SUPPORTING INFORMATION

Facile synthesis of one-dimensional organometallic-organic hybrid polymers based on a diphosphorus complex and flexible bipyridyl linkers

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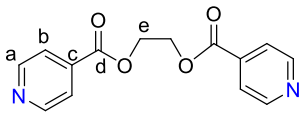
General

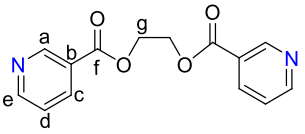
All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. The compounds 1,3-Di(4-pyridyl)ethane (**1**), 1,3-Di(4-pyridyl)propane (**2**) and $Cu(CH_3CN)_4BF_4$ (**B**) were purchased from TCI (**2**) and Sigma-Aldrich (**1**,**4**) and used as received without further purification. The organic linkers edcp-para **3**[1] and **4** as well as the ligand complex $[CpMo_2(CO)_4(\eta^2\text{-}P_2)]$ (**A**)[2,3] were synthesized according to modified literature procedures. Solvents were freshly distilled under argon from CaH_2 (CH_2Cl_2, CH_3CN) and from Na/K alloy (n-pentane). IR spectra were recorded on Varian FTS-800 spectrometer. ^1H, ^{13}C, ^{31}P and ^{19}F NMR spectra were recorded on a Bruker Avance 300 or Avance 400 spectrometers. ^1H and ^{13}C NMR chemical shifts were reported in parts per million (ppm) relative to Me_4Si as external standard. ^{31}P NMR chemical shifts were expressed in ppm relative to external 85% H_3PO_4 and were decoupled from the proton. ^{19}F NMR chemical shifts were reported relative to $CFCl_3$. For the ESI-MS a Finnignan Thermoquest TSQ 7000 mass spectrometer was used. Elemental analyses were performed by the microanalytical laboratory of the Universität Regensburg.

ligand 3



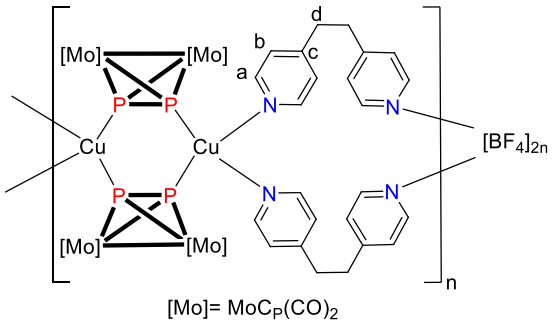
To a stirred suspension of isonicotinoyl chloride hydrochloride (0.513 g, 2.88 mmol) in dry dichloromethane (50 mL) at room temperature was added dropwise triethylamine (0.82 mL, 5.88 mmol). With further stirring at room temperature was added ethylene glycol (0.085 g, 1.37 mmol) and the mixture was refluxed for 12 h. After, the slightly yellowish clear reaction mixture was washed with saturated sodium bicarbonate solution (20 mL), the organic phase was dried over anhydrous K_2CO_3 and filtered. The solvent was then removed under reduced pressure and the product was obtained as white powder (**3**, 0.146 g, 0.54 mmol, 39%). ^1H NMR (300 MHz, CD_3Cl): δ = 4.71 (s, 4H, H_e), 7.85 (m, 4H, H_b), 8.38 (m, 4H, H_a). $^{13}C\{^1H\}$ NMR (75.47 MHz, CD_3Cl): δ = 63.4 (s, C_e), 123.1 (s, C_b), 137.1 (s, C_c), 150.6 (s, C_a), 164.9 (s, C_d).

ligand 4



To a stirred suspension of isonicotinoyl chloride hydrochloride (1.32 g, 7.42 mmol) in dry dichloromethane (50 mL) in an ice path, was added dropwise triethylamine (1.90 mL, 13.62 mmol). The reaction mixture was then warmed to room temperature, ethylene glycol (0.223 g, 3.59 mmol) was added and the mixture was refluxed for 12 h. After cooling, the slightly yellowish clear reaction mixture was washed with saturated $NaHCO_3$ solution (2×20 mL), the organic phase was dried over anhydrous K_2CO_3 and filtered. The solvent was then removed on a rotatory evaporator and the product was obtained as white powder (**4**, 0.863 g, 3.17 mmol, 88%). ^{1}H NMR (300 MHz, CD_3Cl): δ = 4.70 (s, 4H, H_g), 7.39 (s, 2H, H_d), 8.29 (m, 2H, H_c), 8.77 (m, 2H, H_e), 9.22 (m, 2H, H_a). ^{13}C{^{1}H} NMR (75.47 MHz, CD_3Cl): δ = 63.1 (s, C_g), 123.5 (s; C_d), 125.7 (s; C_b), 137.3 (s; C_c), 151.1 (s; C_a), 153.8 (s; C_e), 165.1 (s; C_f).

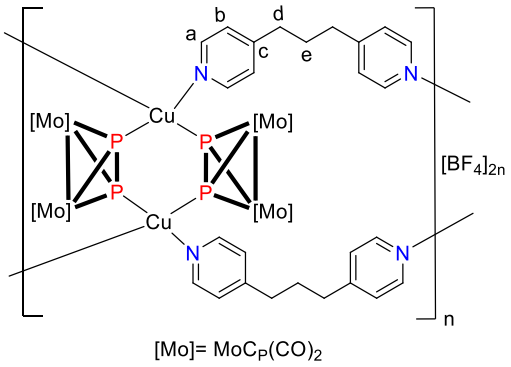
Complex 5



A solution of equimolar amounts of $Cu(CH_3CN)_4BF_4$ (**B**, 0.016 g, 0.05 mmol), $[Cp_2Mo_2(CO)_4(\eta^2\text{-}P_2)]$ (**A**, 0.025 g, 0.05 mmol), and 1,3-Di(4-pyridyl)ethane (**1**, 0.009 g, 0.05 mmol) in CH_2Cl_2 (10 ml) and CH_3CN (5 ml) was stirred for 3 hours at room temperature. The red mixture was filtered off using a teflon capillary to remove any suspended particles and the obtained solution was layered with the same amount of pentane or toluene and kept at room temperature. After five days orange crystals of **5** × 0.6 CH_3CN × 1.98 CH_2Cl_2 were obtained. The crystals were isolated by decanting the mother liquor, washing twice with CH_2Cl_2 (2×3ml) and drying under reduced pressure. The resulting filtrate was isolated, concentrated to about third of its volume and stored in a fridge at -4°C. In two days smaller crystals of the product could be obtained and were isolated using the same procedure used above. All the crystals were collected and the yield was calculated (**5**, 0.039 g, 0.024 mmol, 94%). ^{1}H NMR (300 MHz, CD_3CN): δ = 2.99 (s, 4H, H_d), 5.31 (s, 10H, H_{Cp}), 7.21 (dd, 4H, $^2J_{HH}$ = 4.6 Hz, $^3J_{HH}$ = 1.6 Hz, H_b), 8.38 (dd, 4H, $^2J_{HH}$ = 4.6 Hz, $^3J_{HH}$ = 1.6 Hz, H_a). ^{13}C{^{1}H} NMR (75.47 MHz, CD_3CN): δ = 34.5 (s, C_d), 86.2 (s, C_{Cp}), 124.1 (s, C_b), 149.2 (s, C_a), 150.5 (s, C_c), 225.0 (s, C_{CO}). ^{31}P{^{1}H} NMR (121.49 MHz, CD_3CN): δ = -51.5 (s, $\omega_{1/2}$= 22.4 Hz). ^{19}F{^{1}H} NMR (282.40 MHz, CD_3CN): δ = -150.6 (s, $^{11}BF_4$), -150.5 (s, $^{10}BF_4$). ESI-MS (CH_3CN): m/z (%) = 1246.7.0 (1) $[Cu\{Cp_2Mo_2(CO)_4P_2\}_2(C_{12}H_{12}N_2)]^+$, 1056.6 (9) $[Cu\{Cp_2Mo_2(CO)_4P_2\}_2]^+$, 599.7 (100) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)]^+$. Elemental analysis, calcd. (%) for $C_{52}H_{44}B_2Cu_2F_8Mo_4N_4O_8P_4$ × 0.6 CH_3CN × 1.98 CH_2Cl_2: C 35.74, H 2.71, N 3.48; found: C 37.02, H 2.94, N 3.46. IR (KBr): $\tilde{\nu}$/cm^{-1} = 2952 (w; CH), 2925 (w; CH), 2858 (vw; CH), 1969 (vs; CO), 1920 (vs; CO), 1614 (s; CC, CN), 1499

(vw; CC, CN), 1455 (m; CC, CN), 1422 (m; CC), 1384 (w), 1308 (w), 1242 (m), 1118 (m), 1082 (s; BF), 1034 (m; BF), 942 (vw), 825 (m), 669 (vw), 599 (m, CC), 560 (w; δ(BF)), 524 (m; δ(MoCO), δ(CMoC)), 497(m; δ(BF)).

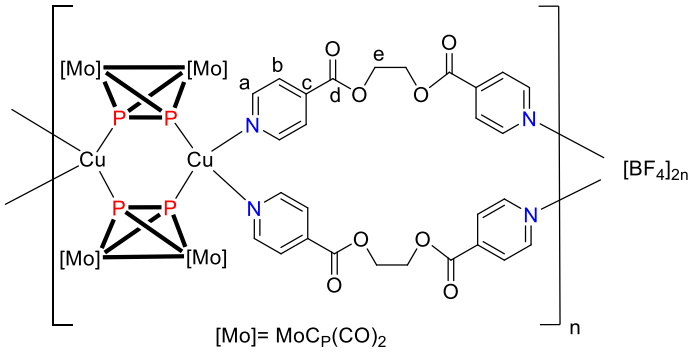
Complex 6



[Mo]= $MoC_P(CO)_2$

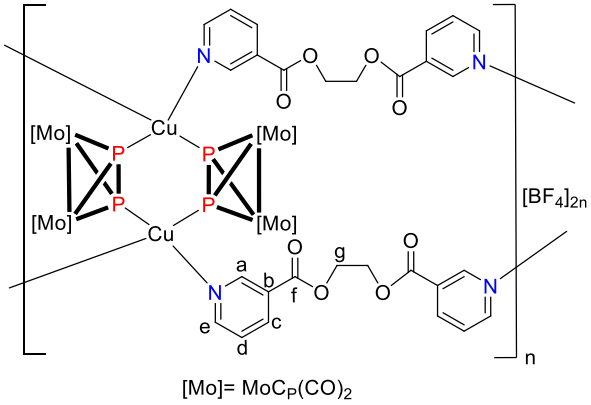
A solution of equimolar amounts of $Cu(CH_3CN)_4BF_4$ (**B**, 0.016 g, 0.05 mmol), $[Cp_2Mo_2(CO)_4(\eta^2\text{-}P_2)]$ (**A**, 0.025 g, 0.05 mmol), and 1,3-Di(4-pyridyl)propane (**2**, 0.010 g, 0.05 mmol) in CH_2Cl_2 (10 ml) and CH_3CN (5 ml) was stirred for 3 hours at room temperature. The red crude mixture was filtered off using a teflon capillary to remove any suspended particles. The obtained solution was layered with the same amount of pentane and kept at room temperature. After four days red crystals of **6** × 0.5 CH_3CN × 0.2 CH_2Cl_2 were obtained. The crystals were isolated by decanting the mother liquor, washed twice with CH_2Cl_2 (2×3ml) and dried under reduced pressure. The resulting filtrate was isolated, concentrated to about third of its volume and stored in a fridge at -4°C. In two days smaller crystals of the product could be obtained and were isolated using the same procedure used above. All the crystals were collected and the yield was calculated (**6**, 0.034 g, 0.020 mmol, 80%). ^{1}H NMR (300 MHz, CD_3CN): δ = 1.99 (m, 2H, H_e), 2.67 (t, 4H, $^2J_{HH}$ = 7.7 Hz, H_d), 5.31 (s, 10H, H_{Cp}), 7.23 (dd, 4H, $^2J_{HH}$ = 4.7 Hz, $^3J_{HH}$ = 1.6 Hz, H_b), 8.40 (dd, 4H, $^2J_{HH}$ = 4.5 Hz, $^3J_{HH}$ = 1.6 Hz, H_a). ^{13}C{^{1}H} NMR (75.47 MHz, CD_3CN): δ = 30.0 (s, C_e), 33.7 (s, C_d), 86.2 (s, C_{Cp}), 124.0 (s, C_b), 149.2 (s, C_a), 151.5 (s, C_c), 225.1 (s, C_{CO}). ^{31}P{^{1}H} NMR (121.49 MHz, CD_3CN): δ = -53.4 (s, $\omega_{1/2}$= 23.6 Hz). ^{19}F{^{1}H} NMR (282.40 MHz, CD_3CN): δ = -150.6 (s, $^{11}BF_4$), -150.5 (s, $^{10}BF_4$). ESI-MS (CH_3CN): m/z (%) = 1056.6 (9) $[Cu\{Cp_2Mo_2(CO)_4P_2\}_2]^+$, 903.0 (10) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(C_{13}H_{14}N_2)_2]^+$, 599.7 (100) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)]^+$. Elemental analysis, calcd. (%) for $C_{54}H_{48}B_2Cu_2F_8Mo_4N_4O_8P_4$ × 0.5 CH_3CN × 0.2 CH_2Cl_2: C 38.39, H 2.96, N 3.97; found: C 38.33, H 2.99, N 3.34. IR (KBr): $\tilde{\nu}$/cm^{-1} = 3112 (w; CH), 2925 (w; CH), 2856 (vw; CH), 1979 (vs; CO), 1920 (vs; CO), 1711 (s; CC, CN), 1613 (s; CC, CN), 1422 (m; CC, CN), 1361 (m), 1304 (m), 1242 (s), 1155 (m), 1124 (m; BF), 1052 (s; BF), 1038 (s; BF), 823 (m), 609 (vw), 561 (m, CC), 519 (m; δ(BF)), 498 (m; δ(MoCO), δ(CMoC)), 450 (m; δ(BF)).

Complex 7



A solution of equimolar amounts of $Cu(CH_3CN)_4BF_4$ (**B**, 0.016 g, 0.05 mmol), $[Cp_2Mo_2(CO)_4(\eta^2\text{-}P_2)]$ (**A**, 0.025 g, 0.05 mmol), and edcp-para (**3**, 0.014 g, 0.05 mmol) in CH_2Cl_2 and CH_3CN was stirred for 3 hours at room temperature. The orange-red crude mixture was filtered off using a teflon capillary to remove any suspended particles. The obtained solution was layered with the same amount of pentane or toluene and kept at room temperature. After two days orange crystals of **7** × 0.1 CH_2Cl_2 were obtained. The crystals were isolated by decanting the mother liquor, washed twice with CH_2Cl_2 (2×3ml) and dried under reduced pressure. The resulting filtrate was isolated, concentrated to about third of its volume and stored in a fridge at -4°C. In two days smaller crystals of the product could be obtained and were isolated using the same procedure used above. All the crystals were collected and the yield was calculated (**7**, 0.031 g, 0.017 mmol, 67%). ^{1}H NMR (400 MHz, CD_3CN): δ = 4.68 (s, 4H, H_e), 5.32 (s, 10H, C_5H_5), 7.85 (m, 4H, H_b), 8.75 (m, 4H, H_a). $^{13}C\{^1H\}$ NMR (100.61 MHz, CD_3CN): δ = 64.3 (s, C_e), 87.5 (s, C_{Cp}), 123.8 (s, C_b), 138.3 (s, C_a), 151.7 (s, C_c), 165.9 (s, C_d), 226.5 (s, C_{CO}). $^{31}P\{^1H\}$ NMR (161.98 MHz, CD_3CN): δ = -48.2 (s, $\omega_{1/2}$= 11.8 Hz). $^{19}F\{^1H\}$ NMR (376.50 MHz, CD_3CN): δ = -151.9 (s, $^{11}BF_4$), -151.8 (s, $^{10}BF_4$). ESI-MS (CH_3CN): m/z (%) = 1478.5 (1) $[Cu_2\{Cp_2Mo_2(CO)_4P_2\}_2(C_{14}H_{12}N_2O_4)(BF_4)]^+$, 1252.7 (1) $[Cu_2\{Cp_2Mo_2(CO)_4P_2\}(C_{14}H_{12}N_2O_4)_2)(BF_4)]^+$, 1056.6 (16) $[Cu\{Cp_2Mo_2(CO)_4P_2\}_2]^+$, 757.1 (6) $[Cu(C_{14}H_{12}N_2O_4)_2(BF_4)]^+$, 599.7 (100) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)]^+$. Elemental analysis, calcd. (%) for $C_{28}H_{22}BCuF_4Mo_2N_2O_8P_2$ × $0.1CH_2Cl_2$: C 36.54, H 2.42, N 3.03; found: C 35.56, H 2.56, N 3.29. IR (KBr): $\tilde{\nu}$/cm^{-1} = 3116 (w; CH), 2963 (w; CH), 2925 (w; CH), 2853 (vw; CH), 1979 (vs; CO), 1922 (vs; CO), 1734 (s; CO), 1634 (m; CC, CN), 1560 (w; CC, CN), 1456 (w; CC, CN), 1417 (m; CC), 1384 (m), 1326 (w), 1299 (m), 1273 (s; COC), 1225 (w), 1124 (s), 1084 (vs; BF), 1061 (s; BF), 1037 (s; BF), 853 (w), 837 (m), 826 (m; δ(CH)), 805 (m), 761 (m), 735 (w), 703 (m), 690 (w), 670 (vw), 656 (vw), 637 (vw), 604 (vw), 561 (m, CC), 521 (m; δ(BF)), 487 (m; δ(MoCO), δ(CMoC)), 457 (m; δ(BF)).

Complex 8



A solution of equimolar amounts of $Cu(CH_3CN)_4BF_4$ (**B**, 0.016 g, 0.05 mmol), $[Cp_2Mo_2(CO)_4(\eta^2\text{-}P_2)]$ (**A**, 0.025 g, 0.05 mmol), and edcp-meta (**4**, 0.014 g, 0.05 mmol) in CH_2Cl_2 (10 ml) and CH_3CN (5 ml) was stirred for 3 hours at room temperature. The orange-red crude mixture was filtered off using a teflon capillary to remove any suspended particles. The obtained solution was layered with the same amount of pentane or toluene and kept at room temperature. After four days orange crystals of **8** × 0.5 CH_2Cl_2 were obtained. The crystals were isolated by decanting the mother liquor, washed twice with CH_2Cl_2 (2×3ml) and dried under reduced pressure. The resulting filtrate was isolated, concentrated to about third of its volume and stored in a fridge at -4°C. In two days smaller crystals of the product could be obtained and were isolated using the same procedure used above. All the crystals were collected and the yield was calculated (**8**, 0.030 g, 0.016 mmol, 65%). ^{1}H NMR (400 MHz, CD_3CN): δ = 4.68 (s, 4H, H_g), 5.32 (s, 10H, C_5H_5), 7.49 (s, 2H, H_d), 8.32 (m, 2H, H_c), 8.76 (m, 2H, H_e), 9.14 (m, 2H, H_a). ^{13}C{^{1}H} NMR (100.61 MHz, CD_3CN): δ = 64.0 (s, C_g), 87.5 (s, C_{Cp}), 124.8 (s, C_d), 127.2 (s, C_b), 138.1 (s, C_c), 151.4 (s, C_a), 154.6 (s, C_e), 166.0 (s, C_f), 226.6 (s, C_{CO}). ^{31}P{^{1}H} NMR (161.98 MHz, CD_3CN): δ = -48.2 (s, $\omega_{1/2}$= 11.1 Hz). ^{19}F{^{1}H} NMR (282.40 MHz, CD_3CN): δ = -150.9 (s, $^{11}BF_4$), -150.8 (s, $^{10}BF_4$). Positive ion ESI-MS (CH_3CN): m/z (%) = 1056.6 (46) $[Cu\{Cp_2Mo_2(CO)_4P_2\}_2]^+$, 830.8 (100) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(C_{14}H_{12}N_2O_4)]^+$, 757.1 (22) $[Cu(C_{14}H_{12}N_2O_4)_2(BF_4)]^+$, 599.8 (58) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)]^+$, 571.7 (26) $[Cu\{Cp_2Mo_2(CO)_4\text{-}P_2\}(CH_3CN)$ - $CO]^+$, 543.8 (48) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)$ - 2 $CO]^+$, 515.8 (11) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)$ - 3 $CO]^+$, 487.7 (12) $[Cu\{Cp_2Mo_2(CO)_4P_2\}(CH_3CN)$ - 4 $CO]^+$, 439.7 (26) $[\{Cp_2Mo_2(CO)_4\text{-}P_2\}$ - 2 $CO]^+$, 375.9 (88) $[Cu(C_{14}H_{12}N_2O_4)(CH_3CN)]^+$, 335.0 (22) $[Cu(C_{14}H_{12}N_2O_4)]^+$, 314.1 (40) $[(C_{14}H_{12}N_2O_4)(CH_3CN)]^+$, 273.1 (82) $[(C_{14}H_{12}N_2O_4)]^+$. Elemental analysis, calcd. (%) for $C_{56}H_{44}B_2Cu_2F_8Mo_4N_4O_{16}P_4 \times CH_2Cl_2$ (1922.25 g.mol^{-1}): C 35.61, H 2.41, N 2.91; found: C 34.87, H 2.48, N 3.11. IR (KBr): $\tilde{\nu}$/cm^{-1} = 3104 (w; CH), 2965 (vw; CH), 2909 (vw; CH), 2853 (vw; CH), 1987 (vs; CO), 1940 (vs; CO), 1927 (vs; CO), 1638 (w; CC, CN), 1601 (m; CC, CN), 1477 (w; CC, CN), 1428 (m; CC), 1339 (m), 1271 (s; COC), 1245 (m), 1199 (m), 1116 (s), 1084 (s; BF), 1046 (s; BF), 1032 (s; BF), 980 (m), 839 (m), 829 (m; δ(CH)), 745 (s), 728 (w), 697 (m), 645 (vw), 562 (m, CC), 521 (s; δ(BF)), 487 (m; δ(MoCO), δ(CMoC)), 457 (s; δ(BF)).

