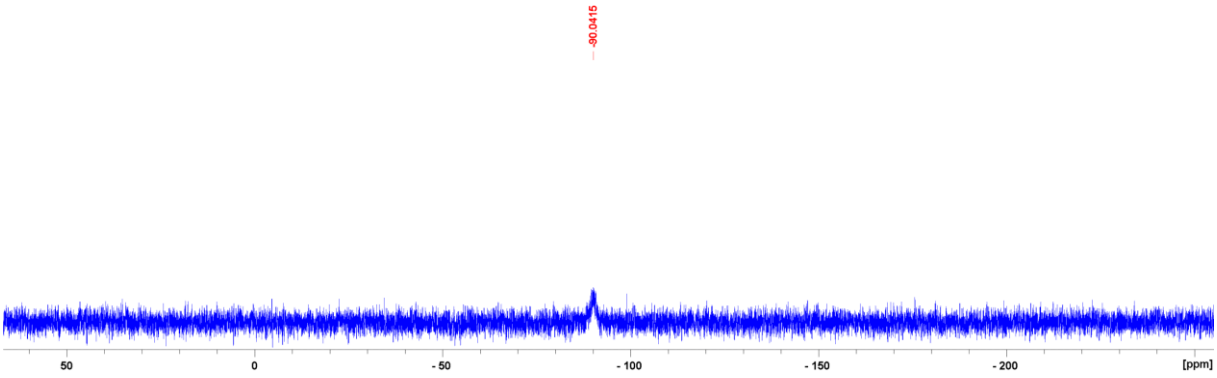


Fig. S7: ^{31}P ^{1}H NMR spectrum of complex **3** in CD_2Cl_2 at 162 MHz.

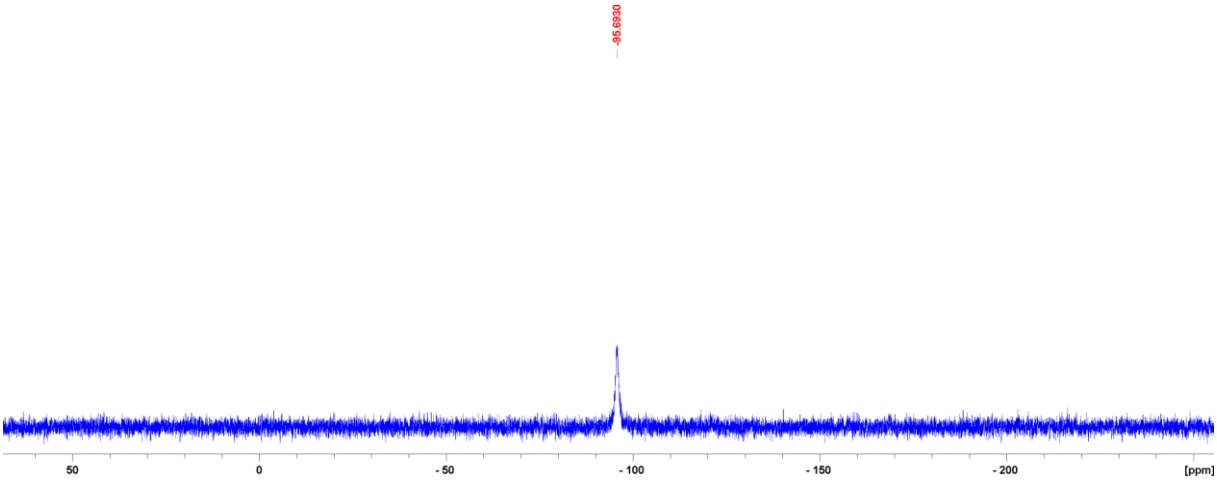


Fig. S8: ^{31}P ^{1}H NMR spectrum of complex **4** in CD_2Cl_2 at 162 MHz.

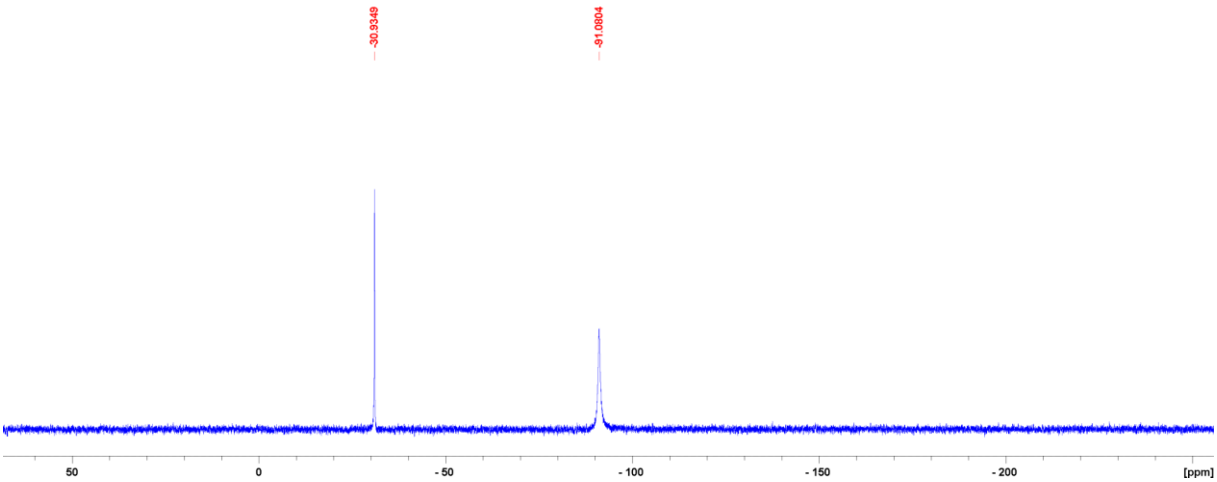


Fig. S9: ^{31}P ^{1}H NMR spectrum of complex **5** in CD_2Cl_2 at 162 MHz.

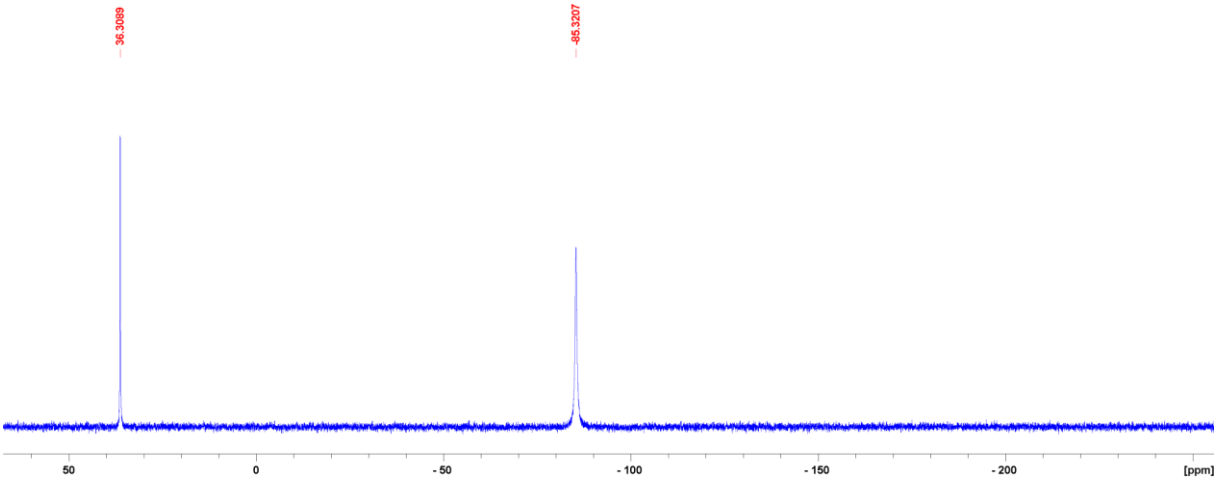


Fig. S10: ^{31}P ^{1}H NMR spectrum of complex **6** in CD_2Cl_2 at 162 MHz.

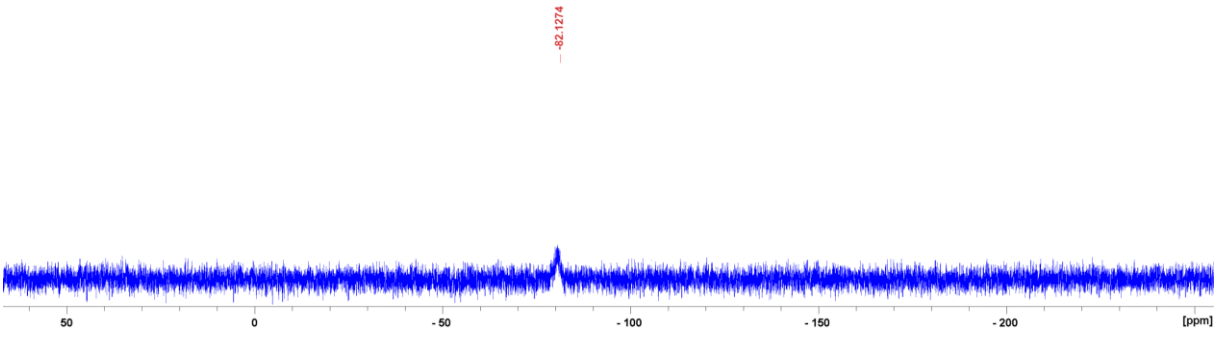


Fig. S11: ^{31}P ^{1}H NMR spectrum of complex **7** in CD_2Cl_2 at 162 MHz.

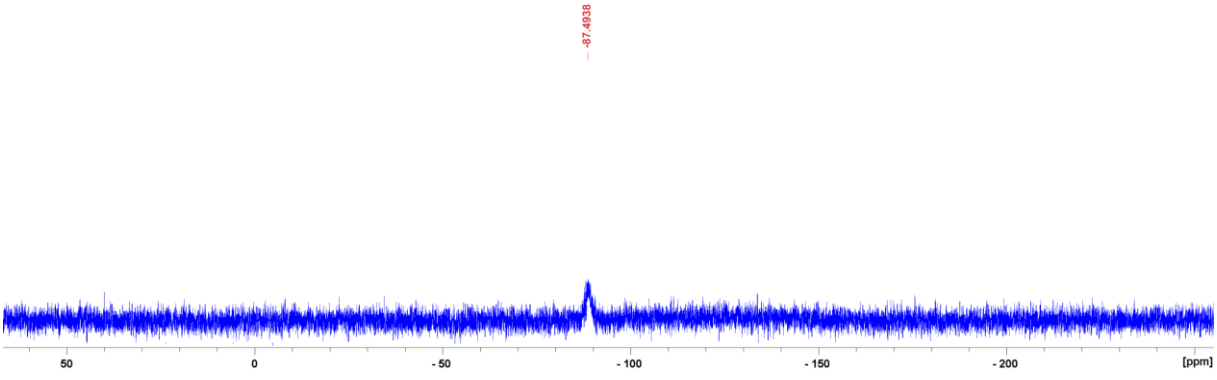


Fig. S12: ^{31}P ^{1}H NMR spectrum of complex **8** in CD_2Cl_2 at 162 MHz.

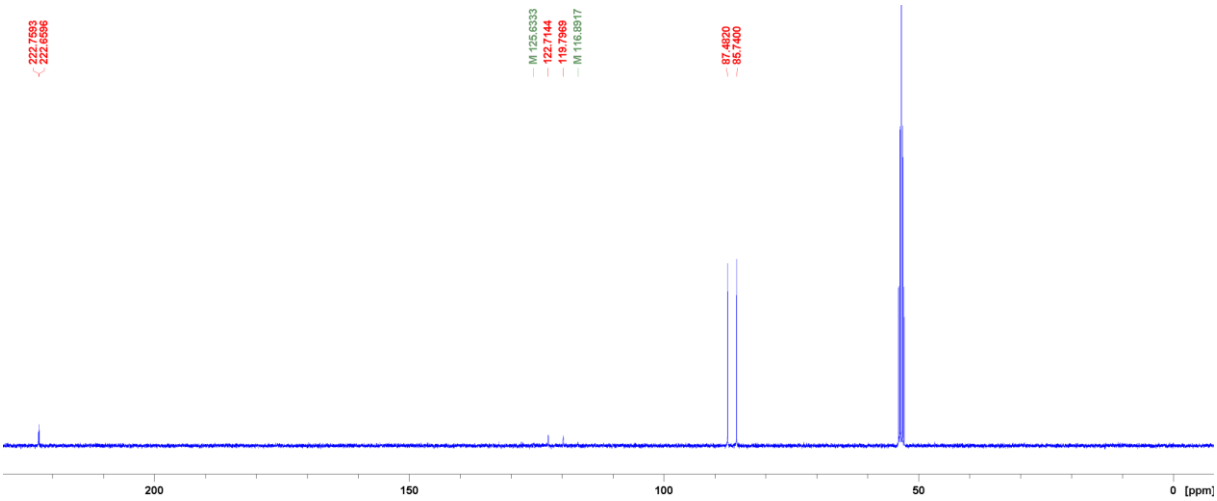


Fig. S13: ^{31}C ^{1}H NMR spectrum of complex **3** in CD_2Cl_2 at 100 MHz.

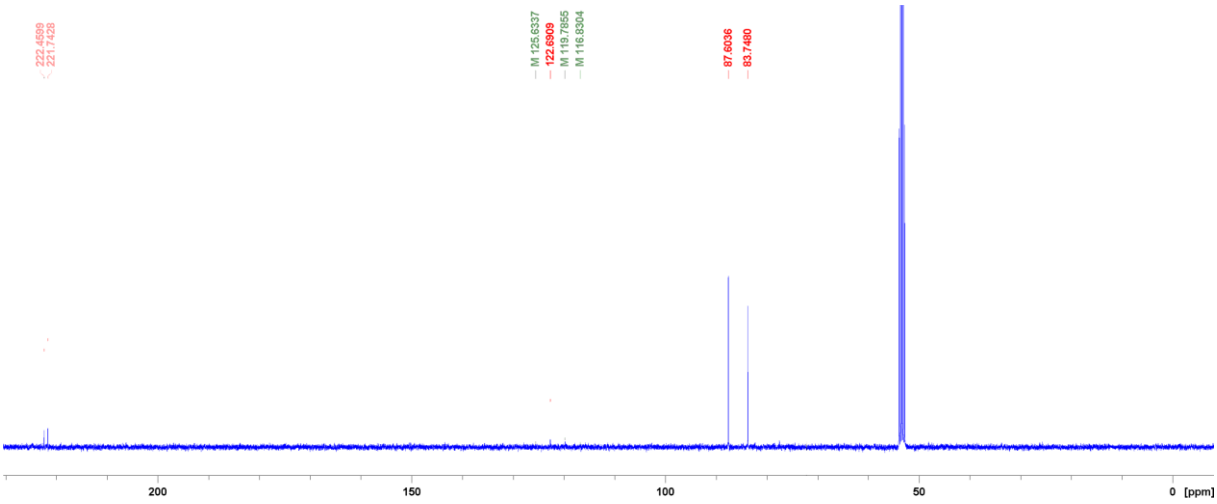


Fig. S14: ^{31}C ^{1}H NMR spectrum of complex **4** in CD_2Cl_2 at 100 MHz.

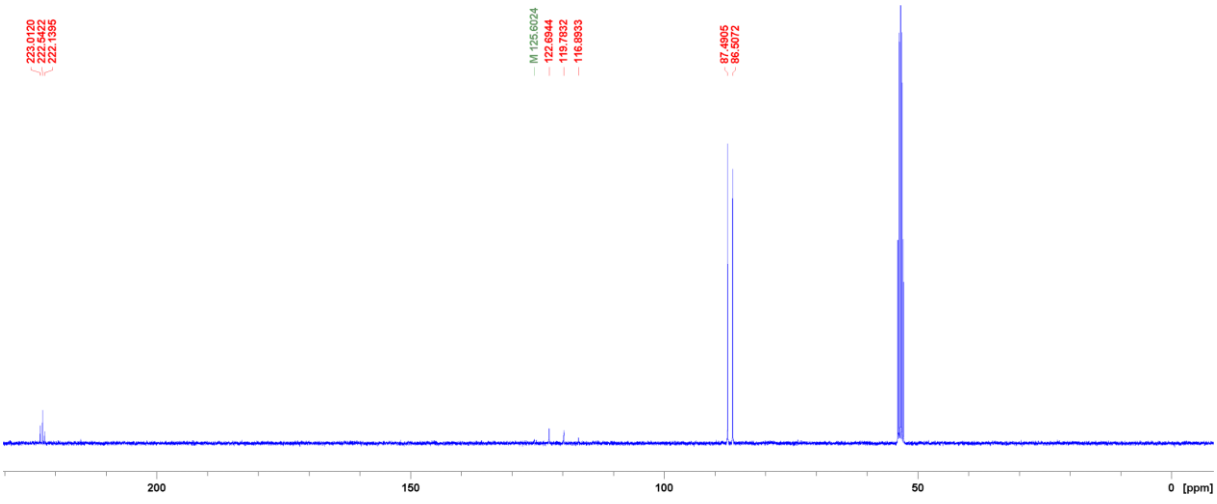


Fig. S15: ^{31}C ^{1}H NMR spectrum of complex **5** in CD_2Cl_2 at 100 MHz.

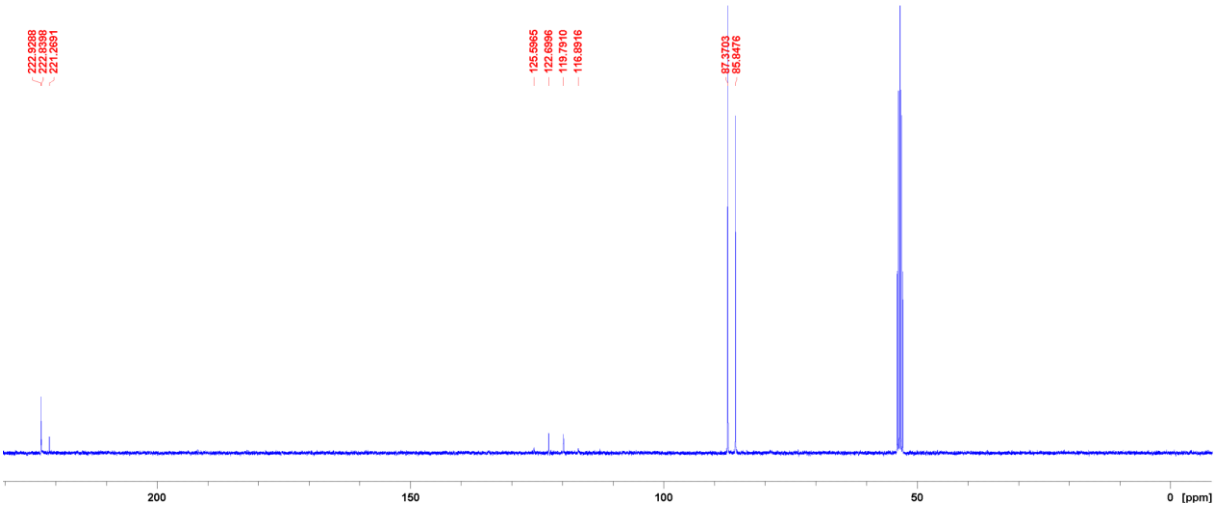


Fig. S16: ^{31}C ^{1}H NMR spectrum of complex **6** in CD_2Cl_2 at 100 MHz.

2.5. IR Spectra:

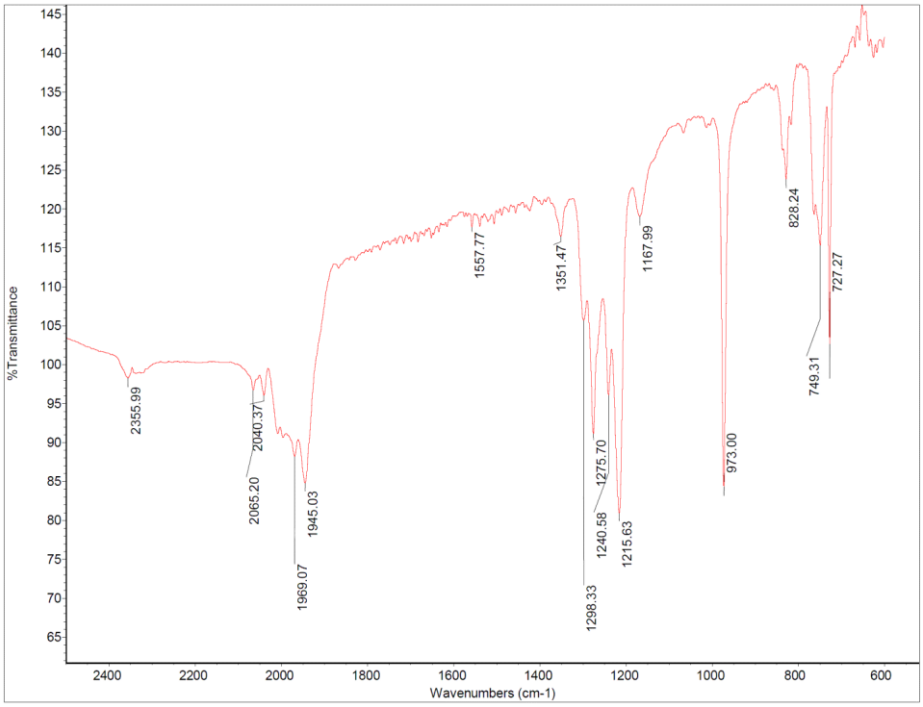


Fig. S17: IR spectrum of complex **3**.

