

Supporting Information for:

Trimetallaborides as Starting Points for the Syntheses of Large Metal-Rich Molecular Borides
and Clusters

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Experimental

Materials: $\text{Li}[\{(\text{CO})_2\text{CpMn}\}_2\text{B}]$ (**1**),¹ dimethylsulfide gold and copper chlorides (DMS–AuCl, DMS–CuCl) and 1,3-(4-tolyl)imidazol-2-ylidene copper chloride (ITol–CuCl),² and $\text{Li}[\{(\text{CO})_2\text{CpMn}\}_2\text{B}\{\text{Pt}(\text{PCy}_3)\}]$ (**6**),³ were prepared by literature methods.

Physical Methods: All manipulations were performed either under an atmosphere of dry argon or in vacuo using standard Schlenk line or glovebox techniques. All solvents (including DMS) were dried and degassed as according to literature methods, and stored under inert environments.⁴ NMR spectra in solution were acquired on a Bruker Avance 400 (¹H: 400.1 MHz, ¹¹B{¹H}: 128.4 MHz, ¹³C{¹H}: 100.6 MHz). ¹H NMR and ¹³C NMR spectra were referenced to external TMS *via* residual protons of the solvent (¹H) or the solvent itself (¹³C) and ¹¹B{¹H} NMR spectra were referenced to external Et₂O·BF₃. IR spectra were acquired on a JASCO FT/IR-6200 type A spectrometer. Elemental analysis was performed on Vario MICRO Cube Elemental Analyzer.

Crystallographic Details: All structures were solved using direct methods, refined with the Shelx software package⁵ and expanded using Fourier techniques. The *ShelXL* was interfaced with *ShelXLe* GUI for most of the refinement steps.⁶ The pictures of molecules were prepared using *Pov-Ray* 3.6.2.⁷ Additional details on refinement can be found in CIF files, which can be obtained from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif under CCDC 1420470 (**2**), CCDC 1420471 (**3**), CCDC 1420472 (**4**), and CCDC 1420473 (**7**).

For 2:

The crystal data of **2** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo_{K α} radiation. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.

Crystal data for **2**: C₂₈H₂₀B₂Cu₂Mn₄O₈, $M_r = 852.90$, orange block, 0.26×0.19×0.12 mm³, Monoclinic space group $P2_1/c$, $a = 12.6570(12)$ Å, $b = 17.3227(16)$ Å, $c = 13.6878(13)$ Å, $\beta = 91.065(4)^\circ$, $V = 3000.6(5)$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.888$ g·cm⁻³, $\mu = 3.072$ mm⁻¹, $F(000) = 1680$, $T = 100(2)$ K, $R_I = 0.0396$, $wR^2 = 0.0780$, 6139 independent reflections [$2\theta \leq 52.74^\circ$] and 397 parameters.

For 3:

The crystal data of **3** were collected on a Bruker X8-Apex II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo_{Kα} radiation. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.

Crystal data for **tsk100**: C₂₈H₂₀Au₂B₂Mn₄O₈, $M_r = 1119.75$, red block, 0.12×0.04×0.03 mm³, Monoclinic space group $C2/c$, $a = 17.4662(13)$ Å, $b = 12.1607(9)$ Å, $c = 15.4013(18)$ Å, $\alpha = 119.822(2)^\circ$, $V = 2838.1(4)$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 2.621$ g·cm⁻³, $\mu = 12.077$ mm⁻¹, $F(000) = 2080$, $T = 100(2)$ K, $R_I = 0.0195$, $wR^2 = 0.0409$, 3023 independent reflections [$2\theta \leq 53.52^\circ$] and 200 parameters.

For 4:

The crystal data of **4** were collected on a Bruker X8-Apex II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo_{Kα} radiation. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.

The displacement parameters of the fragments CuPCy₃ and PtPCy₃ were constrained to the same value.

The U_{ii} displacement parameters of the fragments CuPCy₃ and PtPCy₃ were restrained with ISOR keyword to approximate isotropic behavior.

Crystal data for **4**: $C_{50}H_{76}BCuMn_2O_4P_2Pt$, $M_r = 1182.37$, red block, $0.24 \times 0.18 \times 0.11$ mm³, Triclinic space group $P-1$, $a = 11.1740(8)$ Å, $b = 11.1760(8)$ Å, $c = 19.8602(14)$ Å, $\alpha = 83.931(2)^\circ$, $\beta = 83.831(2)^\circ$, $\gamma = 75.995(2)^\circ$, $V = 2384.3(3)$ Å³, $Z = 2$, $\rho_{calcd} = 1.647$ g·cm⁻³, $\mu = 3.993$ mm⁻¹, $F(000) = 1200$, $T = 100(2)$ K, $R_I = 0.0680$, $wR^2 = 0.0966$, 9725 independent reflections [$2\theta \leq 52.74^\circ$] and 491 parameters.

For 7:

The crystal data of **7** were collected on a Bruker X8APEX diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions.

Crystal data for **7**: $C_{70}H_{83}BCuMn_2N_2O_4PPt$, $M_r = 1426.67$, red block, $0.21 \times 0.15 \times 0.08$ mm³, Triclinic space group $P-1$, $a = 12.516(2)$ Å, $b = 13.405(3)$ Å, $c = 19.099(4)$ Å, $\alpha = 100.262(5)^\circ$, $\beta = 97.963(5)^\circ$, $\gamma = 95.107(5)^\circ$, $V = 3101.3(10)$ Å³, $Z = 2$, $\rho_{calcd} = 1.528$ g·cm⁻³, $\mu = 3.061$ mm⁻¹, $F(000) = 1452$, $T = 100(2)$ K, $R_I = 0.0642$, $wR^2 = 0.0913$, 13026 independent reflections [$2\theta \leq 53.86^\circ$] and 753 parameters.

Computational Details:

For the investigation of potential closed shell interactions, geometry optimization was carried out using the Amsterdam Density Functional (ADF)⁸ program at the OLYP/TZP.⁹ All calculations were conducted within the zeroth-order regular approximation (ZORA) formalism.¹⁰ To obtain

the singlet state, spin-restricted calculations were performed constraining the projection of the total electronic spin along a reference axis to 0. Frequency calculations were conducted to determine if each stationary point corresponds to a minimum. Reported bond orders are of the Mayer bond order type¹¹ and atomic charges were determined according to the Hirshfeld charge analysis.¹² Dispersion was included via the addition of the D3 version of Grimme's dispersion with Becke-Johnson damping.¹³ The Jmol¹⁴ program and the Graphical User Interface (ADF-GUI) – a part of the ADF package, were used for visualization purposes.

For the reported thermochemistry, calculations were performed in the Gaussian 09 software suite.¹⁵ For compound **2** and its related thermochemistry, optimizations were carried out at the B3LYP/6-311+G(d,p) level of theory for all atoms and checked via frequency calculation to ensure the stationary point was a true minimum with no imaginary frequencies. The calculated electronic and free energies at 298.15 K are given in Table 1. For compound **3**, small atoms were calculated at the B3LYP/6-311+G(d,p) level, while Au and Mn were treated at with the LANL2DZ pseudopotential.

Synthetic Details

$\{[(\eta^5\text{-C}_5\text{H}_5)_2(\text{CO})_4\text{Mn}_2]\text{BCu}\}_2$ (**2**): DMS–CuCl (5.0 mg, 0.031 mmol) was added to a solution of **1** (20 mg, 0.031 mmol) in toluene (1 mL) and stirred for 0.5 h at room temperature. The color of the reaction mixture changed from slightly yellow to red and a colorless precipitate formed.

After a complete conversion, indicated by the emergence of a ¹¹B NMR signal at 208 ppm, the solution was filtered and stored at –35 °C. Slow crystallization led to the isolation of red crystals of **2** suitable for X-ray diffraction. For (**2**): 12.1 mg (0.015 mmol, 46%) ¹H NMR (C₆D₆,

400.1 MHz): $\delta = 4.58$ (s, 10H, C_5H_5). $^{11}B\{^1H\}$ NMR (C_6D_6 , 128.4 MHz): $\delta = 208$. $^{13}C\{^1H\}$ NMR (C_6D_6 , 100.6 MHz): $\delta = 225.7$ (CO), 84.3 (s, C_5H_5). FT-IR (hexane): 1957 (br), 1942 (br), 1907 (br), 1878 (br), 1863 (br) cm^{-1} . Elemental analysis: calc'd (%): C: 39.43, H: 2.36; found (%): C: 40.22 H: 2.80.