NMR Spectra

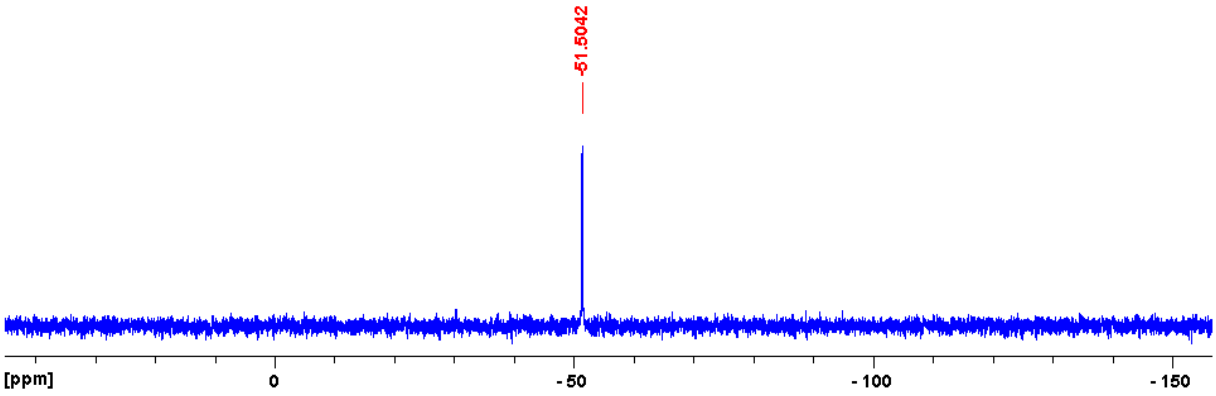


Figure S1: $^{31}P\{^{1}H\}$ NMR spectrum of complex **5** in CD_3CN at 121.49 MHz.

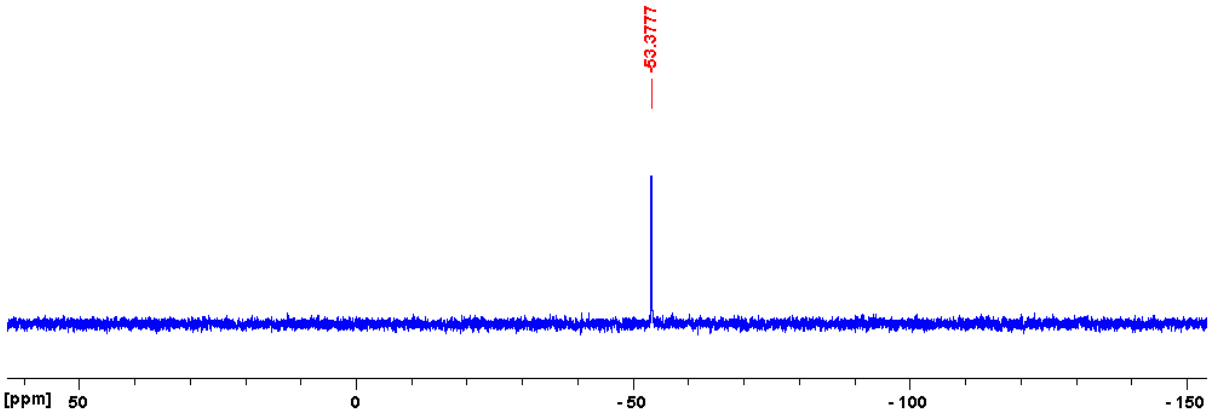


Figure S2: $^{31}P\{^{1}H\}$ NMR spectrum of complex **6** in CD_3CN at 121.49 MHz.

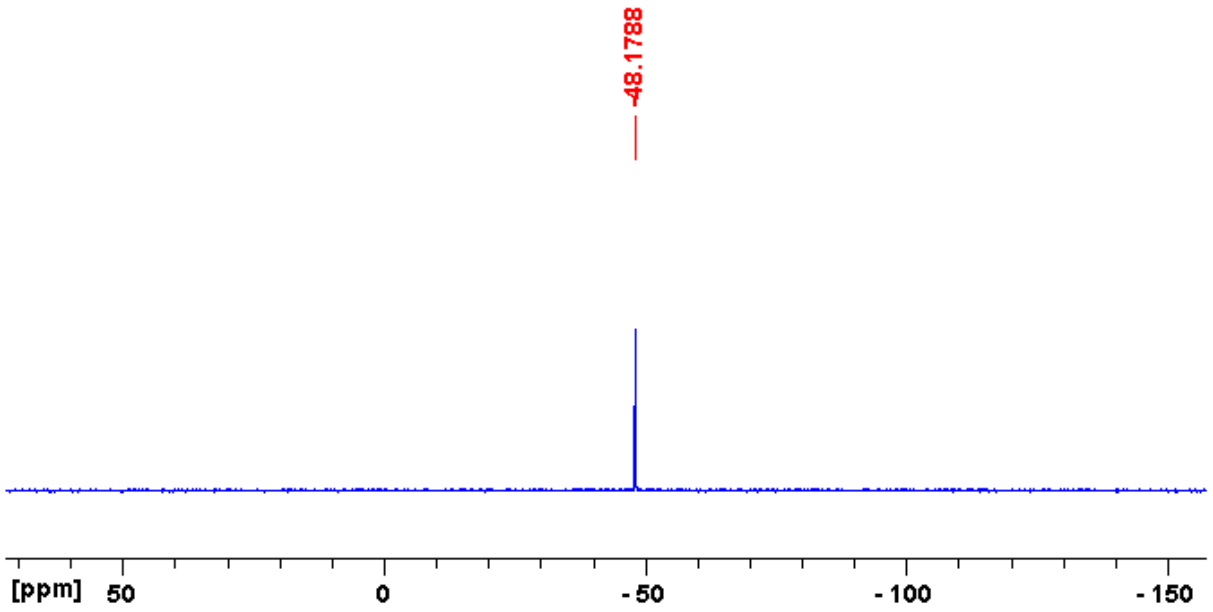


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of complex **7** in CD_3CN at 161.98 MHz.

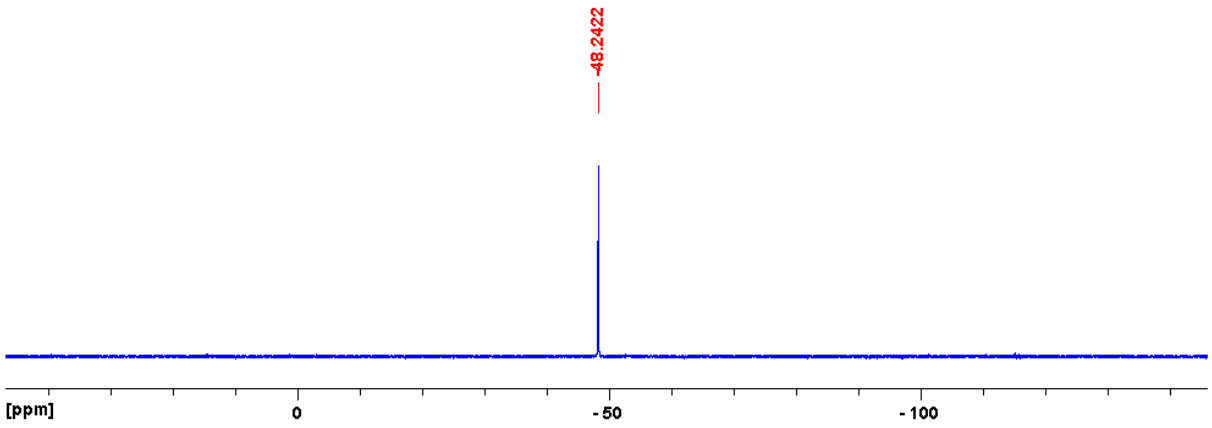


Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum of complex **8** in CD_3CN at 161.98 MHz.

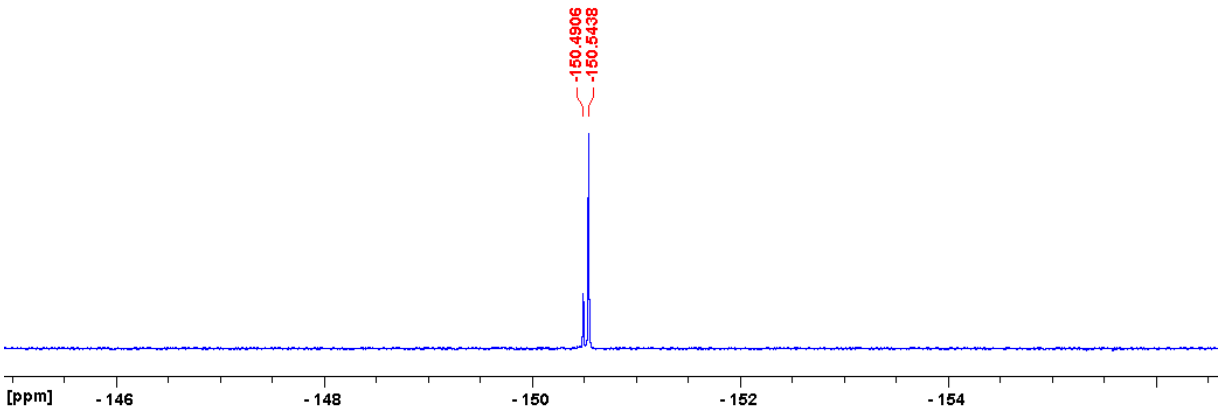


Figure S5: $^{19}F\ \{^{1}H\}$ NMR spectrum of complex **5** in CD_3CN at 282.40 MHz.

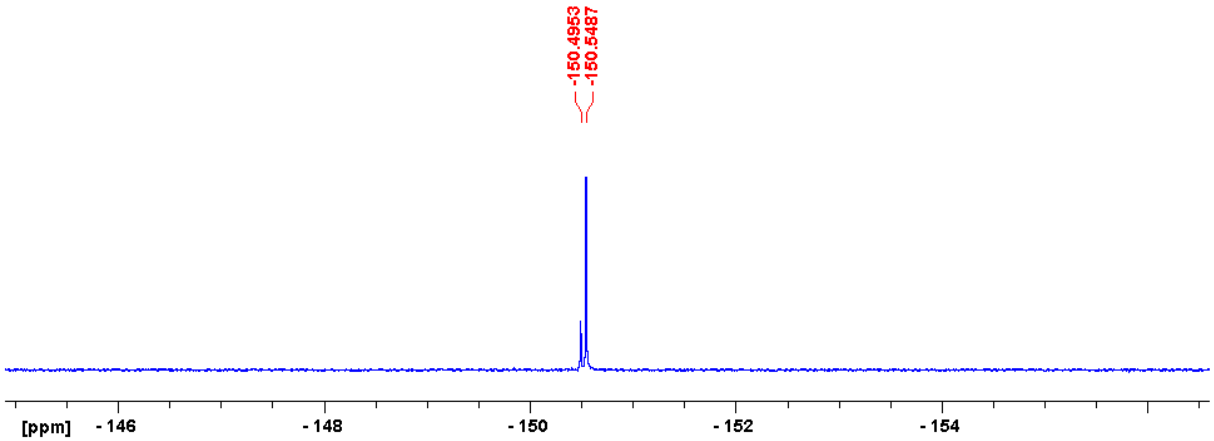


Figure S6: ^{19}F {^{1}H} NMR spectrum of complex **6** in CD_3CN at 282.40 MHz.

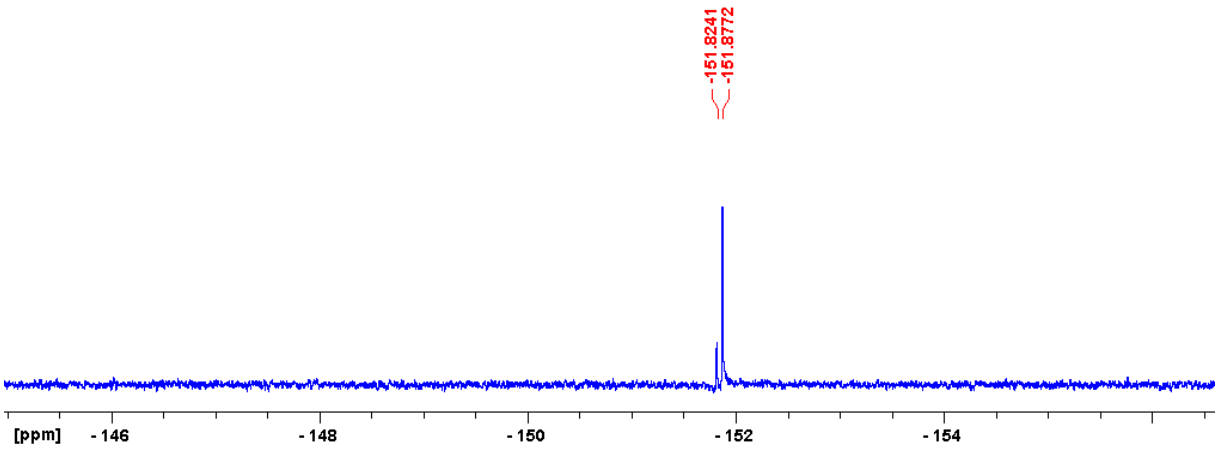


Figure S7: ^{19}F {^{1}H} NMR spectrum of complex **7** in CD_3CN at 376.50 MHz.

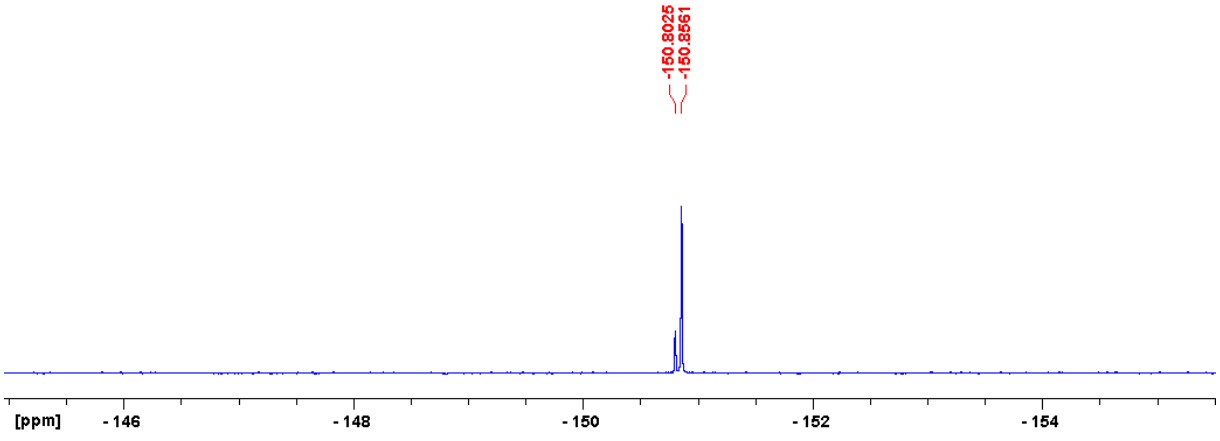
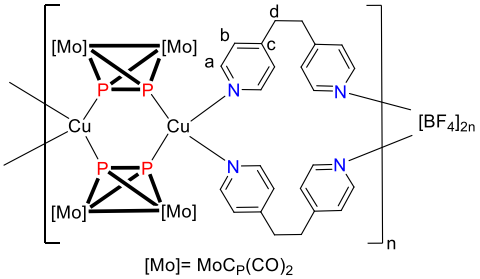


Figure S8: ^{19}F {^{1}H} NMR spectrum of complex **8** in CD_3CN at 282.40 MHz.



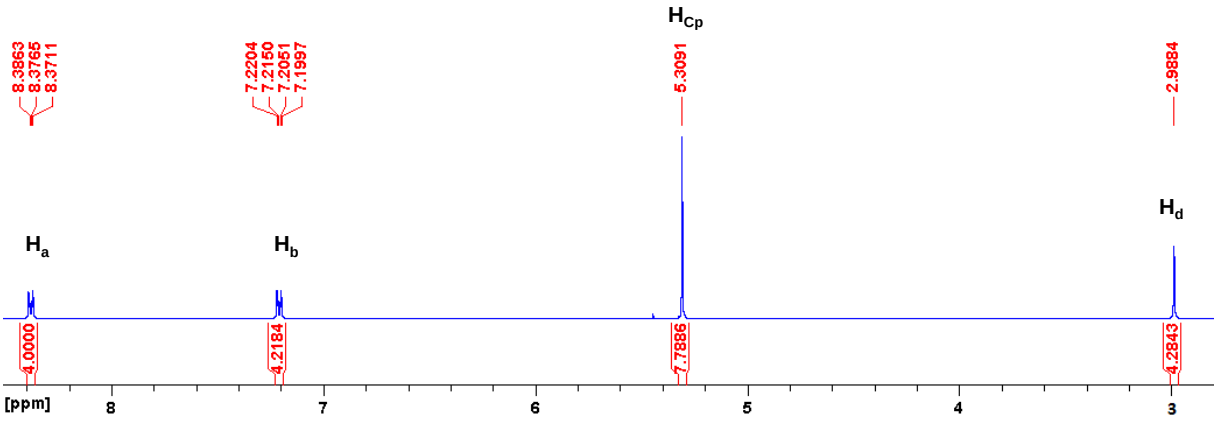
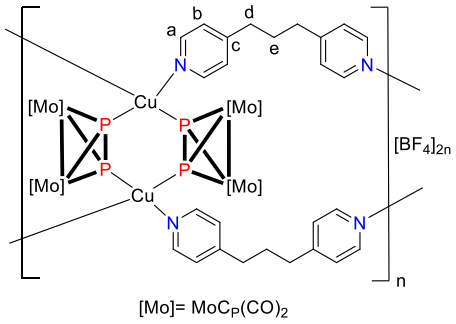


Figure S9: ^{1}H NMR spectrum of complex **5** in CD_3CN at 300 MHz.



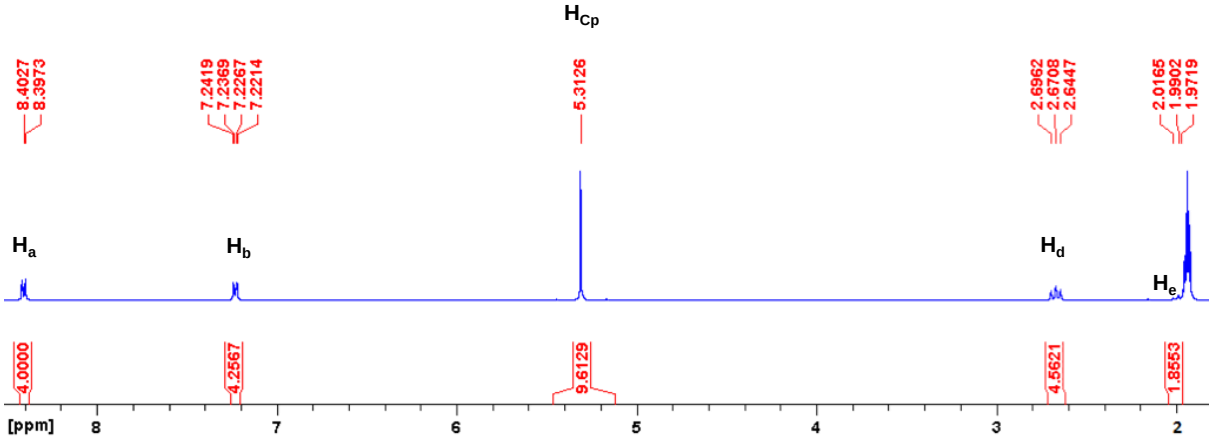


Figure S10: ^{1}H NMR spectrum of complex **6** in CD_3CN at 300 MHz.

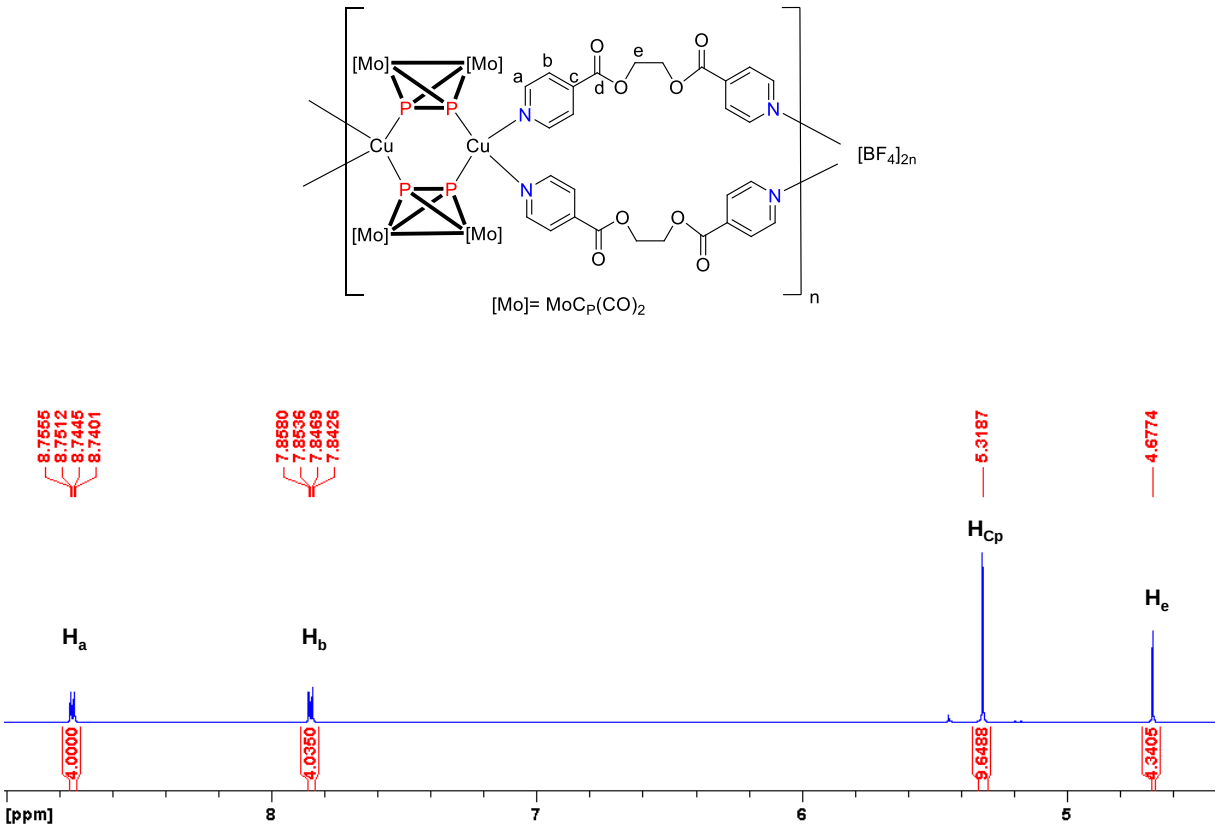


Figure S11: ^{1}H NMR spectrum of complex **7** in CD_3CN at 400 MHz.