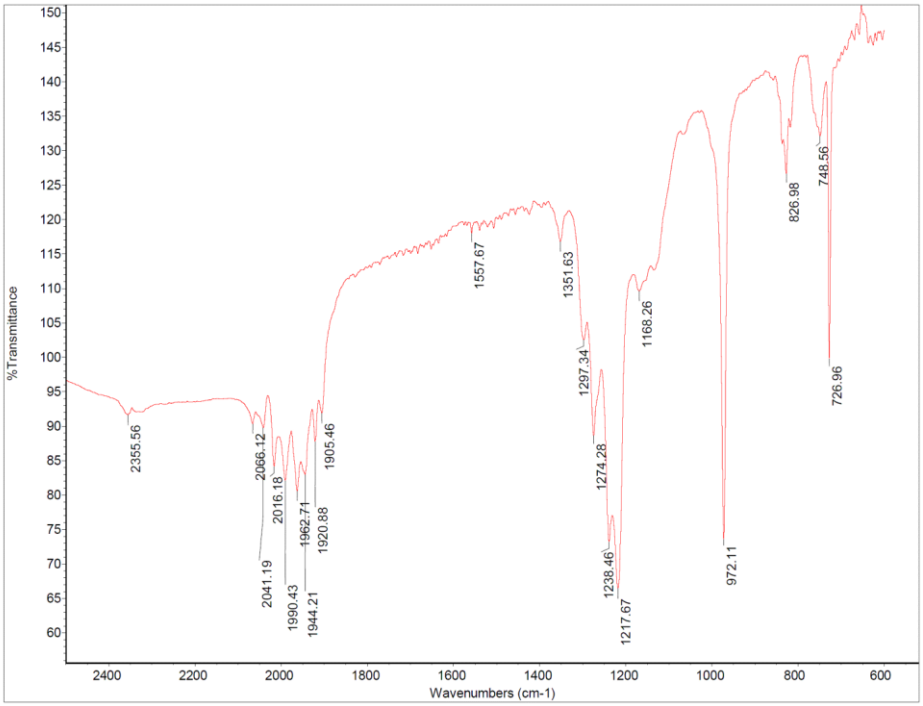


Fig. S18: IR spectrum of complex **4**.

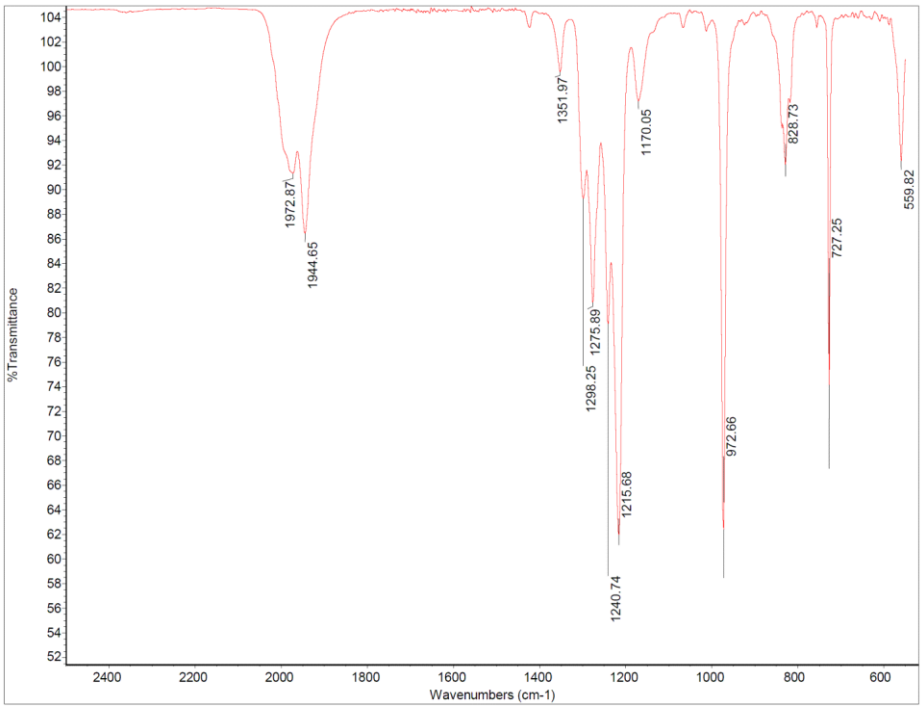


Fig. S19: IR spectrum of complex **5**.

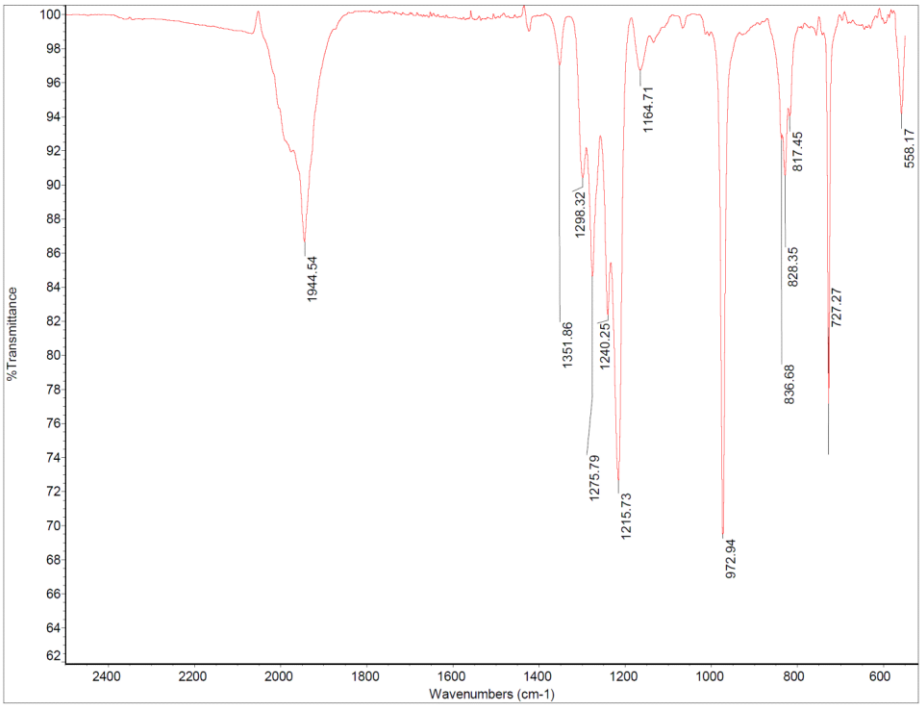


Fig. S20: IR spectrum of complex **6**.

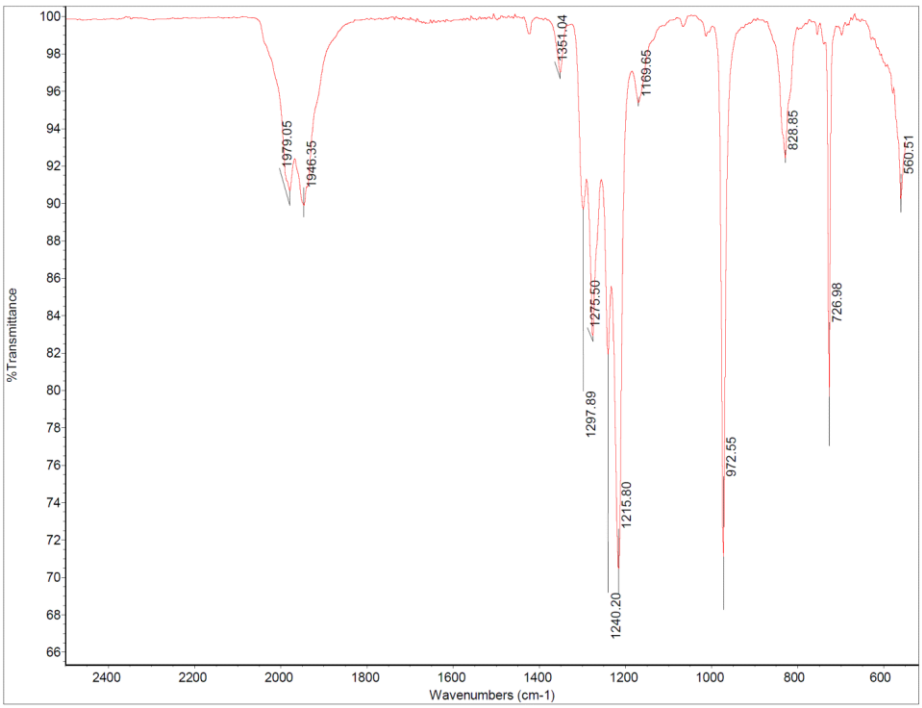


Fig. S21: IR spectrum of complex **7**.

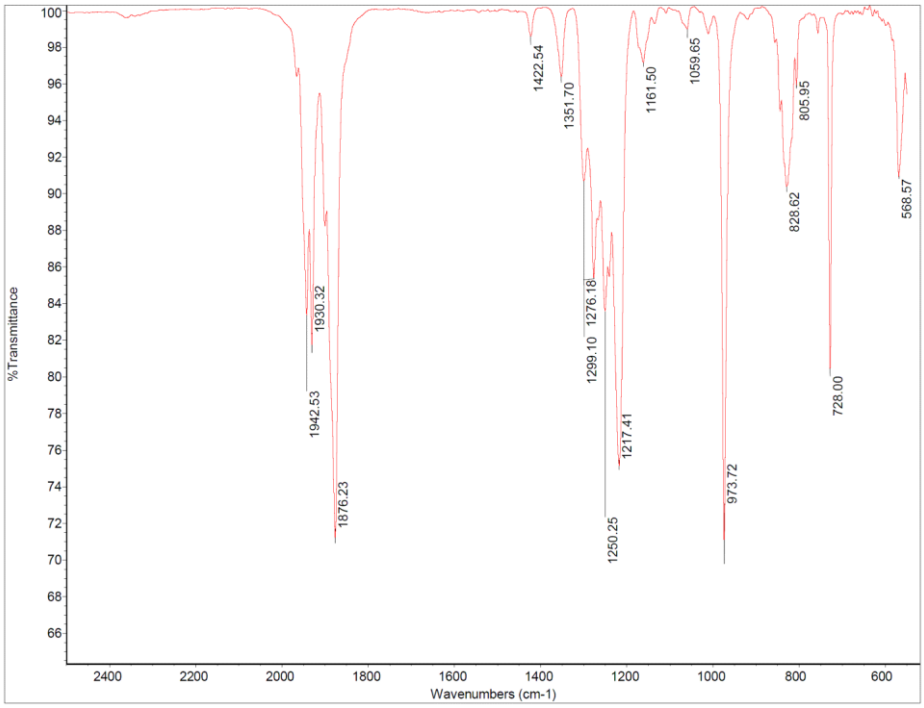


Fig. S22: IR spectrum of complex **8**.

2.5. ESI-MS Spectra:

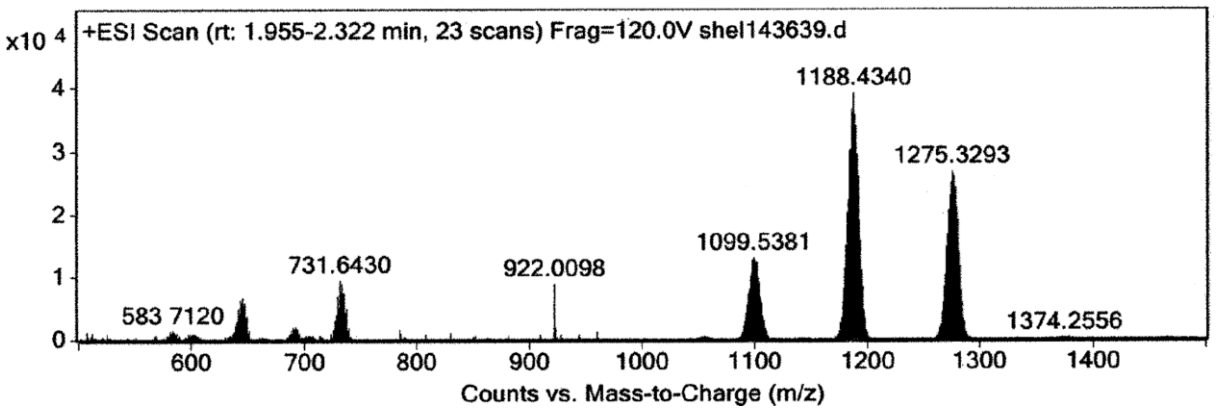


Fig. S23: ESI-MS spectrum of complex **3**.

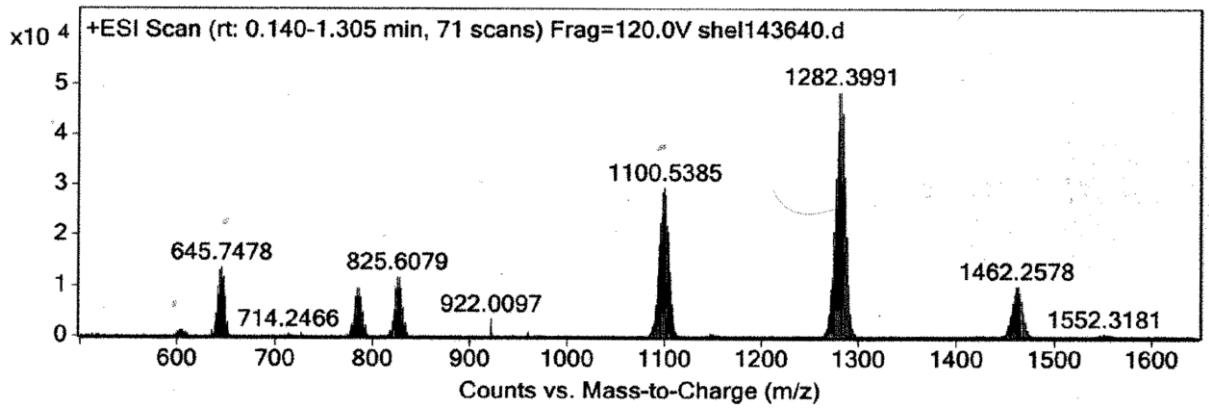


Fig. S24: ESI-MS spectrum of complex **4**.

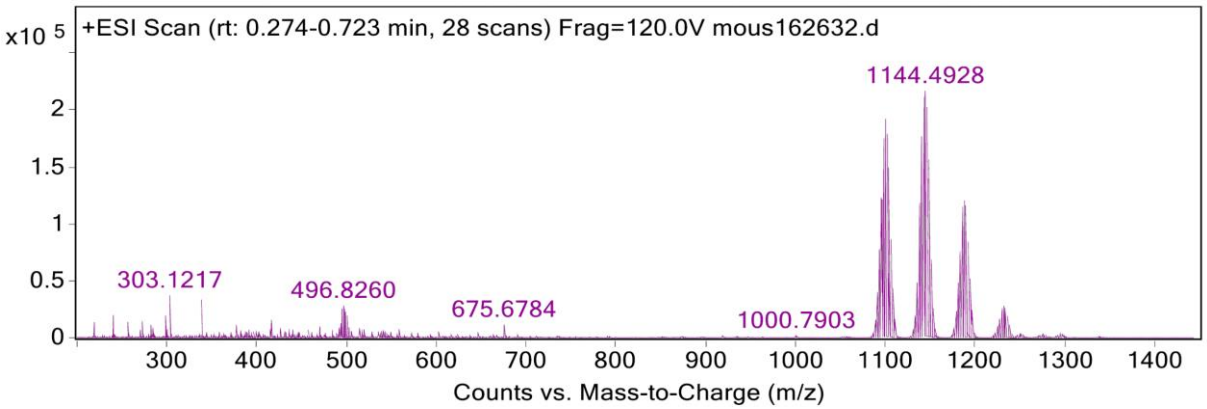


Fig. S25: ESI-MS spectrum of complex **5**.

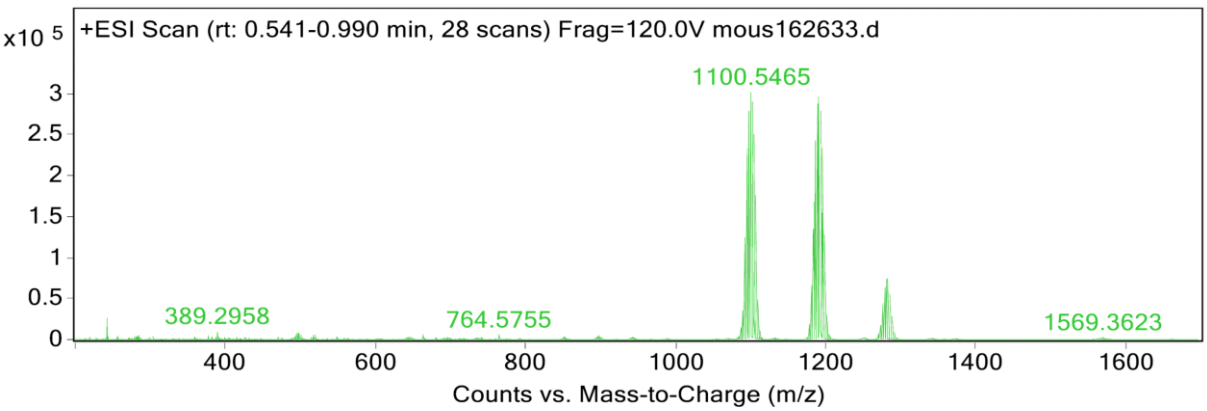


Fig. S26: ESI-MS spectrum of complex **6**.

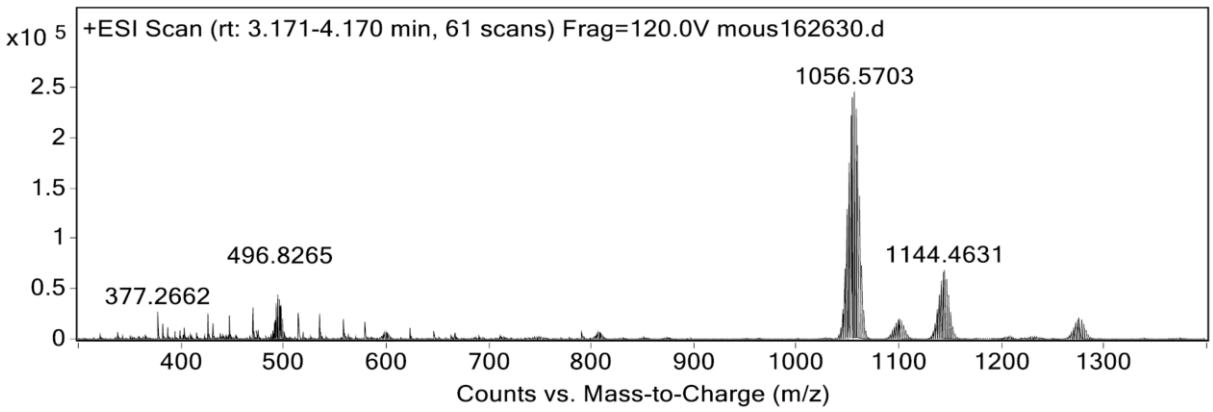


Fig. S27: ESI-MS spectrum of complex **7**.

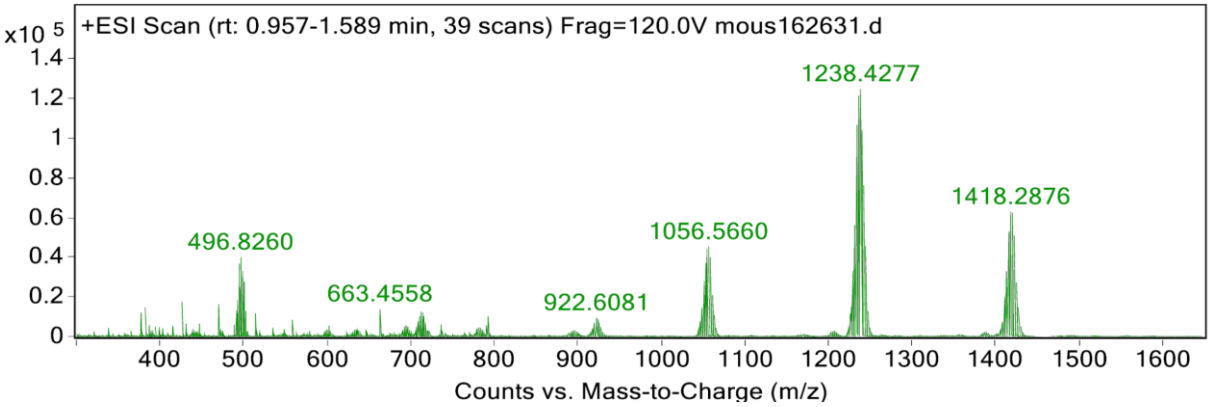


Fig. S28: ESI-MS spectrum of complex **8**.