$\{[(\eta^5-C_5H_5)_2(CO)_4Mn_2]BAu\}_2$ (3): DMS–AuCl (4.6 mg, 0.016 mmol) was added to a solution of **1** (10 mg, 0.016 mmol) in toluene (1 mL) and stirred for 0.5 h at room temperature. The color of the reaction mixture changed from slightly yellow to red and a precipitate was formed. After a complete conversion in the ^{11}B NMR spectrum to a low-field signal at 208 ppm was observed, the solution was filtrated and stored at -35 °C. Slow crystallization led to the isolation of red crystals of **3** suitable for X-ray diffraction. For **3**: 3.2 mg (0.003 mmol, 17%). 1H NMR (C_6D_6 , 400.1 MHz): $\delta = 4.85$ (s, 10H, C_5H_5). $^{11}B\{^1H\}$ NMR (C_6D_6 , 128.4 MHz): $\delta = 208$. $^{13}C\{^1H\}$ NMR (C_6D_6 , 100.6 MHz): $\delta = 232.2$ (CO), 83.9 (s, C_5H_5). FT-IR (hexane): 1986 (br), 1945 (br), 1927 (br), 1913 (br), 1878 (br) cm^{-1} . Elemental analysis: calc'd (%): C: 30.03, H: 1.80; found (%): C: 31.05 H: 1.75.

$\{[(\eta^5-C_5H_5)_2(CO)_4Mn_2B][CuPCy_3][PtPCy_3]\}$ (4): Pt(PCy₃)₂ (21.3 mg, 0.028 mmol) was added to a solution of **(2)** (12 mg, 0.014 mmol) in toluene (1 mL) and stirred for 4 at 60 °C. The color of the reaction mixture remained red, but in the ^{11}B NMR spectrum a low-field shift to 215 ppm was observed. The solution was concentrated and stored at -35 °C. After 4 weeks orange crystals of **4** suitable for X-ray diffraction were obtained. For **4**: 10.2 mg (0.009 mmol, 31%). 1H NMR (C_6D_6 , 400.1 MHz): $\delta = 4.75$ (s, 10H, C_5H_5), 1.23 – 2.41 (br, 66H, PCy₃). $^{11}B\{^1H\}$ NMR (C_6D_6 , 128.4 MHz): $\delta = 215$. $^{13}C\{^1H\}$ NMR (C_6D_6 , 100.6 MHz): $\delta = 236.9$ (CO), 82.3 (s, C_5H_5), 25.0 –

34.9 (br, PCy₃). ³¹P{¹H} NMR (C₆D₆, 162.0 MHz): δ = 63.9 (s, PtPCy₃, ¹J_{P-Pt} = 4421 Hz), 13.4 (s, CuPCy₃). FT-IR (hexane): 1946 (br), 1913 (br), 1873 (br), 1849 (br), 1793 (br), 1768 (br) cm⁻¹. Elemental analysis: calc'd (%): C: 50.79, H: 6.47; found (%) C: 51.06 H: 6.75.

Alternative route to **4**: PCy₃-CuCl (24.0 mg, 0.047 mmol) was added to a solution of **6** (30 mg, 0.047 mmol) in toluene (1 mL) and stirred for 0.5 h at room temperature. The color of the reaction mixture turned yellow and a white precipitate formed. In the ¹¹B NMR spectrum a low-field shift to 216 ppm was observed. The solution was filtered, concentrated and stored at -35 °C. After 12 h yellow crystals of **4** were obtained. Yield: 31 mg, 0.037 mmol, 79%.

(η⁵-C₅H₅)₂(CO)₄Mn₂B(PtPCy₃)(CuITol) (7): ITol-CuCl (3.71 mg, 0.010 mmol) was added to a solution of **6** (10 mg, 0.010 mmol) in toluene (1 mL) and stirred for 2 h at room temperature. The color of the reaction mixture turned red as a white precipitate formed. A downfield shift of the ¹¹B NMR resonance to 226 ppm was observed. The solution was filtered, concentrated and stored at -35 °C. After four weeks, orange crystals of **7** suitable for X-ray diffraction were obtained. For **7**: 7.4 mg (0.006 mmol, 61%). ¹H NMR (C₆D₆, 400.1 MHz): δ = 7.65 (d, 4H, Tol), 7.03 (t, 4H, Tol), 6.47 (s, 2H, NHC), 4.38 (s, 10H, C₅H₅), 2.74 (m, 3H, PCy₃), 2.18 (m, 6H, PCy₃), 1.96 (s, 6H, Tol), 1.77 (m, 6H, PCy₃), 1.63 (m, 6H, PCy₃), 1.36 (m, 6H, PCy₃), 1.20 (m, 6H, PCy₃). ¹¹B{¹H} NMR (C₆D₆, 128.4 MHz): δ = 226. ¹³C{¹H} NMR (C₆D₆, 100.6 MHz): δ = 214.3 (CO), 139.4 (Tol), 138.2 (Tol), 130.8 (Tol), 125.0 (Tol), 121.5 NHC), 82.0 (s, C₅H₅), 34.3 (PCy₃), 30.7 (PCy₃), 28.3 (PCy₃), 27.2 (PCy₃), 20.9 (Tol). ³¹P{¹H} NMR (C₆D₆, 162.0 MHz): δ = 55.3 (s, PtPCy₃, ¹J_{P-Pt} = 4269 Hz). FT-IR (hexane): 1948 (br), 1909 (br), 1859 (br), 1766 (br) cm⁻¹. Elemental analysis: calc'd (%): C: 54.14, H: 5.44, N: 2.25; found (%) C: 54.29 H: 5.53, N: 2.13.

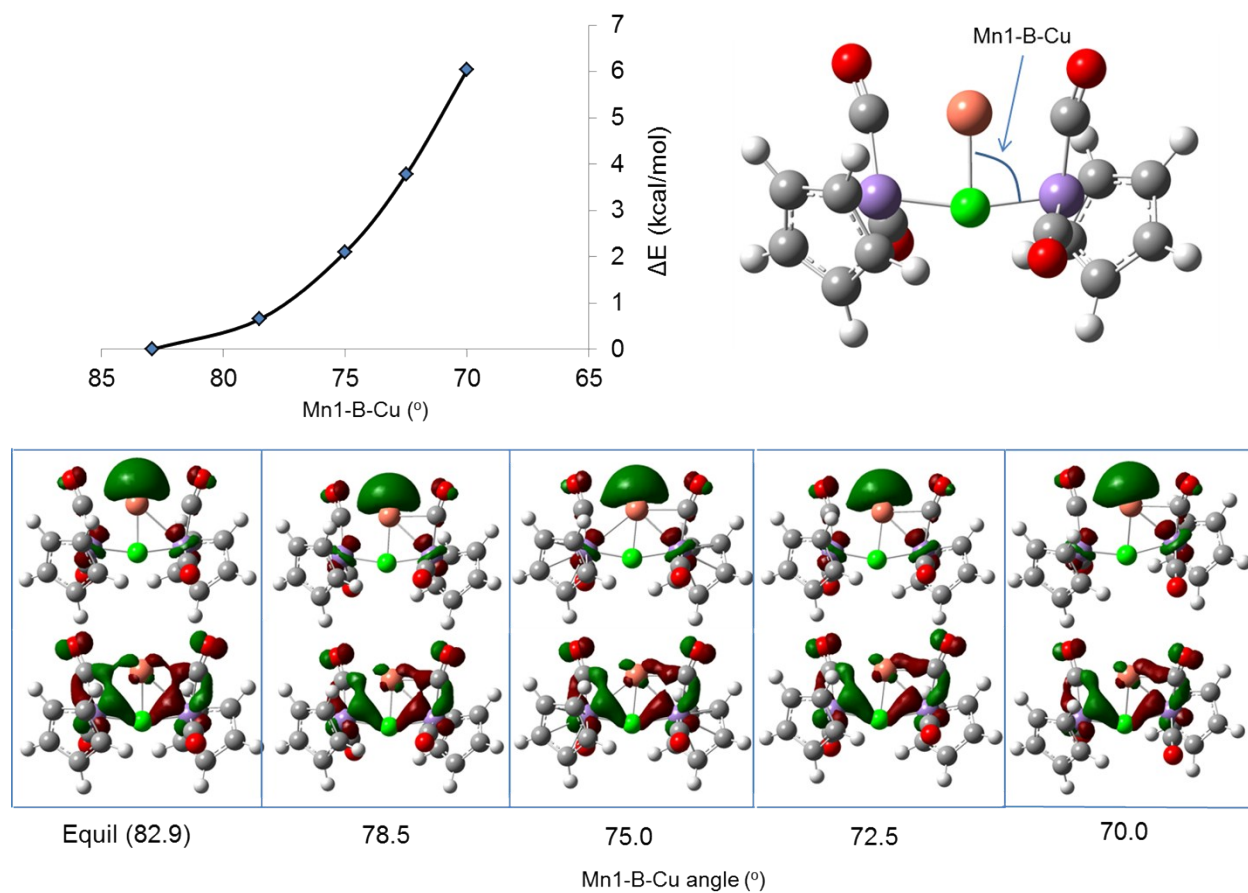
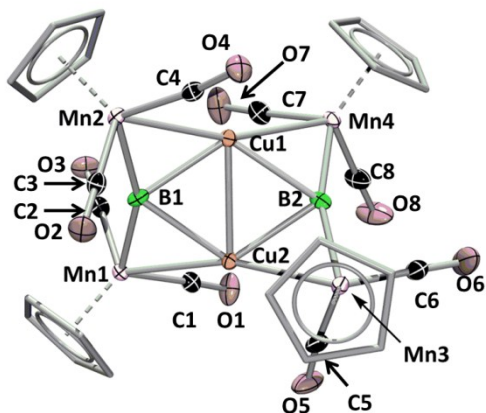