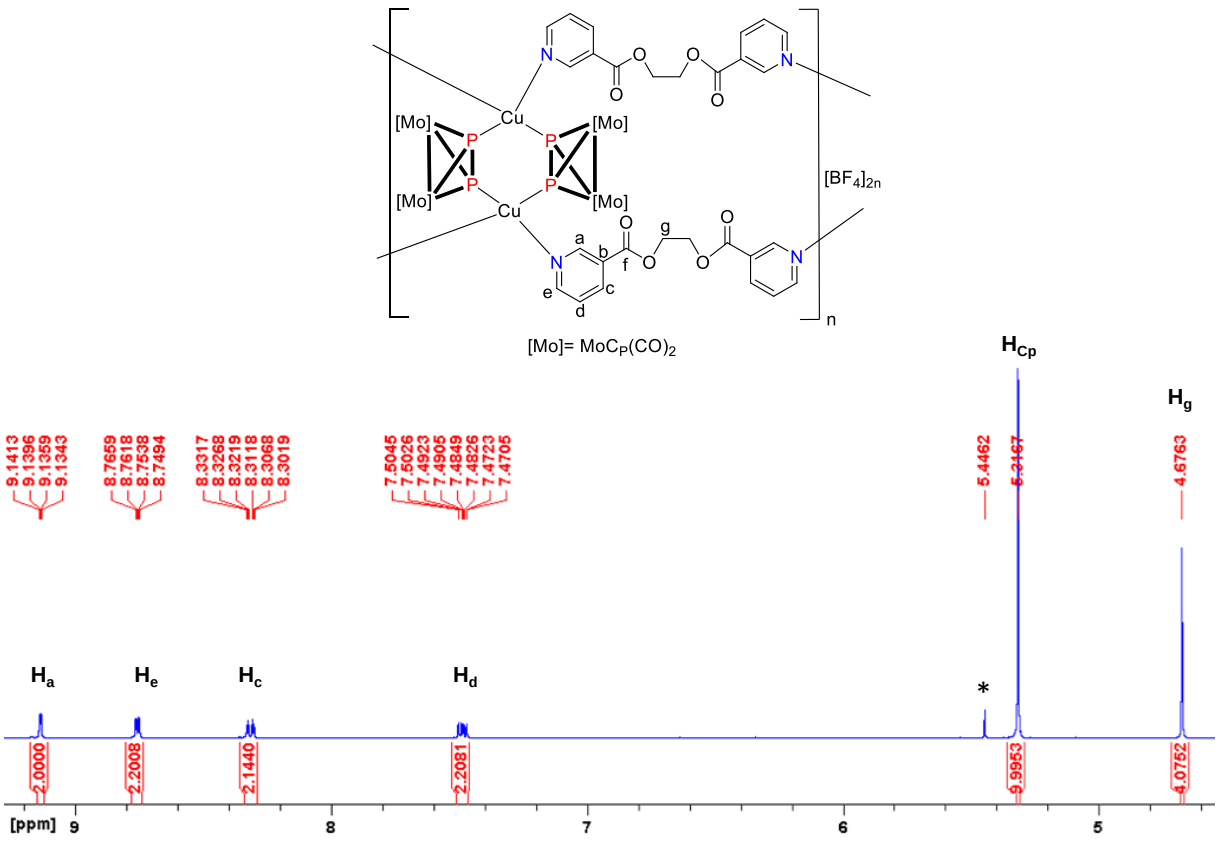


Figure S12: ^{1}H NMR spectrum of complex **8** in CD_3CN at 400 MHz. * CH_2Cl_2 solvent.

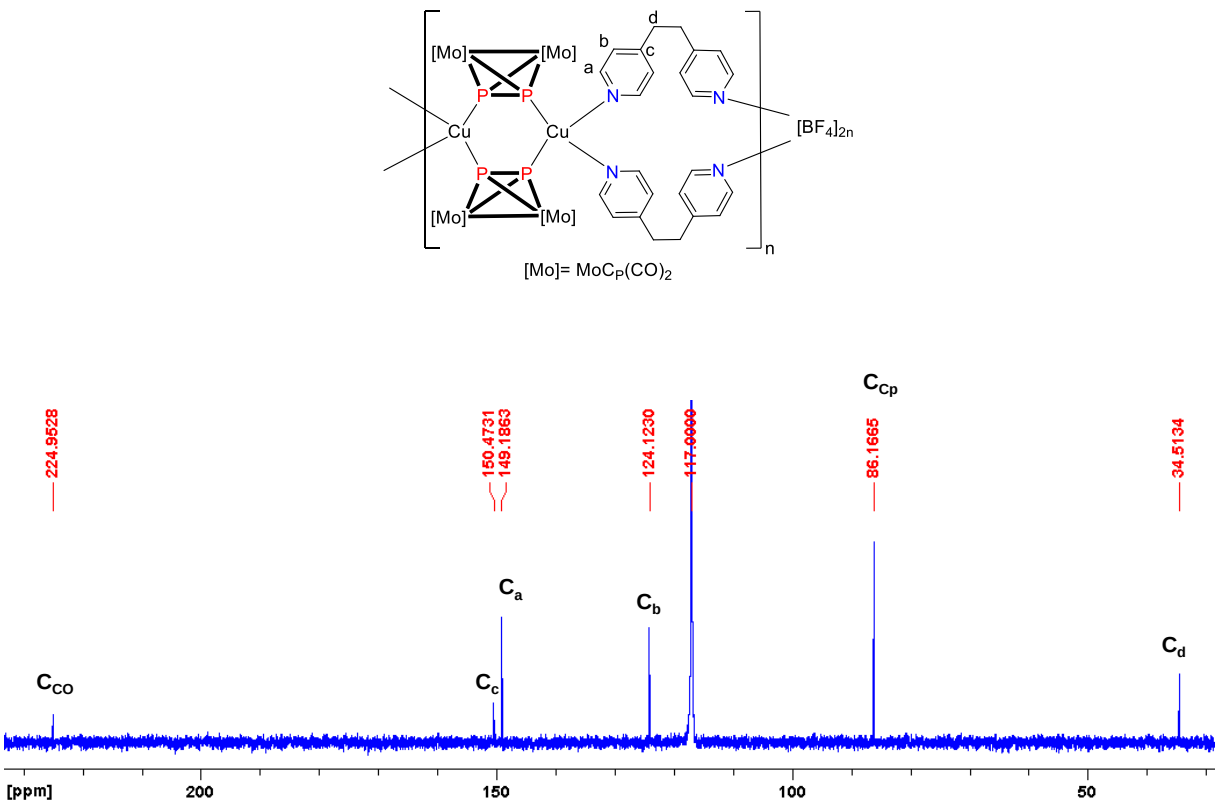


Figure S13: ^{13}C NMR spectrum of complex **5** in CD_3CN at 75.47 MHz.

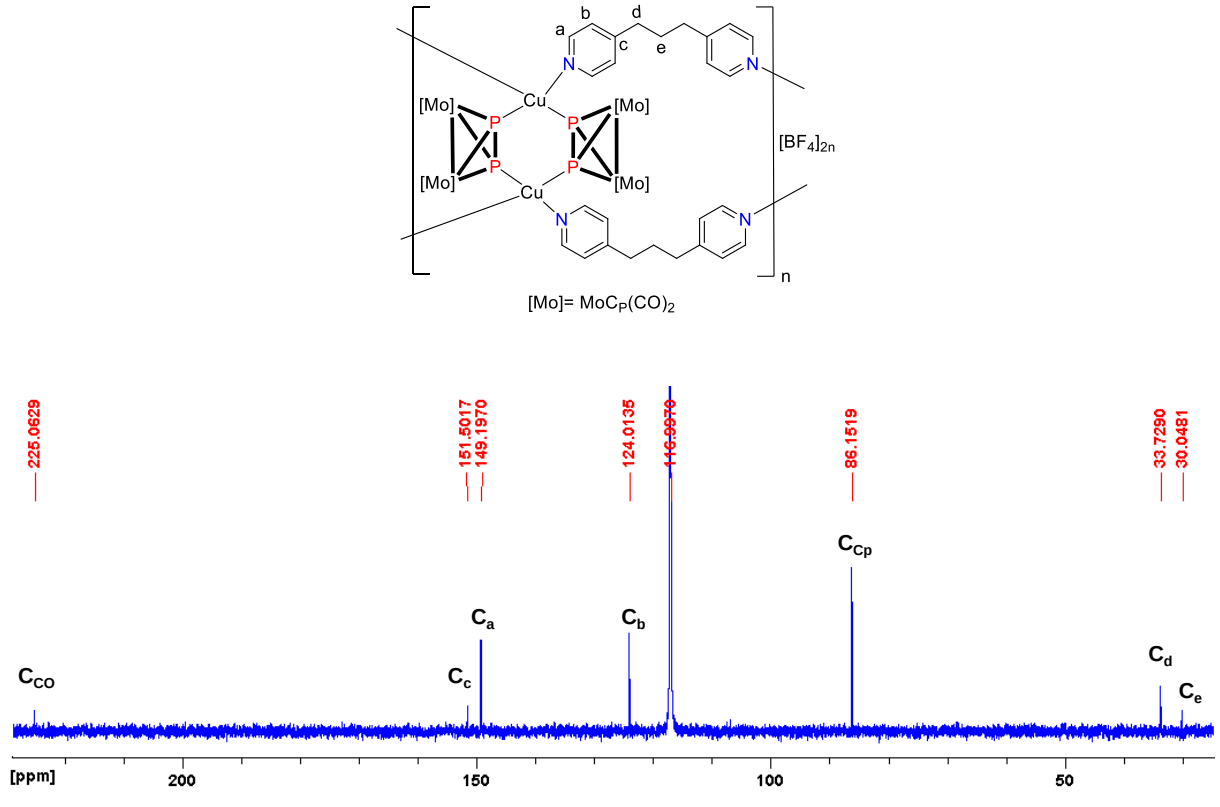


Figure S14: ^{13}C NMR spectrum of complex **6** in CD_3CN at 75.47 MHz.

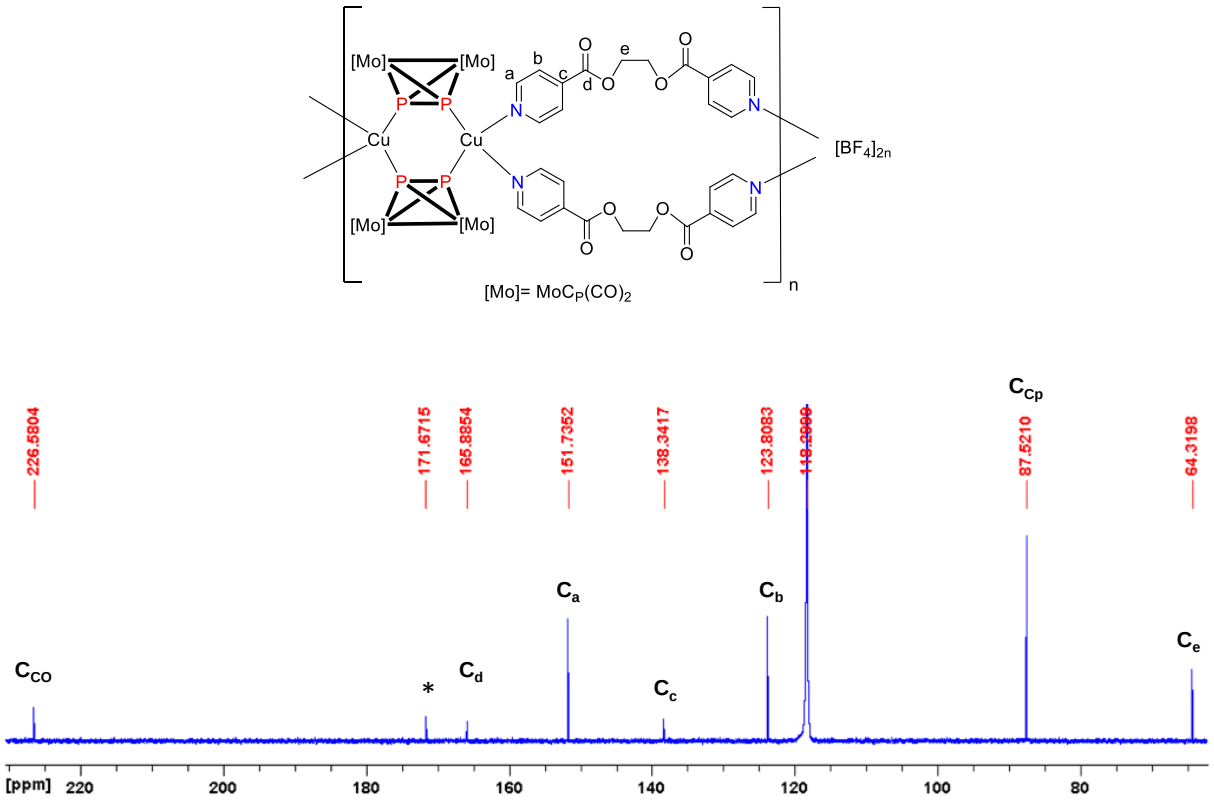


Figure S15: ^{13}C NMR spectrum of complex **7** in CD_3CN at 100.61 MHz. * impurities

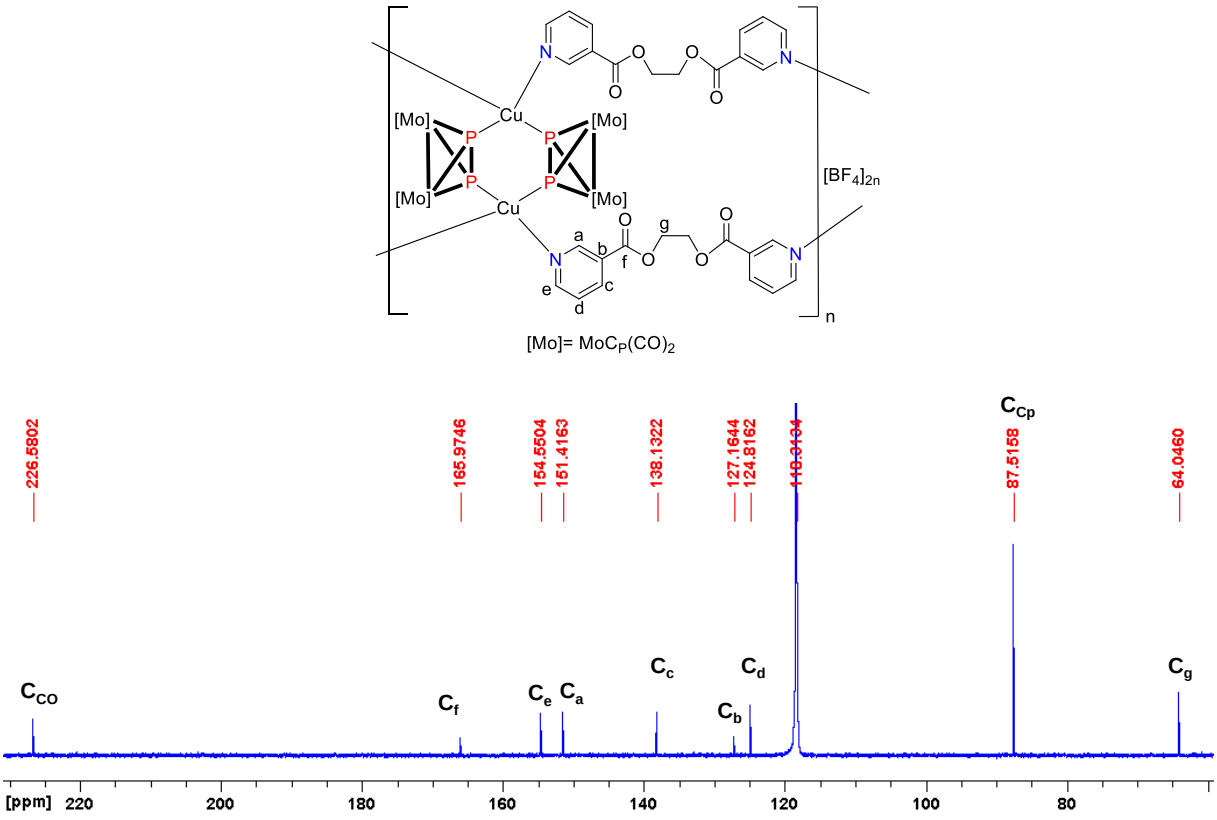


Figure S16: ^{13}C NMR spectrum of complex **8** in CD_3CN at 100.61 MHz.

Crystallographic Studies

Experimental

Single crystals suitable for single crystal X-ray diffraction analysis were obtained for compounds **5-8** as reported above. The crystals were taken out of the Schlenk tube and immediately covered by mineral oil to prevent the loss of solvent. After selection a single crystal was quickly mounted on a pre-centered goniometer head and placed on the goniometer into the stream of nitrogen (T = 123 K). Single crystal data were collected on Agilent Technologies SuperNova diffractometers equipped a SuperNova CuK$_\alpha$ microfocus source (λ = 1.54178 Å) and either with Titan (for **5** and **6**) or Atlas (for **7** and **8**) CCD detector. The data intensities were collected by ω scans of 0.5° (for **7**) or 1° (for **5**, **6**, **8**) frames. Crystallographic data and details of the diffraction experiments are given in Tables S1-S6. The data processing was performed with the *CrysAlis PRO* software.[4] Structures were solved by direct methods with the program SHELXS (**5**, **6**, **7**) or *SUPERFLIP*[5] (**8**) and refined by full-matrix least-squares on F^2 using Olex[6] or SHELXL-13.[7] All non-hydrogen atoms except for some disordered ones were refined in anisotropic approximation. Hydrogen atoms were placed in idealized positions and refined riding on pivot atoms with isotropic displacement parameters.

The crystal structure **5** possesses solvent accessible channels containing several disordered solvent molecules in asymmetric unit. During the refinement six independent CH_2Cl_2 solvent molecule positions and one position of a MeCN molecule were identified by analyzing the geometry and weight of the residual electron density peaks. The solvent molecules are partially occupied and do not add up to an integer value. Several restraints and some constraints had to be applied during the refinement.

In structure of **7** a $\{Cp_2Mo_2(CO)_4P_2\}$ unit is disordered over two positions with a relative weight converged to 0.56/0.44 values so that the disorder does not affect only P atoms. The displacement parameters of heavy atoms were set equal to U_{iso} = 0.04 e·A^{-3}, and the occupancy factors were refined. Their resulting values were fixed, and then a free refinement of the displacement parameters was performed. The spacer molecule is disordered due to its flexibility and adopts twisted configurations in respect to each of two probable positions (relative weight 0.65/0.35) (Figure S20).

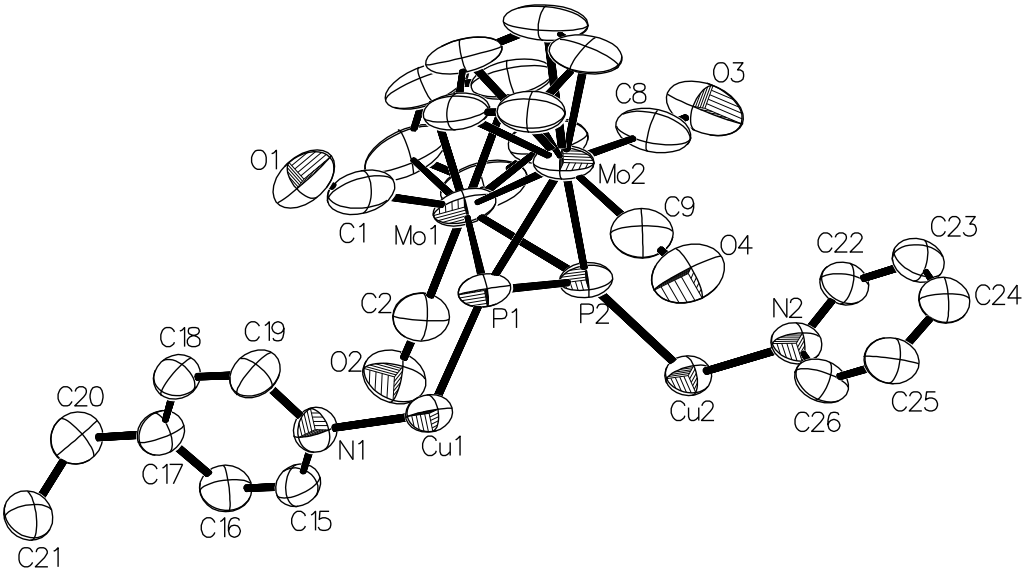
A BF_4^- anion is disordered over close positions or occupies partly few distant positions in crystal structures of **6** and **7**. Solvent CH_2Cl_2 and MeCN molecules are also disordered.

CCDC reference numbers CCDC-1487111-1487114 contain the supplementary crystallographic data for **5**, **6**, **7** and **8**. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retreving.html or from the Cambridge Crystallographic Data Center, 12 union Road, Cambridge CB2 1EZ, UK; Fax: (internat.) + 44-1223-336-033; E-mail: deposit@ccdc.cam.ac.uk.

Table S1. Experimental details

Compound	**5**·0.6 CH_3CN·1.98 CH_2Cl_2	**6**·0.5 CH_3CN·0.2 CH_2Cl_2	**7**·0.1 CH_2Cl_2	2 **8**·CH_2Cl_2
Chemical formula	$C_{55.18}H_{49.76}B_2Cl_{3.96}Cu_2F_8Mo_4N_{4.6}O_8P_4$	$C_{28.2}H_{25.9}BCl_{0.4}CuF_4Mo_2N_{2.5}O_4P_2$	$C_{28.10}H_{22.20}BCl_{0.2}CuF_4Mo_2N_2O_8P_2$	$C_{57}H_{46}B_2Cl_2Cu_2F_8Mo_4N_4O_{16}P_4$
CCDC number	1487111	1487112	1487113	1487114
Molecular weight	1854.04	882.16	927.14	1922.24
Crystal system	trigonal	triclinic	triclinic	monoclinic
Space group	$P3_121$	$P\bar{1}$	$P\bar{1}$	$C2/c$
Temperature (K)	123	123	150	123
a (Å)	13.2466 (4)	12.1500 (5)	11.0510 (3)	23.3364 (11)
b (Å)	13.2466 (4)	12.9837 (5)	12.9411 (3)	15.9366 (4)
c (Å)	38.4491 (11)	13.0995 (5)	14.5125 (4)	20.1067 (7)
α (°)	90	112.581 (4)	107.454 (2)	90
β (°)	90	95.502 (3)	109.734 (2)	116.735 (4)
γ (°)	120	112.579 (4)	92.922 (2)	90
V (Å^3)	5842.9 (4)	1688.53 (13)	1836.64 (8)	6678.3 (5)
Z	3	2	2	4
F(000)	2737	871	912	3784
D_x (Mg m^{-3})	1.581	1.735	1.676	1.912
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	8.31	8.46	7.74	9.13
Crystal shape	plate	prism	rhombic plate	block
Colour	clear orange	red	red	orange
Crystal size (mm)	0.16 × 0.11 × 0.04	0.47 × 0.24 × 0.23	0.26 × 0.13 × 0.09	0.10 × 0.04 × 0.04
T_{min}, T_{max}	0.457, 0.770	0.149, 0.360	0.322, 0.622	0.516, 0.770
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22529, 7682, 5859	10091, 6493, 5960	41379, 7184, 6020	17086, 5936, 4819
R_{int}	0.063	0.068	0.038	0.027
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.624	0.624	0.624	0.597
Range of h, k, l	-12 ≤ h ≤ 15, -14≤ k ≤ 11, -46 ≤ l ≤ 34	-15 ≤ h ≤ 14, -14≤ k ≤ 15, -13 ≤ l ≤ 16	-13 ≤ h ≤ 13, -14≤ k ≤ 15, -17 ≤ l ≤ 17	-26 ≤ h ≤ 27, -19 ≤ k ≤ 16, -24 ≤ l ≤ 24
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.185, 1.00	0.066, 0.189, 1.08	0.055, 0.193, 1.07	0.041, 0.126, 1.06
No. of reflections	7682	6493	7184	5936
No. of parameters	495	442	660	447
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	1.20, -1.05	1.73, -1.98	1.80, -0.58	1.58, -1.44

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.36.28 (release 01-02-2013 CrysAlis171 .NET) (compiled Feb 1 2013, 16:14:44), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008).