3. Crystallographic details

Suitable crystals were selected and mounted on a Gemini Ultra diffractometer equipped with an Atlas^{S2} CCD detector (**3**, **4**), on a SuperNova Dualflex diffractometer equipped with an Atlas^{S2} CCD detector (**7**, **8**) or on a XtaLAB SynergyR DW diffractometer equipped with an HyPix-Arc 150 detector (**5**, **6**) The crystals were kept at a steady T = 123(1) (**3**, **4**, **6**, **7, 8**) K or 100(1) K (**5**) during data collection. Data collection and reduction were performed with CrysAlisPro [Version 1.171.41.76a (**3**, **4**), 1.171.41.90a (**7**, **8**), 1.171.41.93a (**6**), 1.171.41.118a (**5**)].[4] For the compounds **3**, **5**, **6**, **7**, **8** a numerical absorption correction based on a gaussian integration over a multifaceted crystal model and an empirical absorption correction using spherical harmonics, as implemented in SCALE3 ABSPACK scaling algorithm, was applied. For the compound **4** an analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.[5] and an empirical absorption correction using spherical harmonics, as implemented in SCALE3 ABSPACK scaling algorithm, was applied. Using Olex2,[6] the structures were solved with ShelXT[7] and a least-square refinement on F^2 was carried out with ShelXL[8] for all structures. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms at the carbon atoms were located in idealized positions and refined isotropically according to the riding model.
Figures were created with Olex2.[6]

Compound 3: The asymmetric unit contains one unit of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, two molecules of the anion $[Al\{OC(CF_3)_3\}_4]^-$ and two CH_2Cl_2 solvent molecules. In the unit $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ one $CpMo(CO)_2$ group of one complex **A** is disordered over two positions. One of the CH_2Cl_2 solvent molecules is disordered over two positions. For the anions $[Al\{OC(CF_3)_3\}_4]^-$ five $\{OC(CF_3)_3\}$ groups are disordered over two and one over three positions respectively. The restraints SADI, SIMU and DFIX were applied to describe these disorders.

Compound 4: The asymmetric unit contains one unit of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, two molecules of the anion $[Al\{OC(CF_3)_3\}_4]^-$ and 3 CH_2Cl_2 solvent molecules. In the unit $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ three $CpMo(CO)_2$ groups of two complexes **A** are disordered over two positions. Two CH_2Cl_2 solvent molecules are disordered over two positions each. For the anions $[Al\{OC(CF_3)_3\}_4]^-$ ten CF_3 groups of four $\{OC(CF_3)_3\}$ groups are disordered over two positions. Moreover, two more $\{OC(CF_3)_3\}$ groups are disordered over two positions. The restraints SADI, SIMU, DFIX and ISOR were applied to describe these disorders. Further was compound X4 refined as a 2-component inversion twin (BASF 0.38(2)).

Compound 5: The asymmetric unit contains one unit of $[(\eta^2\text{-}\mathbf{D})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, two molecules of $[Al\{OC(CF_3)_3\}_4]^-$ and two CH_2Cl_2 solvent molecules. Both of the η^2-coordinated ligand complexes show a disorder of the PAs units over two positions. However, the too high total phosphorus content indicates an additional substitutional disorder of the PAs units with P_2 units. The occupancy of each mixed P and As position was freely refined and then fixed to the obtained values rounded to two decimals (P5:As5: 0.66:0.44; P6:As6: 0.47:0.53; P7:As7: 0.63:0.37; P8:As8: 0.79:0.21). Moreover, one $CpMo(CO)_2$ group of one complex $\eta^{1:1}$-**A** as well as one CH_2Cl_2 solvent molecule are disordered over two positions. For the anions $[Al\{OC(CF_3)_3\}_4]^-$, three CF_3 groups of one $\{OC(CF_3)_3\}$ group are disordered over two positions. Moreover, five more $\{OC(CF_3)_3\}$ groups are disordered over two positions. The restraints SADI, SIMU, DFIX, RIGU, DANG and ISOR were applied to describe these disorders.

Compound 6: The asymmetric unit contains half of the unit of $[(\eta^2\text{-}\mathbf{E})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, one molecule of $[Al\{OC(CF_3)_3\}_4]^-$ and 0.45 CH_2Cl_2 solvent molecules. The η^2-coordinated ligand at the Cu center shows a substitutional disorder of the Sb atom with a P atom (0.81:0.19) For the anion $[Al\{OC(CF_3)_3\}_4]^-$, three CF_3 groups of one $\{OC(CF_3)_3\}$ group are disordered over two positions. The restraints SADI, DFIX and ISOR were applied to describe these disorders.

Compound 7: The asymmetric unit contains half of the unit of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$, one molecule of $[Al\{OC(CF_3)_3\}_4]^-$ and one $C_6H_5CH_3$ solvent molecule. The η^2-coordinated ligand at the Cu center shows a substitutional disorder of the As_2 unit with a P_2 unit (0.81:0.19). Moreover, one of the $CpMo(CO)_2$ groups of one complex $\eta^{1:1}$-**A** as well as one $C_6H_5CH_3$ solvent molecule are disordered over two positions. For the anion $[Al\{OC(CF_3)_3\}_4]^-$, four $\{OC(CF_3)_3\}$ groups are disordered over two or three positions. The restraints SADI, SIMU, ISOR and FLAT were applied to describe these disorders.

Compound 8: The asymmetric unit contains half of the unit of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$, one molecule of $[Al\{OC(CF_3)_3\}_4]^-$ and one $C_6H_5CH_3$ solvent molecule. The η^2-coordinated ligand at the Cu center shows a substitutional disorder of the Sb_2 unit with a P_2 unit (0.46:0.54). Moreover, are one of the $CpMo(CO)_2$ groups of one complex $\eta^{1:1}$-**A** as well as one $C_6H_5CH_3$ solvent molecule disordered over two positions. For the anion $[Al\{OC(CF_3)_3\}_4]^-$, four $\{OC(CF_3)_3\}$ groups are disordered over two or three positions. The restraints SADI, SIMU, DFIX and FLAT were applied to describe these disorders.

CCDC-2300855 (**3**), CCDC-2300856 (**4**), CCDC-2300857 (**5**), CCDC-2300858 (**6**), CCDC-2300859 (**7**) and CCDC-2300860 (**8**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: + 44-1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table S1. Crystallographic data for compounds **3**-**6**.

Compound	**3**·2 CH_2Cl_2	**4**·3 CH_2Cl_2	**5**·2 CH_2Cl_2	**6**·2 CH_2Cl_2
Data set (internal naming)	PSH_165_mP _abs_gaus	PSH166_Mo_mP _nc_abs_ana	PSH404_Mo_mP _abs	PSH_234b_aP _abs_gauss
CCDC-number	2300855	2300856	2300857	2300858
Formula	$C_{90}H_{44}Ag_2Al_2As_4Cl_4F_{72}Mo_8O_{24}P_4$	$C_{91}H_{46}Ag_2Al_2Cl_6F_{72}Mo_8O_{24}P_4Sb_4$	$C_{90}H_{44}Ag_2Al_2As_{1.71}Cl_4F_{72}Mo_8O_{24}P_{6.29}$	$C_{44.45}H_{20.9}AgAlCl_{0.9}F_{36}Mo_4O_{12}P_{3.19}Sb_{0.81}$
$D_{calc.}$ / g · cm^{-3}	2.269	2.332	2.233	2.260
μ/mm^{-1}	12.401	2.120	1.808	14.051
Formula Weight	4479.83	4752.08	4379.18	2178.84
Colour	clear dark orange	clear dark orange	clear orange	clear orange
Shape	block	plate	block-shaped	block-shaped
Size/mm^3	0.75×0.17×0.15	0.58×0.46×0.14	0.15×0.11×0.07	0.29×0.21×0.10
T/K	123(1)	123(1)	100.0(1)	123.0(1)
Crystal System	monoclinic	monoclinic	monoclinic	triclinic
Space Group	$P2_1/c$	$P2_1$	$P2_1/c$	$P\bar{1}$
a/Å	10.31430(10)	10.54110(10)	10.29414(7)	14.00870(10)
b/Å	59.1705(3)	29.9273(4)	59.0562(5)	14.52390(10)
c/Å	21.48980(10)	21.4675(3)	21.43082(15)	18.68170(10)
α/°	90	90	90	106.0900(10)
β/°	91.0400(10)	92.3940(10)	91.1327(6)	101.8780(10)
γ/°	90	90	90	111.1490(10)
V/$Å^3$	13113.11(16)	6766.37(15)	13025.94(16)	3201.62(5)
Z	4	2	4	2
Z'	1	1	1	1
Wavelength/Å	1.54184	0.71073	0.71073	1.54184
Radiation type	Cu K_α	Mo K_α	Mo K_α	Cu K_α
θ_{min}/°	3.628	2.017	2.233	2.619
θ_{max}/°	71.680	28.282	32.696	74.480
Measured Refl.	80363	46336	189366	66769
Independent Refl.	25149	31124	42599	12933
Reflections with I > 2(I)	22239	28398	33996	12858
R_{int}	0.0562	0.0206	0.0307	0.0282
Parameters	2701	2657	2764	1018
Restraints	1082	1839	849	9
Largest Peak	1.342	1.266	1.795	0.937
Deepest Hole	-1.701	-0.768	-0.918	-0.816
GooF	1.045	1.055	1.043	1.191
wR_2 (all data)	0.1338	0.1100	0.0977	0.0637
wR_2	0.1286	0.1059	0.0929	0.0635
R_1 (all data)	0.0560	0.0499	0.0598	0.0255
R_1	0.0497	0.0441	0.0435	0.0253

Table S2. Crystallographic data for compounds **X7**-**X8**.

Compound	**7**·2 $C_6H_5CH_3$	**8**·2 $C_6H_5CH_3$
Data set (internal naming)	PSH_194_pr_b _mP_abs	PSH224_Mo _mP_abs
CCDC-number	2300859	2300860
Formula	$C_{102}H_{56}Al_2As_{3.24}Cu_2F_{72}Mo_8O_{24}P_{4.76}$	$C_{51}H_{28}AlCuF_{36}Mo_4O_{12}P_{3.08}Sb_{0.92}$
$D_{calc.}$ / g · cm^{-3}	2.123	2.133
μ/mm^{-1}	9.157	1.613
Formula Weight	4372.18	2198.41
Colour	red	intense red
Shape	block	block-shaped
Size/mm^3	0.41×0.31×0.22	0.31×0.26×0.21
T/K	123.01(10)	123.00(10)
Crystal System	monoclinic	monoclinic
Space Group	$P2_1/c$	$P2_1/c$
a/Å	16.6487(2)	16.6787(3)
b/Å	23.0766(2)	23.0865(3)
c/Å	19.1463(2)	19.1437(3)
α/°	90	90
β/°	111.6100(10)	111.768(2)
γ/°	90	90
V/Å^3	6838.89(13)	6845.7(2)
Z	2	4
Z'	0.5	1
Wavelength/Å	1.54184	0.71073
Radiation type	Cu K_α	Mo K_α
θ_{min}/°	3.438	2.602
θ_{max}/°	66.694	30.998
Measured Refl.	66757	85359
Independent Refl.	12040	21810
Reflections with I > 2(I)	11151	17954
R_{int}	0.0918	0.0266
Parameters	1776	2010
Restraints	1302	1275
Largest Peak	1.040	1.283
Deepest Hole	-1.031	-1.125
GooF	1.046	1.069
wR_2 (all data)	0.1386	0.0799
wR_2	0.1346	0.0746
R_1 (all data)	0.0529	0.0508
R_1	0.0500	0.0374

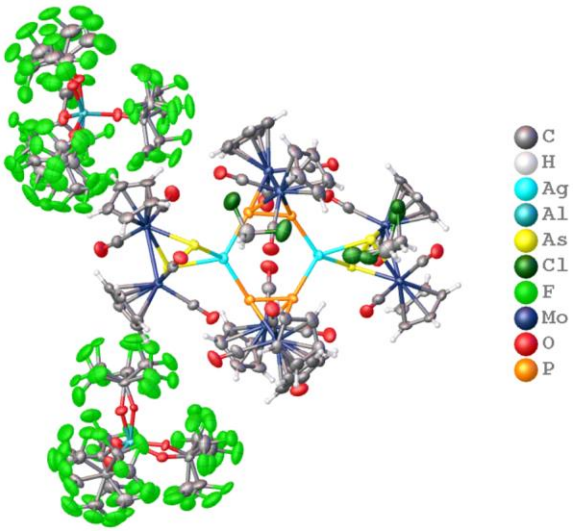


Fig. S29. View of the asymmetric unit of **3**

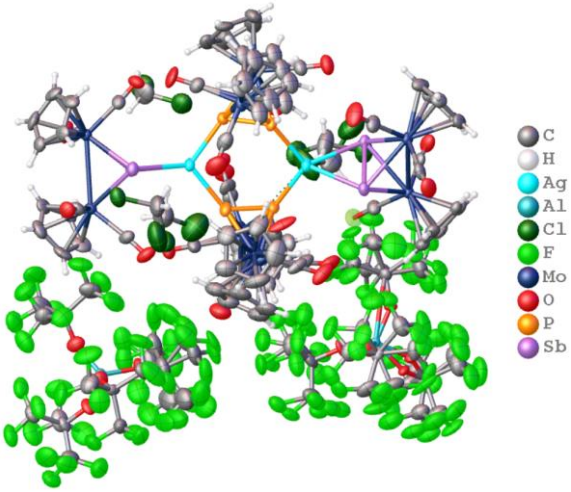


Fig. S30. View of the asymmetric unit of **4**

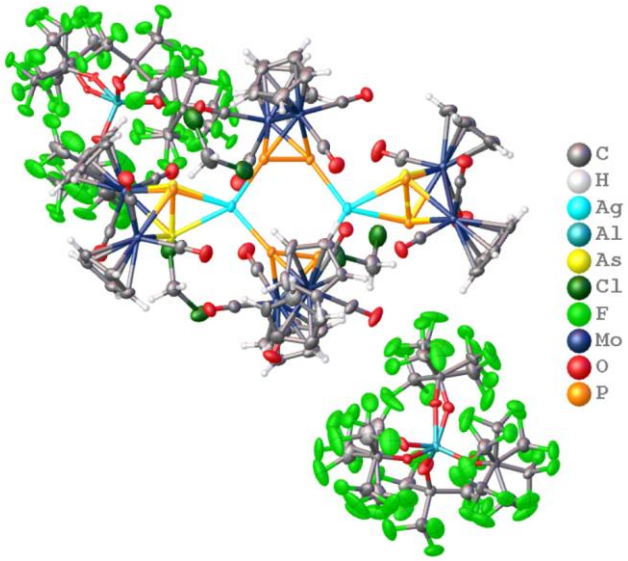


Fig. S31. View of the asymmetric unit of **5**. Next to **5** and **1** also a mixed species may possibly exist (see Fig. S32).

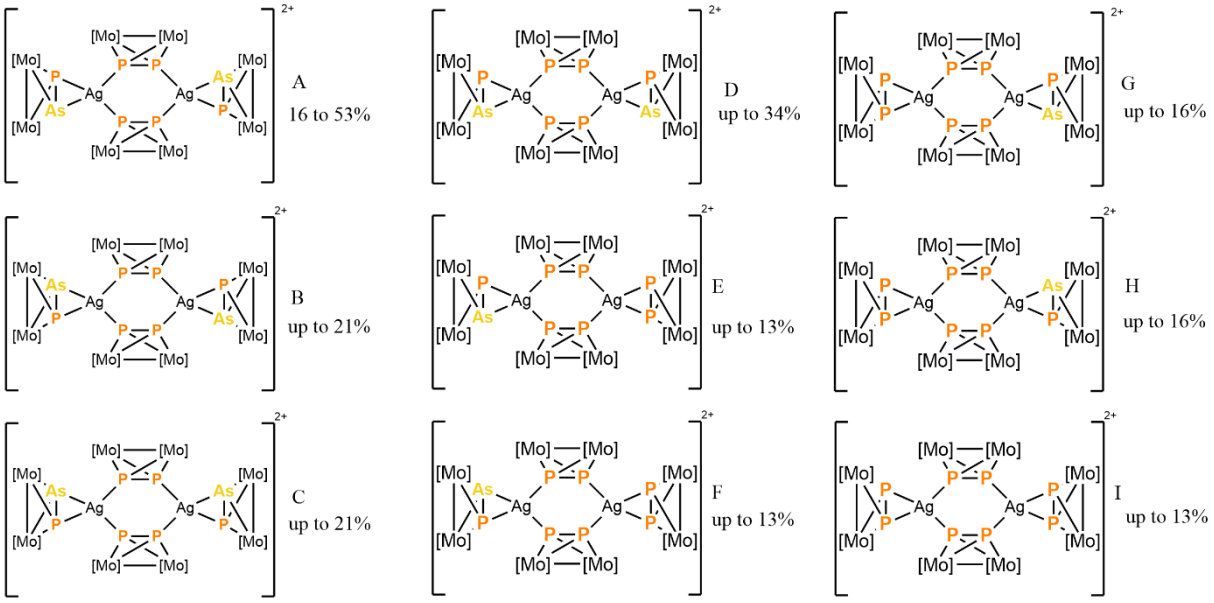


Fig. S32. Possible combination of compounds derived from the disorder of the PAs unit in **5**.

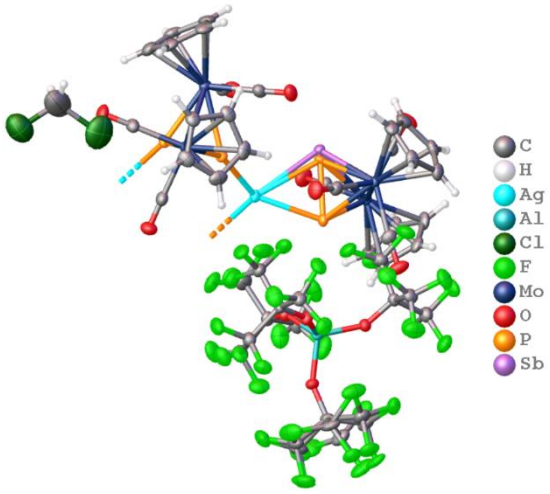


Fig. S33. View of the asymmetric unit of **6**. Next to **6** and **1** also a mixed species may possibly exist (see Fig. S34).

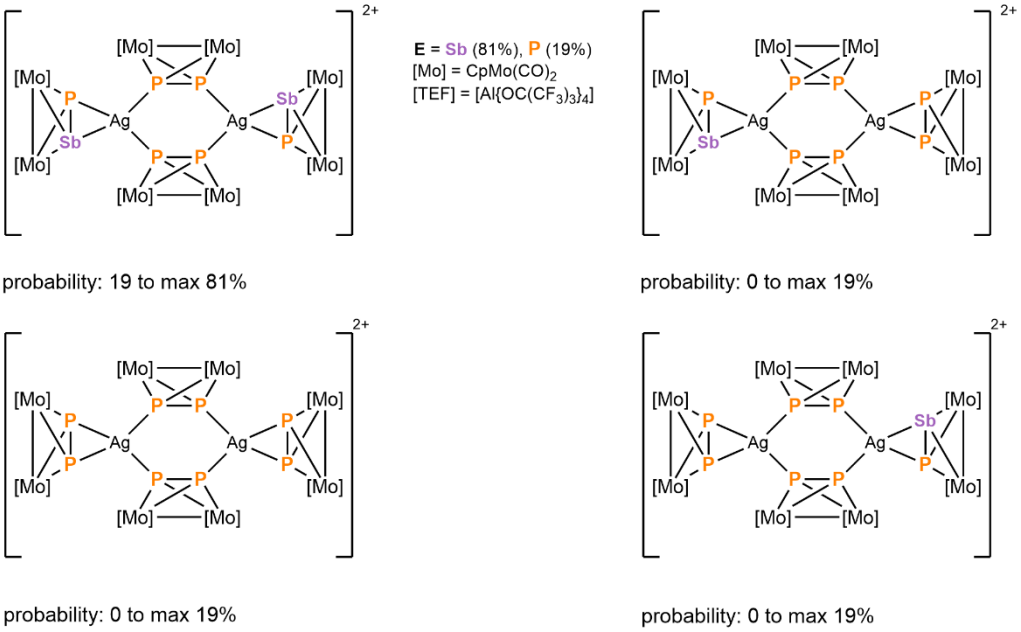


Fig. S34. Possible combination of compounds derived from the disorder of the PSb unit in **6**.

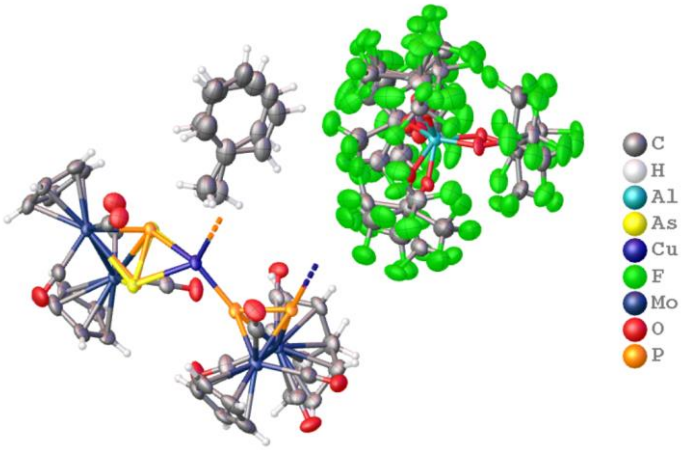


Fig. S35. View of the asymmetric unit of **7.** Next to **7** and **1** also a mixed species may possibly exist (see Fig. S36).