Figure S1. Evaluation of the potential energy changes involved in the movement of the Cu ion in 2a from a centrosymmetric position to a position closer to one of the two Mn atoms. Calculations were carried out at the B3LYP/6-311+G** level for all atoms by fixing the Mn1-B-Cu angle and optimizing around this coordinate. In the Kohn-Sham molecular orbital depictions, the top figure is the LUMO for the partially-optimized structures, and the lower figure is the HOMO. The values of E used for the determination of ΔE are not ZPE-corrected.

Table 1. Energies calculated for the reported thermochemical data. Energies are in Hartrees and calculated in the gas phase at 298.15 K. Optimizations and frequencies calculations were carried out using the B3LYP functional. For copper-containing compounds the 6-311+G(d,p) basis set was used for all atoms. For gold containing compounds the 6-311+G(d,p) basis set was used for all non-metals and the LANL2DZ pseudopotential was used for Mn and Au.

| Compound | E | G |
|---------------------------------------|--------------|--------------|
| 1•Cu⁰ | -4807.864936 | -4807.918751 |
| 1•Au⁰ | -1208.65455 | -1208.710171 |
| 2 | -9615.79298 | -9615.875567 |
| 3 | -2417.380441 | -2417.380441 |
| 1•Cu^{DMS} | -5285.889168 | -5285.952871 |
| 1•Au^{DMS} | -1686.676566 | -1686.740467 |
| 1•Cu^{PMe₃} | -5268.963001 | -5268.029736 |
| 1•Au^{PMe₃} | -1669.758054 | -1669.824634 |
| 1•Cu^{IMe} | -5112.685243 | -5112.752845 |
| 1•Au^{IMe} | -1513.481545 | -1513.548901 |
| | | |
| DMS | -477.991357 | -478.018459 |
| PMe₃ | -461.052417 | -461.081485 |
| IMe | -304.754655 | -304.785764 |

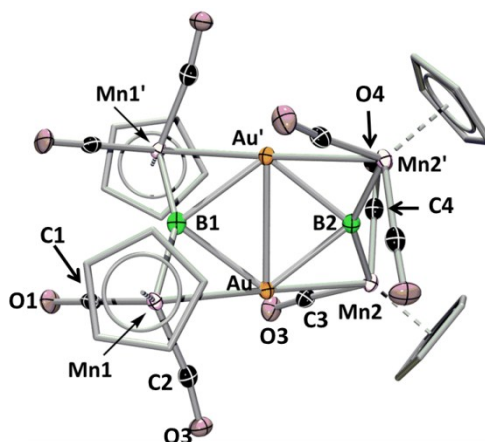
Table 2. Relevant bond lengths and angles for **2**.



| bond | length [Å] | atoms | angle (°) |
|---------|------------|-------------|------------|
| B1-Mn1 | 1.960(3) | B2-Cu1-B1 | 111.13(12) |
| B1-Mn2 | 1.970(3) | Cu1-B1-Cu2 | 67.96(10) |
| B1-Cu1 | 2.186(3) | B1-Cu2-B2 | 112.40(12) |
| B1-Cu2 | 2.238(3) | Cu2-B2-Cu1 | 68.43(10) |
| B2-Mn3 | 1.975(3) | Mn1-B1-Mn2 | 161.95(19) |
| B2-Mn4 | 1.962(3) | Mn3-B2-Mn4 | 157.05(19) |
| B2-Cu1 | 2.240(3) | Mn2-Cu1-Mn4 | 162.90(2) |
| B2-Cu2 | 2.156(3) | Mn1-Cu2-Mn3 | 161.23(2) |
| Cu1-Cu2 | 2.473(1) | | |
| Cu1-Mn2 | 2.458(1) | | |
| Cu1-Mn4 | 2.464(1) | | |
| Cu2-Mn1 | 2.440(1) | | |
| Cu2-Mn3 | 2.462(1) | Mn1-C1-O1 | 173.0(3) |
| Cu1-C4 | 2.430(3) | Mn1-C2-O2 | 177.7(3) |
| Cu1-C7 | 2.264(3) | Mn2-C3-O3 | 178.3(3) |
| Cu2-C1 | 2.315(3) | Mn2-C4-O4 | 174.1(3) |
| Cu2-C5 | 2.281(3) | Mn3-C5-O5 | 171.0(2) |
| | | Mn3-C6-O6 | 178.7(3) |
| C1-O1 | 1.168(4) | Mn4-C7-O7 | 172.8(2) |
| C2-O2 | 1.165(4) | Mn4-C8-O8 | 177.7(3) |
| C3-O3 | 1.157(4) | | |
| C4-O4 | 1.166(3) | | |
| Mn1-C1 | 1.804(3) | | |
| Mn1-C2 | 1.780(3) | | |
| Mn2-C3 | 1.778(3) | | |
| Mn2-C4 | 1.797(3) | | |

| | | | |
|--------|----------|--|--|
| C5-O5 | 1.172(3) | | |
| C6-O6 | 1.162(3) | | |
| C7-O7 | 1.159(4) | | |
| C8-O8 | 1.167(3) | | |
| Mn3-C5 | 1.797(3) | | |
| Mn3-C6 | 1.778(3) | | |
| Mn4-C7 | 1.817(3) | | |
| Mn4-C8 | 1.775(3) | | |

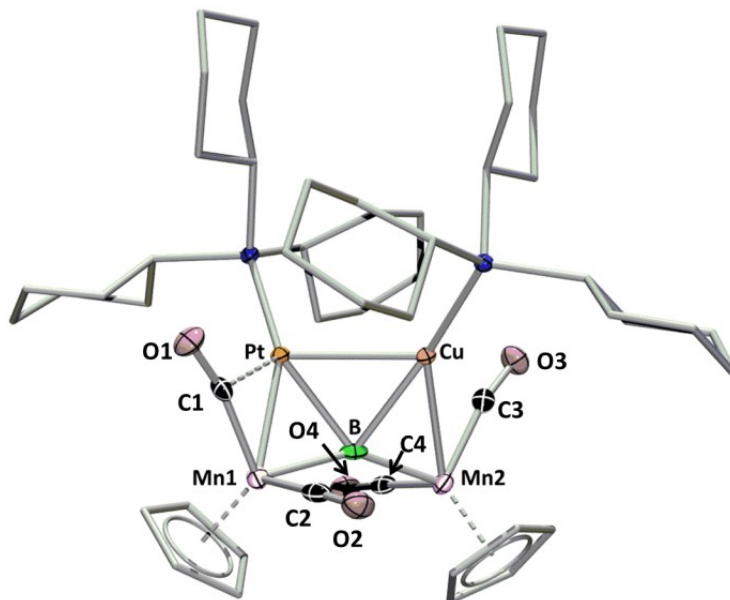
Table 3. Relevant bond lengths and angles for **3**.



| bond | length [Å] | | atoms | angle (°) |
|---------|------------|--|---------------|------------|
| B1-Mn1 | 1.983(2) | | B2-Au-B1 | 104.48(12) |
| B1-Mn1' | 1.983(2) | | Au-B1-Au' | 74.05(16) |
| B1-Au | 2.327(4) | | B1-Au'-B2 | 104.48(12) |
| B1-Au' | 2.327(4) | | Au'-B2-Au | 76.99(17) |
| B2-Mn2 | 1.991(2) | | Mn1-B1-Mn1' | 155.9(3) |
| B2-Mn2' | 1.991(2) | | Mn2-B2-Mn2' | 148.8(3) |
| B2-Au | 2.251(4) | | Mn1-Au-Mn2 | 178.47(2) |
| B2-Au' | 2.251(4) | | Mn1'-Au'-Mn2' | 178.47(2) |
| Au-Au' | 2.803(1) | | | |
| Au-Mn1 | 2.614(1) | | | |
| Au-Mn2 | 2.631(1) | | | |
| | | | | |
| | | | Mn1-C1-O1 | 178.4(3) |

| | | | | |
|--------|----------|--|-----------|----------|
| | | | Mn1-C2-O2 | 169.7(3) |
| C1-O1 | 1.154(4) | | Mn2-C3-O3 | 170.9(3) |
| C2-O2 | 1.156(4) | | Mn2-C4-O4 | 177.8(3) |
| C3-O3 | 1.158(4) | | | |
| C4-O4 | 1.153(4) | | | |
| Mn1-C1 | 1.772(4) | | | |
| Mn1-C2 | 1.830(4) | | | |
| Mn2-C3 | 1.794(4) | | | |
| Mn2-C4 | 1.769(4) | | | |