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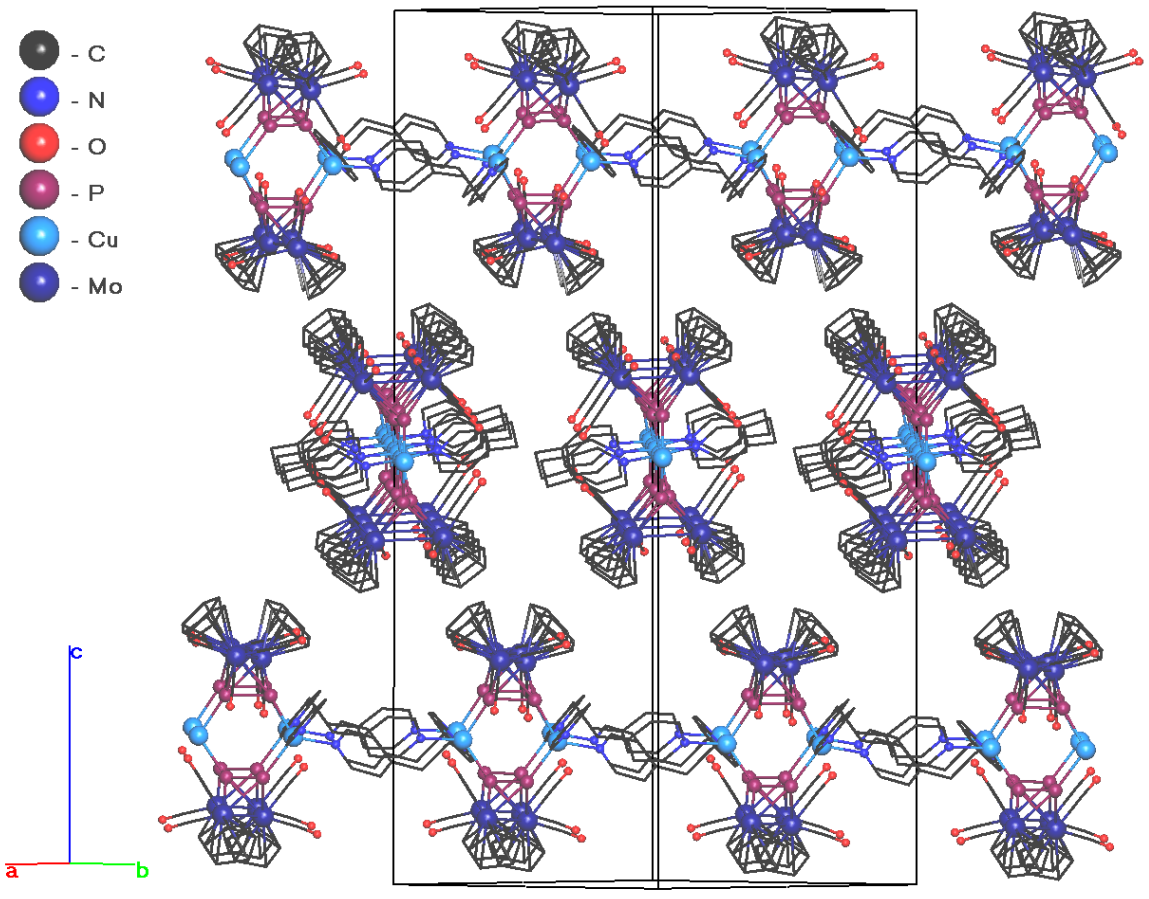


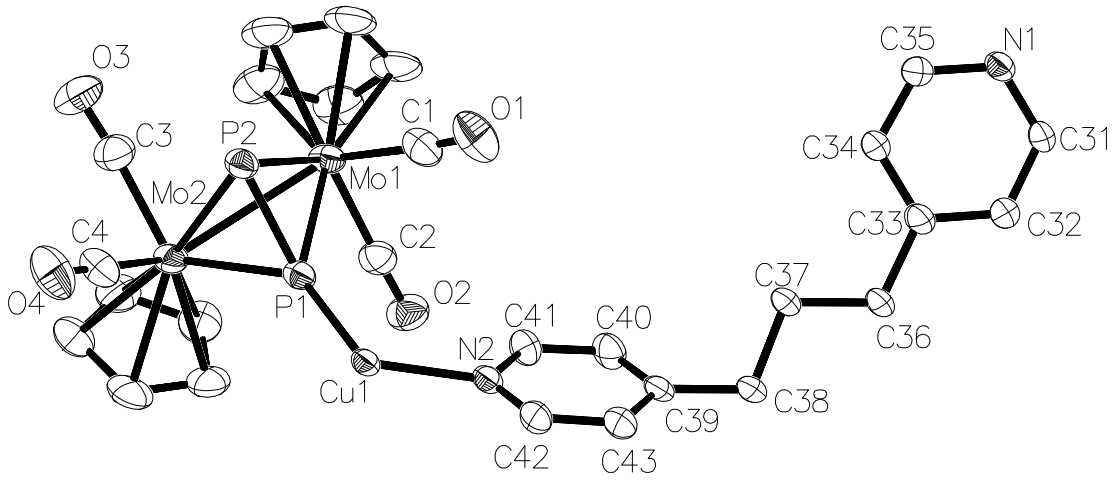
b

Figure S17. Structure of the complex **5**: a) Enumeration scheme and b) crystal packing[8]. Hydrogen atoms as well as solvent molecules have been omitted for clarity.

Table S2. Selected geometric parameters (Å, º) for **5**

Mo1—Mo2	3.0229 (16)	Mo2—C12	2.327 (15)
Mo1—P1	2.527 (3)	Mo2—C13	2.369 (17)
Mo1—P2	2.438 (3)	Mo2—C14	2.294 (13)
Mo1—C1	2.03 (3)	Cu1—P1^{i}	2.272 (3)
Mo1—C2	2.002 (15)	Cu1—P1	2.272 (3)
Mo1—C3	2.326 (16)	Cu1—N1^{i}	2.043 (10)
Mo1—C4	2.367 (17)	Cu1—N1	2.043 (10)
Mo1—C5	2.382 (18)	Cu2—P2^{i}	2.275 (3)
Mo1—C6	2.323 (15)	Cu2—P2	2.275 (3)
Mo1—C7	2.309 (14)	Cu2—N2	2.039 (11)
Mo2—P1	2.452 (3)	Cu2—N2^{i}	2.039 (11)
Mo2—P2	2.517 (3)	P1—P2	2.077 (5)
Mo2—C8	1.98 (2)	O1—C1	1.12 (3)
Mo2—C9	1.974 (18)	O2—C2	1.135 (17)
Mo2—C10	2.284 (11)	O3—C8	1.14 (2)
Mo2—C11	2.313 (13)	O4—C9	1.149 (19)
P1^{i}—Cu1—P1	107.75 (19)	P2—Cu2—P2^{i}	105.4 (2)
N1^{i}—Cu1—P1	112.2 (3)	N2—Cu2—P2^{i}	108.0 (3)
N1—Cu1—P1	110.4 (3)	N2—Cu2—P2	113.3 (3)
N1^{i}—Cu1—P1^{i}	110.4 (3)	N2^{i}—Cu2—P2^{i}	113.3 (3)
N1—Cu1—P1^{i}	112.2 (3)	N2^{i}—Cu2—P2	108.0 (3)
N1^{i}—Cu1—N1	104.0 (6)	N2—Cu2—N2^{i}	108.9 (7)

Symmetry code(s): (i) *y*, *x*, -*z*+1.



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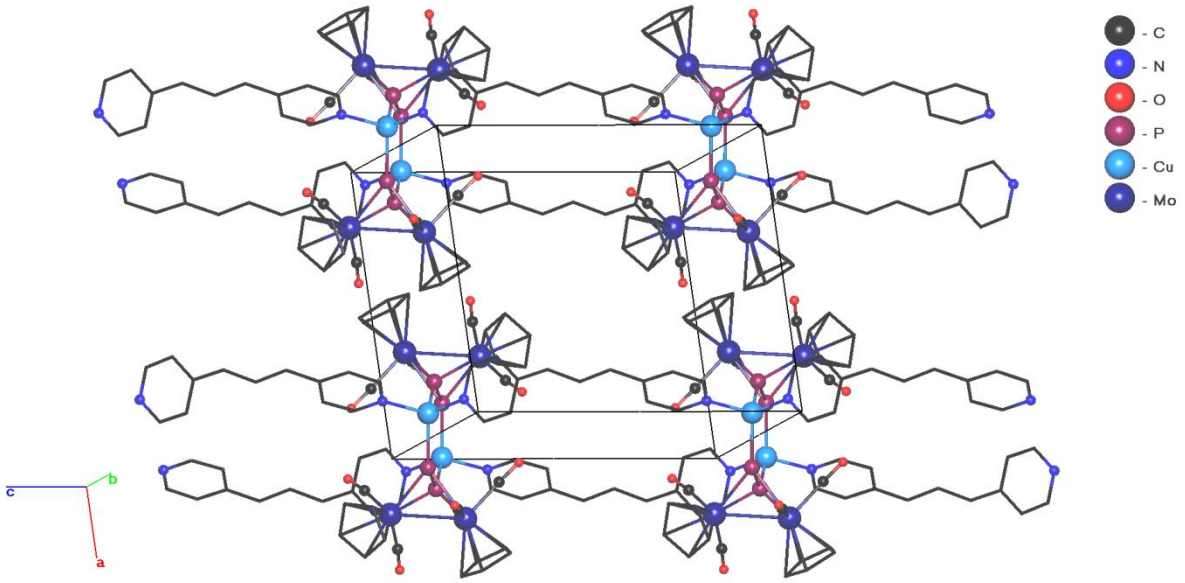


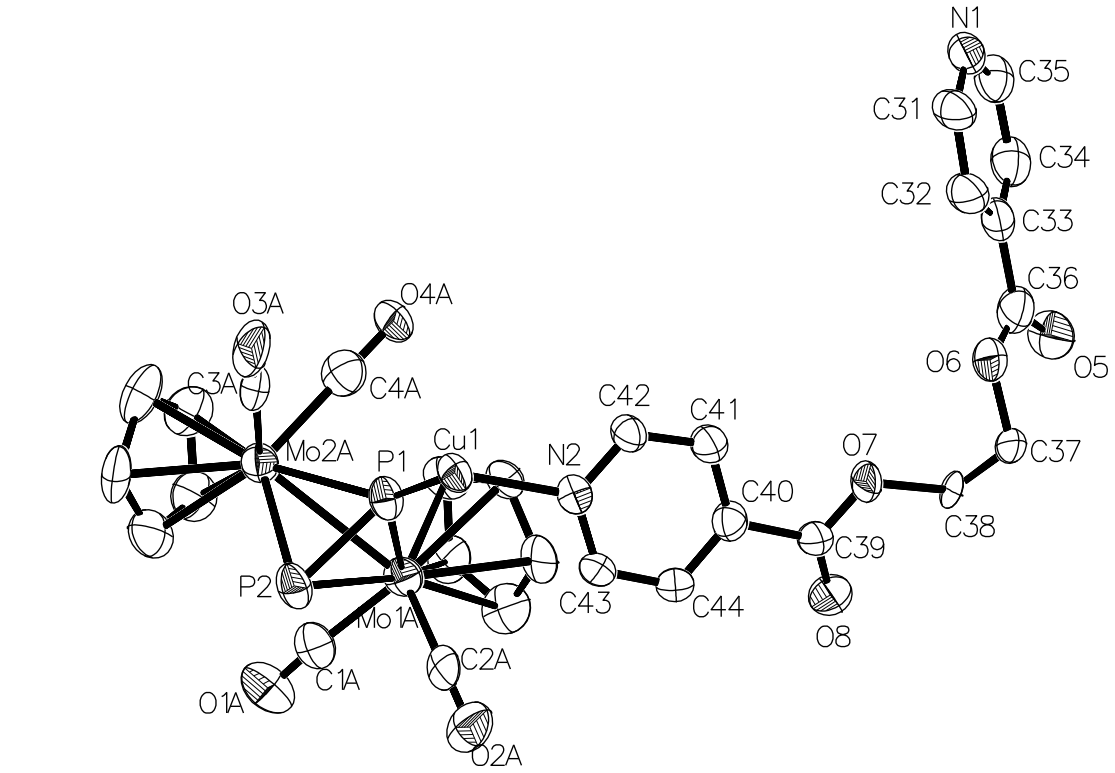
b

Figure S18. Structure of the complex **6**: a) Enumeration scheme and b) crystal packing. Hydrogen atoms, counteranions as well as solvent molecules have been omitted for clarity.

Table S3. Selected geometric parameters (Å, º) for **6**

Cu1—N2^{i}	2.033 (4)	Mo2—C4	1.980 (7)
Cu1—N1	2.054 (4)	Mo2—C25	2.296 (6)
Cu1—P1	2.2702 (14)	Mo2—C21	2.307 (6)
Cu1—P2^{ii}	2.2989 (15)	Mo2—C24	2.319 (6)
Mo1—C2	1.985 (6)	Mo2—C23	2.343 (6)
Mo1—C1	1.997 (7)	Mo2—C22	2.350 (6)
Mo1—C15	2.292 (6)	Mo2—P1	2.4512 (13)
Mo1—C11	2.307 (6)	Mo2—P2	2.5342 (14)
Mo1—C14	2.325 (6)	P1—P2	2.0858 (18)
Mo1—C12	2.342 (7)	P2—Cu1^{ii}	2.2989 (14)
Mo1—C13	2.361 (7)	C1—O1	1.121 (8)
Mo1—P2	2.4590 (13)	C2—O2	1.147 (7)
Mo1—P1	2.5362 (13)	C3—O3	1.133 (8)
Mo1—Mo2	3.0418 (6)	C4—O4	1.147 (8)
Mo2—C3	1.980 (6)		
N2^{i}—Cu1—N1	107.91 (17)	N2^{i}—Cu1—P2^{ii}	108.72 (13)
N2^{i}—Cu1—P1	116.57 (13)	N1—Cu1—P2^{ii}	106.66 (13)
N1—Cu1—P1	109.22 (13)	P1—Cu1—P2^{ii}	107.34 (5)

Symmetry code(s): (i) *x*, *y*, *z*-1; (ii) -*x*+2, -*y*+1, -*z*+2.



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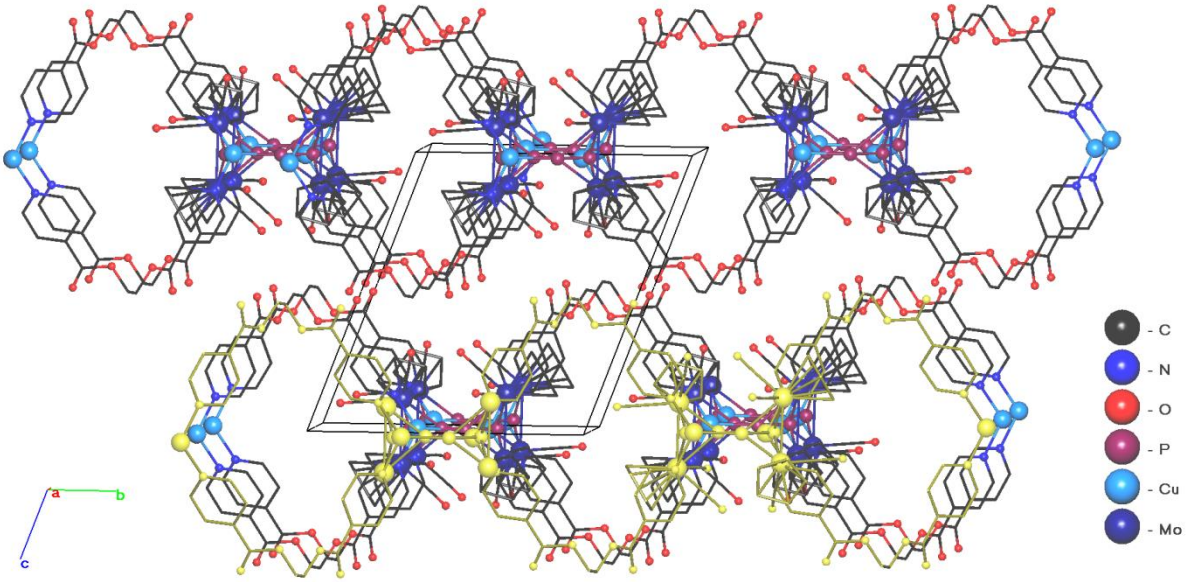
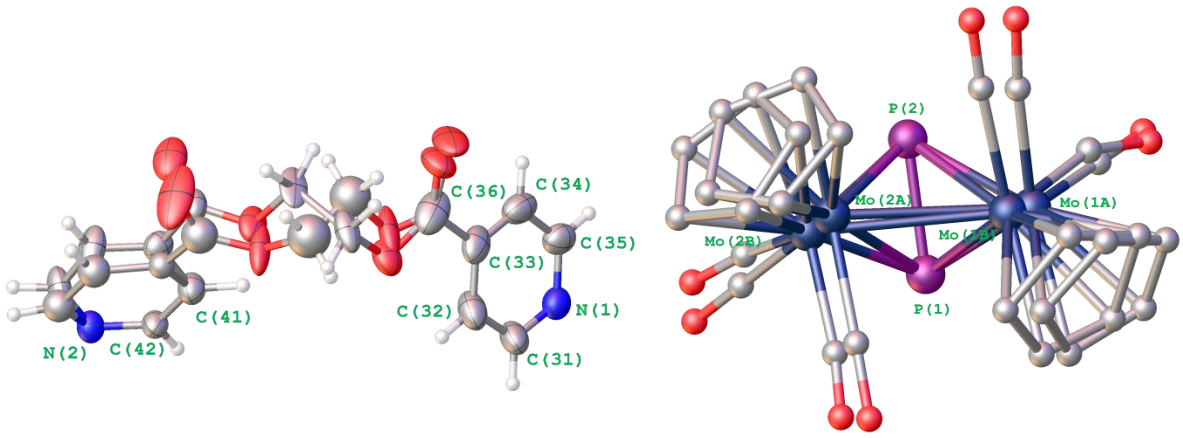


b

Figure S19. Structure of the complex **7**: a) Enumeration scheme and b) crystal packing (one chain is highlighted in yellow). Hydrogen atoms, counteranions as well as solvent molecules have been omitted for clarity.



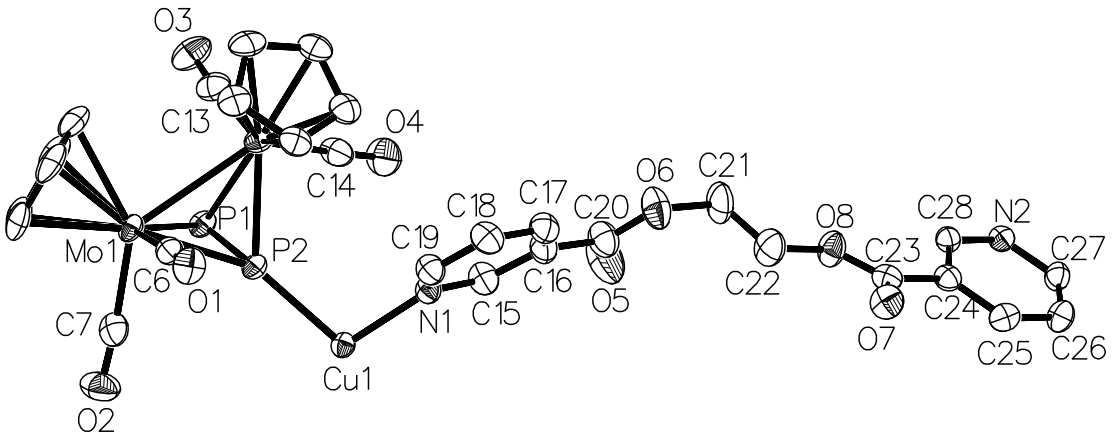
a) b)

Figure S20. The model of the disorder in the crystal structure of polymer **7**. For (a) spacer the minor position (0.35) is refined isotropic. The denoted atoms belong to both orientations. (b) Two positions (denoted as A and B) of the $\{Cp_2Mo_2(CO)_4P_2\}$ unit shown in ball-and-stick representation for clarity. Hydrogen atoms are not shown.

Table S4. Selected geometric parameters (Å, º) for **7**

Cu1—N2^{i}	2.038 (4)	P2—Mo1B	2.490 (4)
Cu1—N1	2.045 (4)	P2—Mo2B	2.573 (3)
Cu1—P2^{ii}	2.2614 (13)	P2—Mo1A	2.584 (3)
Cu1—P1	2.2956 (13)	Mo1A—Mo2A	3.054 (3)
P1—P2	2.0720 (16)	Mo1B—Mo2B	3.052 (3)
P1—Mo1B	2.395 (4)	N1—C31	1.333 (7)
P1—Mo1A	2.497 (3)	N1—C35	1.338 (7)
P1—Mo2A	2.535 (2)	N2—C42	1.326 (6)
P1—Mo2B	2.568 (3)	N2—C43	1.352 (12)
P2—Cu1^{ii}	2.2613 (13)	N2—C43B	1.39 (3)
P2—Mo2A	2.363 (2)	N2—Cu1^{i}	2.038 (4)
N2^{i}—Cu1—N1	109.15 (15)	P2—P1—Mo1A	68.18 (9)
N2^{i}—Cu1—P2^{ii}	110.23 (11)	P2—P1—Mo2A	60.73 (6)
N1—Cu1—P2^{ii}	117.36 (13)	P2—P1—Mo2B	66.36 (7)
N2^{i}—Cu1—P1	102.30 (12)	P1—P2—Cu1^{ii}	125.90 (7)
N1—Cu1—P1	107.61 (12)	P1—P2—Mo2A	69.38 (7)
P2^{ii}—Cu1—P1	109.09 (5)	P1—P2—Mo1B	62.55 (10)
P2—P1—Cu1	124.86 (7)	P1—P2—Mo2B	66.11 (8)
P2—P1—Mo1B	67.30 (11)	P1—P2—Mo1A	63.73 (8)

Symmetry code(s): (i) -*x*+2, -*y*, -*z*; (ii) -*x*+1, -*y*-1, -*z*.