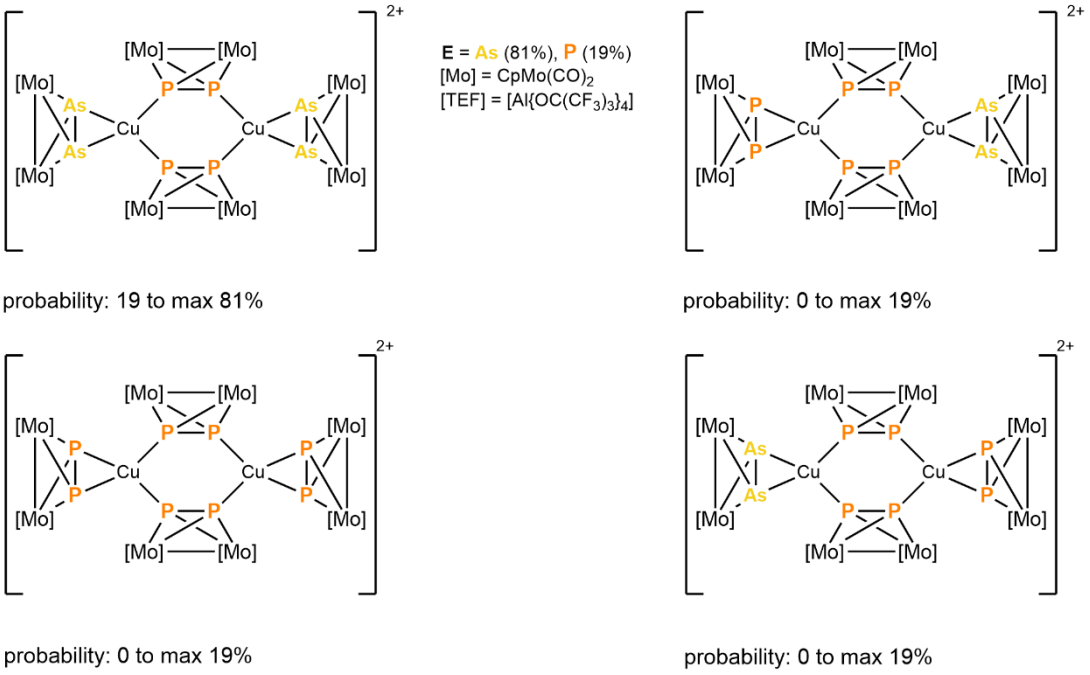


Figure S36. Possible combination of compounds derived from the disorder of the As_2 unit in **7**.

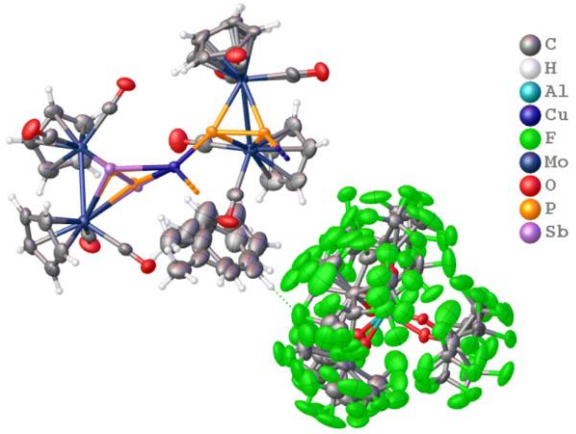


Figure S37. View of the asymmetric unit of **8**. Next to **8** and **1** also a mixed species may possibly exist (see Fig. S38).

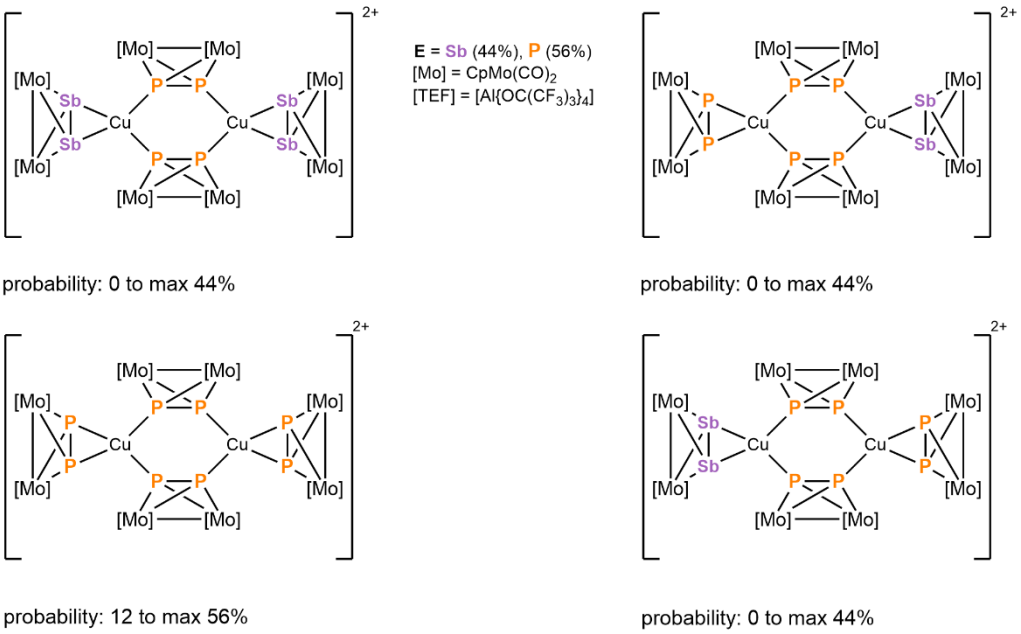


Figure S38. Possible combination of compounds derived from the disorder of the Sb_2 unit in **8**.

Computational details

The DFT calculations have been performed for compounds **A**, **B**, **C,** $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$, $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$, $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ and $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ with Gaussian 09 program package[9] at the BP86[10]/def2-SVP[11] level of theory. The minimum nature of the optimized geometry of compounds has been proven by calculating the vibration spectrum, which shows no imaginary frequencies. All optimized geometries can also be found in a supplemented multi-xyz file as well as in the tables below. Figures were prepared with Chemcraft.[12] For the dicationic species, conformers adopting two conformations of the Ag_2P_4 six-membered ring have been calculated: twisted boat and chair. Interestingly, even though in all cases calculations predict twisted boat conformers to be somewhat more stable experimentally in the solid-state structures of every compound (apart from **4**) chair conformer has been found. This is possibly due to the packing effects. Nevertheless, relative enthalpies and free energies of both twisted boat and chair conformations show a similar trend (Figure S8): for Ag(I) based dimers, formation of complex featuring η^2 coordinated complexes **B** (**3**) from the starting material (**1**) is both exothermic and exergonic, while for the Sb analog (**4**) it is even more exothermic and endergonic; on the other hand, for the Cu(I) based complexes **7**-**8** similar reactions are either slightly endothermic and endergonic or nearly thermodynamically neutral.

Note: Due to limited computational resources, no dispersion correction was applied. Although, because of the structural similarity of the studied complexes dispersion energy contribution are likely to cancel out. This cancellation can be incomplete because of different pnictogen atoms involved. This, in turn, can make an additional contribution to the computed energy errors. Nevertheless, the current results still provide a semi-quantitative explanation for experimentally observed trends.

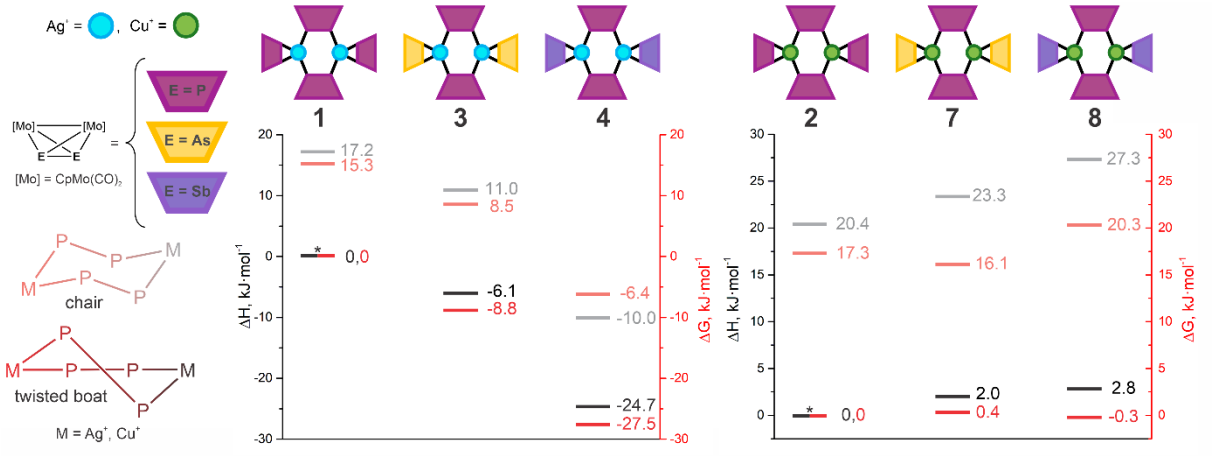
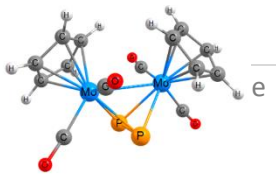


Fig. S39 Summary of the DFT calculations of reactions of Ag(I)-based complex **1** with **B** and **C** leading to the formation of **3** and **4** respectively and Cu(I)-based complex **2** with **B** and **C** leading to the formation of **7** and **8** respectively. For the twisted boat conformers, enthalpies and free energies are shown in black and red; for the chair conformers, enthalpies and free energies are shown in grey and pink respectively. Arbitrary selected zero level in the energy diagrams is indicated with asterisk.

Table S3 Cartesian coordinates of the gas-phase optimized geometry of $[(C_5H_5)_2Mo_2(CO)_4(\mu,\eta^2\text{-}P_2)]$ (**A**) calculated at the BP86/def2-SVP level of theory. E° = -1659.23143939 Hartree

Atom	x	y	z
Mo	-1.536522000	0.066205000	0.023526000
Mo	1.536297000	-0.065524000	0.024890000
P	0.133899000	1.066611000	1.758928000
P	-0.134577000	-1.038612000	1.775217000
O	1.244900000	-3.088730000	-0.791571000
O	3.491967000	-0.996353000	2.303440000
O	-1.243954000	3.075533000	-0.842557000
C	1.303805000	-1.969865000	-0.444600000
C	2.719081000	-0.669278000	1.491653000
C	-1.303182000	1.962427000	-0.477641000
C	1.482868000	1.356342000	-1.914133000
C	3.446551000	0.316718000	-1.230794000
C	2.351535000	0.244942000	-2.159045000
C	2.027049000	2.117147000	-0.824307000
C	3.238134000	1.481538000	-0.403698000
O	-3.491628000	1.039593000	2.284680000
C	-2.026388000	-2.131380000	-0.787199000
C	-2.718950000	0.697007000	1.479061000
C	-1.482785000	-1.389733000	-1.890353000



C	-3.237686000	-1.488994000	-0.377578000	H	-0.577975000	-1.648794000	-2.450839000
C	-2.351890000	-0.283109000	-2.154588000	H	0.578517000	1.606088000	-2.479647000
C	-3.446740000	-0.339038000	-1.225021000	H	1.598741000	3.037355000	-0.409786000
H	-1.597720000	-3.044096000	-0.356785000	H	3.908004000	1.835829000	0.389987000
H	-3.907394000	-1.829669000	0.422184000	H	4.306535000	-0.363063000	-1.190652000
H	-4.307075000	0.340900000	-1.196874000	H	2.225450000	-0.512089000	-2.943590000
H	-2.226123000	0.460258000	-2.952143000				

Table S4 Cartesian coordinates of the gas-phase optimized geometry of $[(C_5H_5)_2Mo_2(CO)_4(\mu,\eta^2\text{-}As_2)]$ (**B**) calculated at the BP86/def2-SVP level of theory. E° = -5448.43845977 Hartree

Atom	x	y	z	C	2.026716000	1.106571000	2.093468000
Mo	1.552015000	0.215161000	-0.074748000	C	2.760364000	-1.246916000	-0.632383000
Mo	-1.551743000	0.214726000	0.073625000	C	1.441396000	2.167605000	1.322884000
As	-0.145825000	-1.608252000	-1.161154000	C	3.246477000	0.716895000	1.452111000
As	0.146687000	-1.603797000	1.166435000	C	2.293197000	2.424949000	0.200942000
O	-1.280059000	1.017698000	3.101482000	C	3.419900000	1.534943000	0.276287000
O	-3.560931000	-2.046051000	0.926600000	H	1.623201000	0.696754000	3.026818000
O	1.276341000	1.011847000	-3.104020000	H	3.945142000	-0.049181000	1.811530000
C	-1.327829000	0.661033000	1.983623000	H	4.275569000	1.513672000	-0.409586000
C	-2.760706000	-1.246890000	0.631198000	H	2.137649000	3.195831000	-0.564568000
C	1.325761000	0.657773000	-1.985424000	H	0.520913000	2.705961000	1.572822000
C	-1.441419000	2.167438000	-1.323773000	H	-0.521245000	2.706826000	-1.572655000
C	-3.420546000	1.532796000	-0.279656000	H	-1.619283000	0.696082000	-3.027650000
C	-2.294964000	2.424038000	-0.203028000	H	-3.942449000	-0.051709000	-1.815709000
C	-2.024640000	1.105681000	-2.095007000	H	-4.277068000	1.510668000	0.405128000
C	-3.244839000	0.714826000	-1.455233000	H	-2.141069000	3.195060000	0.562679000
O	3.560346000	-2.046255000	-0.928059000				

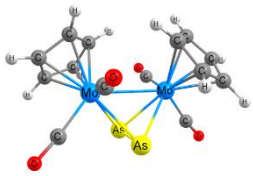


Table S5 Cartesian coordinates of the gas-phase optimized geometry of $[(C_5H_5)_2Mo_2(CO)_4(\mu,\eta^2\text{-}Sb_2)]$ (**C**) calculated at the BP86/def2-SVP level of theory. E° = -1457.45147454 Hartree

Atom	x	y	z	C	2.045078000	1.377809000	2.060333000
Mo	1.584521000	0.433518000	-0.088680000	C	2.827963000	-1.010328000	-0.605142000
Mo	-1.584260000	0.432780000	0.087325000	C	1.415947000	2.403934000	1.277100000
Sb	-0.162729000	-1.536185000	-1.352085000	C	3.270961000	1.016851000	1.410228000
Sb	0.163804000	-1.533324000	1.354734000	C	2.246714000	2.668629000	0.141478000
O	-1.334024000	1.259309000	3.107635000	C	3.404610000	1.818815000	0.219475000
O	-3.669289000	-1.781747000	0.867368000	H	1.673558000	0.984966000	3.013964000
O	1.330588000	1.257875000	-3.109392000	H	3.999878000	0.282437000	1.775786000
C	-1.361906000	0.867929000	1.998239000	H	4.253221000	1.814715000	-0.475429000
C	-2.827759000	-1.011280000	0.603073000	H	2.059124000	3.421107000	-0.635190000
C	1.360151000	0.867439000	-1.999727000	H	0.481556000	2.916085000	1.529659000
C	-1.417351000	2.404849000	-1.276217000	H	-0.483276000	2.918371000	-1.527216000
C	-3.406068000	1.815895000	-0.220953000	H	-1.670895000	0.986708000	-3.014356000
C	-2.249547000	2.667299000	-0.141160000	H	-3.997839000	0.280256000	-1.779432000
C	-2.044322000	1.378539000	-2.061051000	H	-4.255342000	1.809720000	0.473129000
C	-3.270282000	1.015312000	-1.412465000	H	-2.063606000	3.419269000	0.636398000
O	3.669313000	-1.780854000	-0.869956000				

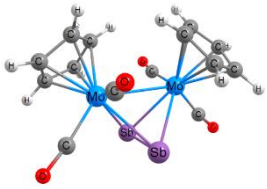
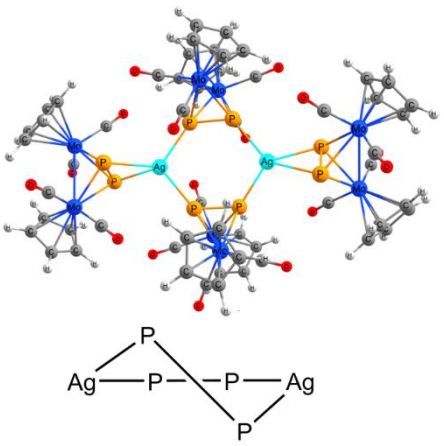


Table S6 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -6930.77205069 Hartree

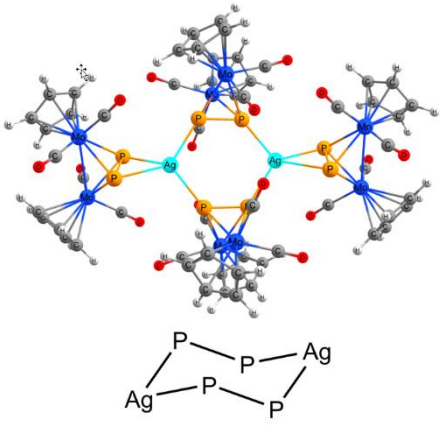
Atom	x	y	z	O	4.257789000	2.672474000	2.562216000
P	-4.991640000	-0.514501000	-0.796727000	C	-7.407033000	0.432759000	-1.909811000
P	5.061291000	0.565351000	-0.784588000	O	-3.412997000	-4.239592000	-1.241502000
P	-4.873415000	0.480340000	1.163586000	O	-3.245586000	4.579429000	0.662604000
P	4.852414000	-0.601428000	1.069319000	C	-4.957203000	-2.322236000	1.840625000
Ag	-2.518994000	0.089917000	-0.002716000	C	-5.406989000	2.250022000	-1.449143000
Ag	2.539285000	0.046852000	-0.087319000	C	7.228646000	-2.894326000	1.361468000
Mo	6.637224000	-1.447328000	-0.439263000	H	6.736094000	-2.891357000	2.341358000
Mo	-6.496567000	-1.508371000	0.915454000	C	7.148200000	3.472740000	0.415626000
Mo	6.614237000	1.281863000	1.024807000	H	6.385204000	4.252332000	0.298173000
Mo	-6.706976000	1.340630000	-0.281125000	O	3.139913000	-4.734251000	0.449690000
Mo	0.287420000	3.653458000	-1.854771000	C	7.851219000	3.144915000	1.633433000
Mo	-0.211759000	3.911633000	1.210258000	H	7.730618000	3.636238000	2.607159000
Mo	-0.384221000	-3.520566000	-1.784441000	C	7.006109000	0.232436000	2.670761000
Mo	0.273048000	-3.747791000	1.293116000	O	7.926549000	0.072218000	-2.886271000
P	-1.017983000	2.090941000	-0.435873000	C	-1.067688000	-1.927188000	-2.749749000
P	1.062718000	2.110840000	0.060098000	C	7.422607000	-0.441866000	-1.969278000
P	-0.981285000	-1.941054000	0.118709000	C	8.755019000	-2.478580000	-0.335242000
P	1.088977000	-2.003159000	-0.390066000	H	9.629801000	-2.106755000	-0.884473000
O	-4.678077000	2.848476000	-2.139365000	C	5.112656000	2.114450000	1.991526000
O	-7.318096000	-0.228123000	3.680035000	C	6.842087000	-3.676094000	0.225385000
O	3.291383000	4.461735000	-1.321051000	H	5.996069000	-4.373906000	0.183463000
O	7.282487000	-0.314092000	3.663378000	C	-0.808309000	2.516683000	2.486431000
O	-7.866504000	-0.025408000	-2.878512000	C	-2.294457000	-3.958242000	-1.397784000
O	1.360805000	1.219542000	-3.539808000	C	2.056097000	-4.371665000	0.700170000
O	-4.081711000	-2.866874000	2.390572000	C	-8.615623000	-2.527054000	1.091980000
C	-6.988028000	-0.653328000	2.645642000	H	-9.374865000	-2.207606000	1.817691000
O	-1.130889000	1.731063000	3.284567000	C	8.801099000	2.113014000	1.321410000
O	-1.467779000	-1.029641000	-3.374721000	H	9.519287000	1.670067000	2.023660000
O	4.532027000	-2.629006000	-2.443590000	C	0.968818000	2.096137000	-2.880947000