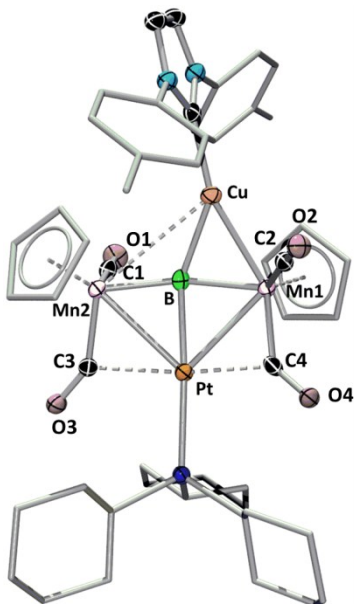
Table 4. Relevant bond lengths and angles in **4**.



| bond | length [Å] | atoms | angle (°) |
|---------|------------|------------|-----------|
| B1-Mn1 | 1.970(6) | Mn1-B1-Mn2 | 149.1(3) |
| B1-Mn2 | 1.970(6) | Cu1-B1-Pt1 | 75.19(18) |
| B1-Cu1 | 2.176(6) | Mn1-B1-Pt1 | 72.02(18) |
| B1-Pt1 | 2.196(5) | Mn1-B1-Cu1 | 130.1(3) |
| Cu1-Mn1 | 2.623(3) | Mn2-B1-Pt1 | 78.3(2) |
| Pt1-Mn1 | 2.456(2) | Mn2-B1-Cu1 | 135.2(3) |
| Pt1-Cu1 | 2.668(3) | | |
| | | | |
| | | Mn1-C1-O1 | 164.7(4) |
| C1-O1 | 1.174(5) | Mn1-C2-O2 | 178.1(4) |
| C2-O2 | 1.176(6) | Mn2-C3-O3 | 164.6(4) |
| C3-O3 | 1.159(5) | Mn2-C4-O4 | 177.8(4) |
| C4-O4 | 1.170(6) | Pt1-C1-O1 | 117.8(4) |
| Mn1-C1 | 1.815(5) | Cu1-C3-O3 | 116.7(4) |
| Mn1-C2 | 1.756(6) | | |
| Mn2-C3 | 1.824(5) | | |
| Mn2-C4 | 1.756(5) | | |
| | | B1-Cu1-P2 | 153.1(3) |
| Pt1-C1 | 2.099(5) | Mn2-Cu1-P2 | 145.0(2) |
| Cu1-C3 | 2.275(5) | B1-Pt1-P1 | 149.2(2) |
| Pt1-P1 | 2.263(7) | Mn1-Pt1-P1 | 155.3(2) |

| | | | |
|--------|----------|--|--|
| Cu1-P2 | 2.259(9) | | |
|--------|----------|--|--|

Table 5. Relevant bond lengths and angles in **7**.



| bond | length [Å] | | atoms | angle (°) |
|---------|------------|--|------------|------------|
| B1-Mn1 | 1.907(5) | | Mn1-B1-Mn2 | 168.2(3) |
| B1-Mn2 | 1.970(5) | | Cu1-B1-Pt1 | 155.1(3) |
| B1-Cu1 | 2.055(5) | | Mn1-B1-Pt1 | 85.6(2) |
| B1-Pt1 | 2.106(5) | | Mn1-B1-Cu1 | 115.2(3) |
| Cu1-Mn1 | 3.347(1) | | Mn2-B1-Pt1 | 83.14(19) |
| Cu1-Mn2 | 2.494(1) | | Mn2-B1-Cu1 | 76.52(17) |
| Pt1-Mn1 | 2.707(1) | | | |
| Pt1-Mn2 | 2.731(1) | | | |
| | | | | |
| C1-O1 | 1.176(5) | | Mn1-C1-O1 | 178.8(4) |
| C2-O2 | 1.169(6) | | Mn1-C3-O3 | 147.6(4) |
| C3-O3 | 1.173(5) | | Mn2-C2-O2 | 176.1(4) |
| C4-O4 | 1.186(5) | | Mn2-C4-O4 | 140.0(3) |
| Mn1-C1 | 1.747(5) | | Pt1-C3-O3 | 129.5(3) |
| Mn1-C3 | 1.853(5) | | Pt1-C4-O4 | 134.5(3) |
| Mn2-C2 | 1.769(5) | | | |
| Mn2-C4 | 1.933(5) | | | |
| | | | | |
| Pt1-C3 | 2.253(4) | | B1-Cu1-C | 147.57(19) |
| Pt1-C4 | 2.059(4) | | Mn2-Cu1-C | 161.21(13) |
| Pt1-P | 2.338(2) | | B1-Pt1-P | 174.51(14) |
| Cu1-C | 1.920(5) | | | |

Table S6. Coordinated for the optimized structures in the presence and absence of dispersion corrections. For the methods employed see the **Computational Details**. Columns are multi-page.

| <u>[(CO)₂CpMn]₂BAu]₂ without dispersion</u> | | | | <u>[(CO)₂CpMn]₂BAu]₂ with dispersion</u> | | | |
|--|----------|----------|----------|---|----------|----------|----------|
| Au | 6.919333 | 10.05712 | 1.93568 | Au | 6.932469 | 10.07047 | 1.920203 |
| Au | 6.716622 | 10.05717 | 4.745432 | Au | 6.704405 | 10.07075 | 4.760564 |
| O | 6.37159 | 5.481425 | 1.325237 | O | 6.440081 | 5.502096 | 1.517156 |
| O | 7.594752 | 8.653916 | -0.8463 | O | 7.74982 | 8.616136 | -0.80423 |
| O | 3.952364 | 10.39174 | 0.566098 | O | 3.893783 | 10.3208 | 0.651448 |
| O | 3.659218 | 12.82483 | 3.751661 | O | 3.819703 | 12.55462 | 4.09245 |
| O | 7.267723 | 5.482672 | 5.354666 | O | 7.19722 | 5.503902 | 5.164335 |
| O | 6.040995 | 8.654205 | 7.527425 | O | 5.885208 | 8.617857 | 7.484893 |
| O | 9.683854 | 10.39102 | 6.11615 | O | 9.74367 | 10.32122 | 6.029062 |
| O | 9.977796 | 12.82098 | 2.928279 | O | 9.816844 | 12.55491 | 2.588559 |
| C | 7.053856 | 6.39898 | 1.588109 | C | 7.122327 | 6.434314 | 1.717276 |
| C | 7.734701 | 8.400316 | 0.294663 | C | 7.844632 | 8.375934 | 0.34266 |
| C | 4.733602 | 11.10739 | 1.073411 | C | 4.655262 | 11.04543 | 1.170774 |
| C | 4.521199 | 12.65567 | 2.96965 | C | 4.57673 | 12.46823 | 3.196416 |
| C | 9.99826 | 8.670789 | 2.667228 | C | 9.798416 | 8.888432 | 2.897067 |
| C | 10.25448 | 8.058899 | 1.409249 | C | 10.23666 | 8.26974 | 1.696779 |
| C | 9.984742 | 6.666656 | 1.52248 | C | 10.06303 | 6.862901 | 1.824999 |
| C | 9.556411 | 6.417547 | 2.862034 | C | 9.506856 | 6.613459 | 3.113924 |
| C | 9.559178 | 7.655694 | 3.567372 | C | 9.336199 | 7.864859 | 3.774347 |
| C | 7.438416 | 13.23868 | 0.570259 | C | 7.300568 | 13.09514 | 0.652513 |
| C | 6.976609 | 14.22861 | 1.481271 | C | 6.953077 | 14.04226 | 1.653554 |
| C | 5.618898 | 14.52081 | 1.16311 | C | 5.597059 | 14.42374 | 1.448585 |
| C | 5.241332 | 13.7223 | 0.049651 | C | 5.103919 | 13.72097 | 0.316735 |
| C | 6.368591 | 12.92304 | -0.31135 | C | 6.160501 | 12.89342 | -0.1692 |
| C | 6.584395 | 6.399575 | 5.092244 | C | 6.514527 | 6.435743 | 4.963984 |
| C | 5.901568 | 8.400455 | 6.386449 | C | 5.791018 | 8.377461 | 6.337979 |
| C | 8.902709 | 11.10672 | 5.608788 | C | 8.982014 | 11.04583 | 5.510003 |
| C | 9.115768 | 12.65329 | 3.710774 | C | 9.059882 | 12.46866 | 3.484647 |
| C | 3.638312 | 8.669873 | 4.013991 | C | 3.837795 | 8.888585 | 3.783054 |
| C | 3.382288 | 8.057372 | 5.271718 | C | 3.399506 | 8.269906 | 4.983331 |
| C | 3.652712 | 6.665289 | 5.157947 | C | 3.573732 | 6.863111 | 4.855375 |
| C | 4.081216 | 6.416895 | 3.818313 | C | 4.130269 | 6.613681 | 3.566613 |
| C | 4.077931 | 7.65534 | 3.113483 | C | 4.300602 | 7.865048 | 2.906045 |
| C | 6.198372 | 13.23861 | 6.109698 | C | 6.335933 | 13.09383 | 6.029368 |
| C | 6.66104 | 14.22832 | 5.198845 | C | 6.682538 | 14.04154 | 5.028563 |
| C | 8.018705 | 14.52002 | 5.517601 | C | 8.038354 | 14.42385 | 5.233293 |
| C | 8.395415 | 13.7214 | 6.631252 | C | 8.532259 | 13.72103 | 6.364767 |