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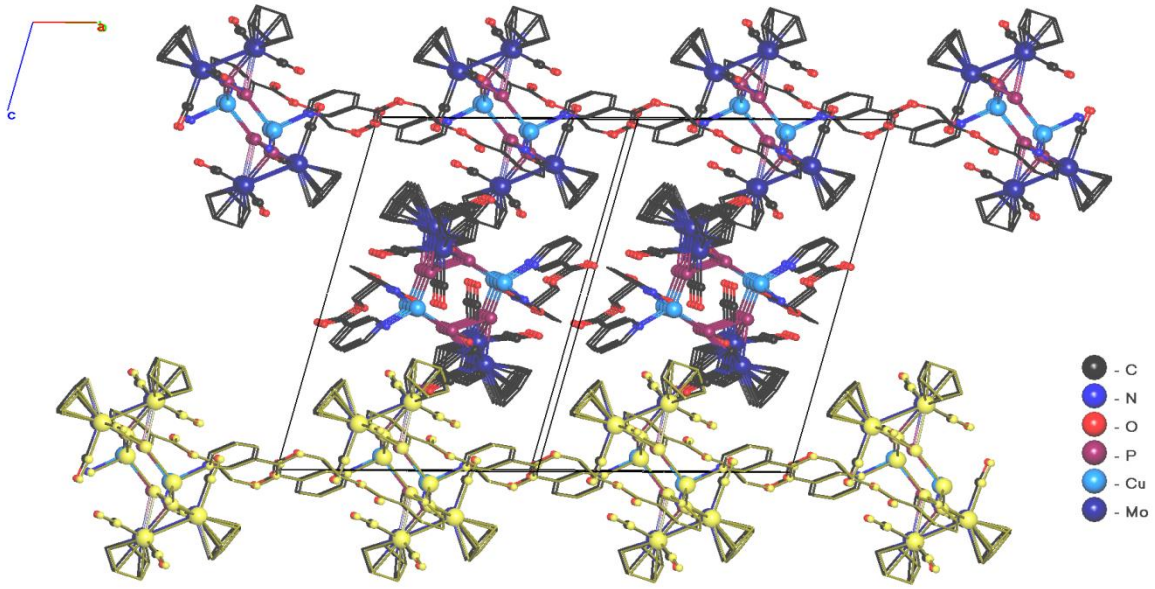


b

Figure S21. Structure of the complex **8**: a) Enumeration scheme and b) crystal packing (one chain is highlighted in yellow). Hydrogen atoms as well as solvent molecules have been omitted for clarity.

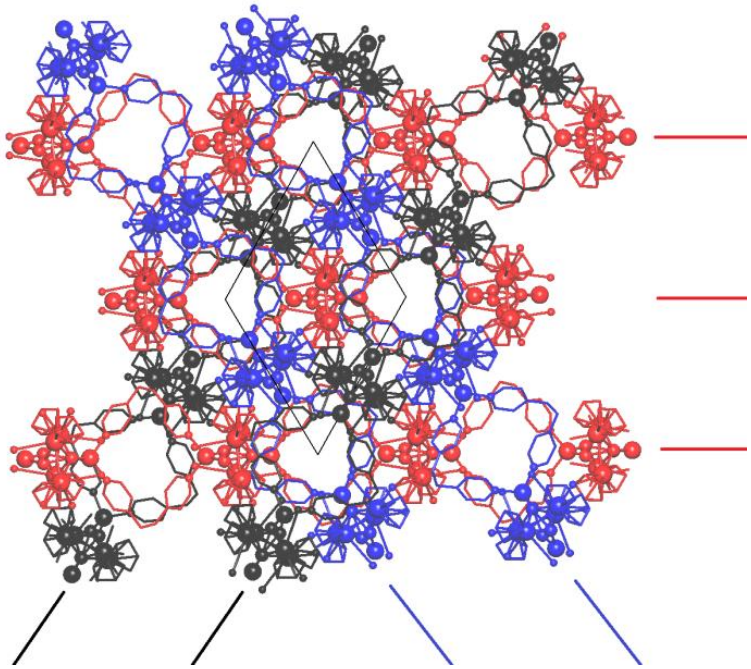
Table S5. Selected geometric parameters (Å, º) for **8**.

Mo1—P1	2.4437 (15)	Mo2—C14	1.988 (7)
Mo1—P2	2.5507 (12)	Cu1—P1	2.2362 (15)
Mo1—C1	2.346 (6)	Cu1—N2	2.042 (4)
Mo1—C2	2.325 (5)	Cu1—P2^{i}	2.3069 (13)
Mo1—C3	2.293 (5)	Cu1—N1^{ii}	2.062 (3)
Mo1—C4	2.315 (5)	Cl1—C67	1.770 (7)
Mo1—C5	2.344 (5)	P1—P2	2.0823 (17)
Mo1—C6	1.987 (5)	O1—C6	1.148 (6)
Mo1—C7	2.008 (5)	O2—C7	1.137 (7)
Mo2—P1	2.5426 (12)	O3—C13	1.147 (8)
Mo2—P2	2.4543 (12)	O4—C14	1.148 (9)
Mo2—C8	2.334 (6)	O5—C20	1.209 (9)
Mo2—C9	2.382 (5)	O6—C21	1.437 (9)
Mo2—C10	2.360 (5)	O6—C20	1.342 (8)
Mo2—C11	2.304 (5)	O7—C23	1.206 (7)
Mo2—C12	2.298 (5)	O8—C22	1.450 (9)
Mo2—C13	1.987 (6)	O8—C23	1.338 (6)
P1—Cu1—N2	122.13 (11)	Mo1—P2—P1	62.71 (5)
P1—Cu1—P2^{i}	110.03 (5)	Mo1—P2—Cu1^{i}	155.76 (6)
P1—Cu1—N1^{ii}	112.26 (13)	Mo2—P2—P1	67.60 (4)
P2^{i}—Cu1—N2	108.89 (12)	Mo2—P2—Cu1^{i}	129.51 (6)
N1^{ii}—Cu1—N2	97.98 (15)	Cu1^{i}—P2—P1	124.00 (7)
P2^{i}—Cu1—N1^{ii}	103.58 (11)	C20—O6—C21	117.3 (6)
Mo1—P1—Mo2	74.93 (4)	C22—O8—C23	116.6 (5)
Mo1—P1—Cu1	144.23 (6)	F1—B1—F2	107.6 (5)
Mo1—P1—P2	68.07 (5)	F1—B1—F3	109.6 (5)
Mo2—P1—Cu1	140.46 (7)	F1—B1—F4	108.7 (6)
Mo2—P1—P2	63.18 (4)	F2—B1—F3	112.9 (6)
Cu1—P1—P2	125.22 (6)	F2—B1—F4	109.6 (6)
Mo1—P2—Mo2	74.61 (3)	F3—B1—F4	108.4 (6)

Symmetry code(s): (i) -*x*+1, -*y*, -*z*; (ii) *x*+1/2, *y*+1/2, *z*.

Crystal packing in 5-8.

Polymers chains in **5-8** are arranged in different fashion. In **6** and **7** the chains are parallel (*cf.* Figs. S18b and S19b). In **5** and **8** they are arranged in layers and have different directions of their propagation (Fig. S22).



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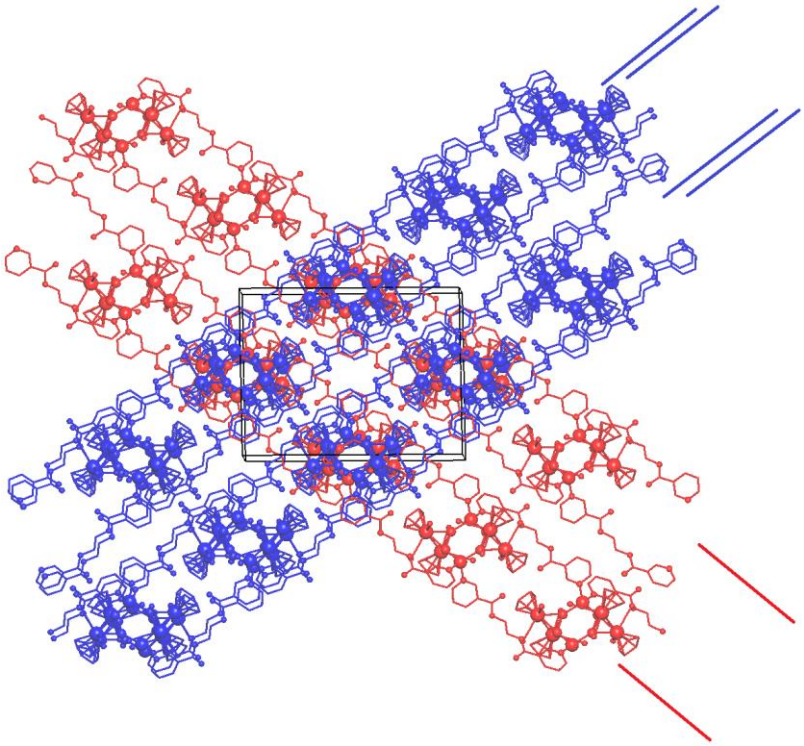

b

Figure S22*:* Comparative orientation of the chains in crystal packing: a) three orientations in **5** and b) two orientations in **8**. The co-directed chains and their schematic directions are shown in similar colour.

In **5**, according to a trigonal space group three orientations of the chains intersect at 60 degrees (Fig. S22a). In this structure, the counteranions BF_4^- and solvated CH_2Cl_2 molecules are located in the interstitial space between the chains. The $Cu_2(\mathbf{1})_2$ meshes are too small to accommodate counteranions, MeCN or CH_2Cl_2 molecules.

In **6**, the arrangement of the chains is parallel, with a relative shift of half of the repeating unit for neighbouring chains. Such orientation of the chains can be favoured by slipped Cp...Cp stacking (dot-to-plane distance 3.20 Å) between the complexes **A** of the neighbouring chains. The other interchain interaction is a stacking between molecules of an organic linker featured with a longer dot-to-plane distance of 3.58 Å. Both types of contacts join all chains in different directions and result in 3D structure. With not very large size of a $Cu_2(\mathbf{A})_2(\mathbf{2})_2$ mesh, the counteranions BF_4^- occupy the space above and below the meshes and, being disordered, do not show significant intermolecular interactions. Solvated CH_2Cl_2 and MeCN molecules are found in-between the parallel chains.

In **7**, the meshes $Cu_2(\mathbf{3})_2$ are large enough to include one BF_4^- counteranion, which is disordered in the centre of the mesh. One more BF_4^- anion and solvated CH_2Cl_2 molecules are disordered in the interchain space. In agreement with the observed disorder, no significant intermolecular interactions of the BF_4^- anions and the polymer are found. There is also a relative shift for the neighbouring chains, which affords more dense packing. However, no interchain intermolecular interactions like π…π stacking is observed, due to non-parallel orientation of Cp and py aromatic systems.

In **8**, the meshes $Cu_2(\mathbf{A})_2(\mathbf{4})_2$ are not available for either anions or solvates, since they are blocked by the carbonyl groups of two complexes **A** from above and from below, which point into the mesh. The chains are joint via slipped Cp...Cp stacking (3.31 Å) that together with different directions of the chains leads to a 3D framework. The counteranions BF_4^- and solvate molecules are located between the chains.

Table S6. $^{31}P\{^1H\}$ and $^{19}F\{^1H\}$ data, minimum and maximum data for selected bond lengths [Å], angles [°] for the complexes **C**, **5**-**8**.

Compd.	$\delta^{31}P$ [ppm]	$\delta^{19}F$ [ppm]	P-P	Cu-P	Cu-Cu	Cu-N	N-Cu-N	N-Cu-P
C	-49.1	−150.6	2.094(2)-2.159(2)	2.2603(15)-2.3849(18)	4.696	2.033 (4)-2.054 (4)	107.91 (17)	106.66 (13)-116.57 (13)
5	-51.5	-150.6 -150.5	2.077 (5)	2.272 (3)-2.275 (3)	4.760	2.039 (11)-2.043 (10)	104.0 (6)-108.9 (7)	108.0 (3)-113.3 (3)
6	-53.4	-150.6 -150.5	2.0858 (18)	2.2702 (14)-2.2989 (15)	4.786	2.033 (4)-2.054 (4)	107.91 (17)	108.72 (13)-116.57 (13)
7	-48.2	-150.9 -150.8	2.0720 (16)	2.2613 (13)-2.2956 (13)	4.713	2.038 (4)-2.045 (4)	109.15 (15)	102.30 (12)-117.36 (13)
8	-48.2	-150.9 -150.8	1.148 (6)	2.2362 (15)-2.3069 (13)	4.676	2.042 (4)-2.062 (3)	97.98 (15)	103.58 (11)-122.13 (11)

DFT calculations

All calculations have been performed with the TURBOMOLE program package[9] at the RI[9]-B3LYP[10]/def2-TZVP[11] level of theory. The geometries were optimized in the gas phase using the Multipole Accelerated Resolution of Identity (MARI-J)[12] approximation during the geometry optimization steps. The solvent effects were incorporated as single point calculations (without the RI approximation) on the gas phase optimized geometries via the Conductor-like Screening Model (COSMO)[13] using the dielectric constant of CH_2Cl_2 (ε = 8.930). For the reaction energies the SCF energies, corrected for the "outlying charge" were used.

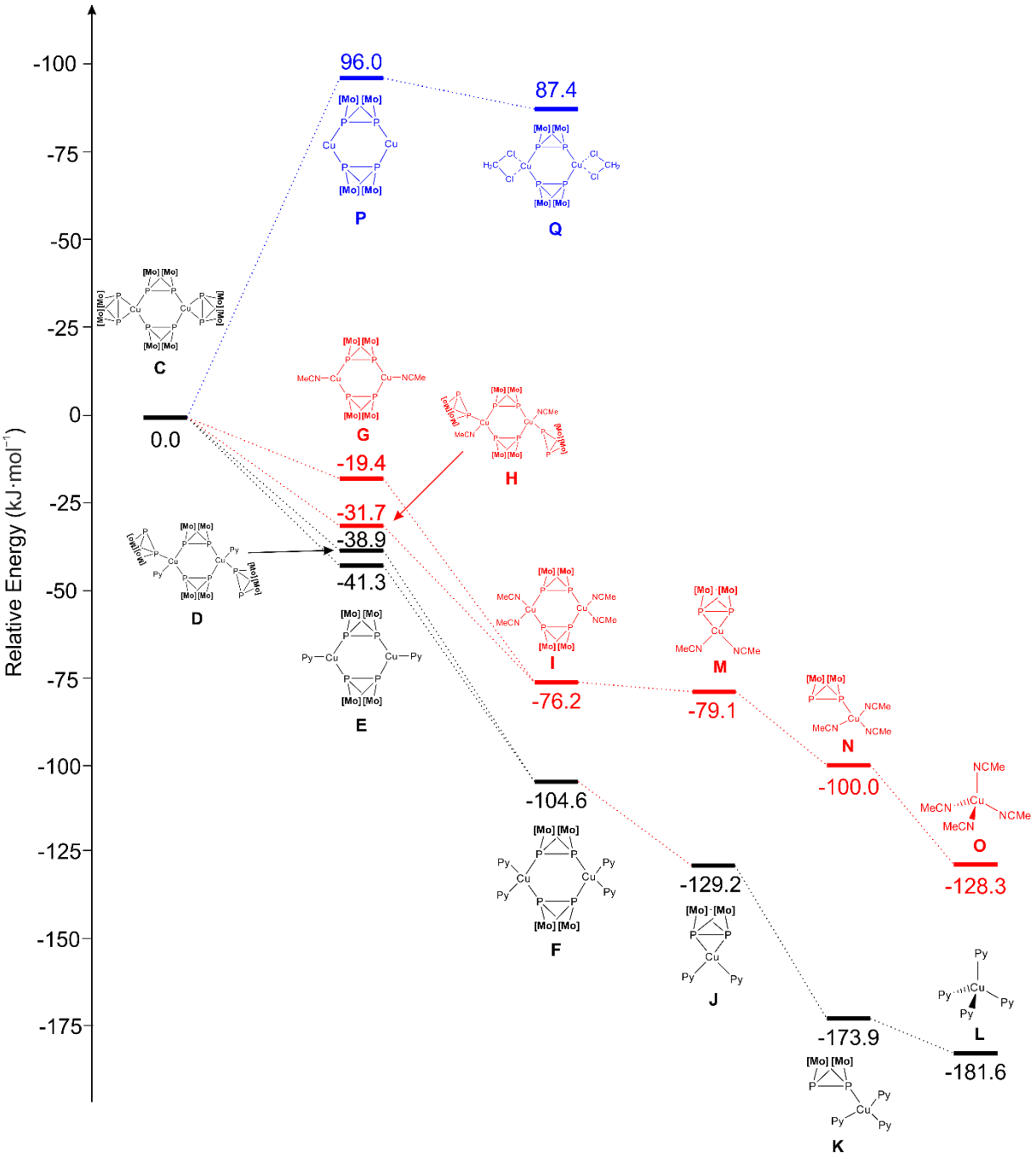

Figure S23*:* Energy profile of the reaction **C** with pyridine, CH_3CN and CH_2Cl_2. Positive charges, ligands added or cleaved are not depicted. Relative energies were calculated at the COSMO (ε=8.930) B3LYP/def2-TZVP level. **[Mo]** = $CpMo(CO)_2$.

Table S7. Cartesian coordinates of the optimized geometry of **C**.

Atom	x	y	z
Mo	-0.3264904	-2.4965863	-2.9013340
Mo	2.0536149	-0.5733682	-3.4677720
Mo	-3.3881681	3.6785692	-4.1955568
Mo	-5.2695370	3.3947766	-1.7311651
Cu	-1.5683765	1.4421752	-1.1297655
P	1.1320881	-1.4190194	-1.2154689
P	-0.0337023	-0.0185693	-2.2428210
P	-2.7905649	3.5314870	-1.7012871
P	-3.5258093	1.7458921	-2.6353320
O	-1.8964321	-0.9473475	-5.1445279
O	-2.8803747	-2.1852202	-1.1091366
O	3.7063384	1.3869704	-1.6545201
O	3.9711624	-2.9435763	-2.7038020
O	-3.0467542	6.6898397	-3.3495600
O	-0.2691622	3.4810622	-4.3483263
O	-7.0002138	1.4805400	-3.5303960
O	-5.3690063	1.1450824	0.4468750
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C	-1.2425251	-4.5645264	-3.4625245
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C	1.0023605	-4.2674323	-3.8738239
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C	2.8977490	-0.9859356	-5.6405543
C	3.4663071	0.2201819	-5.1430496
C	2.4081732	1.1693034	-5.0042687
C	1.2042928	0.5456963	-5.4119032
C	1.5062978	-0.7836836	-5.8128190
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C	-1.9290658	-2.2453664	-1.7396895
C	3.0796986	0.6442126	-2.2513094
C	3.2544652	-2.0779787	-2.9382533
C	-3.3028685	2.6807045	-6.3249313
C	-3.2641746	4.0994738	-6.4893383
C	-4.5188970	4.6141463	-6.0641072
C	-5.3262328	3.5283734	-5.6450771
C	-4.5713982	2.3340643	-5.7994858
C	-6.0434554	5.6661235	-2.0711323
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C	-7.1142114	4.2618405	-0.5976388
C	-5.9463256	4.7759943	0.0452621
C	-5.2883827	5.6369919	-0.8676775
C	-3.1743441	5.5813398	-3.6098606
C	-1.4107190	3.5549539	-4.2434626
C	-6.3278019	2.1604083	-2.9000597
C	-5.2941201	1.9475427	-0.3666210
H	-0.9723401	-5.0114797	-1.2869404
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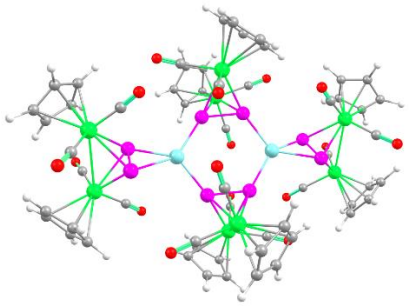

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H	-5.8266737	6.2643084	-2.9393211
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H	-7.8572872	3.6211019	-0.1518802
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Mo	-2.0536383	0.5734857	3.4678536
Mo	3.3881686	-3.6787068	4.1955262
Mo	5.2694604	-3.3947213	1.7310998
Cu	1.5683325	-1.4421073	1.1298619
P	-1.1320715	1.4191329	1.2155596
P	0.0336688	0.0186393	2.2429148
P	2.7904940	-3.5314433	1.7012853
P	3.5257538	-1.7459075	2.6354431
O	1.8964741	0.9473339	5.1445778
O	2.8804199	2.1851640	1.1092501
O	-3.7064375	-1.3866919	1.6545018
O	-3.9710755	2.9438182	2.7039782
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O	0.2691662	-3.4812121	4.3484252
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O	5.3688583	-1.1448335	-0.4467494
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C	1.2426571	4.5645517	3.4626243
C	0.2830199	4.2666807	4.4703543
C	-1.0022292	4.2675289	3.8739651
C	-0.8446016	4.5529204	2.4905664
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C	-3.4663543	-0.2200888	5.1430977
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C	3.2642253	-4.0997879	6.4892800
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C	6.0433780	-5.6661079	2.0708166
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C	7.1140930	-4.2616787	0.5974305
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C	5.2882653	-5.6368484	0.8673914
C	3.1743409	-5.5814321	3.6096928
C	1.4107190	-3.5550850	4.2435109
C	6.3277642	-2.1604746	2.9000908

C	5.2939970	-1.9473657	0.3666778
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H	2.3017127	4.6963958	3.6123375
H	0.4955924	4.1191965	5.5170981
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H	-1.6385241	4.6449606	1.7685027
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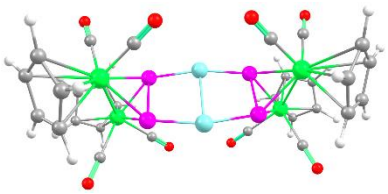
H	-0.2354614	-1.0127075	5.4389108
H	-0.8105660	1.4961663	6.2207524
H	2.5250181	-1.9877583	6.5992011
H	2.4577061	-4.6715287	6.9183299
H	4.8177434	-5.6500964	6.0962455
H	6.3483214	-3.5931630	5.3140263
H	4.9188651	-1.3357877	5.5932154
H	5.8266213	-6.2643823	2.9389500
H	7.9446932	-4.6497462	2.6307213
H	7.8571583	-3.6208994	0.1517131
H	5.6424170	-4.5742443	-1.0597362
H	4.3940942	-6.2050584	0.6723538

ENERGIES [a.u.]:
Total energy = -9918.7916635134
Total energy + OC corr. = -9918.7864197660

Table S8. Cartesian coordinates of the optimized geometry of **P**.