C	2.180319000	4.138707000	-1.482156000
C	7.789405000	-3.418729000	-0.833719000
H	7.808247000	-3.899244000	-1.820073000
C	5.291412000	-2.147666000	-1.697331000
C	-1.102444000	5.592149000	-2.081604000
H	-1.483103000	6.201050000	-1.254047000
C	-0.461745000	-4.592509000	-3.826060000
H	-1.305005000	-4.480525000	-4.519349000
C	8.414081000	-2.160632000	1.017907000
H	8.984747000	-1.508838000	1.688861000
C	-0.316820000	-5.613183000	-2.821569000
H	-1.038096000	-6.408964000	-2.595180000
C	-7.592255000	-3.508353000	1.325804000
H	-7.445794000	-4.077856000	2.252268000
C	7.664123000	2.642637000	-0.630629000
H	7.362991000	2.671388000	-1.684932000
C	-8.536359000	1.774573000	1.219559000
H	-9.055287000	1.019994000	1.821240000
C	-8.007970000	3.244582000	-0.501629000
H	-8.062000000	3.812174000	-1.439195000
C	-1.783097000	4.486229000	-2.693900000
H	-2.763098000	4.086270000	-2.407611000
C	-0.976965000	4.017742000	-3.780934000
H	-1.242034000	3.208394000	-4.473298000
C	-7.416040000	-2.784209000	-0.877389000
H	-7.100595000	-2.691227000	-1.923735000
C	0.970389000	-5.452873000	-2.210518000
H	1.392583000	-6.102082000	-1.434779000
C	-7.412501000	2.562872000	1.641132000
H	-6.921413000	2.506662000	2.620303000
C	-8.511825000	-2.086066000	-0.265596000
H	-9.181666000	-1.376563000	-0.764178000
C	-0.550934000	-5.398839000	0.583989000
C	8.691120000	1.808386000	-0.072722000
H	9.316007000	1.099391000	-0.627229000
C	0.212896000	4.830987000	-3.843308000
H	1.006361000	4.764656000	-4.598360000
C	0.129305000	5.800834000	-2.783128000
H	0.857731000	6.598766000	-2.588979000
C	1.109065000	5.911101000	1.074612000
H	1.434427000	6.399671000	0.149561000
C	-6.849659000	-3.666826000	0.097467000
H	-6.021316000	-4.365271000	-0.074898000
C	1.852190000	4.933227000	1.818487000
H	2.831327000	4.519683000	1.552641000
C	-7.086296000	3.474464000	0.585881000
H	-6.298414000	4.237594000	0.616133000
C	1.621148000	-4.327601000	-2.811847000
H	2.625017000	-3.952009000	-2.581356000
C	-8.898284000	2.189927000	-0.101411000
H	-9.740134000	1.804025000	-0.690913000
C	-0.865202000	-2.817505000	3.195257000
H	-1.704707000	-2.115094000	3.138158000
C	0.741255000	-3.793051000	-3.808427000
H	0.968501000	-2.953777000	-4.478261000
C	-0.977798000	-4.240969000	3.231341000
H	-1.915347000	-4.809764000	3.211790000
C	-0.106612000	5.389289000	2.988263000
H	-0.867853000	5.415695000	3.778104000
C	0.526574000	-2.472149000	3.286922000
H	0.938608000	-1.455205000	3.295628000
C	-0.099957000	6.186818000	1.790511000
H	-0.865803000	6.920331000	1.506752000
C	0.351277000	-4.788916000	3.353329000
H	0.605544000	-5.850843000	3.462626000
O	-1.021529000	-6.448303000	0.355758000
C	1.278302000	-3.686194000	3.394720000
H	2.364541000	-3.761441000	3.531689000
C	1.109978000	4.613876000	2.999981000
H	1.435696000	3.931224000	3.794914000
C	-2.123303000	4.296830000	0.824889000

Table S7 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -6930.76530980 Hartree

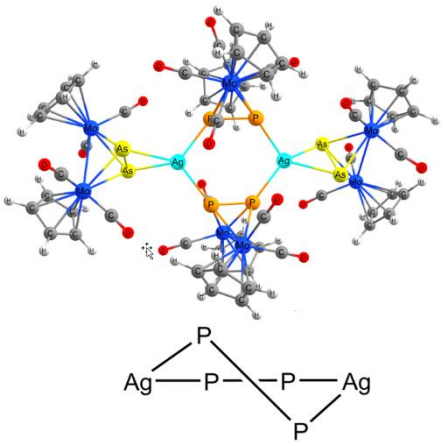
Atom	x	y	z
Ag	2.474390000	0.051986000	-0.266162000
Mo	6.573005000	1.437698000	0.628315000
Ag	-2.474033000	-0.051189000	0.266196000
Mo	-6.588859000	1.325536000	0.771556000
Mo	-6.571986000	-1.436950000	-0.629534000
Mo	6.588273000	-1.327081000	-0.768302000
Mo	-0.233505000	-3.962019000	-1.145981000
Mo	0.234464000	3.962368000	1.144701000
Mo	-0.472664000	3.572881000	-1.851924000
Mo	0.471167000	-3.572773000	1.851189000
P	-4.940074000	-0.634934000	1.065280000
P	-4.870001000	0.487014000	-0.827155000
P	4.869478000	-0.484629000	0.828416000
P	4.941017000	0.634128000	-1.065795000
P	1.094677000	-2.093277000	-0.177207000
P	0.942409000	2.072435000	-0.464791000
P	-1.094398000	2.093608000	0.177080000
P	-0.942660000	-2.072182000	0.463080000
O	7.528374000	-0.088023000	3.217947000
O	-3.152645000	-4.727642000	-0.230352000
O	1.655482000	-1.111513000	3.411220000
O	4.354195000	2.748872000	2.425236000
O	-4.352293000	-2.744104000	-2.428355000
O	-7.614824000	-0.157747000	3.360200000
O	3.433068000	-4.394514000	1.141386000
O	-7.528216000	0.091860000	-3.217029000
O	-4.353969000	2.674515000	2.512368000
O	-3.433984000	4.394655000	-1.139763000
O	-1.658926000	1.111495000	-3.410270000
O	3.152311000	4.728988000	0.225743000
C	-5.144323000	-2.220246000	-1.751984000
O	7.618787000	0.152097000	-3.357507000
O	-1.379889000	-1.967353000	-3.293437000
C	5.145803000	2.223471000	1.749563000
C	-5.165967000	2.128333000	1.871836000
C	7.146092000	0.428497000	2.244722000
C	-2.077168000	-4.400209000	-0.550277000
O	4.354200000	-2.675358000	-2.510656000
C	-2.335156000	4.063211000	-1.362279000
C	1.220880000	-1.990197000	2.784798000
C	-0.868063000	-5.524388000	2.252068000
C	7.208147000	-0.349554000	-2.387747000
C	-1.223422000	1.990235000	-2.784550000
C	-7.145609000	-0.425879000	-2.244580000
C	2.077278000	4.401260000	0.546823000
C	2.334078000	-4.063023000	1.363073000
C	-1.538212000	-4.397673000	2.837623000
C	8.511760000	2.049899000	-0.659404000
C	-8.509399000	-2.052125000	0.658701000
C	0.400427000	-5.671459000	2.900115000
C	-6.943877000	3.514779000	0.038699000
C	-7.205778000	0.345525000	2.390613000
C	-8.514613000	1.909811000	-0.551616000
C	0.866206000	5.524440000	-2.254524000
C	-0.983102000	-2.669029000	-2.456770000
C	-7.401478000	-2.846156000	1.109032000
C	7.783068000	3.346122000	1.127005000
C	-8.739261000	-2.353541000	-0.721505000
C	7.389804000	-2.670865000	1.032749000
C	6.954057000	3.647743000	-0.016240000
C	5.165892000	-2.129396000	-1.869530000
C	8.740458000	2.354141000	0.720369000
C	1.799482000	-4.927517000	-1.939672000
C	-0.079512000	-6.253886000	-1.624310000
C	-0.520809000	4.644457000	-3.901558000
C	-8.749623000	2.272339000	0.812710000
C	8.512365000	-1.912178000	0.556886000
C	-7.783790000	3.267852000	1.187174000
C	7.404359000	2.843183000	-1.112343000
C	0.517004000	-4.644514000	3.900798000
C	-0.403031000	5.671496000	-2.901101000
C	6.939431000	-3.515675000	-0.031628000
C	-6.951996000	-3.648356000	0.010863000
C	-7.393512000	2.671055000	-1.026845000
C	-7.782059000	-3.344546000	-1.131030000
C	0.912664000	-4.702232000	-3.040551000
C	1.535640000	4.397656000	-2.840748000
C	0.686760000	3.855767000	-3.858466000
O	1.384704000	1.968501000	3.290826000
C	7.780391000	-3.271984000	-1.180024000
C	-0.258338000	-5.523618000	-2.851611000
C	1.190339000	-5.892165000	-1.068912000
C	-0.690528000	-3.855856000	3.856380000
C	-1.797940000	4.926960000	1.941048000
C	8.747570000	-2.277365000	-0.806690000
C	0.986329000	2.669878000	2.454654000
C	-1.190500000	5.891729000	1.069236000
C	-0.909452000	4.702350000	3.040729000
C	0.079953000	6.254210000	1.622784000
C	0.260865000	5.524300000	2.849987000
H	9.107531000	1.367116000	-1.275512000
H	7.006215000	2.860929000	-2.134198000
H	6.145868000	4.389237000	-0.048618000



H	7.733817000	3.829429000	2.110907000
H	9.540118000	1.940187000	1.348231000
H	6.980898000	-2.641327000	2.049969000
H	6.122891000	-4.245367000	0.033457000
H	7.733463000	-3.793930000	-2.144117000
H	9.555901000	-1.898375000	-1.445547000
H	9.115505000	-1.214790000	1.148831000
H	2.782715000	-4.460122000	-1.811442000
H	1.641544000	-6.317355000	-0.165697000
H	-0.771937000	-7.003385000	-1.219727000
H	-1.102595000	-5.620257000	-3.545815000
H	1.112278000	-4.050895000	-3.901013000
H	-1.279641000	-6.187819000	1.483737000
H	1.134081000	-6.465557000	2.710182000
H	1.345334000	-4.522825000	4.610074000
H	-0.935171000	-3.015394000	4.518451000
H	-2.540558000	-4.039314000	2.574652000
H	-2.781126000	4.459035000	1.814277000
H	-1.107507000	4.051084000	3.901605000
H	1.106040000	5.621535000	3.542991000
H	0.771427000	7.003980000	1.217087000
H	-1.643162000	6.316512000	0.166562000
H	1.278708000	6.187937000	-1.486748000
H	2.538288000	4.039304000	-2.578910000
H	0.930612000	3.015252000	-4.520759000
H	-1.349953000	4.522743000	-4.609881000
H	-1.136423000	6.465648000	-2.710386000
H	-6.128583000	4.245931000	-0.025615000
H	-6.985116000	2.643843000	-2.044339000
H	-9.117017000	1.212516000	-1.144420000
H	-9.557039000	1.891068000	1.451365000
H	-7.737111000	3.788295000	2.152093000
H	-9.104723000	-1.370747000	1.276794000
H	-9.539573000	-1.938484000	-1.347808000
H	-7.733582000	-3.825829000	-2.115962000
H	-6.143580000	-4.389696000	0.041020000
H	-7.002406000	-2.865934000	2.130491000

Table S8 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -14509.1885344 Hartree

Atom	x	y	z
As	-5.029909000	-0.629130000	-0.897961000
As	5.110999000	0.651369000	-0.902919000
As	-4.934729000	0.616080000	1.202987000
As	4.909755000	-0.676411000	1.135602000
Ag	-2.543083000	0.080720000	-0.006965000
Ag	2.565937000	0.040502000	-0.087422000
Mo	6.764329000	-1.436432000	-0.514335000
Mo	-6.618170000	-1.470394000	0.975269000
Mo	6.739893000	1.291928000	1.020818000
Mo	-6.826373000	1.317492000	-0.434920000
Mo	0.271230000	3.676547000	-1.811708000
Mo	-0.215162000	3.869729000	1.260207000
Mo	-0.365881000	-3.508541000	-1.786270000
Mo	0.254696000	-3.765321000	1.295231000
P	-1.013933000	2.075939000	-0.418092000
P	1.068332000	2.101723000	0.069647000
P	-0.985809000	-1.945933000	0.125304000
P	1.089267000	-2.003316000	-0.361701000
O	-4.749206000	2.836049000	-2.230319000
O	-7.428976000	-0.049617000	3.671524000
O	3.271810000	4.498082000	-1.278716000
O	7.401141000	-0.307938000	3.656665000
O	-7.869453000	-0.176868000	-3.008544000
O	1.360843000	1.283199000	-3.543514000
O	-4.206646000	-2.808142000	2.473801000
C	-7.089556000	-0.523578000	2.660083000
O	-1.119499000	1.640689000	3.288513000
O	-1.443634000	-1.005671000	-3.360998000
O	4.628538000	-2.686522000	-2.442497000
O	4.398142000	2.738176000	2.527325000
C	-7.438777000	0.327420000	-2.047855000
O	-3.399282000	-4.234335000	-1.272848000
O	-3.253171000	4.527042000	0.722614000
C	-5.076486000	-2.262301000	1.913782000
C	-5.490671000	2.223666000	-1.564332000
C	7.427160000	-2.898240000	1.250483000
H	6.945530000	-2.951890000	2.234438000
C	7.332323000	3.480698000	0.475003000
H	6.593822000	4.288430000	0.396446000
O	3.143822000	-4.718543000	0.490136000
C	8.041791000	3.091408000	1.669314000
H	7.950350000	3.553322000	2.660358000
C	7.114291000	0.235928000	2.663970000
O	7.981139000	0.108694000	-2.980008000
C	-1.045472000	-1.908386000	-2.741565000
C	7.491577000	-0.411157000	-2.056773000
C	8.923477000	-2.366986000	-0.440355000
H	9.779136000	-1.943104000	-0.981883000
C	5.240721000	2.149853000	1.966662000
C	7.072213000	-3.666199000	0.093538000
H	6.262105000	-4.404397000	0.036968000
C	-0.801982000	2.445766000	2.507272000
C	-2.279241000	-3.954187000	-1.419947000
C	2.053375000	-4.367407000	0.726501000
C	-8.772036000	-2.390623000	1.194590000
H	-9.529165000	-1.990452000	1.881399000
C	8.952838000	2.039718000	1.307485000
H	9.668227000	1.552961000	1.983027000
C	0.962613000	2.144668000	-2.868300000
C	2.161805000	4.170995000	-1.439137000
C	8.001261000	-3.339490000	-0.960923000
H	8.037533000	-3.793235000	-1.959299000
C	5.394026000	-2.170446000	-1.724376000
C	-1.145740000	5.600455000	-1.995085000
H	-1.533282000	6.186314000	-1.154220000
C	-0.415657000	-4.559449000	-3.839588000
H	-1.252646000	-4.445644000	-4.540140000
C	8.575025000	-2.101338000	0.922499000
H	9.119246000	-1.445466000	1.610973000
C	-0.274276000	-5.589142000	-2.843977000
H	-0.992818000	-6.391421000	-2.632354000
C	-7.790070000	-3.389063000	1.520353000
H	-7.676254000	-3.889722000	2.490050000
C	7.807105000	2.671647000	-0.608166000
H	7.499219000	2.752312000	-1.657898000
C	-8.709681000	1.747349000	0.996131000
H	-9.205171000	1.010255000	1.637614000
C	-8.215700000	3.129054000	-0.808574000
H	-8.275184000	3.630655000	-1.782627000
C	-1.812739000	4.499323000	-2.630791000
H	-2.788781000	4.081956000	-2.355094000
C	-1.001503000	4.065338000	-3.728298000
H	-1.256808000	3.267923000	-4.437968000
C	-7.560357000	-2.845395000	-0.730762000
H	-7.235492000	-2.853702000	-1.778407000
C	1.006097000	-5.426937000	-2.218737000
H	1.425181000	-6.081422000	-1.445724000
C	-7.640397000	2.621229000	1.388662000
H	-7.178599000	2.662381000	2.382789000
C	-8.635610000	-2.061393000	-0.191831000
H	-9.272950000	-1.371434000	-0.755902000
C	-0.540024000	-5.413838000	0.549014000
C	8.814325000	1.787018000	-0.094665000
H	9.409770000	1.081049000	-0.683956000
C	0.177338000	4.895394000	-3.774266000
H	0.970510000	4.855825000	-4.531499000
C	0.082362000	5.840711000	-2.693004000
H	0.800234000	6.643867000	-2.481885000
C	1.106049000	5.870999000	1.165844000
H	1.437129000	6.375304000	0.251342000
C	-7.039367000	-3.668368000	0.320316000
H	-6.239493000	-4.412165000	0.215471000
C	1.846026000	4.882206000	1.898149000
H	2.828419000	4.474654000	1.634152000
C	-7.335860000	3.477296000	0.280442000
H	-6.593539000	4.285416000	0.278343000
C	1.655897000	-4.291828000	-2.802287000
H	2.656842000	-3.915031000	-2.560310000
C	-9.058538000	2.054947000	-0.357703000
H	-9.865473000	1.588840000	-0.937948000
C	-0.950476000	-2.900384000	3.190375000
H	-1.814058000	-2.228274000	3.127616000
C	0.782054000	-3.752766000	-3.801833000
H	1.010467000	-2.905566000	-4.461233000
C	-1.013682000	-4.326422000	3.207363000
H	-1.930008000	-4.927878000	3.164776000
C	-0.121147000	5.317390000	3.063132000
H	-0.887070000	5.330070000	3.848771000
C	0.427469000	-2.508573000	3.308426000
H	0.801855000	-1.477542000	3.338132000
C	-0.107989000	6.134116000	1.878373000
H	-0.872517000	6.871761000	1.601946000
C	0.331051000	-4.830493000	3.342773000
H	0.619376000	-5.884600000	3.442886000
O	-0.996305000	-6.465715000	0.302579000
C	1.219265000	-3.697027000	3.413852000
H	2.304904000	-3.737532000	3.569270000



C	1.096150000	4.543175000	3.069358000	C	-2.128924000	4.250828000	0.881767000
H	1.417553000	3.848557000	3.855713000				

Table S9 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -14509.1818669 Hartree

Atom	x	y	z
Ag	2.494143000	0.051241000	-0.280899000
Mo	6.694266000	1.419293000	0.683390000
Ag	-2.493224000	-0.047550000	0.276490000
Mo	-6.696278000	1.326008000	0.820793000
Mo	-6.691105000	-1.413752000	-0.689594000
Mo	6.695598000	-1.336926000	-0.796823000
Mo	-0.266537000	-3.918670000	-1.176227000
Mo	0.269022000	3.921195000	1.166752000
Mo	-0.494289000	3.616660000	-1.825624000
Mo	0.489093000	-3.615548000	1.818206000
As	-4.991511000	-0.729646000	1.150048000
As	-4.900975000	0.578214000	-0.911557000
As	4.897221000	-0.564718000	0.921567000
As	4.997616000	0.719969000	-1.153527000
P	1.079968000	-2.080310000	-0.179086000
P	0.948156000	2.075477000	-0.507513000
P	-1.076502000	2.080819000	0.173274000
P	-0.946567000	-2.072075000	0.495958000
O	7.557609000	-0.142124000	3.281610000
O	-3.161905000	-4.725236000	-0.219370000
O	1.665656000	-1.195310000	3.445875000
O	4.477635000	2.829516000	2.406027000
O	-4.472118000	-2.803183000	-2.426182000
O	-7.670872000	-0.183837000	3.411236000
O	3.449963000	-4.388088000	1.053319000
O	-7.560541000	0.170185000	-3.272081000
O	-4.445791000	2.720628000	2.504005000
O	-3.453906000	4.383808000	-1.050715000
O	-1.674206000	1.195675000	-3.449634000
O	3.158263000	4.736799000	0.198759000
C	-5.256786000	-2.239975000	-1.771616000
O	7.690896000	0.145065000	-3.395516000
O	-1.494390000	-1.872116000	-3.227171000
C	5.261052000	2.258698000	1.756536000
C	-5.257002000	2.148848000	1.883281000
C	7.195696000	0.386320000	2.305314000
C	-2.094799000	-4.385271000	-0.552603000
O	4.450332000	-2.735411000	-2.483449000
C	-2.354054000	4.072271000	-1.296006000
C	1.233468000	-2.056338000	2.793504000
C	-0.821827000	-5.595516000	2.174526000
C	7.279316000	-0.352810000	-2.422490000
C	-1.240238000	2.056762000	-2.798535000
C	-7.196283000	-0.366784000	-2.301315000
C	2.093546000	4.393610000	0.536126000
C	2.349856000	-4.074206000	1.294564000
C	-1.498016000	-4.495714000	2.802923000
C	8.672601000	1.953525000	-0.574319000
C	-8.665284000	-1.964116000	0.567690000
C	0.455880000	-5.747050000	2.802827000
C	-7.140647000	3.521655000	0.171613000
C	-7.266483000	0.324750000	2.440696000
C	-8.639108000	1.875611000	-0.488989000
C	0.810178000	5.600088000	-2.186871000
C	-1.062403000	-2.595425000	-2.426569000
C	-7.605979000	-2.831328000	0.998913000
C	7.997265000	3.245590000	1.238128000
C	-8.898413000	-2.207608000	-0.823756000
C	7.537690000	-2.698332000	0.972072000
C	7.198265000	3.617892000	0.095824000
C	5.259526000	-2.162100000	-1.861425000
C	8.902398000	2.211412000	0.815072000
C	1.755532000	-4.843619000	-2.043781000
C	-0.107131000	-6.193056000	-1.724812000
C	-0.586279000	4.749319000	-3.841196000
C	-8.891457000	2.173339000	0.888083000
C	8.631743000	-1.883552000	0.524112000
C	-7.970792000	3.195386000	1.305744000
C	7.615728000	2.817635000	-1.017544000
C	0.572788000	-4.749986000	3.833113000
C	-0.469524000	5.747536000	-2.812037000
C	7.123955000	-3.527541000	-0.120572000
C	-7.190359000	-3.619127000	-0.123977000
C	-7.551585000	2.702898000	-0.929898000
C	-7.992916000	-3.235967000	-1.260146000
C	0.841631000	-4.593625000	-3.117076000
C	1.487822000	4.501654000	-2.816094000
C	0.633210000	3.977925000	-3.838341000
O	1.511792000	1.877157000	3.211192000
C	7.959172000	-3.220264000	-1.256350000
C	-0.318815000	-5.429378000	-2.926175000
C	1.172341000	-5.837092000	-1.187624000
C	-0.644535000	-3.975216000	3.827758000
C	-1.753008000	4.840300000	2.040237000
C	8.885491000	-2.199409000	-0.848652000
C	1.074005000	2.599801000	2.413093000
C	-1.174458000	5.836096000	1.183566000
C	-0.835784000	4.591513000	3.110997000
C	0.105473000	6.194661000	1.717895000
C	0.322086000	5.430354000	2.917971000
H	9.237080000	1.255567000	-1.202428000
H	7.236724000	2.889756000	-2.044332000
H	6.434687000	4.405597000	0.072751000
H	7.964127000	3.707487000	2.232820000
H	9.673130000	1.741589000	1.439727000
H	7.130109000	-2.720141000	1.990108000
H	6.337221000	-4.291256000	-0.082186000
H	7.935363000	-3.715722000	-2.235042000
H	9.682842000	-1.773975000	-1.471823000
H	9.205750000	-1.182965000	1.140375000
H	2.739710000	-4.374628000	-1.926223000
H	1.645801000	-6.283712000	-0.306435000
H	-0.784852000	-6.959322000	-1.326813000
H	-1.177957000	-5.512382000	-3.603670000
H	1.016464000	-3.916225000	-3.962690000
H	-1.235008000	-6.240700000	1.391658000
H	1.196607000	-6.525735000	2.579485000
H	1.408248000	-4.640281000	4.535937000
H	-0.890964000	-3.158902000	4.518745000
H	-2.507851000	-4.142454000	2.562822000
H	-2.736427000	4.369175000	1.924823000
H	-1.006761000	3.912822000	3.956359000
H	1.182755000	5.514773000	3.593346000
H	0.780332000	6.962898000	1.318824000
H	-1.651075000	6.282292000	0.303858000
H	1.223504000	6.247112000	-1.405594000
H	2.499239000	4.151406000	-2.578249000
H	0.880131000	3.161706000	-4.529265000
H	-1.423247000	4.636730000	-4.541767000
H	-1.211869000	6.524302000	-2.587379000
H	-6.359519000	4.291435000	0.140455000
H	-7.146586000	2.739533000	-1.948537000
H	-9.210247000	1.178953000	-1.112295000
H	-9.684516000	1.735404000	1.508057000
H	-7.947705000	3.679375000	2.290171000
H	-9.229233000	-1.273888000	1.204792000
H	-9.671536000	-1.732467000	-1.441394000
H	-7.961743000	-3.687271000	-2.259751000
H	-6.425449000	-4.405775000	-0.111233000
H	-7.224106000	-2.913755000	2.023857000