| | | | |
|----|----------|----------|----------|
| C | 7.267651 | 12.92257 | 6.991781 |
| B | 6.818351 | 8.152177 | 3.340486 |
| B | 6.818249 | 11.88867 | 3.340343 |
| Mn | 5.740913 | 12.44048 | 1.719253 |
| Mn | 8.16072 | 7.731144 | 1.918566 |
| Mn | 7.896068 | 12.43966 | 4.96145 |
| Mn | 5.476246 | 7.730787 | 4.762421 |
| H | 10.12886 | 9.718144 | 2.899426 |
| H | 10.59317 | 8.570888 | 0.516409 |
| H | 10.08769 | 5.928836 | 0.73647 |
| H | 9.281899 | 5.456385 | 3.276559 |
| H | 9.335396 | 7.791301 | 4.616089 |
| H | 8.432654 | 12.81387 | 0.547592 |
| H | 7.565108 | 14.69653 | 2.256143 |
| H | 4.986975 | 15.24343 | 1.665613 |
| H | 4.272542 | 13.71593 | -0.4348 |
| H | 6.405148 | 12.19916 | -1.11668 |
| H | 3.507574 | 9.717301 | 3.782178 |
| H | 3.043462 | 8.568852 | 6.164795 |
| H | 3.550113 | 5.927166 | 5.943719 |
| H | 4.356223 | 5.455999 | 3.403478 |
| H | 4.301694 | 7.791572 | 2.064846 |
| H | 5.203939 | 12.81425 | 6.13185 |
| H | 6.073042 | 14.69647 | 4.423747 |
| H | 8.651121 | 15.24242 | 5.015405 |
| H | 9.363939 | 13.71474 | 7.116229 |
| H | 7.230536 | 12.19875 | 7.797141 |

| | | | |
|----|----------|----------|----------|
| C | 7.476358 | 12.8926 | 6.850699 |
| B | 6.818321 | 8.183076 | 3.340322 |
| B | 6.818487 | 11.79473 | 3.340453 |
| Mn | 5.664857 | 12.34976 | 1.836354 |
| Mn | 8.180451 | 7.798831 | 2.007192 |
| Mn | 7.971904 | 12.34994 | 4.844801 |
| Mn | 5.455927 | 7.799785 | 4.673478 |
| H | 9.788884 | 9.944518 | 3.097124 |
| H | 10.60822 | 8.788438 | 0.824737 |
| H | 10.28811 | 6.120714 | 1.073512 |
| H | 9.225354 | 5.653712 | 3.517882 |
| H | 8.967286 | 8.012591 | 4.77573 |
| H | 8.255264 | 12.60437 | 0.558897 |
| H | 7.604731 | 14.39631 | 2.432311 |
| H | 5.03502 | 15.12493 | 2.048886 |
| H | 4.103782 | 13.77799 | -0.08715 |
| H | 6.097288 | 12.20116 | -0.99624 |
| H | 3.847088 | 9.944642 | 3.582894 |
| H | 3.027546 | 8.788557 | 5.85523 |
| H | 3.348818 | 6.120948 | 5.606937 |
| H | 4.412282 | 5.653983 | 3.162887 |
| H | 4.669698 | 8.01276 | 1.904728 |
| H | 5.381568 | 12.60241 | 6.123068 |
| H | 6.030407 | 14.39553 | 4.250186 |
| H | 8.599713 | 15.1257 | 4.633136 |
| H | 9.532438 | 13.77862 | 6.768468 |
| H | 7.540282 | 12.20008 | 7.677473 |

[(CO)₂CpMn]₂BCu]₂ without dispersion

| | | | |
|----|----------|----------|----------|
| Cu | 10.35544 | 16.44941 | 3.281967 |
| Cu | 8.697267 | 18.27904 | 3.055855 |
| O | 8.002471 | 18.99922 | 5.972949 |
| O | 7.700556 | 14.85315 | 6.042224 |
| O | 7.281647 | 12.92061 | 3.249838 |
| O | 10.90908 | 15.89732 | 6.224251 |
| O | 11.8681 | 19.00633 | -0.04353 |
| O | 7.737252 | 19.27889 | 0.363198 |
| O | 11.3576 | 13.50575 | 3.406043 |
| O | 11.25919 | 19.90623 | 6.268798 |
| C | 7.663531 | 18.19857 | 5.179968 |

[(CO)₂CpMn]₂BAu]₂ dispersion

| | | | |
|----|----------|----------|----------|
| Cu | 10.29852 | 16.42076 | 3.399325 |
| Cu | 8.673323 | 18.18454 | 2.910584 |
| O | 8.451097 | 18.80216 | 6.027508 |
| O | 7.841427 | 14.62563 | 5.794591 |
| O | 6.846282 | 13.31701 | 2.857463 |
| O | 10.67062 | 16.17629 | 6.334405 |
| O | 12.09412 | 19.16185 | 0.133762 |
| O | 7.818899 | 19.10257 | 0.201583 |
| O | 11.02561 | 13.35061 | 3.682856 |
| O | 11.44845 | 20.12103 | 6.05289 |
| C | 7.951595 | 18.06562 | 5.263792 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 7.420963 | 15.6916 | 5.277191 | C | 7.541428 | 15.57129 | 5.177282 |
| C | 8.026462 | 13.67858 | 2.755702 | C | 7.794685 | 13.91934 | 2.522161 |
| C | 11.29078 | 16.63963 | 5.398581 | C | 11.11962 | 16.81024 | 5.455329 |
| C | 11.14215 | 19.40383 | 0.792906 | C | 11.23639 | 19.47007 | 0.875892 |
| C | 8.643573 | 19.48267 | 1.095618 | C | 8.687958 | 19.33573 | 0.969368 |
| C | 10.48794 | 14.09498 | 2.875323 | C | 10.27644 | 13.98551 | 3.038937 |
| C | 11.55181 | 19.08912 | 5.480731 | C | 11.63141 | 19.21064 | 5.338459 |
| C | 4.940371 | 17.85913 | 4.523682 | C | 5.374806 | 18.30797 | 4.212698 |
| C | 5.411026 | 18.26321 | 3.236506 | C | 5.81013 | 18.08675 | 2.872931 |
| C | 5.199725 | 15.96909 | 3.228823 | C | 5.185983 | 16.05893 | 3.774314 |
| C | 5.564026 | 17.09409 | 2.436991 | C | 5.692595 | 16.68866 | 2.605666 |
| C | 9.970148 | 15.74951 | 0.128543 | C | 9.991249 | 16.20217 | 0.504598 |
| C | 4.81942 | 16.4478 | 4.521274 | C | 4.988916 | 17.06244 | 4.772064 |
| C | 9.10116 | 13.61381 | 0.054281 | C | 9.749315 | 13.94615 | 0.076465 |
| C | 8.012255 | 14.54174 | 0.075397 | C | 8.474953 | 14.56605 | -0.04627 |
| C | 8.54982 | 15.8572 | 0.117077 | C | 8.621591 | 15.95807 | 0.212676 |
| C | 9.687995 | 21.53931 | 3.599595 | C | 9.619146 | 21.18928 | 3.709612 |
| C | 8.905405 | 21.88856 | 2.463472 | C | 8.659711 | 21.50505 | 2.70932 |
| C | 9.784617 | 22.16385 | 1.374478 | C | 9.349363 | 22.00764 | 1.56409 |
| C | 11.11514 | 21.97773 | 1.84283 | C | 10.73594 | 21.99046 | 1.858121 |
| C | 11.05814 | 21.60026 | 3.215363 | C | 10.90709 | 21.49286 | 3.182849 |
| C | 14.1419 | 18.52595 | 4.640445 | C | 14.0745 | 18.30923 | 4.433264 |
| C | 13.77887 | 18.71924 | 3.27367 | C | 13.61159 | 18.55027 | 3.104712 |
| C | 13.48992 | 17.44137 | 2.714521 | C | 13.1365 | 17.31603 | 2.580082 |
| C | 13.67542 | 16.46433 | 3.733518 | C | 13.30891 | 16.31687 | 3.580919 |
| C | 14.08749 | 17.13618 | 4.923848 | C | 13.89825 | 16.93276 | 4.724421 |
| C | 10.3036 | 14.36461 | 0.087163 | C | 10.68337 | 14.96144 | 0.428686 |
| Mn | 6.889833 | 16.95569 | 4.150027 | Mn | 7.036227 | 16.95829 | 4.2165 |
| Mn | 9.138313 | 14.74956 | 1.901106 | Mn | 9.172712 | 14.82807 | 1.934305 |
| Mn | 10.05529 | 20.10143 | 1.989532 | Mn | 9.983208 | 20.01089 | 1.971183 |
| Mn | 12.11373 | 17.84758 | 4.355961 | Mn | 12.01238 | 17.8471 | 4.306875 |
| B | 8.260385 | 16.07597 | 3.068155 | B | 8.289227 | 16.06318 | 3.099165 |
| B | 10.79672 | 18.68023 | 3.168658 | B | 10.7377 | 18.66662 | 3.143942 |
| H | 4.734113 | 18.51582 | 5.360128 | H | 5.378986 | 19.25872 | 4.727 |
| H | 5.588654 | 19.28149 | 2.914726 | H | 6.129087 | 18.83846 | 2.166969 |
| H | 5.202555 | 14.93429 | 2.913783 | H | 5.021284 | 14.99902 | 3.890581 |
| H | 5.866858 | 17.07871 | 1.399802 | H | 5.945152 | 16.19848 | 1.679235 |
| H | 10.67032 | 16.57172 | 0.112529 | H | 10.41667 | 17.16199 | 0.735928 |
| H | 4.494161 | 15.83526 | 5.35312 | H | 4.637867 | 16.89747 | 5.779818 |
| H | 9.02033 | 12.53471 | 0.01595 | H | 9.962923 | 12.89476 | -0.04623 |
| H | 6.96042 | 14.28489 | 0.038079 | H | 7.548992 | 14.06397 | -0.28826 |