Atom	x	y	z
Mo	-0.5261045	-2.7570301	-3.1039268
Mo	2.0102233	-0.9297257	-3.5487212
Cu	-0.7661148	0.8448208	-0.6399638
P	0.9914889	-1.8311788	-1.4044228
P	-0.1264821	-0.3249574	-2.4912771
O	-1.9912916	-1.1791287	-5.4170630
O	-3.0479846	-2.3510816	-1.2741698
O	3.6627437	0.8069371	-1.5175397
O	3.8416229	-3.4132000	-2.8670554
C	-0.8810316	-4.9986181	-2.5120419
C	-1.5471261	-4.7436501	-3.7498879
C	-0.5468453	-4.4766522	-4.7279895
C	0.7213875	-4.5692971	-4.1032727
C	0.5139327	-4.8853057	-2.7331034
C	2.8828919	-1.3125829	-5.7138063
C	3.5334097	-0.1833960	-5.1391598
C	2.5534475	0.8444486	-4.9835335
C	1.3149042	0.3448494	-5.4568993
C	1.5190865	-0.9853431	-5.9142498
C	-1.4532201	-1.7185148	-4.5683973
C	-2.1258583	-2.4605503	-1.9360297
C	3.0494285	0.1564079	-2.2254098
C	3.1619554	-2.5236476	-3.0850190
H	-1.3541428	-5.2814616	-1.5855278
H	-2.6078430	-4.8133985	-3.9289078
H	-0.7253496	-4.2929433	-5.7755807
H	1.6752720	-4.4739632	-4.5928348



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H	2.7360968	1.8430701	-4.6206985
H	0.3894244	0.8947928	-5.5064356
H	0.7811302	-1.6131454	-6.3832855
Mo	0.5260896	2.7570485	3.1039249
Mo	-2.0102026	0.9297037	3.5487055
Cu	0.7661148	-0.8448097	0.6399459
P	-0.9914898	1.8311799	1.4044144
P	0.1265124	0.3249759	2.4912652
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O	3.0479553	2.3511627	1.2741397
O	-3.6626105	-0.8070901	1.5175508
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C	0.8809926	4.9986516	2.5120762
C	1.5470738	4.7436724	3.7499249
C	0.5467804	4.4766385	4.7280079
C	-0.7214457	4.5692738	4.1032715
C	-0.5139715	4.8853139	2.7331132
C	-2.8829051	1.3125824	5.7137687
C	-3.5333568	0.1833406	5.1391524
C	-2.5533381	-0.8444539	4.9835663
C	-1.3148260	-0.3447728	5.4569247
C	-1.5190823	0.9854234	5.9142297
C	1.4532017	1.7185312	4.5683944
C	2.1258386	2.4606087	1.9360167
C	-3.0493396	-0.1565059	2.2254091
C	-3.1619898	2.5235740	3.0849725
H	1.3541115	5.2815174	1.5855731
H	2.6077864	4.8134397	3.9289625
H	0.7252708	4.2929237	5.7755998
H	-1.6753359	4.4739054	4.5928140
H	-1.2855442	5.0568659	2.0005380
H	-3.3616734	2.2358354	5.9991326
H	-4.5871861	0.0959616	4.9297585
H	-2.7359297	-1.8430972	4.6207618
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H	-0.7811637	1.6132775	6.3832575

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  ENERGIES [a.u.]:
    Total energy            =    -6599.7233882376
    Total energy + OC corr. =    -6599.7181189281
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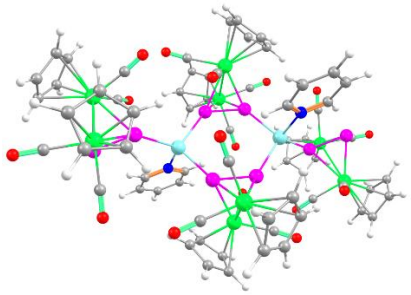
Table S9. Cartesian coordinates of the optimized geometry of **D**.

Atom	x	y	z
Cu	2.4162102	-0.7497163	0.4295194
Mo	-0.2720325	1.7706638	3.6359032
Mo	-0.8559770	-1.2771862	3.6212289
Mo	6.7667950	0.3897100	-0.7567142
Mo	6.1599951	1.6325689	2.0269061
P	0.6965237	-0.0777708	2.0949280
P	-1.2933362	0.4714633	1.7652932
P	4.6231241	0.2338528	0.6770746



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Mo	0.2720387	-1.7708139	-3.6356820
Mo	0.8558876	1.2770234	-3.6211470
Mo	-6.7668555	-0.3897552	0.7566679
Mo	-6.1599241	-1.6321812	-2.0270914
P	-0.6965060	0.0776519	-2.0947339
P	1.2933803	-0.4715230	-1.7651491
P	-4.6230884	-0.2337667	-0.6769472
P	-6.2911608	0.8528401	-1.3437194
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O	-3.8476389	-0.5006043	4.1952070
O	1.4497963	3.5503494	1.7291149
O	2.4047220	1.0620419	5.1142764
N	2.5146132	-2.8778702	0.7223525
C	1.4670446	-3.6516892	0.4010842
O	9.0736007	0.7707208	2.8350075
C	2.5977700	-5.6446976	1.0812638
O	4.9594240	2.6355087	-2.0033180
C	3.6841172	-4.8506722	1.4219126
O	5.2061152	-1.8286740	-2.3113899
C	1.4652766	-5.0288591	0.5621248
C	3.6017222	-3.4790830	1.2273760
C	-1.9806386	2.0456865	5.3328858
C	-2.4503717	2.6581717	4.1397289
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C	9.0849688	-0.1897532	-0.4486370
C	-1.5097050	-2.4118580	2.1277119
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C	8.5301353	1.5575295	-1.8325333
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C	-0.9746988	-2.1427992	5.8283143
C	8.2785067	0.3488504	-2.5374261
C	0.8253686	2.8434787	2.3848427
C	5.5792181	0.6701182	3.6734548
C	4.8792812	3.5801758	1.4426198
O	5.2654553	0.1634511	4.6509323
C	8.0085559	1.0440542	2.5122094
C	1.4336858	1.2653083	4.5397680
C	7.0559635	3.8219538	2.1352894
C	4.9071145	3.4359708	2.8526335
C	6.2575451	3.5867607	3.2896849
O	1.8769155	3.1360780	-1.3187916
O	3.8475238	0.5004421	-4.1952488
O	-1.4497221	-3.5504854	-1.7288249
O	-2.4048659	-1.0624287	-5.1138726
O	-9.0734438	-0.7700984	-2.8352573

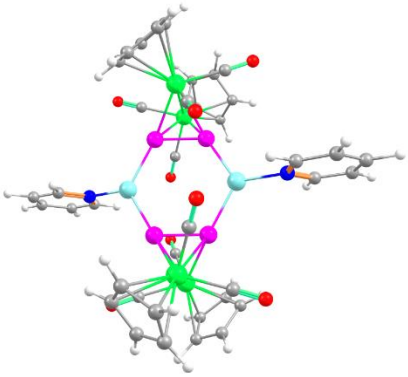
O	-4.9596173	-2.6357033	2.0031789
O	-5.2062464	1.8284668	2.3116512
C	1.9805733	-2.0458979	-5.3327284
C	2.4503695	-2.6583204	-4.1395657
C	-1.0721642	2.1146132	-4.7876736
C	0.5472316	-3.7675221	-4.8125898
C	-9.0321597	-1.2272494	0.5492641
C	0.8061271	-2.7232447	-5.7422581
C	0.9429063	3.2232207	-4.9049882
C	-0.3317780	3.2018272	-4.2612432
C	2.7558858	0.7416879	-3.9442392
C	1.5719334	-3.7224252	-3.8191008
C	-0.2673240	1.4651461	-5.7623383
C	-9.0849920	0.1898355	0.4485360
C	1.5096652	2.4117641	-2.1277021
C	-6.2069085	-3.8251979	-1.0017322
C	-5.7351342	0.9957797	1.7212676
C	-8.6266917	0.7330121	1.6726744
C	-8.5303100	-1.5577033	1.8321669
C	-5.5794304	-1.8039266	1.5092182
C	0.9744606	2.1425561	-5.8282683
C	-8.2786856	-0.3491554	2.5372854
C	-0.8253086	-2.8436088	-2.3845590
C	-5.5789828	-0.6694215	-3.6733984
C	-4.8792462	-3.5798824	-1.4430670
O	-5.2651039	-0.1625269	-4.6507212
C	-8.0084352	-1.0435268	-2.5124206
C	-1.4337595	-1.2655827	-4.5394390
C	-7.0558988	-3.8215415	-2.1358712
C	-4.9070183	-3.4354516	-2.8530604
C	-6.2574289	-3.5861706	-3.2901941
N	-2.5144824	2.8778859	-0.7221961
C	-1.4668458	3.6516312	-0.4009739
C	-2.5974550	5.6447053	-1.0811521
C	-3.6838714	4.8507538	-1.4217524
C	-1.4649899	5.0287991	-0.5620362
C	-3.6015684	3.4791625	-1.2271898
H	-4.4327498	2.8343821	-1.4809157
H	-4.5884126	5.2792528	-1.8317117
H	-2.6310238	6.7180243	-1.2183679
H	-0.5877922	5.5984762	-0.2859759
H	-0.5975739	3.1473020	-0.0057381
H	4.4328591	-2.8342547	1.4811290
H	4.5886782	-5.2791164	1.8318862
H	2.6313963	-6.7180122	1.2184976
H	0.5881056	-5.5985856	0.2860806
H	0.5977236	-3.1474171	0.0058836
H	4.0008383	3.5448233	0.8205763
H	4.0532250	3.2802395	3.4903946
H	6.6027237	3.5827377	4.3105427
H	8.1174834	4.0111231	2.1327508
H	6.5095223	4.0183069	-0.0135156
H	9.3619246	1.9268413	0.1987463
H	9.4494460	-0.7500176	0.3961064
H	8.4023215	2.5536843	-2.2248773
H	7.9448409	0.2666782	-3.5586514
H	8.5880796	-1.7809340	-1.9231090

H	2.4590548	-1.2394042	-5.8604839
H	3.3400187	-2.3879537	-3.5970733
H	0.2325733	-2.5155158	-6.6314626
H	-0.2407374	-4.4992305	-4.8840960
H	1.6851716	-4.4077041	-2.9951135
H	-0.6847462	3.9150272	-3.5346952
H	1.7175434	3.9587877	-4.7629033
H	1.7880045	1.9089414	-6.4963120
H	-0.5659019	0.6337462	-6.3768728
H	-2.0841464	1.8509338	-4.5294432
H	-0.2326994	2.5152402	6.6317304
H	0.2407177	4.4990222	4.8844698
H	-1.6851035	4.4076024	2.9953916
H	-3.3400009	2.3878340	3.5971878
H	-2.4591556	1.2391775	5.8605876
H	-1.7882782	-1.9092062	6.4963230
H	-1.7177347	-3.9589903	4.7628419
H	0.5656489	-0.6340244	6.3770652
H	2.0839929	-1.8511697	4.5296857
H	0.6846297	-3.9152180	3.5347830
H	-4.0008325	-3.5446500	-0.8209739
H	-4.0531059	-3.2796214	-3.4907663
H	-6.6025649	-3.5819726	-4.3110659
H	-8.1174218	-4.0106953	-2.1334031
H	-6.5095500	-4.0182331	0.0129250
H	-8.4025496	-2.5539316	2.2243421
H	-9.3619833	-1.9266362	-0.1992276
H	-9.4493923	0.7502591	-0.3961360
H	-8.5881316	1.7807457	1.9233092
H	-7.9450751	-0.2671721	3.5585440

```
  ENERGIES [a.u.]:
    Total energy            =   -10415.2687684366
    Total energy + OC corr. =   -10415.2632382259
```

Table S10. Cartesian coordinates of the optimized geometry of **E**.

Atom	x	y	z
Mo	3.1829676	0.6078542	2.3466042
Mo	0.6759189	-0.3596793	3.9292186
Cu	-0.8600106	2.0110030	0.4495462
P	0.8154972	1.0850192	1.7998884
P	1.2729018	-0.9530361	1.6000462
O	4.3693251	-2.2815006	2.7504582
O	3.9664701	0.3238242	-0.6745570
O	0.3957601	2.5897118	4.9971424
O	-2.3820016	-0.2279335	3.2551132
C	3.7382702	1.9852779	4.2584857
C	4.8764458	1.2324826	3.8780058
C	5.2609288	1.6355776	2.5683892
C	4.3416769	2.6411231	2.1406258
C	3.4033763	2.8497284	3.1815330
C	3.9024607	-1.2470450	2.6004210
C	3.6313353	0.4105032	0.4161843
C	1.2996441	-0.8289163	6.1640565
C	2.1814589	-1.5976316	5.3650619



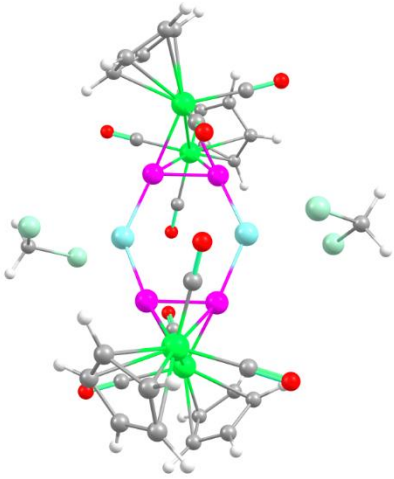
C	1.4056430	-2.5373134	4.6340753
C	0.0460691	-2.3588122	4.9906436
C	-0.0260759	-1.2967021	5.9424702
C	0.5100477	1.5318185	4.5747277
C	-1.2550674	-0.2615912	3.4510406
H	3.2462112	1.9469808	5.2148438
H	5.3972963	0.5165657	4.4936296
H	6.1282762	1.2936366	2.0276687
H	4.3850679	3.1813558	1.2088373
H	2.6013210	3.5689714	3.1770935
H	1.5859513	-0.0586233	6.8622626
H	3.2547153	-1.5187223	5.3534809
H	1.7912480	-3.2836116	3.9595725
H	-0.7835733	-2.9527334	4.6429098
H	-0.9128322	-0.9573026	6.4524380
Cu	0.8602832	-2.0108267	-0.4495973
P	-1.2729105	0.9532245	-1.6005245
N	-2.0448357	3.5280334	1.1178215
Mo	-3.1830267	-0.6077110	-2.3467195
Mo	-0.6759654	0.3593759	-3.9294885
P	-0.8155611	-1.0847766	-1.7998471
C	-3.7384407	-1.9854611	-4.2582949
C	-4.8765234	-1.2323560	-3.8781281
C	-5.2612450	-1.6351083	-2.5684698
C	-4.3422604	-2.6407600	-2.1404030
C	-3.4038704	-2.8497839	-3.1811391
C	-3.9025282	1.2471172	-2.6006069
C	-3.6314122	-0.4101061	-0.4162521
C	-1.3003129	0.8280649	-6.1642050
C	-2.1816729	1.5972291	-5.3651459
C	-1.4054040	2.5369322	-4.6346739
C	-0.0459933	2.3580142	-4.9916621
C	0.0255893	1.2956210	-5.9432162
C	-0.5100191	-1.5323184	-4.5743586
C	1.2550118	0.2615209	-3.4512349
N	2.0452061	-3.5275720	-1.1176777
O	-4.3694692	2.2815482	-2.7505978
O	-3.9667261	-0.3232346	0.6744144
O	-0.3957060	-2.5903726	-4.9963734
O	2.3819557	0.2280776	-3.2553143
H	-3.2462347	-1.9474573	-5.2145882
H	-5.3971413	-0.5164618	-4.4939731
H	-6.1285584	-1.2928583	-2.0278899
H	-4.3858889	-3.1807895	-1.2085068
H	-2.6019755	-3.5692046	-3.1764683
H	-1.5870456	0.0576323	-6.8620817
H	-3.2549422	1.5185913	-5.3532169
H	-1.7906302	3.2835563	-3.9603145
H	0.7839067	2.9518423	-4.6443844
H	0.9121131	0.9558717	-6.4533535
C	-1.7292763	4.8109656	0.8719536
C	-3.1642295	3.2745872	1.8172609
C	-2.5062887	5.8708709	1.3079020
H	-0.8228180	4.9874215	0.3066218
C	-3.6621052	5.6025893	2.0304460
C	-3.9941735	4.2790223	2.2880217
H	-4.2906838	6.4089851	2.3852229

H	-4.8836271	4.0207244	2.8461301
H	-3.3964422	2.2335759	2.0019678
C	1.7309658	-4.8104177	-0.8696526
C	3.1634269	-3.2742141	-1.8190180
C	2.5081521	-5.8703154	-1.3053030
H	0.8254251	-4.9868143	-0.3028346
C	3.6627448	-5.6021257	-2.0298435
C	3.9934651	-4.2786526	-2.2896144
H	4.2914280	-6.4085180	-2.3844471
H	4.8819636	-4.0204184	-2.8492734
H	3.3946507	-2.2332763	-2.0053662
H	-2.2063659	6.8850852	1.0825173
H	2.2092982	-6.8844487	-1.0781371

ENERGIES [a.u.]:
Total energy = -7096.2378770909
Total energy + OC corr. = -7096.2324007340

Table S11. Cartesian coordinates of the optimized geometry of **Q**.

Atom	x	y	z
Mo	-0.5805847	-2.6565041	-3.0569569
Mo	2.0132843	-0.9376895	-3.4348171
Cu	-1.1607667	1.2534512	-0.9495391
P	0.8951878	-1.7747744	-1.2865853
P	-0.0920728	-0.2415633	-2.3524071
O	-1.9507361	-0.9152530	-5.3004140
O	-3.1280666	-2.2016053	-1.2808870
O	3.7167943	0.7203815	-1.3854764
O	3.7024426	-3.4780338	-2.6373781
C	-1.0241036	-4.9011564	-2.5307034
C	-1.6530611	-4.5920363	-3.7748263
C	-0.6226680	-4.3332725	-4.7231567
C	0.6273063	-4.4874692	-4.0741955
C	0.3785423	-4.8306887	-2.7177386
C	2.8989782	-1.3695251	-5.5840924
C	3.5911611	-0.2667536	-5.0073023
C	2.6562217	0.8040005	-4.8718643
C	1.4034518	0.3581994	-5.3609320
C	1.5547350	-0.9821661	-5.8083798
C	-1.4399903	-1.5182020	-4.4736420
C	-2.1854048	-2.3246605	-1.9138785
C	3.0705296	0.1018988	-2.0955981
C	3.0675603	-2.5642000	-2.9013988
H	-1.5280957	-5.1876807	-1.6218422
H	-2.7112571	-4.6193590	-3.9778199
H	-0.7713946	-4.1149448	-5.7686512
H	1.5947121	-4.4117579	-4.5397145
H	1.1273963	-5.0440432	-1.9730738
H	3.3396871	-2.3155390	-5.8555321
H	4.6441970	-0.2255106	-4.7811311
H	2.8779356	1.7943033	-4.5081825
H	0.5034407	0.9470507	-5.4244534
H	0.7959480	-1.5792040	-6.2839314
Mo	0.5808125	2.6564408	3.0570210
Mo	-2.0132089	0.9379527	3.4351732

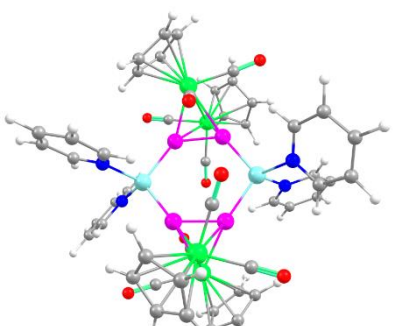


Cu	1.1604041	-1.2538202	0.9502013
P	-0.8947456	1.7740708	1.2868429
P	0.0922759	0.2411489	2.3533725
O	1.9497363	0.9162564	5.3020472
O	3.1287819	2.2000680	1.2820583
O	-3.7170793	-0.7200478	1.3860323
O	-3.7017955	3.4783258	2.6366681
C	1.0236871	4.9007546	2.5290687
C	1.6536300	4.5925436	3.7729301
C	0.6240050	4.3342590	4.7222056
C	-0.6264930	4.4878041	4.0741233
C	-0.3788044	4.8301789	2.7172474
C	-2.8991338	1.3704626	5.5842784
C	-3.5914449	0.2677222	5.0075842
C	-2.6567092	-0.8032544	4.8725088
C	-1.4039292	-0.3576214	5.3617195
C	-1.5550081	0.9828683	5.8088713
C	1.4394899	1.5188216	4.4746902
C	2.1859279	2.3236527	1.9146579
C	-3.0706116	-0.1016874	2.0960715
C	-3.0671118	2.5644774	2.9011317
H	1.5269243	5.1868127	1.6196448
H	2.7119658	4.6201140	3.9751566
H	0.7735845	4.1165292	5.7677055
H	-1.5935363	4.4122493	4.5404238
H	-1.1282698	5.0429875	1.9730422
H	-3.3397214	2.3166086	5.8554524
H	-4.6444683	0.2266577	4.7813156
H	-2.8785849	-1.7936065	4.5090577
H	-0.5040448	-0.9466369	5.4255202
H	-0.7961586	1.5798317	6.2844165
C	-3.5718392	3.0901467	-2.5084634
Cl	-1.8746116	3.6411357	-2.4316568
Cl	-3.7835892	1.5179435	-1.6750327
H	-3.8427969	2.9581573	-3.5490907
H	-4.1931349	3.8226361	-2.0072540
C	3.5713199	-3.0918305	2.5083215
Cl	1.8744555	-3.6434098	2.4287535
Cl	3.7841842	-1.5196014	1.6751486
H	3.8406106	-2.9596878	3.5493610
H	4.1937264	-3.8241068	2.0081742

```
  ENERGIES [a.u.]:
    Total energy            =    -8518.9690244703
    Total energy + OC corr. =    -8518.9643258092
```

Table S12. Cartesian coordinates of the optimized geometry of **F**.