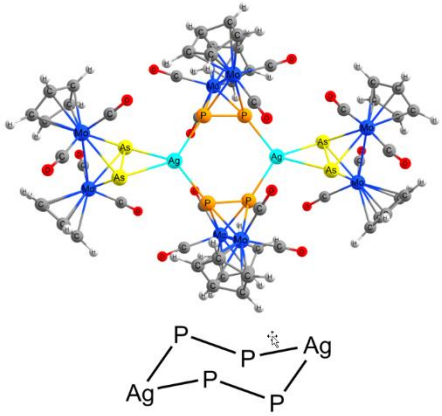


Table S10 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -6527.22294853 Hartree

Atom	x	y	z
Sb	-5.115666000	-0.701923000	-1.166482000
Sb	5.165704000	0.670101000	-1.181788000
Sb	-5.077628000	0.748683000	1.272948000
Sb	5.093344000	-0.709229000	1.293024000
Ag	-2.594038000	0.046033000	-0.003424000
Ag	2.616456000	-0.024515000	-0.021582000
Mo	7.025021000	-1.467113000	-0.590459000
Mo	-6.927376000	-1.431917000	0.841723000
Mo	7.000438000	1.412183000	0.807707000
Mo	-7.017579000	1.409343000	-0.639932000
Mo	0.279503000	3.704117000	-1.639310000

Mo	-0.214681000	3.747227000	1.437270000
Mo	-0.306333000	-3.582731000	-1.668128000
Mo	0.149481000	-3.783011000	1.446064000
P	-0.995342000	2.029184000	-0.326496000
P	1.085849000	2.044385000	0.167295000
P	-1.020345000	-1.982212000	0.185056000
P	1.073703000	-2.049922000	-0.200899000
O	-4.845617000	2.982114000	-2.267209000
O	-7.840892000	-0.008981000	3.498828000
O	3.280132000	4.510214000	-1.086814000
O	7.836942000	0.058592000	3.525558000
O	-7.976419000	-0.033013000	-3.270297000
O	1.370105000	1.392978000	-3.478601000
O	-4.630335000	-2.882681000	2.411246000
C	-7.440533000	-0.473544000	2.502561000
O	-1.086022000	1.406073000	3.349514000
O	-1.340944000	-1.112937000	-3.321630000
O	4.850225000	-3.014002000	-2.236565000
O	4.738513000	3.002106000	2.286949000
C	-7.554483000	0.440134000	-2.286986000
O	-3.354487000	-4.329840000	-1.281289000
O	-3.259566000	4.391160000	0.926389000
C	-5.446916000	-2.281512000	1.823617000
C	-5.613038000	2.333381000	-1.663982000
C	7.881075000	-2.767779000	1.219842000
H	7.464568000	-2.818233000	2.233318000
C	7.590042000	3.558550000	0.123443000
H	6.861714000	4.376514000	0.054745000
O	3.139953000	-4.600329000	0.906940000
C	8.365385000	3.210637000	1.287224000
H	8.343343000	3.718831000	2.259327000
C	7.462516000	0.497354000	2.507501000
O	8.047447000	-0.106388000	-3.240356000
C	-0.960287000	-2.002882000	-2.672526000
C	7.605303000	-0.547950000	-2.251392000
C	9.249503000	-2.213680000	-0.569125000
H	10.044201000	-1.756962000	-1.173177000
C	5.538754000	2.345166000	1.736546000
C	7.538722000	-3.624186000	0.120893000
H	6.795070000	-4.430964000	0.142821000
C	-0.782032000	2.256059000	2.610082000
C	-2.230706000	-4.044301000	-1.382926000
C	2.017939000	-4.298879000	1.042935000
C	-9.138217000	-2.210558000	0.949600000
H	-9.911555000	-1.744548000	1.573928000
C	9.234430000	2.124755000	0.917960000
H	9.984337000	1.657837000	1.569587000
C	0.971943000	2.223046000	-2.764831000
C	2.169278000	4.187396000	-1.251524000
C	8.388258000	-3.285752000	-0.992834000
H	8.416973000	-3.791687000	-1.965963000
C	5.617330000	-2.374530000	-1.623689000
C	-1.153826000	5.622545000	-1.733396000
H	-1.550731000	6.162506000	-0.866650000
C	-0.249280000	-4.675912000	-3.698061000
H	-1.061131000	-4.596992000	-4.432174000
C	8.942040000	-1.900057000	0.793007000
H	9.460352000	-1.166068000	1.419471000
C	-0.122422000	-5.679444000	-2.674227000
H	-0.829629000	-6.493650000	-2.470427000
C	-8.240717000	-3.254346000	1.369595000
H	-8.216155000	-3.726157000	2.359810000
C	7.984439000	2.693969000	-0.951191000
H	7.629594000	2.746959000	-1.987768000
C	-8.963754000	1.818944000	0.710551000
H	-9.469542000	1.085991000	1.348255000
C	-8.427034000	3.178212000	-1.100760000
H	-8.457947000	3.660415000	-2.085777000
C	-1.809255000	4.550460000	-2.428026000
H	-2.786686000	4.116460000	-2.183537000
C	-0.988292000	4.179126000	-3.541131000
H	-1.233751000	3.417378000	-4.292265000
C	-7.845377000	-2.807847000	-0.881278000
H	-7.476257000	-2.889579000	-1.910972000
C	1.130101000	-5.472570000	-2.005243000
H	1.536348000	-6.098728000	-1.202418000
C	-7.932435000	2.725539000	1.129203000
H	-7.528608000	2.809678000	2.145603000
C	-8.899412000	-1.940995000	-0.435596000
H	-9.457366000	-1.236873000	-1.062307000
C	-0.499720000	-5.465240000	0.641250000
C	9.004941000	1.812099000	-0.459553000
H	9.550070000	1.070144000	-1.052780000
C	0.183949000	5.019431000	-3.538584000
H	0.980931000	5.024336000	-4.292789000
C	0.075919000	5.907848000	-2.411200000
H	0.785728000	6.705058000	-2.155196000
C	1.122288000	5.740195000	1.444923000
H	1.483509000	6.271649000	0.557737000
C	-7.438414000	-3.619463000	0.229637000
H	-6.683127000	-4.415162000	0.200594000
C	1.837723000	4.726050000	2.166480000
H	2.829164000	4.325958000	1.922611000
C	-7.601296000	3.566013000	0.014740000
H	-6.881110000	4.393905000	0.026496000
C	1.775039000	-4.336226000	-2.589917000
H	2.762286000	-3.939202000	-2.324658000
C	-9.263278000	2.092473000	-0.661843000
H	-10.037205000	1.599306000	-1.264183000
C	-1.346820000	-3.116972000	3.218052000
H	-2.300517000	-2.598478000	3.063120000
C	0.926353000	-3.839801000	-3.632614000
H	1.159172000	-3.001941000	-4.302352000
C	-1.179925000	-4.530749000	3.270509000
H	-1.978590000	-5.275692000	3.163946000
C	-0.162017000	5.135433000	3.287823000
H	-0.949329000	5.127459000	4.052059000
C	-0.061144000	-2.504868000	3.434463000
H	0.133287000	-1.425513000	3.474052000
C	-0.111372000	5.988238000	2.129489000
H	-0.863173000	6.739710000	1.855631000
C	0.211163000	-4.810570000	3.517230000
H	0.653647000	-5.804448000	3.661667000
O	-0.889216000	-6.541775000	0.382929000
C	0.899905000	-3.546938000	3.633905000
H	1.960724000	-3.411826000	3.880372000
C	1.050901000	4.355430000	3.303634000
H	1.344978000	3.636613000	4.079085000
C	-2.131094000	4.123648000	1.073624000

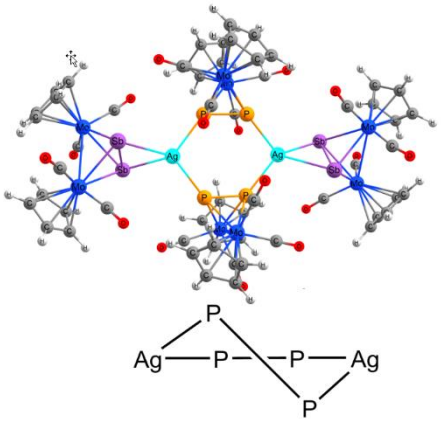
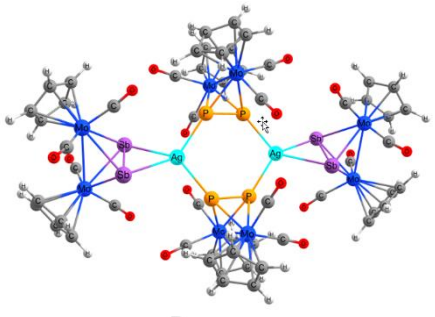


Table S11 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Ag_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -6527.21601975 Hartree

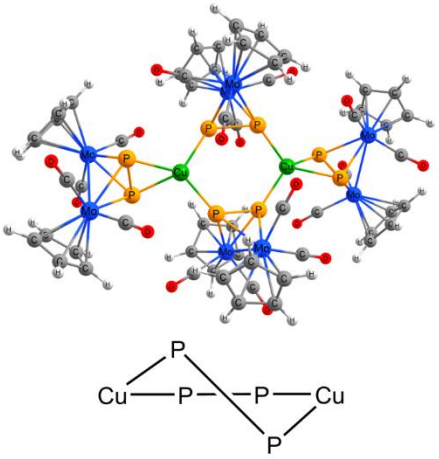
Atom	x	y	z
Ag	2.528493000	0.048121000	-0.283946000
Mo	6.923645000	1.435573000	0.711903000
Ag	-2.528651000	-0.047626000	0.284411000
Mo	-6.899639000	1.384907000	0.811614000
Mo	-6.923475000	-1.436127000	-0.711902000
Mo	6.899503000	-1.384985000	-0.812400000
Mo	-0.303918000	-3.842461000	-1.240851000
Mo	0.303707000	3.842798000	1.241247000
Mo	-0.495761000	3.700111000	-1.752576000
Mo	0.496057000	-3.699966000	1.752816000
Sb	-5.096915000	-0.816987000	1.321563000
Sb	-4.971671000	0.656377000	-1.100327000
Sb	4.971743000	-0.656808000	1.099978000
Sb	5.096897000	0.817079000	-1.321677000
P	1.058597000	-2.061722000	-0.171191000
P	0.957821000	2.081708000	-0.533714000
P	-1.058049000	2.061617000	0.171284000
P	-0.957265000	-2.081092000	0.534186000
O	7.793231000	-0.105777000	3.314919000
O	-3.161024000	-4.741668000	-0.250528000
O	1.647060000	-1.363917000	3.515196000
O	4.753393000	2.957327000	2.397628000
O	-4.753385000	-2.958356000	-2.397406000
O	-7.905484000	-0.021482000	3.443157000
O	3.457441000	-4.394954000	0.924410000
O	-7.792883000	0.105039000	-3.315091000
O	-4.652556000	2.865326000	2.422754000
O	-3.457526000	4.394147000	-0.924717000
O	-1.645494000	1.363700000	-3.515328000
O	3.160916000	4.743182000	0.252286000
C	-5.508335000	-2.333138000	-1.760845000
O	7.904720000	0.021885000	-3.443926000
O	-1.666910000	-1.711460000	-3.111932000
C	5.508451000	2.332315000	1.760997000
C	-5.451509000	2.247586000	1.826784000
C	7.406529000	0.407131000	2.336784000
C	-2.107351000	-4.372314000	-0.593388000
O	4.651993000	-2.865246000	-2.423112000
C	-2.354874000	4.106879000	-1.188163000
C	1.225253000	-2.189753000	2.812021000
C	-0.777447000	-5.721197000	2.008878000
C	7.466975000	-0.434322000	-2.458894000
C	-1.224144000	2.189663000	-2.812026000
C	-7.406240000	-0.407832000	-2.336908000
C	2.107292000	4.373336000	0.594729000



C	2.354924000	-4.107326000	1.188022000
C	-1.465952000	-4.670416000	2.704460000
C	8.903126000	1.890344000	-0.570801000
C	-8.903109000	-1.890668000	0.570632000
C	0.508436000	-5.885321000	2.616399000
C	-7.390777000	3.564505000	0.156444000
C	-7.467495000	0.434524000	2.458155000
C	-8.840444000	1.881058000	-0.519999000
C	0.777106000	5.721801000	-2.007990000
C	-1.174638000	-2.470559000	-2.380873000
C	-7.887222000	-2.816320000	0.984554000
C	8.318457000	3.183394000	1.274276000
C	-9.163978000	-2.112242000	-0.819373000
C	7.771615000	-2.738090000	0.950266000
C	7.524436000	3.614332000	0.151316000
C	5.451078000	-2.247535000	-1.827296000
C	9.164213000	2.111500000	0.819225000
C	1.712706000	-4.679569000	-2.211586000
C	-0.121288000	-6.076570000	-1.926417000
C	-0.617925000	4.945935000	-3.699749000
C	-9.112448000	2.171516000	0.854407000
C	8.840250000	-1.881577000	0.519096000
C	-8.221981000	3.217779000	1.281724000
C	7.887239000	2.816183000	-0.984312000
C	0.618701000	-4.945804000	3.699930000
C	-0.508527000	5.885480000	-2.616160000
C	7.390801000	-3.564861000	-0.158208000
C	-7.524184000	-3.614760000	-0.150793000
C	-7.771728000	2.737242000	-0.951623000
C	-8.318082000	-3.184196000	-1.273993000
C	0.766258000	-4.382095000	-3.244340000
C	1.466334000	4.671275000	-2.703256000
C	0.612845000	4.194137000	-3.748662000
O	1.665830000	1.711836000	3.112998000
C	8.222007000	-3.217521000	-1.283291000
C	-0.375558000	-5.247706000	-3.074987000
C	1.166397000	-5.731056000	-1.401393000
C	-0.611774000	-4.193571000	3.749440000
C	-1.713364000	4.679738000	2.211090000
C	9.112348000	-2.171352000	-0.855439000
C	1.173979000	2.470933000	2.381661000
C	-1.166753000	5.731370000	1.401279000
C	-0.767378000	4.382225000	3.244273000
C	0.120659000	6.076902000	1.926940000
C	0.374450000	5.247928000	3.075541000
H	9.422319000	1.177601000	-1.220622000
H	7.515278000	2.941095000	-2.008632000
H	6.804255000	4.442435000	0.152403000
H	8.322488000	3.629246000	2.276734000
H	9.920930000	1.595255000	1.424003000
H	7.373718000	-2.799524000	1.970555000
H	6.631056000	-4.356321000	-0.136486000
H	8.220020000	-3.701526000	-2.267903000
H	9.901170000	-1.714770000	-1.467286000
H	9.386929000	-1.172319000	1.149637000
H	2.696982000	-4.209231000	-2.094353000
H	1.669369000	-6.219945000	-0.559742000
H	-0.776665000	-6.876361000	-1.557993000
H	-1.250714000	-5.305380000	-3.734418000
H	0.907604000	-3.653481000	-4.052855000
H	-1.186343000	-6.328293000	1.194034000
H	1.260376000	-6.636537000	2.342199000
H	1.458956000	-4.861504000	4.400562000
H	-0.865202000	-3.422598000	4.488332000
H	-2.484069000	-4.322831000	2.492934000
H	-2.697598000	4.209425000	2.093410000
H	-0.909107000	3.653552000	4.052665000
H	1.249305000	5.305607000	3.735378000
H	0.776150000	6.876790000	1.558927000
H	-1.669346000	6.220292000	0.559418000
H	1.185420000	6.329087000	-1.192997000
H	2.484472000	4.324053000	-2.491224000
H	0.866904000	3.423262000	-4.487437000
H	-1.457798000	4.861357000	-4.400810000
H	-1.260873000	6.636427000	-2.342333000
H	-6.630951000	4.355871000	0.134301000
H	-7.373890000	2.798165000	-1.971968000
H	-9.387198000	1.171522000	-1.150165000
H	-9.901305000	1.715305000	1.466484000
H	-8.219925000	3.702280000	2.266093000
H	-9.422509000	-1.177836000	1.220192000
H	-9.920630000	-1.596208000	-1.424413000
H	-8.321930000	-3.630334000	-2.276324000
H	-6.803956000	-4.442821000	-0.151531000
H	-7.515323000	-2.940851000	2.008945000

Table S12 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -9917.75870728 Hartree