| | | | |
|---|----------|----------|----------|
| H | 7.988637 | 16.77783 | 0.087248 |
| H | 9.313525 | 21.29475 | 4.58395 |
| H | 7.823852 | 21.94477 | 2.431322 |
| H | 9.493222 | 22.45367 | 0.372314 |
| H | 12.01661 | 22.11636 | 1.25755 |
| H | 11.90478 | 21.42244 | 3.861716 |
| H | 14.42024 | 19.30453 | 5.340784 |
| H | 13.75306 | 19.66267 | 2.746107 |
| H | 13.21644 | 17.24931 | 1.686548 |
| H | 13.53463 | 15.3964 | 3.624776 |
| H | 14.30057 | 16.66921 | 5.877516 |
| H | 11.30702 | 13.95529 | 0.082898 |

| | | | |
|---|----------|----------|----------|
| H | 7.846601 | 16.70383 | 0.179782 |
| H | 9.411623 | 20.78733 | 4.686753 |
| H | 7.591591 | 21.36888 | 2.794113 |
| H | 8.898629 | 22.30768 | 0.629307 |
| H | 11.52876 | 22.28757 | 1.186068 |
| H | 11.84352 | 21.3549 | 3.696919 |
| H | 14.47527 | 19.05234 | 5.107805 |
| H | 13.60096 | 19.49643 | 2.587427 |
| H | 12.73162 | 17.16995 | 1.593324 |
| H | 13.02813 | 15.27738 | 3.498083 |
| H | 14.12464 | 16.44343 | 5.660386 |
| H | 11.73528 | 14.81333 | 0.623772 |

$\{(CO)_2CpMn\}_2B\{Cu(PCy_3)\}\{Pt(PCy_3)\}$
without dispersion

| | | | |
|----|----------|----------|----------|
| Mn | 6.287589 | 6.960661 | 6.74922 |
| Mn | 6.70913 | 7.077202 | 2.918896 |
| B | 6.890715 | 6.700542 | 4.885858 |
| O | 7.563701 | 5.010592 | 8.592955 |
| C | 7.279923 | 5.711871 | 7.668762 |
| O | 4.00894 | 5.211083 | 6.18188 |
| C | 4.978744 | 5.856994 | 6.385287 |
| O | 8.682635 | 5.660192 | 1.267116 |
| C | 7.926956 | 6.144436 | 2.036841 |
| O | 8.618316 | 9.17798 | 3.660191 |
| C | 7.886359 | 8.292803 | 3.400032 |
| C | 6.675194 | 8.336058 | 8.420368 |
| H | 7.309969 | 8.088915 | 9.262211 |
| C | 7.09113 | 8.972069 | 7.217682 |
| H | 8.089916 | 9.309669 | 6.979264 |
| C | 5.959444 | 9.087 | 6.365626 |
| H | 5.951059 | 9.556413 | 5.393219 |
| C | 4.845301 | 8.516761 | 7.042202 |
| H | 3.827477 | 8.464088 | 6.675003 |
| C | 5.288052 | 8.051301 | 8.322008 |
| H | 4.675754 | 7.567442 | 9.072837 |
| C | 4.6103 | 6.512156 | 2.599164 |
| H | 4.118981 | 5.643583 | 3.011317 |
| C | 5.278232 | 6.602385 | 1.343489 |
| H | 5.415275 | 5.798181 | 0.631924 |
| C | 5.742418 | 7.938114 | 1.175363 |