Atom	x	y	z
Mo	3.0402559	0.8098872	2.3222763
Mo	0.6504993	-0.4351053	3.8328466
Cu	-1.0327764	2.1294779	0.4843300
P	0.6336963	1.0880822	1.7376819
P	1.2855000	-0.8931686	1.4667031



O	4.4313809	-1.9913566	2.6220487
O	3.9240060	0.6811840	-0.6805103
O	0.1093933	2.4511384	4.9498221
O	-2.4176320	-0.5210826	3.2054569
N	-2.6705310	2.6089503	1.6534027
C	3.4406459	2.1541005	4.2821653
C	4.6485700	1.5059412	3.8952031
C	5.0198217	1.9860097	2.5998128
C	4.0200951	2.9300739	2.1868432
C	3.0475721	3.0282157	3.2231433
C	3.8708848	-0.9782423	2.5066985
C	3.5338601	0.7018760	0.4109465
C	1.3165769	-0.9011080	6.0427866
C	2.2582698	-1.5794534	5.2169834
C	1.5543573	-2.5630843	4.4574526
C	0.1790994	-2.5016089	4.8237841
C	0.0250350	-1.4709893	5.8112818
C	0.3262267	1.4036537	4.4919073
C	-1.2712848	-0.4684517	3.3693561
C	-5.0296913	2.5124037	2.1376552
C	-4.8591992	3.3373604	3.2495528
C	-3.5744979	3.7915232	3.5511903
C	-2.5153540	3.4076931	2.7339471
C	-3.9179067	2.1726885	1.3718284
H	2.9320846	2.0388618	5.2326366
H	5.2203600	0.8072994	4.4989633
H	5.9228178	1.7277159	2.0555673
H	4.0325359	3.5039550	1.2656298
H	2.1810636	3.6811235	3.2277280
H	1.5443181	-0.1219138	6.7642951
H	3.3289939	-1.4102675	5.2003442
H	1.9988804	-3.2603627	3.7550881
H	-0.6093421	-3.1522974	4.4589265
H	-0.8920931	-1.2114356	6.3307339
H	-5.7102100	3.6205703	3.8694138
H	-3.3872042	4.4352921	4.4099681
H	-1.4993330	3.7430488	2.9434558
H	-4.0157882	1.5295858	0.4983050
Cu	1.0297367	-2.1259161	-0.4943229
P	-1.4542006	0.8083412	-1.3817587
N	-0.3583280	3.9812048	-0.2198733
Mo	-2.9019841	-1.0961240	-2.4027901
Mo	-0.8107459	0.7169909	-3.7768517
P	-0.4849196	-1.0009643	-1.8515637
C	-3.0857232	-2.2023876	-4.5325580
C	-4.3871391	-1.8697445	-4.0583728
C	-4.6197945	-2.5906103	-2.8448031
C	-3.4421445	-3.3651220	-2.5710019
C	-2.4983597	-3.1210178	-3.6091392
C	-4.0745626	0.4995190	-2.2954913
C	-3.2759436	-1.4125774	-0.4894634
C	-1.6135345	1.2462197	-5.9263400
C	-2.6638409	1.6017170	-5.0321145
C	-2.1824187	2.6353843	-4.1709500
C	-0.8386944	2.9266678	-4.5416742
C	-0.4787256	2.0666094	-5.6337198
C	-0.0743514	-0.9251282	-4.6099993

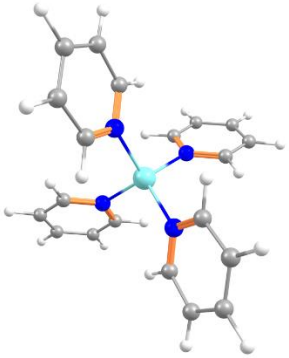
C	1.0318026	1.1915435	-3.2475206
N	2.8590513	-2.5834885	-1.3441193
N	0.1923569	-3.9969882	-0.0713200
O	-4.8259060	1.3865865	-2.2478571
O	-3.5626528	-1.6861007	0.6010870
O	0.3707438	-1.8450041	-5.1661815
O	2.1114133	1.5502555	-3.0188671
C	3.1857991	-2.2250255	-2.6051635
C	3.7719130	-3.2875848	-0.6366469
H	-2.6364918	-1.8573375	-5.4569607
H	-5.1030919	-1.2218353	-4.5556997
H	-5.5404659	-2.5959941	-2.2697852
H	-3.3118580	-4.0505795	-1.7393439
H	-1.5199034	-3.5796781	-3.7062700
H	-1.6752629	0.5155640	-6.7276131
H	-3.6687693	1.1949043	-5.0350534
H	-2.7559773	3.1346015	-3.3970272
H	-0.2088975	3.6950522	-4.1041856
H	0.4607558	2.0772258	-6.1773980
C	5.0128566	-3.6516608	-1.1509191
C	5.3389527	-3.2785652	-2.4556003
C	4.4045903	-2.5514707	-3.1933280
H	6.3025174	-3.5489047	-2.8881719
H	4.6108136	-2.2363609	-4.2155697
H	2.4349420	-1.6570271	-3.1527314
H	3.4873132	-3.5614731	0.3795609
C	0.8929984	4.1460393	-0.7017318
C	-1.1788644	5.0542275	-0.2244202
C	1.3607694	5.3635256	-1.1909600
H	1.5305830	3.2615102	-0.6928633
C	0.5072341	6.4682616	-1.1863604
C	-0.7882981	6.3061473	-0.6939207
H	0.8446810	7.4356525	-1.5593391
H	-1.4932412	7.1367086	-0.6697397
H	-2.1840898	4.8918781	0.1663791
C	-0.8062893	-4.1432413	0.8266725
C	0.6264990	-5.1036274	-0.7128311
C	-1.3916781	-5.3744320	1.1129329
H	-1.1412815	-3.2322831	1.3236413
C	-0.9325309	-6.5134114	0.4489356
C	0.0962308	-6.3710325	-0.4830488
H	-1.3677915	-7.4919701	0.6533897
H	0.4891915	-7.2285975	-1.0285106
H	1.4304894	-4.9558986	-1.4348667
H	-6.0117987	2.1315189	1.8598209
H	2.3799654	5.4383594	-1.5695877
H	5.7082852	-4.2174602	-0.5318328
H	-2.1958914	-5.4333759	1.8460623

```
  ENERGIES [a.u.]:
    Total energy            =    -7596.1076096115
    Total energy + OC corr. =    -7596.1022451337
```

Table S13. Cartesian coordinates of the optimized geometry of **G**.

Atom	x	y	z

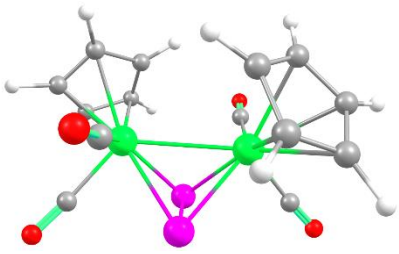
Cu	0.0014887	0.0012940	-0.0003740
N	1.8479997	-0.5335972	-0.8953553
N	-0.9221308	-1.8199013	0.5737735
C	2.2825306	0.0593914	-2.0173699
C	2.6307934	-1.4751535	-0.3460464
C	3.8537678	-1.8503634	-0.8817237
C	4.2953299	-1.2285417	-2.0423522
C	3.4909147	-0.2551498	-2.6204943
H	5.2445845	-1.4976094	-2.4873112
H	3.7893763	0.2556749	-3.5259869
H	1.6312088	0.8109484	-2.4455404
H	2.2547607	-1.9447678	0.5547268
C	-1.5337378	-1.9540224	1.7600705
C	-0.9235550	-2.8792082	-0.2501703
C	-2.1600955	-3.1245448	2.1606832
H	-1.5139991	-1.0884026	2.4102284
C	-2.1589951	-4.2140120	1.2993632
C	-1.5265148	-4.0865318	0.0695471
H	-2.6390818	-5.1422800	1.5809626
H	-1.4963935	-4.9066186	-0.6351384
H	-0.4167521	-2.7489055	-1.1985692
H	4.4427107	-2.6158917	-0.3947562
H	-2.6366501	-3.1750911	3.1303632
N	-1.2211633	1.0858498	-1.3518411
C	-0.9866673	2.3834382	-1.6014489
C	-2.2444438	0.5039206	-1.9949956
C	-1.7457554	3.1334720	-2.4872608
C	-3.0544890	1.1789355	-2.8955900
C	-2.8014278	2.5206724	-3.1496325
H	-0.1602663	2.8326378	-1.0642686
H	-2.4181150	-0.5414389	-1.7726194
H	-1.5096359	4.1765564	-2.6492769
H	-3.8667019	0.6577786	-3.3840985
H	-3.4143167	3.0767634	-3.8471958
N	0.2981587	1.2697695	1.6726083
C	-0.7209310	1.9719418	2.1916588
C	1.4991602	1.3919658	2.2574390
C	-0.5845327	2.8025369	3.2938891
C	1.7246395	2.2001365	3.3614983
C	0.6627323	2.9201638	3.8932278
H	-1.6785627	1.8626234	1.6974155
H	2.3069989	0.8209648	1.8173060
H	-1.4422740	3.3442424	3.6692053
H	2.7156083	2.2604173	3.7907814
H	0.8044247	3.5599361	4.7546686



ENERGIES [a.u.]:
Total energy = -2633.3233206540
Total energy + OC corr. = -2633.3200145458

Table S14. Cartesian coordinates of the optimized geometry of **A**.

Atom	x	y	z
Mo	-1.5559117	0.0069760	0.5627777
Mo	1.5450011	0.0355811	0.5903500
P	-0.1014059	-0.9509053	2.3433128

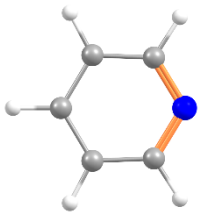


P	0.0584393	1.1212438	2.2682024
O	-3.5539242	0.9665254	2.7784009
O	3.5006702	-0.7570687	2.9074333
O	-1.3936560	2.9857481	-0.3975426
O	1.3989772	-3.0060285	-0.1504782
C	-1.4078539	1.9016248	-0.0066421
C	-2.7806282	0.6360565	1.9977310
C	1.4064083	-1.8960040	0.1595571
C	2.7422922	-0.4854632	2.0902803
C	-3.1897906	-1.6541534	0.1882583
H	-3.8314388	-1.9907621	0.9863549
C	-1.9637984	-2.2476329	-0.1966415
H	-1.5029277	-3.1072839	0.2599873
C	-1.4590155	-1.5271671	-1.3131714
H	-0.5573355	-1.7551500	-1.8545987
C	-2.3696635	-0.4837465	-1.6116833
H	-2.2787171	0.2245844	-2.4194398
C	-3.4486431	-0.5568100	-0.6886788
H	-4.3253070	0.0696120	-0.6840515
C	1.9689463	2.2284682	-0.3251941
H	1.5003623	3.1191554	0.0582383
C	3.1870178	1.6655529	0.1251271
H	3.8139241	2.0602499	0.9081661
C	3.4611270	0.5067462	-0.6636878
H	4.3369665	-0.1172640	-0.5966977
C	2.3994219	0.3654253	-1.5987278
H	2.3229700	-0.4004951	-2.3537152
C	1.4843292	1.4275605	-1.3948497
H	0.5931639	1.6148245	-1.9683777

```
  ENERGIES [a.u.]:
    Total energy            =    -1659.5155691591
    Total energy + OC corr. =    -1659.5158776158
```

Table S15. Cartesian coordinates of the optimized geometry of pyridine.

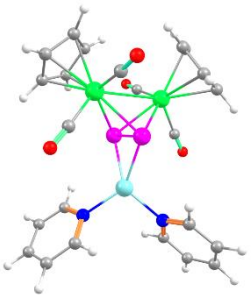
Atom	x	y	z
C	0.0000000	0.0000000	-1.1904960
C	-1.1939104	0.0000000	-0.4809940
C	-1.1396955	0.0000000	0.9089368
N	0.0000000	0.0000000	1.6012270
C	1.1396955	0.0000000	0.9089368
C	1.1939104	0.0000000	-0.4809940
H	0.0000000	0.0000000	-2.2736241
H	-2.1495526	0.0000000	-0.9894902
H	-2.0547335	0.0000000	1.4929940
H	2.0547335	0.0000000	1.4929940
H	2.1495526	0.0000000	-0.9894902



```
  ENERGIES [a.u.]:
    Total energy            =     -248.2308381719
    Total energy + OC corr. =     -248.2309957123
```

Table S16. Cartesian coordinates of the optimized geometry of **L**.

Atom	x	y	z
Mo	0.4418213	-1.4346952	2.1810316
Mo	2.4336333	-1.0290349	-0.1814003
Cu	-1.1369483	0.9732167	-0.7912543
P	-0.0400380	-1.1265678	-0.3286726
P	0.6678698	0.5877299	0.7639565
O	0.0356331	-4.3715040	1.1344482
O	-2.6764927	-1.1139326	2.2079764
O	4.0846037	0.8425717	1.7307840
O	2.5088979	1.2558115	-2.3265039
C	0.2732704	-0.6011488	4.3744468
C	0.2428627	-2.0282513	4.4279264
C	1.5170955	-2.4993923	4.0073130
C	2.3273964	-1.3779725	3.7027704
C	1.5564667	-0.2051356	3.9240661
C	3.1603044	-3.3219778	0.1153192
C	4.2969213	-2.4800077	0.0369922
C	4.3215454	-1.8822504	-1.2531942
C	3.1825994	-2.3607565	-1.9702824
C	2.4686323	-3.2435128	-1.1233827
C	0.1843234	-3.2844264	1.4685017
C	-1.5382766	-1.2315024	2.1550107
C	3.4401887	0.1796740	1.0519984
C	2.4547834	0.4451200	-1.5190326
H	-0.5263331	0.0592683	4.6682393
H	-0.5741990	-2.6355733	4.7811474
H	1.8247548	-3.5320970	3.9686918
H	3.3594263	-1.4072684	3.3987967
H	1.9020314	0.8081758	3.8045038
H	2.8910934	-3.9450914	0.9505274
H	5.0403314	-2.3465871	0.8065031
H	5.0920894	-1.2353401	-1.6391063
H	2.9350175	-2.1253700	-2.9925875
H	1.5771159	-3.7896124	-1.3831757
N	-2.5780023	2.1838642	0.0943923
C	-3.8717275	2.0428953	-0.2332799
C	-2.2562081	3.1138110	1.0063638
C	-4.8776410	2.8107835	0.3310980
C	-3.1996194	3.9282508	1.6126856
C	-4.5369703	3.7741787	1.2715992
H	-4.1023676	1.2867052	-0.9729262
H	-1.2053381	3.1995211	1.2526998
H	-5.9054248	2.6520341	0.0345666
H	-2.8856057	4.6659145	2.3385754
H	-5.2984800	4.3922199	1.7294391
N	-1.3760035	1.2023998	-2.8446952
C	-1.3447624	2.4260509	-3.3948574
C	-1.5548576	0.1499693	-3.6573775
C	-1.4851896	2.6413626	-4.7564522
C	-1.7111848	0.2787439	-5.0284812
C	-1.6738733	1.5477367	-5.5913818
H	-1.2011590	3.2567815	-2.7156204
H	-1.5704030	-0.8236048	-3.1838109
H	-1.4469148	3.6486877	-5.1479942

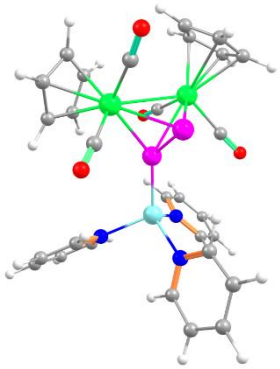


H	-1.8573312	-0.6027938	-5.6377428
H	-1.7893574	1.6819286	-6.6591588

ENERGIES [a.u.]:
Total energy = -3796.3670245090
Total energy + OC corr. = -3796.3639158288

Table S17. Cartesian coordinates of the optimized geometry of **M**.

Atom	x	y	z
Mo	0.9483645	0.2245688	2.9956542
Mo	2.9958206	0.4427695	0.6643485
Cu	-1.2071593	0.0771111	-1.0318264
P	0.5352280	0.3700991	0.4579003
P	1.1580102	2.1286081	1.4016329
O	0.5098595	-2.7599014	2.1309706
O	-2.1648230	0.5918689	2.9506009
O	4.5052403	2.6248055	2.3477192
O	3.0175506	2.3972018	-1.7862745
C	0.7505629	1.2552841	5.1076404
C	0.7375343	-0.1612194	5.2886743
C	2.0200160	-0.6515910	4.9180803
C	2.8171782	0.4496817	4.5184083
C	2.0300863	1.6281375	4.6308365
C	3.7527327	-1.7781669	1.2662678
C	4.8743508	-0.9220261	1.1441004
C	4.9544358	-0.4806084	-0.2060795
C	3.8645001	-1.0703997	-0.9148729
C	3.1240791	-1.8643734	-0.0054964
C	0.6755428	-1.6534700	2.4058761
C	-1.0263644	0.4573865	2.9215865
C	3.9081916	1.8514027	1.7452452
C	2.9833073	1.7193627	-0.8619028
H	-0.0607622	1.9288610	5.3315670
H	-0.0746297	-0.7445148	5.6901708
H	2.3414365	-1.6792185	4.9744308
H	3.8512153	0.4080611	4.2228157
H	2.3614585	2.6315134	4.4216438
H	3.4518687	-2.3034655	2.1560927
H	5.5734529	-0.6779022	1.9278083
H	5.7299584	0.1372566	-0.6278420
H	3.6646633	-0.9624871	-1.9684328
H	2.2561719	-2.4570716	-0.2405971
N	-2.8103798	-1.0941207	-0.2744591
C	-2.6043445	-2.3169309	0.2382105
C	-4.0603514	-0.6095260	-0.2490157
C	-3.6203028	-3.0901958	0.7790165
C	-5.1335767	-1.3144339	0.2740837
C	-4.9120490	-2.5810198	0.7978924
H	-1.5852162	-2.6813387	0.2221672
H	-4.1983351	0.3823498	-0.6595231
H	-3.3944356	-4.0689828	1.1799793
H	-6.1204122	-0.8717895	0.2705748
H	-5.7277095	-3.1572461	1.2153104

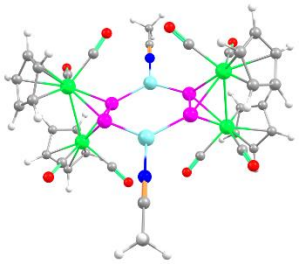


N	-0.5634010	-0.8095366	-2.8828878
C	-1.0526427	-1.9743944	-3.3299022
C	0.3555311	-0.1863946	-3.6354340
C	-0.6494476	-2.5558934	-4.5231099
C	0.8134260	-0.6953301	-4.8417824
C	0.3029509	-1.9047211	-5.2960289
H	-1.7976549	-2.4529243	-2.7063813
H	0.7313375	0.7547527	-3.2538200
H	-1.0788726	-3.4982692	-4.8353920
H	1.5532615	-0.1478663	-5.4101797
H	0.6384059	-2.3293842	-6.2334779
N	-2.0663522	1.9191895	-1.7239602
C	-2.7444372	1.9551371	-2.8808943
C	-1.9561444	3.0597867	-1.0280760
C	-3.3314427	3.1085093	-3.3780370
C	-2.5120537	4.2579810	-1.4523360
C	-3.2140615	4.2855434	-2.6496065
H	-2.8129579	1.0217817	-3.4260121
H	-1.3931281	3.0051531	-0.1052964
H	-3.8661288	3.0791348	-4.3178504
H	-2.3894478	5.1488115	-0.8513428
H	-3.6587053	5.2046037	-3.0091762

ENERGIES [a.u.]:
Total energy = -4044.6065239058
Total energy + OC corr. = -4044.6034381387

Table S18. Cartesian coordinates of the optimized geometry of **H**.

Atom	x	y	z
Mo	-0.7732099	-2.3626126	-3.1198463
Mo	2.0647026	-1.0659028	-3.2399527
Cu	-1.1408656	1.5898188	-1.0825238
P	0.6698667	-1.7765831	-1.1968990
P	0.0256723	-0.0774559	-2.2447970
O	-1.6289284	-0.3410395	-5.3776366
O	-3.3892663	-1.5039297	-1.6166099
O	3.9147215	0.1011080	-0.9914787
O	3.2252692	-3.8900745	-2.4699636
C	-1.6091715	-4.5183252	-2.7055509
C	-2.0886131	-4.0811549	-3.9775739
C	-0.9649764	-3.9702897	-4.8443388
C	0.1938655	-4.3425755	-4.1192559
C	-0.2037389	-4.6733208	-2.7956881
C	3.0384874	-1.5261483	-5.3460281
C	3.8452175	-0.5767378	-4.6575889
C	3.0793296	0.6208160	-4.5222437
C	1.8150699	0.4037783	-5.1238314
C	1.7921666	-0.9199597	-5.6400386
C	-1.2944089	-1.0500650	-4.5427910
C	-2.4083498	-1.7815678	-2.1332384
C	3.1991247	-0.3233392	-1.7750190
C	2.7727459	-2.8704012	-2.7291362
H	-2.2166627	-4.7384268	-1.8426904



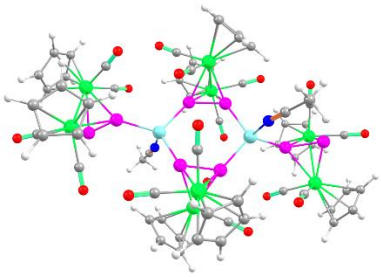
H	-3.1198387	-3.9295647	-4.2517859
H	-1.0002947	-3.7029954	-5.8884066
H	1.1918709	-4.4128451	-4.5158686
H	0.4462748	-5.0219563	-2.0104670
H	3.3463433	-2.5165962	-5.6409509
H	4.8706950	-0.7144198	-4.3558647
H	3.4215413	1.5436123	-4.0825197
H	1.0234851	1.1291561	-5.2126369
H	0.9893968	-1.3660425	-6.2011156
Mo	0.7018094	2.4927896	3.0549888
Mo	-1.9994803	0.9535340	3.3357767
Cu	1.1376331	-1.5851087	1.0913175
P	-0.7733818	1.7449255	1.2183157
P	0.0683677	0.1304223	2.2605835
O	1.9302644	0.5803285	5.2357177
O	3.2505263	1.9820908	1.2973803
O	-3.7666277	-0.6044205	1.2630035
O	-3.5019316	3.5934482	2.5019149
C	1.2812155	4.7258982	2.6079776
C	1.8703426	4.3422219	3.8507710
C	0.8111149	4.1125945	4.7739199
C	-0.4167660	4.3579662	4.1111228
C	-0.1258799	4.7294665	2.7704675
C	-2.8943563	1.4162071	5.4749145
C	-3.6431506	0.3642198	4.8753382
C	-2.7738156	-0.7608781	4.7441365
C	-1.5045754	-0.3987112	5.2580512
C	-1.5806288	0.9442477	5.7170172
C	1.4669401	1.2469289	4.4280630
C	2.3021278	2.1154507	1.9200149
C	-3.0904742	-0.0181110	1.9729249
C	-2.9307909	2.6404917	2.7795538
H	1.8163591	5.0099360	1.7163284
H	2.9247105	4.3016767	4.0703494
H	0.9294088	3.8517332	5.8134982
H	-1.3949109	4.3217964	4.5584078
H	-0.8492212	5.0061618	2.0215501
H	-3.2801725	2.3854617	5.7477714
H	-4.6923710	0.3905262	4.6303838
H	-3.0497595	-1.7313577	4.3644960
H	-0.6428457	-1.0414781	5.3284330
H	-0.7942153	1.4886320	6.2102967
N	-2.4836810	2.7087369	-2.0012255
C	-3.2888978	3.3360176	-2.5256259
C	-4.3066338	4.1276700	-3.1874893
H	-3.8695009	5.0568938	-3.5559255
H	-4.7208791	3.5700279	-4.0286240
H	-5.1072641	4.3635786	-2.4850311
N	2.4927814	-2.7416356	1.9428013
C	3.3046014	-3.3895595	2.4306459
C	4.3306164	-4.2070101	3.0467859
H	3.8698514	-5.0515583	3.5612940
H	5.0130208	-4.5832069	2.2833396
H	4.8929987	-3.6130047	3.7686047

ENERGIES [a.u.]:

```
Total energy            =    -6865.2453565826
Total energy + OC corr. =    -6865.2400973697
```

Table S19. Cartesian coordinates of the optimized geometry of **I**.