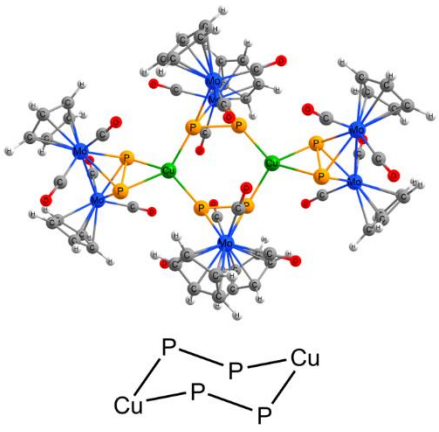
Atom	x	y	z
P	4.638940000	-0.669845000	0.691383000
P	-4.673046000	0.730335000	0.669952000
P	4.469131000	0.586945000	-1.109473000
P	-4.429849000	-0.697587000	-0.993318000
Cu	2.409611000	0.042240000	0.036857000
Cu	-2.418027000	0.068331000	0.125092000
Mo	-6.283167000	-1.284747000	0.557356000
Mo	6.086820000	-1.425070000	-1.188064000
Mo	-6.157139000	1.204324000	-1.273157000
Mo	6.364303000	1.224047000	0.373196000
Mo	-0.278760000	3.430384000	1.933107000
Mo	0.254515000	3.751476000	-1.114402000
Mo	0.405808000	-3.370310000	1.832886000
Mo	-0.402978000	-3.545648000	-1.208689000
P	1.064096000	1.899797000	0.502868000
P	-1.014618000	1.919843000	-0.015730000
P	0.955865000	-1.783128000	-0.072332000
P	-1.098633000	-1.808099000	0.520407000
O	4.454004000	2.465036000	2.527456000
O	6.808968000	0.209346000	-3.788933000
O	-3.281085000	4.217454000	1.372523000
O	-6.754966000	-0.729479000	-3.692598000
O	7.612379000	-0.489766000	2.710956000
O	-1.335157000	0.974745000	3.597511000
O	3.634311000	-2.597404000	-2.752136000
C	6.516756000	-0.349248000	-2.808163000
O	1.218203000	1.638439000	-3.238464000
O	1.541957000	-0.918792000	3.447733000
O	-4.258720000	-2.276640000	2.740454000
O	-3.738403000	2.321334000	-2.933666000
C	7.121286000	0.097938000	1.832239000
O	3.401951000	-4.099170000	1.158576000
O	3.261481000	4.460406000	-0.481868000
C	4.517365000	-2.115919000	-2.157372000
C	5.130879000	1.962671000	1.717215000
C	-6.912446000	-2.926978000	-1.050088000
H	-6.408200000	-3.068214000	-2.013566000
C	-6.699926000	3.460616000	-1.007438000
H	-5.941502000	4.252746000	-0.985359000
O	-3.125143000	-4.702247000	-0.135169000
C	-7.370289000	2.957533000	-2.182282000
H	-7.222517000	3.301128000	-3.213882000
C	-6.506938000	-0.053986000	-2.774679000
O	-7.553898000	0.571398000	2.770955000
C	1.121038000	-1.796361000	2.809332000
C	-7.055004000	-0.071896000	1.936786000
C	-8.440827000	-2.238841000	0.552524000
H	-9.306979000	-1.767491000	1.035104000
C	-4.613374000	1.868778000	-2.303083000
C	-6.570654000	-3.570138000	0.183186000
H	-5.752117000	-4.286893000	0.325906000
C	0.881313000	2.393598000	-2.417329000
C	2.293654000	-3.807626000	1.363895000
C	-2.086670000	-4.282279000	-0.473442000
C	8.195949000	-2.403228000	-1.590584000
H	8.925745000	-1.985964000	-2.296605000
C	-8.331517000	1.981761000	-1.747242000
H	-9.033168000	1.441618000	-2.396185000
C	-0.947381000	1.852559000	2.938016000
C	-2.170289000	3.898489000	1.544921000
C	-7.519073000	-3.142574000	1.184212000
H	-7.569471000	-3.490783000	2.223637000
C	-4.980959000	-1.864558000	1.920112000
C	1.037207000	5.413726000	2.213152000
H	1.399912000	6.055955000	1.402892000
C	0.581447000	-4.454786000	3.864028000
H	1.441576000	-4.321659000	4.532470000
C	-8.071718000	-2.110679000	-0.824228000
H	-8.609153000	-1.531273000	-1.583466000
C	0.437198000	-5.475616000	2.859774000
H	1.175360000	-6.248589000	2.609667000
C	7.161356000	-3.346680000	-1.913864000
H	6.975853000	-3.785042000	-2.902582000
C	-7.246049000	2.793312000	0.135845000
H	-6.971838000	2.976941000	1.181877000
C	8.144190000	1.854888000	-1.119349000
H	8.635050000	1.192004000	-1.840617000
C	7.692618000	3.071981000	0.808950000
H	7.786713000	3.502155000	1.814067000



C	1.753293000	4.319212000	2.803854000
H	2.746391000	3.956590000	2.515802000
C	0.960460000	3.796016000	3.875301000
H	1.252630000	2.980837000	4.549526000
C	7.078257000	-2.930088000	0.372891000
H	6.804851000	-2.981629000	1.433728000
C	-0.870260000	-5.352759000	2.287686000
H	-1.294134000	-6.013182000	1.522503000
C	7.013323000	2.698706000	-1.383870000
H	6.485589000	2.781371000	-2.341836000
C	8.149844000	-2.152165000	-0.182505000
H	8.844275000	-1.517957000	0.379654000
C	0.560449000	-5.183789000	-0.649639000
C	-8.259864000	1.885074000	-0.320860000
H	-8.901869000	1.264924000	0.314420000
C	-0.258203000	4.564539000	3.949143000
H	-1.053029000	4.453013000	4.697454000
C	-0.203911000	5.561590000	2.912965000
H	-0.959904000	6.337131000	2.733701000
C	-1.061349000	5.751936000	-0.954489000
H	-1.382950000	6.231663000	-0.023532000
C	6.470325000	-3.673526000	-0.689163000
H	5.649789000	-4.393067000	-0.578162000
C	-1.806880000	4.780992000	-1.704903000
H	-2.783513000	4.366570000	-1.432986000
C	6.734197000	3.455419000	-0.200089000
H	5.949290000	4.214681000	-0.096122000
C	-1.536492000	-4.249582000	2.913835000
H	-2.555635000	-3.900281000	2.713161000
C	8.557594000	2.079557000	0.232353000
H	9.417083000	1.611976000	0.730200000
C	0.440059000	-2.445778000	-3.166805000
H	1.219653000	-1.675343000	-3.168263000
C	-0.645940000	-3.692771000	3.888062000
H	-0.879766000	-2.864598000	4.569218000
C	0.659368000	-3.855318000	-3.282631000
H	1.635644000	-4.342764000	-3.388520000
C	0.145015000	5.247548000	-2.878715000
H	0.903453000	5.281351000	-3.671000000
C	-0.974382000	-2.213574000	-3.099598000
H	-1.466588000	-1.236475000	-3.016558000
C	0.143850000	6.033815000	-1.673952000
H	0.911778000	6.763885000	-1.386737000
C	-0.628350000	-4.504760000	-3.297293000
H	-0.810869000	-5.578389000	-3.432474000
O	1.094440000	-6.212948000	-0.483507000
C	-1.635859000	-3.481273000	-3.185567000
H	-2.721349000	-3.639291000	-3.212012000
C	-1.071578000	4.472216000	-2.893511000
H	-1.402466000	3.794729000	-3.690361000
C	2.150344000	4.156702000	-0.682448000

Table S13 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{A})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -9917.75074088 Hartree

Atom	x	y	z
Cu	2.418560000	-0.011710000	-0.086388000
Mo	6.233455000	1.298606000	0.835956000
Cu	-2.418591000	0.011593000	0.086844000
Mo	-6.266681000	1.285338000	0.867921000
Mo	-6.233350000	-1.298527000	-0.835990000
Mo	6.266656000	-1.285394000	-0.867805000
Mo	-0.088944000	-3.941556000	-0.962367000
Mo	0.088765000	3.941357000	0.962273000
Mo	-0.126217000	3.119129000	-2.015957000
Mo	0.126435000	-3.119146000	2.015819000
P	-4.585801000	-0.669851000	0.916173000
P	-4.561316000	0.661867000	-0.844697000
P	4.561570000	-0.661820000	0.844949000
P	4.585689000	0.669811000	-0.916018000
P	1.091036000	-1.933240000	-0.074370000
P	1.018103000	1.841491000	-0.226115000
P	-1.090611000	1.932801000	0.074025000
P	-1.017716000	-1.841434000	0.226011000
O	7.185589000	-0.465212000	3.272355000
O	-3.134190000	-4.584018000	-0.464863000
O	1.263445000	-0.527459000	3.382914000
O	3.989238000	2.423762000	2.727512000
O	-3.989289000	-2.422924000	-2.728213000
O	-7.161987000	-0.474448000	3.327778000
O	3.112696000	-4.133577000	1.907057000
O	-7.185533000	0.466019000	-3.271822000
O	-4.015770000	2.528360000	2.671306000
O	-3.112612000	4.133102000	-1.907291000
O	-1.263315000	0.527664000	-3.383426000
O	3.133985000	4.584291000	0.465191000
C	-4.790949000	-1.968291000	-2.015400000
O	7.161951000	0.474805000	-3.327378000
O	-0.799512000	-2.387832000	-3.604342000
C	4.790940000	1.968893000	2.014919000
C	-4.827553000	2.022404000	1.999491000
C	6.804898000	0.144381000	2.354440000
C	-2.014524000	-4.293086000	-0.636697000
O	4.016093000	-2.528573000	-2.671560000
C	-2.012396000	3.740944000	-1.904084000
C	0.843778000	-1.455688000	2.819767000
C	-1.373749000	-4.931793000	2.486838000
C	6.799425000	-0.136635000	-2.402397000
C	-0.843559000	1.455757000	-2.820131000
C	-6.804882000	-0.143878000	-2.354083000
C	2.014370000	4.293215000	0.636933000
C	2.012555000	-3.741211000	1.903965000
C	-2.054847000	-3.702087000	2.780158000
C	8.167289000	2.033470000	-0.388282000
C	-8.166271000	-2.034285000	0.389058000
C	-0.230011000	-5.020651000	3.344127000
C	-6.748521000	3.524555000	0.408528000
C	-6.799441000	0.136783000	2.402677000
C	-8.236070000	1.919635000	-0.363729000
C	1.374026000	4.931790000	-2.486622000
C	-0.571906000	-2.894512000	-2.585131000
C	-7.060852000	-2.876917000	0.747252000
C	7.454799000	3.138041000	1.529529000
C	-8.405425000	-2.189673000	-1.013619000
C	7.164267000	-2.793499000	0.750370000
C	6.621353000	3.561862000	0.429735000
C	4.827771000	-2.022541000	-1.999656000
C	8.405393000	2.190201000	1.014416000
C	2.007974000	-5.049730000	-1.166346000
C	0.046582000	-6.284304000	-1.108042000
C	0.204450000	3.854363000	-4.184179000
C	-8.472323000	2.100180000	1.036395000
C	8.235919000	-1.919533000	0.364000000
C	-7.556776000	3.095024000	1.524328000
C	7.061963000	2.875558000	-0.748066000
C	-0.205136000	-3.853231000	4.184330000
C	0.229887000	5.021302000	-3.343322000
C	6.748399000	-3.524552000	-0.408153000
C	-6.621213000	-3.562177000	-0.431503000
C	-7.164447000	2.793649000	-0.750056000
C	-7.455363000	-3.137209000	-1.530307000
C	1.393592000	-4.951688000	-2.454991000
C	2.054799000	3.702154000	-2.780955000
C	1.340032000	3.038163000	-3.829363000
O	0.799294000	2.388053000	3.604475000
C	7.556746000	-3.095168000	-1.523947000
C	0.170024000	-5.716848000	-2.424230000
C	1.181797000	-5.880026000	-0.335867000
C	-1.340683000	-3.037401000	3.828524000
C	-2.008472000	5.049040000	1.166508000
C	8.472253000	-2.100268000	-1.036089000
C	0.571750000	2.894493000	2.585113000
C	-1.182597000	5.879556000	0.335972000
C	-1.393898000	4.951110000	2.455074000
C	-0.047352000	6.284071000	1.107987000
C	-0.170504000	5.716555000	2.424180000
H	8.755366000	1.416356000	-1.076878000
H	6.658781000	3.002247000	-1.760133000
H	5.813133000	4.302150000	0.480121000
H	7.412969000	3.514985000	2.559208000
H	9.207184000	1.710396000	1.590614000
H	6.766800000	-2.912597000	1.765700000
H	5.984697000	-4.311539000	-0.429701000
H	7.526401000	-3.498756000	-2.543844000
H	9.251520000	-1.603190000	-1.628373000
H	8.809207000	-1.269694000	1.034334000
H	2.958264000	-4.589871000	-0.873708000
H	1.406834000	-6.193495000	0.689316000
H	-0.753935000	-6.957285000	-0.774422000
H	-0.510495000	-5.887767000	-3.267934000
H	1.805468000	-4.418433000	-3.320894000
H	-1.700488000	-5.691380000	1.768343000
H	0.474210000	-5.861059000	3.396756000
H	0.511572000	-3.651464000	4.990399000
H	-1.630873000	-2.093247000	4.306837000
H	-2.980169000	-3.348283000	2.309480000
H	-2.958727000	4.589017000	0.874017000
H	-1.805541000	4.417773000	3.321046000
H	0.510071000	5.887643000	3.267804000



H	0.752949000	6.957259000	0.774274000
H	-1.407819000	6.193019000	-0.689169000
H	1.701234000	5.690934000	-1.767866000
H	2.980293000	3.347949000	-2.310906000
H	1.629832000	2.094208000	-4.308307000
H	-0.512721000	3.653124000	-4.989968000
H	-0.474232000	5.861845000	-3.395149000
H	-5.984744000	4.311473000	0.430156000
H	-6.767052000	2.912877000	-1.765396000
H	-8.809447000	1.269921000	-1.034102000
H	-9.251547000	1.603002000	1.628651000
H	-7.526329000	3.498450000	2.544287000
H	-8.753798000	-1.417813000	1.078693000
H	-9.207562000	-1.709192000	-1.588771000
H	-7.414292000	-3.513172000	-2.560375000
H	-5.813013000	-4.302395000	-0.483105000
H	-6.656914000	-3.004558000	1.758900000

Table S14 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -17496.1721556 Hartree

Atom	x	y	z
As	4.697337000	-0.709216000	0.815565000
As	-4.742736000	0.815952000	0.762416000
As	4.510395000	0.657009000	-1.193021000
As	-4.463508000	-0.784522000	-1.058556000
Cu	2.412735000	0.054981000	0.060072000
Cu	-2.425617000	0.073126000	0.143778000
Mo	-6.407757000	-1.296806000	0.584895000
Mo	6.198462000	-1.446940000	-1.175276000
Mo	-6.280904000	1.192907000	-1.302386000
Mo	6.500273000	1.244505000	0.375070000
Mo	-0.264144000	3.442785000	1.956229000
Mo	0.230244000	3.758286000	-1.099904000
Mo	0.386891000	-3.362693000	1.859139000
Mo	-0.375984000	-3.545016000	-1.192978000
P	1.059013000	1.910808000	0.511604000
P	-1.026321000	1.930562000	0.018438000
P	0.965108000	-1.779489000	-0.042296000
P	-1.096778000	-1.801576000	0.523126000
O	4.596292000	2.636830000	2.439318000
O	6.863887000	0.122210000	-3.828613000
O	-3.270218000	4.240239000	1.429651000
O	-6.815447000	-0.745730000	-3.730451000
O	7.689135000	-0.418797000	2.776501000
O	-1.320958000	0.992999000	3.629129000
O	3.734335000	-2.720228000	-2.637619000
C	6.580225000	-0.407672000	-2.827886000
O	1.152635000	1.632778000	-3.229141000
O	1.533575000	-0.915585000	3.472916000
O	-4.375801000	-2.340249000	2.734858000
O	-3.865598000	2.404046000	-2.899011000
C	7.206845000	0.148126000	1.877630000
O	3.386987000	-4.113615000	1.221810000
O	3.254214000	4.448066000	-0.525190000
C	4.617162000	-2.192517000	-2.080376000
C	5.263326000	2.069473000	1.663003000
C	-7.059405000	-2.952273000	-1.002380000
H	-6.550288000	-3.137865000	-1.955855000
C	-6.903929000	3.430501000	-1.091227000
H	-6.175120000	4.250513000	-1.092611000
O	-3.146018000	-4.642412000	-0.180423000
C	-7.556808000	2.874580000	-2.250630000
H	-7.422230000	3.196798000	-3.290803000
C	-6.577982000	-0.071852000	-2.806764000
O	-7.664832000	0.564402000	2.799295000
C	1.107787000	-1.791865000	2.835305000
C	-7.159129000	-0.076290000	1.965224000
C	-8.589004000	-2.181052000	0.560375000
H	-9.449013000	-1.674930000	1.017982000
C	-4.733561000	1.906471000	-2.290664000
C	-6.757183000	-3.576929000	0.251903000
H	-5.966391000	-4.318052000	0.423542000
C	0.830531000	2.394154000	-2.407306000
C	2.277470000	-3.817908000	1.414013000
C	-2.092190000	-4.244091000	-0.495841000
C	8.334523000	-2.351252000	-1.573738000
H	9.050349000	-1.913645000	-2.281670000
C	-8.479858000	1.873977000	-1.787765000
H	-9.163150000	1.293608000	-2.421311000
C	-0.932209000	1.869120000	2.967653000
C	-2.157755000	3.920138000	1.589368000
C	-7.707164000	-3.100373000	1.227276000
H	-7.784184000	-3.424140000	2.272859000
C	-5.096610000	-1.899329000	1.926254000
C	1.078505000	5.409802000	2.219588000
H	1.445405000	6.043064000	1.404148000
C	0.527512000	-4.447313000	3.892345000
H	1.384626000	-4.328627000	4.567350000
C	-8.195545000	-2.096090000	-0.813346000
H	-8.703716000	-1.520871000	-1.595279000
C	0.373363000	-5.465583000	2.886856000
H	1.099829000	-6.251233000	2.642066000
C	7.333039000	-3.331769000	-1.894121000
H	7.160948000	-3.779051000	-2.881171000
C	-7.424838000	2.774250000	0.071575000
H	-7.164313000	3.001148000	1.112702000
C	8.299780000	1.763202000	-1.134804000
H	8.752854000	1.068765000	-1.850952000
C	7.919772000	3.025654000	0.781658000
H	8.039533000	3.462658000	1.780990000
C	1.784415000	4.309860000	2.812641000
H	2.773335000	3.936206000	2.522920000
C	0.989725000	3.802272000	3.890349000
H	1.274807000	2.987335000	4.567947000
C	7.238859000	-2.911276000	0.392620000
H	6.975348000	-2.975758000	1.455361000
C	-0.928042000	-5.320154000	2.305200000
H	-1.357948000	-5.973279000	1.537096000
C	7.213758000	2.661780000	-1.405586000
H	6.693872000	2.767283000	-2.365674000
C	8.281894000	-2.098223000	-0.165973000
H	8.953897000	-1.439464000	0.394746000
C	0.540400000	-5.194403000	-0.593273000
C	-8.404318000	1.817619000	-0.359220000
H	-9.023633000	1.193818000	0.294422000
C	-0.218978000	4.585935000	3.966321000
H	-1.011173000	4.488004000	4.719319000
C	-0.157643000	5.576724000	2.924322000
H	-0.904608000	6.360921000	2.744947000
C	-1.080548000	5.761089000	-0.925636000
H	-1.390665000	6.241909000	0.008630000
C	6.654727000	-3.676815000	-0.668607000
H	5.860588000	-4.425465000	-0.556345000
C	-1.836799000	4.791849000	-1.667543000
H	-2.812532000	4.380636000	-1.387124000
C	6.978662000	3.444590000	-0.227968000
H	6.238610000	4.248645000	-0.129878000
C	-1.580079000	-4.205942000	2.926444000
H	-2.592572000	-3.840010000	2.720097000
C	8.728781000	1.981551000	0.213378000
H	9.566580000	1.478400000	0.713432000
C	0.551671000	-2.493668000	-3.141341000
H	1.350490000	-1.743395000	-3.130081000
C	-0.686528000	-3.664266000	3.906636000
H	-0.910966000	-2.831860000	4.585819000
C	0.738865000	-3.908916000	-3.232538000
H	1.705500000	-4.421365000	-3.303600000
C	0.103303000	5.253714000	-2.863040000
H	0.852719000	5.285941000	-3.663937000
C	-0.858073000	-2.225339000	-3.117382000
H	-1.325574000	-1.234147000	-3.063646000
C	0.117293000	6.040287000	-1.658404000
H	0.889841000	6.768802000	-1.379772000
C	-0.563907000	-4.526537000	-3.274721000
H	-0.769172000	-5.597142000	-3.401064000
O	1.049509000	-6.233300000	-0.409159000
C	-1.548640000	-3.477178000	-3.206105000
H	-2.636497000	-3.609523000	-3.262954000
C	-1.115232000	4.481234000	-2.863974000
H	-1.457739000	3.805165000	-3.657163000
C	2.136524000	4.155206000	-0.70205000

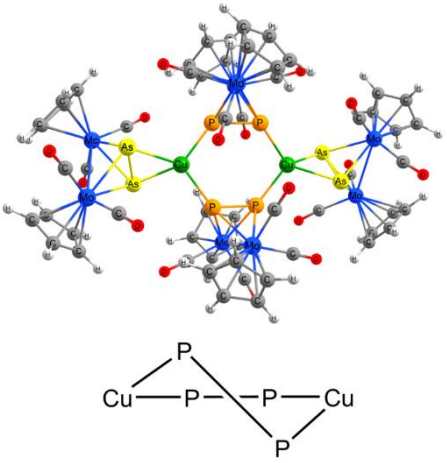


Table S15 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{B})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -17496.1637615 Hartree

Atom	x	y	z
Cu	2.406941000	-0.004499000	-0.136321000
Mo	6.350176000	1.306952000	0.842625000
Cu	-2.406780000	0.004806000	0.136845000