$\{(CO)_2CpMn\}_2B\{Cu(PCy_3)\}\{Pt(PCy_3)\}$
with dispersion

| | | | |
|----|----------|----------|----------|
| Mn | 6.366275 | 7.108947 | 6.803667 |
| Mn | 6.631512 | 7.090449 | 3.050144 |
| B | 6.845865 | 6.774829 | 4.961521 |
| O | 7.576569 | 5.229126 | 8.741378 |
| C | 7.242279 | 5.854066 | 7.782785 |
| O | 3.96756 | 5.560998 | 6.187802 |
| C | 4.966142 | 6.134366 | 6.448388 |
| O | 8.242864 | 5.407217 | 1.26035 |
| C | 7.664645 | 5.998494 | 2.111356 |
| O | 8.634511 | 9.119402 | 3.695164 |
| C | 7.873001 | 8.260539 | 3.435069 |
| C | 7.096173 | 8.494541 | 8.265531 |
| H | 7.775724 | 8.2056 | 9.053452 |
| C | 7.471157 | 8.950857 | 6.973085 |
| H | 8.474559 | 9.074619 | 6.600224 |
| C | 6.282847 | 9.153398 | 6.219617 |
| H | 6.238869 | 9.492107 | 5.200017 |
| C | 5.176996 | 8.821758 | 7.050599 |
| H | 4.133797 | 8.8634 | 6.771686 |
| C | 5.678471 | 8.414366 | 8.324415 |
| H | 5.090823 | 8.079336 | 9.166283 |
| C | 4.588579 | 6.465397 | 2.920894 |
| H | 4.204551 | 5.557497 | 3.356109 |
| C | 5.124055 | 6.632827 | 1.611769 |
| H | 5.23866 | 5.858434 | 0.869425 |
| C | 5.536059 | 7.985368 | 1.460052 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| H | 6.295472 | 8.321586 | 0.326826 | H | 6.009293 | 8.414655 | 0.589028 |
| C | 5.366701 | 8.66954 | 2.337301 | C | 5.25611 | 8.654331 | 2.685577 |
| H | 5.5708 | 9.718564 | 2.515918 | H | 5.470423 | 9.691691 | 2.898548 |
| C | 4.661646 | 7.792891 | 3.21036 | C | 4.666613 | 7.720484 | 3.581233 |
| H | 4.232646 | 8.049069 | 4.16615 | H | 4.361787 | 7.910849 | 4.593879 |
| Pt | 8.583301 | 5.997659 | 5.998525 | Pt | 8.46559 | 5.894509 | 6.02665 |
| P | 10.96603 | 5.755214 | 6.051831 | P | 10.67215 | 5.407695 | 5.811623 |
| C | 11.76907 | 7.09929 | 7.165109 | C | 11.59041 | 6.534574 | 6.973077 |
| H | 12.65771 | 6.601218 | 7.571334 | H | 12.48472 | 5.989553 | 7.290895 |
| C | 10.84984 | 7.474194 | 8.347164 | C | 10.71527 | 6.820296 | 8.196337 |
| H | 9.957175 | 7.966141 | 7.948626 | H | 9.830298 | 7.357047 | 7.844491 |
| H | 10.49249 | 6.58478 | 8.869641 | H | 10.34668 | 5.899286 | 8.641785 |
| C | 11.54913 | 8.409608 | 9.346571 | C | 11.45194 | 7.66535 | 9.226034 |
| H | 12.37968 | 7.875002 | 9.831043 | H | 12.3167 | 7.105682 | 9.605596 |
| H | 10.84698 | 8.674452 | 10.14789 | H | 10.79606 | 7.858317 | 10.0818 |
| C | 12.085 | 9.675683 | 8.670306 | C | 11.9301 | 8.975193 | 8.612647 |
| H | 11.24049 | 10.29317 | 8.331817 | H | 11.05673 | 9.572525 | 8.322488 |
| H | 12.64588 | 10.28618 | 9.389712 | H | 12.49325 | 9.562647 | 9.345455 |
| C | 12.96858 | 9.325656 | 7.4695 | C | 12.78153 | 8.710552 | 7.376958 |
| H | 13.89416 | 8.847938 | 7.823048 | H | 13.69978 | 8.189311 | 7.676433 |
| H | 13.27561 | 10.23903 | 6.9433 | H | 13.08526 | 9.654822 | 6.912452 |
| C | 12.26161 | 8.387795 | 6.474837 | C | 12.03455 | 7.856668 | 6.356762 |
| H | 11.41195 | 8.918806 | 6.029053 | H | 11.14705 | 8.398697 | 6.01914 |
| H | 12.95733 | 8.158434 | 5.663831 | H | 12.66563 | 7.686086 | 5.48333 |
| C | 11.92842 | 5.848837 | 4.410335 | C | 11.42993 | 5.630652 | 4.150609 |
| H | 12.96705 | 6.05271 | 4.704581 | H | 12.50925 | 5.732126 | 4.305127 |
| C | 11.4456 | 6.994332 | 3.497072 | C | 10.89415 | 6.871991 | 3.446334 |
| H | 11.4119 | 7.946625 | 4.023647 | H | 10.95074 | 7.754024 | 4.073838 |
| H | 10.42052 | 6.783454 | 3.189366 | H | 9.836627 | 6.70293 | 3.253399 |
| C | 12.33257 | 7.13687 | 2.249141 | C | 11.6402 | 7.105042 | 2.138605 |
| H | 11.93648 | 7.943461 | 1.619133 | H | 11.24076 | 7.996781 | 1.644481 |
| H | 13.34352 | 7.449379 | 2.551327 | H | 12.69584 | 7.308184 | 2.362779 |
| C | 12.41584 | 5.833793 | 1.446612 | C | 11.53347 | 5.900209 | 1.211259 |
| H | 13.13838 | 5.937378 | 0.626415 | H | 12.1699 | 6.040071 | 0.330425 |
| H | 11.44277 | 5.63431 | 0.983129 | H | 10.50466 | 5.81932 | 0.859448 |
| C | 12.80485 | 4.652043 | 2.341341 | C | 11.91155 | 4.605452 | 1.922586 |
| H | 13.85302 | 4.760583 | 2.656961 | H | 12.98856 | 4.605262 | 2.136671 |
| H | 12.75234 | 3.714448 | 1.772967 | H | 11.71724 | 3.750908 | 1.269274 |
| C | 11.91634 | 4.536706 | 3.594919 | C | 11.16343 | 4.433485 | 3.241972 |
| H | 10.88631 | 4.312098 | 3.296329 | H | 10.08744 | 4.382122 | 3.068325 |
| H | 12.26391 | 3.687532 | 4.187523 | H | 11.45806 | 3.49651 | 3.71051 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 11.63868 | 4.142326 | 6.826475 | C | 11.27035 | 3.734913 | 6.327613 |
| H | 11.24894 | 3.388992 | 6.128231 | H | 10.68351 | 3.049092 | 5.711195 |
| C | 13.17537 | 3.992884 | 6.885998 | C | 12.75327 | 3.476413 | 6.073103 |
| H | 13.59317 | 4.732512 | 7.579899 | H | 13.34643 | 4.147684 | 6.701773 |
| H | 13.63838 | 4.186803 | 5.915074 | H | 13.0203 | 3.691257 | 5.038993 |
| C | 13.59257 | 2.592311 | 7.370831 | C | 13.10974 | 2.03196 | 6.412966 |
| H | 13.29401 | 1.844001 | 6.62217 | H | 12.55873 | 1.363327 | 5.739512 |
| H | 14.68762 | 2.542477 | 7.435274 | H | 14.17626 | 1.858753 | 6.233042 |
| C | 12.96305 | 2.240636 | 8.723057 | C | 12.75072 | 1.699391 | 7.855791 |
| H | 13.22085 | 1.211316 | 9.004541 | H | 12.97533 | 0.649549 | 8.072045 |
| H | 13.38948 | 2.890118 | 9.501511 | H | 13.37336 | 2.305513 | 8.526151 |
| C | 11.44104 | 2.419049 | 8.689319 | C | 11.28271 | 1.996901 | 8.134288 |
| H | 11.01507 | 2.239575 | 9.684874 | H | 11.04709 | 1.801234 | 9.18535 |
| H | 11.00284 | 1.662127 | 8.024905 | H | 10.66024 | 1.324662 | 7.536206 |
| C | 11.03134 | 3.820596 | 8.206935 | C | 10.93518 | 3.439637 | 7.78668 |
| H | 9.943192 | 3.906905 | 8.176228 | H | 9.885043 | 3.653386 | 7.985051 |
| H | 11.38275 | 4.551435 | 8.944772 | H | 11.52541 | 4.103999 | 8.423272 |
| Cu | 7.073072 | 4.731977 | 3.968425 | Cu | 7.246295 | 4.886642 | 3.964276 |
| P | 6.678317 | 2.395 | 3.847934 | P | 7.08158 | 2.695818 | 3.982913 |
| C | 8.015852 | 1.448373 | 2.879456 | C | 8.563593 | 1.728685 | 3.446326 |
| H | 8.839348 | 1.464665 | 3.605293 | H | 9.379761 | 2.143243 | 4.043354 |
| C | 8.550905 | 2.170569 | 1.626808 | C | 8.894566 | 1.971683 | 1.975547 |
| H | 8.804209 | 3.205433 | 1.860148 | H | 8.955983 | 3.039104 | 1.770367 |
| H | 7.781621 | 2.212592 | 0.848515 | H | 8.083138 | 1.573024 | 1.360847 |
| C | 9.782502 | 1.449134 | 1.054269 | C | 10.18805 | 1.263813 | 1.588495 |
| H | 10.61291 | 1.522019 | 1.770538 | H | 11.0155 | 1.690738 | 2.162441 |
| H | 10.11308 | 1.966983 | 0.145108 | H | 10.40503 | 1.442934 | 0.530497 |
| C | 9.502939 | -0.0277 | 0.752933 | C | 10.10332 | -0.23067 | 1.8721 |
| H | 8.783495 | -0.10143 | -0.0756 | H | 9.325997 | -0.67484 | 1.237587 |
| H | 10.41884 | -0.52632 | 0.411116 | H | 11.04728 | -0.72289 | 1.615408 |
| C | 8.936882 | -0.75005 | 1.980816 | C | 9.754355 | -0.48236 | 3.333862 |
| H | 9.713942 | -0.81772 | 2.75577 | H | 10.57125 | -0.11406 | 3.967473 |
| H | 8.666181 | -1.78309 | 1.724925 | H | 9.657876 | -1.55604 | 3.527381 |
| C | 7.705415 | -0.02799 | 2.554993 | C | 8.462735 | 0.230363 | 3.725455 |
| H | 6.898205 | -0.0792 | 1.814494 | H | 7.637396 | -0.18874 | 3.141769 |
| H | 7.349508 | -0.56468 | 3.440196 | H | 8.237419 | 0.04299 | 4.774629 |
| C | 5.033533 | 1.883642 | 3.018648 | C | 5.766084 | 2.054124 | 2.84198 |
| H | 5.114778 | 0.795191 | 2.901659 | H | 6.128195 | 1.089098 | 2.475738 |
| C | 4.879051 | 2.509292 | 1.617263 | C | 5.633642 | 3.014102 | 1.66086 |
| H | 5.722998 | 2.239478 | 0.979358 | H | 6.604899 | 3.222669 | 1.215805 |
| H | 4.899017 | 3.599556 | 1.709684 | H | 5.27257 | 3.964568 | 2.054809 |