Atom	x	y	z
Cu	2.4356401	-0.6167777	0.3381259
Mo	-0.1906370	1.7189123	3.5509297
Mo	-0.7737473	-1.3364238	3.6153884
Mo	6.7471232	0.7135739	-0.7503711
Mo	6.2170110	1.4101690	2.2280108
P	0.7416705	-0.1629451	2.0402007
P	-1.2552065	0.3732054	1.7482226
P	4.6374479	0.3253487	0.6715538
P	6.2807187	-0.9117613	1.0837507
Cu	-2.3542184	0.5154541	-0.4119161
Mo	0.4343634	-2.0143419	-3.5170340
Mo	0.5444650	1.0762184	-3.7794902
Mo	-6.8026479	-0.1652812	0.6958012
Mo	-6.2522152	-1.4755376	-2.0682946
P	-0.7323797	-0.1997523	-2.0901053
P	1.3326715	-0.4222611	-1.8297577
P	-4.6171998	-0.2760038	-0.6625234
P	-6.0997981	1.0190753	-1.3818782
O	-1.9181084	-3.2101586	1.3775818
O	-3.7515470	-0.5316138	4.2291926
O	1.3971650	3.4347289	1.4661736
O	2.5477242	1.0596583	4.9269260
O	9.0959712	0.3075152	2.8462413
O	4.7680416	2.9886683	-1.6358005
O	5.3218192	-1.3639645	-2.5983635
C	-1.8316907	2.0186067	5.3093683
C	-2.3464183	2.6167231	4.1277677
C	1.1859434	-2.1745423	4.7261499
C	-0.4160240	3.7306318	4.7120370
C	8.9798155	1.5859097	-0.3964260
C	-0.6412825	2.6987531	5.6645488
C	-0.8407853	-3.2476023	4.9475585
C	0.4076885	-3.2609638	4.2542740
C	-2.6650393	-0.7871386	3.9697946
C	-1.4785472	3.6742047	3.7601114
C	0.4292732	-1.4890890	5.7143379
C	9.0916443	0.1806265	-0.5833920
C	-1.4922109	-2.4882721	2.1569608
C	6.2837919	3.7395825	1.5792563
C	5.7919539	-0.5805325	-1.9008670
C	8.6361557	-0.1234002	-1.8880877
C	8.4456128	2.1462364	-1.5824964
C	5.4590494	2.1435860	-1.2773997
C	-0.8197674	-2.1439898	5.8444430
C	8.2303994	1.0937196	-2.5147692
C	0.8195604	2.7593463	2.1899979
C	5.5757919	0.1818022	3.6622542
C	4.9710150	3.4569681	2.0426465
O	5.2129808	-0.4874362	4.5183210



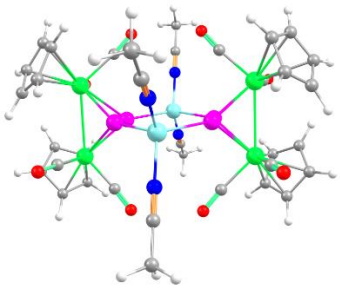
C	8.0404840	0.6730630	2.5889854
C	1.5529992	1.2482199	4.3849519
C	7.1850252	3.5268767	2.6518644
C	5.0612802	3.0786080	3.4061219
C	6.4338884	3.1226527	3.7918104
O	1.0510780	3.3418210	-1.6695736
O	3.6472094	0.8933725	-4.2618404
O	-0.3863958	-3.9215766	-1.1678725
O	-2.5214508	-2.0577617	-4.5543047
O	-8.9793360	-0.2343540	-3.0237292
O	-5.2183798	-2.5294325	2.0289890
O	-5.1079407	1.9371180	2.2699583
C	1.9491255	-2.0432037	-5.4038486
C	2.6618469	-2.5261250	-4.2728779
C	-1.5236721	1.4383989	-4.9561695
C	0.9162716	-3.9713231	-4.6907511
C	-9.1257380	-0.7842061	0.3916583
C	0.8735235	-2.9286186	-5.6584673
C	0.2970201	2.8047235	-5.3214375
C	-0.9432273	2.6865995	-4.6241527
C	2.5228202	0.9253555	-4.0428002
C	2.0302136	-3.7146616	-3.8357546
C	-0.6503746	0.7788769	-5.8629330
C	-9.0417269	0.6323456	0.3022836
C	0.8936186	2.4733664	-2.3972911
C	-6.5991583	-3.6283898	-1.0179165
C	-5.6861229	1.1396834	1.6755824
C	-8.5843909	1.1223354	1.5487931
C	-8.7095059	-1.1679725	1.6901683
C	-5.7605553	-1.6607497	1.5082954
C	0.4715372	1.6152489	-6.0830036
C	-8.3741121	0.0076245	2.4162983
C	-0.1215575	-3.1702024	-1.9896102
C	-5.4387886	-0.6076023	-3.6650965
C	-5.2414728	-3.5605062	-1.4314449
O	-4.9742102	-0.1465958	-4.6063990
C	-7.9773018	-0.6464475	-2.6498023
C	-1.4537091	-1.9882903	-4.1356246
C	-7.4155960	-3.5350129	-2.1719854
C	-5.2194135	-3.4364105	-2.8434123
C	-6.5677292	-3.4215939	-3.3098155
H	4.0646018	3.5466920	1.4672952
H	4.2368815	2.8302342	4.0530139
H	6.8252292	2.9399246	4.7790795
H	8.2504519	3.6904683	2.6271093
H	6.5429593	4.0907173	0.5953421
H	9.2950200	2.1333416	0.4746133
H	9.4899117	-0.5222469	0.1291387
H	8.2730105	3.1945566	-1.7663505
H	7.8843785	1.2038147	-3.5292109
H	8.6357594	-1.0999856	-2.3446432
H	2.2131415	-1.1839835	-5.9952593
H	3.5449635	-2.0848305	-3.8447680
H	0.1708345	-2.8562166	-6.4731146
H	0.2678186	-4.8312134	-4.6540993
H	2.3582599	-4.3417003	-3.0231831
H	-1.3824026	3.4373260	-3.9885607

H	0.9502501	3.6617414	-5.3225471
H	1.2932052	1.4122555	-6.7510291
H	-0.8348862	-0.1695068	-6.3367445
H	-2.4787721	1.0699600	-4.6199157
H	-0.0346250	2.5010432	6.5338096
H	0.3753713	4.4614143	4.7422664
H	-1.6176878	4.3482183	2.9310453
H	-3.2553294	2.3395336	3.6220663
H	-2.2904409	1.2190587	5.8645502
H	-1.6027356	-1.8817550	6.5378719
H	-1.6306830	-3.9745935	4.8535196
H	0.7642653	-0.6465865	6.2941182
H	2.1907306	-1.9313818	4.4227334
H	0.7168865	-3.9950797	3.5287694
H	-4.3813702	-3.6252381	-0.7854702
H	-4.3397223	-3.3920148	-3.4630264
H	-6.8860466	-3.3898437	-4.3388627
H	-8.4922723	-3.5891922	-2.1926377
H	-6.9454608	-3.7660727	-0.0082112
H	-8.6915589	-2.1738953	2.0779509
H	-9.4895979	-1.4447227	-0.3760224
H	-9.3169527	1.2289864	-0.5512673
H	-8.4585347	2.1602427	1.8113709
H	-8.0765126	0.0521450	3.4509285
N	-2.5556023	2.5691089	-0.7065169
C	-2.8862280	3.6610842	-0.8293185
C	-3.3191798	5.0374860	-0.9869541
H	-2.4549819	5.6920380	-1.1063721
H	-3.9602894	5.1256177	-1.8650821
H	-3.8845580	5.3507267	-0.1083622
N	2.8227608	-2.6593252	0.5386685
C	3.2921810	-3.6941332	0.7001595
C	3.9042402	-4.9936168	0.9085237
H	4.3842504	-5.0229147	1.8875856
H	3.1495675	-5.7791859	0.8559613
H	4.6603871	-5.1731889	0.1432382

ENERGIES [a.u.]:
Total energy = -10184.2816996812
Total energy + OC corr. = -10184.2765113837

Table S20. Cartesian coordinates of the optimized geometry of **J**.

Atom	x	y	z
Mo	-0.6585612	-2.5292607	-3.0097615
Mo	1.9897396	-0.9389751	-3.3240779
Cu	-1.2551694	1.6829722	-1.1857747
P	0.7891156	-1.7196153	-1.1688390
P	-0.0763777	-0.1357089	-2.2174651
O	-1.9001697	-0.6532296	-5.2072539
O	-3.2583959	-2.0113638	-1.3404088
O	3.8118467	0.5739475	-1.2734773
O	3.5141828	-3.5584594	-2.4846308
C	-1.1840708	-4.7665126	-2.5103775



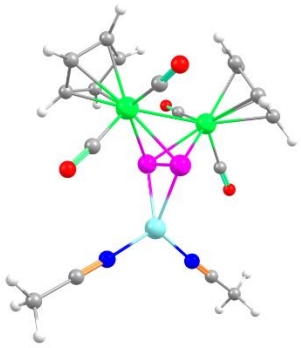
C	-1.7885204	-4.4262038	-3.7585380
C	-0.7406492	-4.1950996	-4.6926914
C	0.4956140	-4.3970537	-4.0318967
C	0.2216039	-4.7426980	-2.6806266
C	2.8763289	-1.3700447	-5.4787396
C	3.6034245	-0.3026861	-4.8820119
C	2.7069625	0.7992348	-4.7363974
C	1.4423435	0.4078272	-5.2393805
C	1.5491278	-0.9307577	-5.7054390
C	-1.4240244	-1.3027690	-4.3902248
C	-2.2797291	-2.1443635	-1.9197637
C	3.0999286	0.0101713	-1.9709331
C	2.9256127	-2.6137001	-2.7623139
H	-1.7090964	-5.0364450	-1.6086357
H	-2.8445968	-4.4130690	-3.9725677
H	-0.8700303	-3.9577347	-5.7365081
H	1.4701890	-4.3466379	-4.4853950
H	0.9568212	-4.9814823	-1.9305087
H	3.2825693	-2.3294561	-5.7564592
H	4.6549715	-0.3041085	-4.6463482
H	2.9621651	1.7726426	-4.3503856
H	0.5618734	1.0257225	-5.2960125
H	0.7712239	-1.4941538	-6.1906874
Mo	0.6592001	2.5293475	3.0092492
Mo	-1.9891404	0.9393293	3.3243373
Cu	1.2551702	-1.6841431	1.1852591
P	-0.7885434	1.7190223	1.1687650
P	0.0769799	0.1354607	2.2178768
O	1.9002319	0.6546859	5.2081921
O	3.2593831	2.0095694	1.3411163
O	-3.8105685	-0.5754221	1.2745138
O	-3.5136066	3.5581488	2.4830585
C	1.1852034	4.7660109	2.5078979
C	1.7892434	4.4268181	3.7565616
C	0.7410722	4.1967841	4.6906410
C	-0.4949634	4.3982449	4.0292752
C	-0.2205326	4.7426022	2.6777697
C	-2.8758495	1.3717189	5.4787155
C	-3.6028931	0.3039621	4.8826262
C	-2.7063999	-0.7980207	4.7377467
C	-1.4418082	-0.4062506	5.2405109
C	-1.5486532	0.9326074	5.7057799
C	1.4242283	1.3037368	4.3906937
C	2.2805460	2.1432575	1.9200409
C	-3.0989515	-0.0109173	1.9716980
C	-2.9250140	2.6135821	2.7614116
H	1.7105208	5.0349724	1.6060331
H	2.8452584	4.4137303	3.9709049
H	0.8701078	3.9603844	5.7347198
H	-1.4696790	4.3483695	4.4825382
H	-0.9555020	4.9807662	1.9272111
H	-3.2821329	2.3312847	5.7558411
H	-4.6544295	0.3052010	4.6469150
H	-2.9615640	-1.7716721	4.3523267
H	-0.5613294	-1.0240940	5.2975769
H	-0.7708130	1.4963260	6.1907519
N	-0.7799756	3.4817173	-2.0706542

C	-0.6542298	4.4935036	-2.5977346
C	-0.5034546	5.7732999	-3.2662156
H	0.5388673	6.0926790	-3.2339144
H	-0.8168672	5.6874329	-4.3074832
H	-1.1210435	6.5249631	-2.7728451
N	-3.2605437	1.4879305	-1.5007939
C	-4.3853580	1.3125451	-1.6413177
C	-5.8061871	1.0779840	-1.8116458
H	-6.0532006	1.0419115	-2.8733763
H	-6.0762954	0.1282362	-1.3482498
H	-6.3753335	1.8809072	-1.3415708
N	3.2603137	-1.4892931	1.5015362
C	4.3851186	-1.3145735	1.6429549
C	5.8059450	-1.0808155	1.8143718
H	6.0518972	-1.0430245	2.8762867
H	6.3749774	-1.8850047	1.3463265
H	6.0772529	-0.1321071	1.3495428
N	0.7787189	-3.4822611	2.0707290
C	0.6518977	-4.4938219	2.5979812
C	0.4997198	-5.7733762	3.2665964
H	-0.5398927	-6.0996781	3.2195588
H	1.1294261	-6.5217845	2.7836970
H	0.7972222	-5.6837021	4.3121957

ENERGIES [a.u.]:
Total energy = -7130.7451512399
Total energy + OC corr. = -7130.7397320200

Table S21. Cartesian coordinates of the optimized geometry of **N**.

Atom	x	y	z
Mo	-0.0307916	-0.6974814	1.8761685
Mo	1.7159020	-0.7522287	-0.7002920
Cu	-1.7529885	1.5098373	-1.2198060
P	-0.7569544	-0.6330484	-0.5904073
P	0.1974090	1.1168567	0.2035037
O	-0.7767211	-3.6892693	1.2545197
O	-3.0875315	-0.0946946	2.2067387
O	3.7180848	1.1564163	0.7971060
O	1.7689048	1.2353801	-3.1215598
C	0.1129457	0.4064134	3.9492689
C	-0.0307438	-0.9944589	4.1909335
C	1.1455198	-1.6341663	3.7122237
C	2.0074907	-0.6418862	3.1844205
C	1.3663588	0.6188973	3.3258117
C	2.2826029	-3.0532606	-0.1967349
C	3.4683743	-2.3397818	-0.4985454
C	3.3926727	-1.8995068	-1.8485104
C	2.1428922	-2.3467432	-2.3772041
C	1.4608042	-3.0524126	-1.3565682
C	-0.5082639	-2.5885581	1.4301186
C	-1.9760060	-0.3190724	2.0360069
C	2.9488216	0.4873708	0.2726158
C	1.7219596	0.5415969	-2.2097051

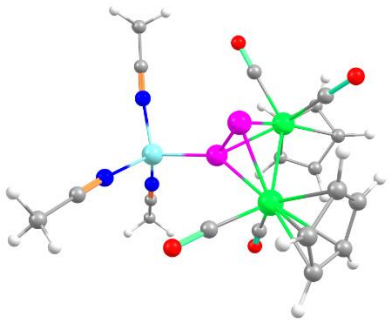


H	-0.5903393	1.1728185	4.2317335
H	-0.8512590	-1.4728123	4.6999984
H	1.3594588	-2.6889287	3.7781771
H	2.9936956	-0.8079174	2.7866992
H	1.7794325	1.5726247	3.0424612
H	2.0619254	-3.5476807	0.7334369
H	4.3039615	-2.1900227	0.1662838
H	4.1648823	-1.3791291	-2.3908484
H	1.7981711	-2.2091880	-3.3891367
H	0.5034764	-3.5370277	-1.4524240
N	-1.5215430	2.1617524	-3.0890306
C	-1.2899940	2.5490828	-4.1432864
C	-0.9824843	3.0360599	-5.4736474
H	0.0814210	2.9031531	-5.6744909
H	-1.5596242	2.4815563	-6.2146471
H	-1.2314144	4.0953155	-5.5483387
N	-3.4514492	2.1202251	-0.3745034
C	-4.4358678	2.3797526	0.1533782
C	-5.6784045	2.6961249	0.8298317
H	-6.5170078	2.5721620	0.1435738
H	-5.8110653	2.0279854	1.6818199
H	-5.6567141	3.7278936	1.1828567

ENERGIES [a.u.]:
Total energy = -3565.3731524323
Total energy + OC corr. = -3565.3704186749

Table S22. Cartesian coordinates of the optimized geometry of **O**.

Atom	x	y	z
Mo	0.4022808	-0.5049781	2.2676089
Mo	1.9548338	1.1913852	0.1669718
Cu	-1.9704827	-0.1309614	-1.7243871
P	-0.2947165	0.2178335	-0.0945240
P	-0.3029830	1.7112816	1.3624660
O	1.0363784	-3.0227704	0.4999269
O	-2.6037836	-1.3871417	2.3033907
O	2.7002023	3.1620173	2.4987553
O	0.9586418	3.6501099	-1.4997188
C	0.0633682	-0.3152780	4.5930466
C	0.5995760	-1.6096975	4.3156039
C	1.9245009	-1.4288675	3.8318502
C	2.2051187	-0.0401586	3.8157746
C	1.0517367	0.6486526	4.2812651
C	3.5524524	-0.6235131	0.0264273
C	4.2508645	0.5966251	0.1980266
C	3.9999951	1.4180282	-0.9360393
C	3.1326976	0.6924119	-1.8077350
C	2.8550386	-0.5614201	-1.2106848
C	0.7972139	-2.0763089	1.1081141
C	-1.5073542	-1.0505317	2.2407271
C	2.3786724	2.4397061	1.6664528
C	1.2881042	2.7596333	-0.8530332
H	-0.9110666	-0.1093085	5.0054432

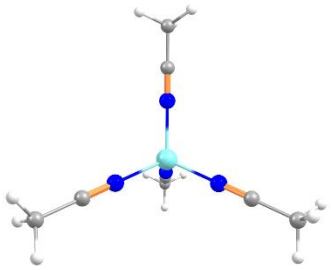


H	0.1124613	-2.5535866	4.4968422
H	2.6099078	-2.2170846	3.5645295
H	3.1419749	0.4127311	3.5409556
H	0.9600324	1.7145576	4.4065120
H	3.5755146	-1.4654490	0.6964632
H	4.8952522	0.8469369	1.0254759
H	4.4332081	2.3857992	-1.1278900
H	2.7819538	1.0259507	-2.7708016
H	2.2476348	-1.3448358	-1.6315813
N	-3.7789522	-0.4208001	-0.8279434
C	-4.7144261	-0.5959126	-0.1879101
C	-5.8844367	-0.8204689	0.6394583
H	-6.5286905	-1.5714774	0.1810105
H	-5.5696857	-1.1704837	1.6234427
H	-6.4453457	0.1080113	0.7519878
N	-1.6308936	-1.7579611	-2.9129095
C	-1.4844354	-2.7060722	-3.5420788
C	-1.3007988	-3.9075594	-4.3354941
H	-0.5152347	-4.5252689	-3.8985588
H	-2.2286302	-4.4802482	-4.3616611
H	-1.0195647	-3.6416667	-5.3551187
N	-2.0013799	1.5852152	-2.8223308
C	-1.9362217	2.6298640	-3.2921227
C	-1.8394674	3.9568863	-3.8700193
H	-1.6789332	3.8857207	-4.9463497
H	-2.7597890	4.5117110	-3.6840600
H	-1.0023441	4.4887420	-3.4155767

ENERGIES [a.u.]:
Total energy = -3698.1200823790
Total energy + OC corr. = -3698.1173772914

Table S23. Cartesian coordinates of the optimized geometry of **K**.

Atom	x	y	z
Cu	0.0013598	0.0000431	0.0009097
N	0.4842122	1.7721078	-0.8738994
C	0.7562738	2.7716495	-1.3670873
C	1.1004951	4.0363178	-1.9910669
H	2.1690525	4.2260500	-1.8828671
H	0.8508567	4.0078120	-3.0523810
H	0.5463132	4.8477983	-1.5178835
N	-1.9938033	-0.3386085	-0.2113643
C	-3.1187628	-0.5291174	-0.3318110
C	-4.5420994	-0.7701366	-0.4842614
H	-4.8016450	-0.8093370	-1.5428554
H	-4.8110775	-1.7185194	-0.0176316
H	-5.1083707	0.0320720	-0.0095849
N	0.4704886	0.0691294	1.9792690
C	0.7346669	0.1079030	3.0950822
C	1.0688785	0.1569588	4.5068563
H	0.1574638	0.2106499	5.1034625
H	1.6253488	-0.7376090	4.7889597
H	1.6808841	1.0355744	4.7141800



N	1.0422656	-1.5031571	-0.8915680
C	1.6291595	-2.3506943	-1.3951256
C	2.3717082	-3.4230096	-2.0322919
H	3.2637959	-3.6554700	-1.4495016
H	1.7500581	-4.3165000	-2.1010658
H	2.6724772	-3.1219068	-3.0364728

```
ENERGIES [a.u.]:
  Total energy            =    -2171.3448622088
  Total energy + OC corr. =    -2171.3419431462
```

Table S24. Cartesian coordinates of the optimized geometry of **acetonitrile**.

Atom	x	y	z
N	0.0000000	0.0000000	-2.1163973
C	0.0000000	0.0000000	-0.9667009
C	0.0000000	0.0000000	0.4886653
H	0.5118299	-0.8865154	0.8648109
H	0.5118299	0.8865154	0.8648109
H	-1.0236598	0.0000000	0.8648109

```
ENERGIES [a.u.]:
  Total energy            =     -132.7388821149
  Total energy + OC corr. =     -132.7390157726
```

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