Mo	-6.373026000	1.287838000	0.904651000
Mo	-6.349376000	-1.305880000	-0.844184000
Mo	6.372775000	-1.289228000	-0.902232000
Mo	-0.150161000	-3.894251000	-1.032917000
Mo	0.151965000	3.894414000	1.031926000
Mo	-0.220730000	3.225076000	-1.967218000
Mo	0.218349000	-3.225227000	1.966780000
As	-4.630538000	-0.760634000	1.024666000
As	-4.587647000	0.725514000	-0.911706000
As	4.587641000	-0.723636000	0.913428000
As	4.630815000	0.759525000	-1.025228000
P	1.087321000	-1.938688000	-0.107527000
P	1.005575000	1.853009000	-0.303463000
P	-1.086566000	1.938632000	0.108419000
P	-1.005353000	-1.852849000	0.301446000
O	7.266966000	-0.469937000	3.280141000
O	-3.170951000	-4.546024000	-0.409107000
O	1.420433000	-0.713156000	3.423619000
O	4.127046000	2.508084000	2.709527000
O	-4.125228000	-2.502650000	-2.712752000
O	-7.258580000	-0.454364000	3.378088000
O	3.195918000	-4.221188000	1.655438000
O	-7.267065000	0.474398000	-3.278906000
O	-4.119351000	2.586378000	2.661756000
O	-3.197741000	4.221092000	-1.651056000
O	-1.425751000	0.712892000	-3.421457000
O	3.171294000	4.547774000	0.402598000
C	-4.911903000	-2.011720000	-2.004970000
O	7.259554000	0.449595000	-3.377606000
O	-0.982894000	-2.195412000	-3.546121000
C	4.913257000	2.015497000	2.002373000
C	-4.927446000	2.049776000	2.006735000
C	6.887831000	0.140951000	2.360563000
C	-2.059609000	-4.254677000	-0.625933000
O	4.119260000	-2.589049000	-2.658592000
C	-2.097706000	3.834017000	-1.725132000
C	0.973342000	-1.606890000	2.826970000
C	-1.252812000	-5.068614000	2.413521000
C	6.887380000	-0.147934000	-2.445564000
C	-0.977344000	1.606664000	-2.825839000
C	-6.887653000	-0.137781000	-2.360304000
C	2.060489000	4.255930000	0.621444000
C	2.095755000	-3.834175000	1.727750000
C	-1.919986000	-3.861023000	2.811241000
C	8.303067000	1.988957000	-0.381668000
C	-8.301052000	-1.991055000	0.380150000
C	-0.065281000	-5.199418000	3.203224000
C	-6.899730000	3.517690000	0.468021000
C	-6.886816000	0.144433000	2.446704000
C	-8.352639000	1.890889000	-0.326080000
C	1.248789000	5.069157000	-2.416692000
C	-0.708138000	-2.761927000	-2.570824000
C	-7.225324000	-2.877378000	0.721516000
C	7.634898000	3.091273000	1.555080000
C	-8.547861000	-2.115336000	-1.024644000
C	7.298345000	-2.791018000	0.705488000
C	6.814050000	3.558138000	0.464690000
C	4.927282000	-2.051973000	-2.003868000
C	8.548804000	2.116311000	1.023035000
C	1.929506000	-4.990420000	-1.423001000
C	-0.028895000	-6.226204000	-1.294850000
C	-0.007200000	4.079846000	-4.106224000
C	-8.593281000	2.050261000	1.075954000
C	8.351949000	-1.891484000	0.329559000
C	-7.700531000	3.060149000	1.576717000
C	7.227780000	2.874746000	-0.725833000
C	0.001505000	-4.080743000	4.105142000
C	0.060152000	5.198948000	-3.204886000
C	6.898220000	-3.518716000	-0.462147000
C	-6.812343000	-3.558001000	-0.470862000
C	-7.299537000	2.791559000	-0.700699000
C	-7.634145000	-3.088932000	-1.559568000
C	1.232496000	-4.833252000	-2.662807000
C	1.916121000	3.861780000	-2.814779000
C	1.147971000	3.251823000	-3.858122000
O	0.990795000	2.196549000	3.543713000
C	7.699346000	-3.063307000	-1.571491000
C	0.011025000	-5.598715000	-2.588994000
C	1.155860000	-5.857899000	-0.580731000
C	-1.152864000	-3.251967000	3.855863000
C	-1.927708000	4.988771000	1.427649000
C	8.592593000	-2.053128000	-1.072213000
C	0.713593000	2.762622000	2.568854000
C	-1.157330000	5.856603000	0.582789000
C	-1.226882000	4.832754000	2.665463000
C	0.029220000	6.226270000	1.293239000
C	-0.006345000	5.599308000	2.587784000
H	8.868168000	1.363215000	-1.081480000
H	6.833111000	3.037968000	-1.736097000
H	6.034704000	4.328017000	0.526973000
H	7.608994000	3.454769000	2.590023000
H	9.335640000	1.601970000	1.589937000
H	6.908757000	-2.933921000	1.720845000
H	6.149605000	-4.319964000	-0.492693000
H	7.677912000	-3.457019000	-2.595397000
H	9.362938000	-1.535600000	-1.658592000
H	8.910817000	-1.237408000	1.007634000
H	2.899486000	-4.544521000	-1.177077000
H	1.447466000	-6.220373000	0.410942000
H	-0.807365000	-6.915018000	-0.941976000
H	-0.722884000	-5.730217000	-3.394133000
H	1.590211000	-4.263254000	-3.529458000
H	-1.617002000	-5.789205000	1.673272000
H	0.642073000	-6.038238000	3.171919000
H	0.758827000	-3.921047000	4.883024000
H	-1.419254000	-2.338068000	4.402034000
H	-2.870504000	-3.488654000	2.410382000
H	-2.898010000	4.541851000	1.184830000
H	-1.581505000	4.262830000	3.533439000
H	0.729778000	5.731836000	3.390731000
H	0.805981000	6.915707000	0.937835000
H	-1.452208000	6.218438000	-0.408145000
H	1.613549000	5.790316000	-1.677274000
H	2.867386000	3.490177000	-2.414994000
H	1.414137000	2.337847000	-4.404271000
H	-0.765460000	3.919401000	-4.883038000
H	-0.647651000	6.037366000	-3.172942000
H	-6.151521000	4.319270000	0.499780000
H	-6.910069000	2.936198000	-1.715858000
H	-8.911228000	1.237584000	-1.005131000
H	-9.363311000	1.531426000	1.661590000
H	-7.679224000	3.452312000	2.601221000
H	-8.865679000	-1.366954000	1.081801000
H	-9.335293000	-1.599962000	-1.589776000
H	-7.608961000	-3.450150000	-2.595326000
H	-6.032865000	-4.327553000	-0.535417000
H	-6.829849000	-3.042802000	1.731108000

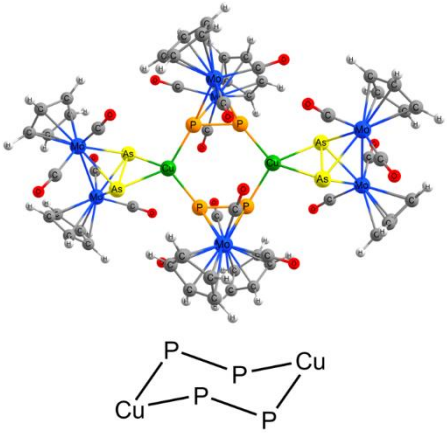
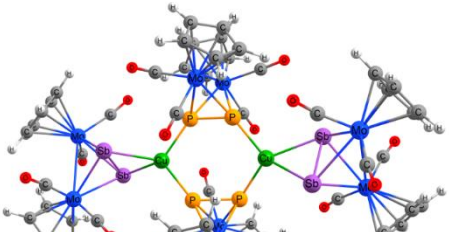


Table S16 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the twisted boat conformation calculated at the BP86/def2-SVP level of theory. E° = -9514.19793771 Hartree

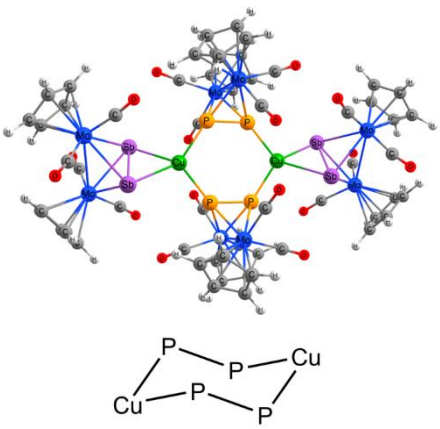
Atom	x	y	z
Sb	-4.821893000	-0.732441000	-1.063872000
Sb	4.877952000	0.863785000	-0.998767000
Sb	-4.622109000	0.737800000	1.331139000
Sb	4.583711000	-0.880448000	1.198884000
Cu	-2.425145000	0.068409000	-0.092225000
Cu	2.446057000	0.051557000	-0.165197000
Mo	6.680969000	-1.368131000	-0.595274000
Mo	-6.458585000	-1.491220000	1.084164000
Mo	6.541765000	1.255481000	1.230035000
Mo	-6.752566000	1.320191000	-0.400238000
Mo	0.222898000	3.489310000	-1.925701000
Mo	-0.166165000	3.720459000	1.154671000
Mo	-0.333284000	-3.404016000	-1.836129000
Mo	0.271693000	-3.529175000	1.252877000
P	-1.039958000	1.914901000	-0.479211000
P	1.061453000	1.928239000	-0.055531000
P	-0.996595000	-1.780740000	0.004597000
P	1.088740000	-1.819964000	-0.460866000
O	-4.837878000	2.901089000	-2.311615000
O	-7.153180000	-0.062982000	3.803792000
O	3.233538000	4.318687000	-1.479537000
O	7.127280000	-0.536668000	3.752313000
O	-7.919066000	-0.208312000	-2.894734000
O	1.272200000	1.094821000	-3.681906000
O	-4.028401000	-2.912704000	2.462743000
C	-6.836614000	-0.527692000	2.777828000
O	-0.950702000	1.515400000	3.257100000
O	-1.440847000	-0.994946000	-3.532273000
O	4.653417000	-2.626846000	-2.628464000
O	4.164453000	2.606119000	2.766268000
C	-7.421753000	0.299104000	-1.965688000
O	-3.354173000	-4.171946000	-1.324199000
O	-3.224224000	4.366609000	0.736458000
C	-4.890373000	-2.315429000	1.938930000
C	-5.500490000	2.248610000	-1.597405000
C	7.390966000	-2.943636000	1.051988000
H	6.891167000	-3.145363000	2.007193000



C	7.202695000	3.471388000	0.956056000
H	6.491337000	4.306726000	0.960656000
O	3.130244000	-4.568742000	0.448442000
C	7.872353000	2.924826000	2.108502000
H	7.770113000	3.269515000	3.145058000
C	6.849145000	0.069851000	2.791011000
O	7.910121000	0.365917000	-2.919694000
C	-1.029189000	-1.856754000	-2.865697000
C	7.391745000	-0.215272000	-2.047065000
C	8.899478000	-2.131135000	-0.510643000
H	9.740318000	-1.594635000	-0.969106000
C	5.008003000	2.040575000	2.178266000
C	7.141168000	-3.613936000	-0.191844000
H	6.398863000	-4.405244000	-0.356227000
C	-0.681578000	2.309565000	2.446286000
C	-2.238587000	-3.872871000	-1.470945000
C	2.048632000	-4.191523000	0.685567000
C	-8.630192000	-2.320775000	1.416456000
H	-9.346431000	-1.872433000	2.117158000
C	8.762772000	1.895392000	1.641395000
H	9.451383000	1.314881000	2.268959000
C	0.886020000	1.950577000	-2.992842000
C	2.119967000	3.988320000	-1.609436000
C	8.078188000	-3.114595000	-1.165861000
H	8.187631000	-3.461792000	-2.200899000
C	5.364072000	-2.091562000	-1.865483000
C	-1.178127000	5.425070000	-2.094405000
H	-1.542324000	6.021628000	-1.250535000
C	-0.371216000	-4.538126000	-3.845653000
H	-1.205301000	-4.456611000	-4.554194000
C	8.481723000	-2.032069000	0.854669000
H	8.946986000	-1.413085000	1.629266000
C	-0.230414000	-5.526787000	-2.808867000
H	-0.946660000	-6.323453000	-2.569703000
C	-7.671103000	-3.343170000	1.740532000
H	-7.535438000	-3.813537000	2.722425000
C	7.682852000	2.784605000	-0.208574000
H	7.417646000	3.011097000	-1.248565000
C	-8.571498000	1.714219000	1.125411000
H	-8.995207000	0.983850000	1.823200000
C	-8.245125000	3.044801000	-0.756261000
H	-8.383007000	3.504040000	-1.743117000
C	-1.870390000	4.327225000	-2.707294000
H	-2.848051000	3.927409000	-2.412141000
C	-1.087294000	3.875201000	-3.817976000
H	-1.366676000	3.075677000	-4.516093000
C	-7.516924000	-2.888097000	-0.537601000
H	-7.249798000	-2.958055000	-1.599140000
C	1.046128000	-5.335109000	-2.185068000
H	1.463818000	-5.957336000	-1.385154000
C	-7.527951000	2.653332000	1.423945000
H	-7.029732000	2.769102000	2.394247000
C	-8.540477000	-2.046832000	0.014761000
H	-9.178161000	-1.358491000	-0.550269000
C	-0.555787000	-5.206059000	0.607100000
C	8.651771000	1.815021000	0.216672000
H	9.242499000	1.169254000	-0.442001000
C	0.098635000	4.692263000	-3.896335000
H	0.874623000	4.638947000	-4.670396000
C	0.036920000	5.647107000	-2.820974000
H	0.767038000	6.445184000	-2.633731000
C	1.108169000	5.747006000	0.979948000
H	1.379791000	6.253050000	0.047114000
C	-6.980818000	-3.690293000	0.524053000
H	-6.213883000	-4.467678000	0.416160000
C	1.904514000	4.775991000	1.675980000
H	2.878435000	4.387025000	1.359702000
C	-7.325741000	3.476018000	0.265897000
H	-6.627113000	4.318900000	0.191642000
C	1.694773000	-4.222358000	-2.811798000
H	2.694686000	-3.833342000	-2.584680000
C	-9.007055000	1.949360000	-0.217548000
H	-9.823005000	1.425758000	-0.732415000
C	-0.849761000	-2.519710000	3.124041000
H	-1.681393000	-1.809822000	3.049947000
C	0.823584000	-3.726636000	-3.835820000
H	1.052663000	-2.906564000	-4.528427000
C	-0.975520000	-3.940484000	3.210211000
H	-1.919813000	-4.497785000	3.212988000
C	-0.002256000	5.180677000	2.944190000
H	-0.724671000	5.184298000	3.770155000
C	0.544266000	-2.183159000	3.199364000
H	0.962178000	-1.168958000	3.175210000
C	-0.068818000	5.991759000	1.757560000
H	-0.861421000	6.713272000	1.520089000
C	0.348881000	-4.495016000	3.348211000
H	0.594564000	-5.554439000	3.495190000
O	-1.022709000	-6.262294000	0.408349000
C	1.285768000	-3.399816000	3.346194000
H	2.371555000	-3.480993000	3.483844000
C	1.228117000	4.429406000	2.888493000
H	1.609765000	3.745534000	3.656801000
C	-2.093542000	4.092969000	0.851616000

Table S17 Cartesian coordinates of the gas-phase optimized geometry of $[(\eta^2\text{-}\mathbf{C})_2(\eta^{1:1}\text{-}\mathbf{A})_2Cu_2]^{2+}$ in the chair conformation calculated at the BP86/def2-SVP level of theory. E° = -9514.18841075 Hartree

Atom	x	y	z
Cu	2.394163000	-0.021523000	-0.212394000
Mo	6.606594000	1.349698000	0.778476000
Cu	-2.392926000	0.028658000	0.214765000
Mo	-6.605547000	1.367728000	0.891197000
Mo	-6.589786000	-1.340574000	-0.811306000
Mo	6.593105000	-1.390963000	-0.870547000
Mo	-0.303962000	-3.771568000	-1.166674000
Mo	0.322594000	3.772583000	1.168696000
Mo	-0.305584000	3.432509000	-1.838961000
Mo	0.281181000	-3.424844000	1.847562000
Sb	-4.745704000	-0.820842000	1.237811000
Sb	-4.662910000	0.800135000	-1.067844000
Sb	4.662663000	-0.770421000	1.084687000
Sb	4.748147000	0.805690000	-1.251633000
P	1.052500000	-1.948913000	-0.142769000
P	1.008383000	1.858326000	-0.427618000
P	-1.044791000	1.951129000	0.159403000
P	-1.008990000	-1.852894000	0.414447000
O	7.528062000	-0.314310000	3.286288000
O	-3.263700000	-4.469098000	-0.335421000
O	1.523901000	-1.090182000	3.542679000
O	4.476183000	2.756829000	2.605245000
O	-4.436237000	-2.685478000	-2.658178000
O	-7.540318000	-0.230557000	3.437602000
O	3.229909000	-4.373216000	1.255368000
O	-7.519841000	0.366169000	-3.287116000
O	-4.385084000	2.803001000	2.576314000
O	-3.244526000	4.378702000	-1.198307000
O	-1.580112000	1.100581000	-3.513951000
O	3.257756000	4.502717000	0.278780000
C	-5.181861000	-2.125554000	-1.952911000
O	7.537065000	0.155030000	-3.445642000
O	-1.367597000	-1.813727000	-3.386768000
C	5.211711000	2.173312000	1.908606000
C	-5.170469000	2.199720000	1.947475000
C	7.125365000	0.244679000	2.340738000
C	-2.173700000	-4.164359000	-0.627113000
O	4.361703000	-2.831499000	-2.536279000
C	-2.154620000	4.002574000	-1.392620000
C	1.066071000	-1.908076000	2.853059000
C	-1.147333000	-5.328826000	2.177319000
C	7.122364000	-0.354799000	-2.477054000
C	-1.107838000	1.917391000	-2.832651000
C	-7.114865000	-0.208647000	-2.352087000
C	2.176345000	4.188118000	0.590509000
C	2.137410000	-3.996325000	1.432435000
C	-1.796649000	-4.182107000	2.747096000
C	8.564315000	1.891981000	-0.507321000
C	-8.546212000	-1.929127000	0.456707000
C	0.088208000	-5.528835000	2.872708000
C	-7.164218000	3.571161000	0.385536000
C	-7.128071000	0.299483000	2.478825000
C	-8.580195000	1.897586000	-0.379807000
C	1.112335000	5.341152000	-2.192481000
C	-0.993633000	-2.486918000	-2.517133000
C	-7.505069000	-2.857964000	0.792670000
C	7.990894000	3.083023000	1.408711000
C	-8.817663000	-2.056647000	-0.943115000
C	7.517399000	-2.810248000	0.813029000
C	7.175450000	3.559911000	0.320451000
C	5.150963000	-2.226130000	-1.914199000
C	8.841937000	2.045459000	0.888660000
C	1.720000000	-4.824338000	-1.868535000
C	-0.230664000	-6.064658000	-1.659493000
C	-0.265128000	4.524095000	-3.879084000
C	-8.837921000	2.090410000	1.014424000
C	8.564993000	-1.916947000	0.406763000
C	-7.968596000	3.130318000	1.496969000
C	7.531655000	2.824445000	-0.859061000
C	0.203829000	-4.515631000	3.887052000
C	-0.135301000	5.537624000	-2.866802000



C	7.132431000	-3.590315000	-0.327479000
C	-7.137397000	-3.565299000	-0.400499000
C	-7.540209000	2.807345000	-0.768849000
C	-7.954313000	-3.074574000	-1.481458000
C	0.900314000	-4.549487000	-3.009499000
C	1.755064000	4.196118000	-2.772922000
C	0.912515000	3.692753000	-3.815195000
O	1.473464000	1.820492000	3.349275000
C	7.938985000	-3.176164000	-1.447561000
C	-0.315016000	-5.317796000	-2.886385000
C	1.024898000	-5.766036000	-1.038232000
C	-0.970249000	-3.681075000	3.803307000
C	-1.697257000	4.788771000	1.938192000
C	8.818549000	-2.136079000	-0.984362000
C	1.063488000	2.491478000	2.494123000
C	-1.045025000	5.743484000	1.088482000
C	-0.836104000	4.525513000	3.051140000
C	0.225262000	6.061864000	1.669030000
C	0.361403000	5.314509000	2.891170000
H	9.083388000	1.220026000	-1.199406000
H	7.142539000	2.995203000	-1.870220000
H	6.442868000	4.375080000	0.373589000
H	8.004431000	3.477578000	2.432373000
H	9.613543000	1.509257000	1.456119000
H	7.134791000	-2.924511000	1.834596000
H	6.388840000	-4.397130000	-0.331113000
H	7.929488000	-3.613350000	-2.453794000
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H	9.111353000	-1.229956000	1.061595000
H	2.717537000	-4.405792000	-1.691586000
H	1.410401000	-6.219599000	-0.118526000
H	-0.975714000	-6.784935000	-1.297464000
H	-1.127717000	-5.371141000	-3.621785000
H	1.173376000	-3.902273000	-3.852604000
H	-1.553726000	-5.971115000	1.388760000
H	0.797960000	-6.349225000	2.704898000
H	1.006879000	-4.432554000	4.630211000
H	-1.208770000	-2.838321000	4.464606000
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H	-1.070253000	3.872165000	3.901234000
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H	0.945492000	6.795800000	1.284976000
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H	1.530362000	5.985041000	-1.411366000
H	2.738199000	3.800609000	-2.490885000
H	1.142234000	2.850740000	-4.480550000
H	-1.080271000	4.438844000	-4.608715000
H	-0.844326000	6.355989000	-2.686549000
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H	-7.117570000	-3.045670000	1.801438000

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