| | | | |
|---|----------|----------|----------|
| C | 3.576873 | 2.081403 | 0.918343 |
| H | 3.500267 | 2.599281 | -0.04666 |
| H | 3.624466 | 1.006861 | 0.687991 |
| C | 2.337834 | 2.359994 | 1.77436 |
| H | 1.437504 | 1.981618 | 1.273665 |
| H | 2.199306 | 3.445171 | 1.88086 |
| C | 2.482215 | 1.724717 | 3.158973 |
| H | 1.62467 | 1.986333 | 3.791995 |
| H | 2.468974 | 0.62946 | 3.058531 |
| C | 3.775652 | 2.156241 | 3.87251 |
| H | 3.711353 | 3.220654 | 4.123586 |
| H | 3.835179 | 1.616868 | 4.819875 |
| C | 6.59932 | 1.435924 | 5.501148 |
| H | 5.978855 | 0.556674 | 5.275809 |
| C | 5.907978 | 2.261754 | 6.605843 |
| H | 4.950148 | 2.659428 | 6.275029 |
| H | 6.532901 | 3.128364 | 6.830664 |
| C | 5.70191 | 1.446198 | 7.89167 |
| H | 5.231541 | 2.086995 | 8.647463 |
| H | 4.997211 | 0.623203 | 7.699596 |
| C | 7.021567 | 0.880679 | 8.424353 |
| H | 7.646422 | 1.708163 | 8.783776 |
| H | 6.839697 | 0.228185 | 9.288225 |
| C | 7.770053 | 0.10938 | 7.33309 |
| H | 7.218996 | -0.81196 | 7.093025 |
| H | 8.754488 | -0.21082 | 7.698041 |
| C | 7.953639 | 0.928608 | 6.041109 |
| H | 8.606392 | 1.787168 | 6.241714 |
| H | 8.468306 | 0.299107 | 5.311831 |

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|---|----------|----------|----------|
| C | 4.661084 | 2.477896 | 0.618183 |
| H | 4.563649 | 3.193751 | -0.20528 |
| H | 5.068039 | 1.553044 | 0.189456 |
| C | 3.297217 | 2.187935 | 1.234184 |
| H | 2.623021 | 1.75602 | 0.487236 |
| H | 2.847352 | 3.131967 | 1.565972 |
| C | 3.428088 | 1.256018 | 2.433404 |
| H | 2.449345 | 1.08817 | 2.895396 |
| H | 3.79697 | 0.279124 | 2.095847 |
| C | 4.395229 | 1.823802 | 3.468284 |
| H | 4.001712 | 2.777056 | 3.831224 |
| H | 4.466485 | 1.15425 | 4.326713 |
| C | 6.712636 | 2.035021 | 5.654731 |
| H | 6.368786 | 1.002646 | 5.534442 |
| C | 5.632565 | 2.867465 | 6.337701 |
| H | 4.756487 | 2.997376 | 5.711174 |
| H | 6.049676 | 3.86063 | 6.501951 |
| C | 5.240782 | 2.237957 | 7.667853 |
| H | 4.468206 | 2.8481 | 8.146014 |
| H | 4.800992 | 1.249752 | 7.477356 |
| C | 6.44539 | 2.099556 | 8.590759 |
| H | 6.759439 | 3.094604 | 8.904849 |
| H | 6.170421 | 1.5433 | 9.493738 |
| C | 7.616759 | 1.413892 | 7.895642 |
| H | 7.375103 | 0.356858 | 7.720419 |
| H | 8.496537 | 1.435908 | 8.542841 |
| C | 7.94565 | 2.058835 | 6.552761 |
| H | 8.236541 | 3.104795 | 6.680983 |
| H | 8.788522 | 1.543918 | 6.094642 |

$\{(\text{CO})_2\text{CpMn}\}_2\text{B}\{\text{Cu}(\text{ITol})\}\{\text{Pt}(\text{PCy}_3)\}$
without dispersion

| | | | |
|----|----------|----------|----------|
| Pt | 7.308311 | 1.493381 | 4.291855 |
| Mn | 9.759415 | 1.309359 | 5.881208 |
| P | 6.844125 | 3.256043 | 2.762623 |
| B | 8.051362 | 0.33368 | 5.872384 |
| O | 10.93763 | -1.31679 | 5.323704 |
| C | 10.42937 | -0.27323 | 5.549484 |
| Cu | 7.321874 | -0.5418 | 7.790088 |
| Mn | 6.40038 | -0.69807 | 5.502085 |

$\{(\text{CO})_2\text{CpMn}\}_2\text{B}\{\text{Cu}(\text{ITol})\}\{\text{Pt}(\text{PCy}_3)\}$
with dispersion

| | | | |
|----|----------|----------|----------|
| Pt | 7.485754 | 1.508704 | 4.489575 |
| Mn | 9.078792 | 1.865788 | 6.631013 |
| P | 6.710268 | 3.087914 | 3.018777 |
| B | 8.12828 | 0.328734 | 6.084 |
| O | 11.37727 | 0.140499 | 6.189053 |
| C | 10.43549 | 0.836874 | 6.34099 |
| Cu | 7.279841 | -0.88252 | 7.486118 |
| Mn | 7.226307 | -1.05984 | 5.068857 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| O | 4.425984 | 0.64102 | 7.231789 | O | 4.627276 | -1.67192 | 6.254357 |
| C | 5.271975 | 0.09706 | 6.611148 | C | 5.707793 | -1.36496 | 5.882531 |
| O | 10.50001 | 1.971519 | 3.114644 | O | 9.962827 | 3.346053 | 4.265641 |
| C | 9.99461 | 1.703125 | 4.149592 | C | 9.331817 | 2.660167 | 5.004132 |
| O | 4.48735 | 0.685909 | 3.698146 | O | 5.15369 | -0.00408 | 3.282635 |
| C | 5.549819 | 0.555278 | 4.244665 | C | 6.139965 | 0.055021 | 3.955514 |
| C | 9.305363 | 3.109904 | 7.063585 | C | 7.739404 | 3.231547 | 7.616642 |
| H | 8.403212 | 3.698168 | 6.971198 | H | 6.801197 | 3.546748 | 7.190891 |
| C | 10.52216 | 3.295735 | 6.342184 | C | 9.010416 | 3.854757 | 7.429825 |
| H | 10.70788 | 4.055506 | 5.595579 | H | 9.201066 | 4.737495 | 6.840701 |
| C | 11.4578 | 2.317989 | 6.775939 | C | 9.984808 | 3.085232 | 8.111036 |
| H | 12.4702 | 2.195637 | 6.411052 | H | 11.04723 | 3.278631 | 8.13287 |
| C | 10.81029 | 1.510679 | 7.756414 | C | 9.317069 | 1.9684 | 8.710257 |
| H | 11.25523 | 0.67885 | 8.28129 | H | 9.784456 | 1.186987 | 9.290527 |
| C | 9.488954 | 2.009474 | 7.942731 | C | 7.927954 | 2.075954 | 8.411102 |
| H | 8.758126 | 1.637237 | 8.647668 | H | 7.149952 | 1.410691 | 8.728005 |
| C | 6.506463 | -2.75544 | 6.109488 | C | 8.148497 | -2.92318 | 5.314614 |
| H | 6.576248 | -3.12539 | 7.124395 | H | 8.131992 | -3.49474 | 6.229781 |
| C | 7.606807 | -2.49246 | 5.232612 | C | 9.136991 | -1.9597 | 4.951409 |
| H | 8.656991 | -2.58169 | 5.470802 | H | 9.989987 | -1.66984 | 5.535063 |
| C | 7.075367 | -2.11893 | 3.972126 | C | 8.794041 | -1.44388 | 3.673637 |
| H | 7.652751 | -1.83416 | 3.102214 | H | 9.316557 | -0.65675 | 3.153287 |
| C | 5.650535 | -2.16107 | 4.06161 | C | 7.593446 | -2.08353 | 3.243252 |
| H | 4.955847 | -1.91567 | 3.26983 | H | 7.056579 | -1.8783 | 2.33013 |
| C | 5.297851 | -2.5589 | 5.372456 | C | 7.200004 | -3.00288 | 4.247651 |
| H | 4.290171 | -2.67843 | 5.75109 | H | 6.312014 | -3.61752 | 4.230703 |
| C | 5.037344 | 3.78693 | 2.975689 | C | 4.878252 | 3.086241 | 3.092414 |
| H | 4.554601 | 2.825231 | 2.76887 | H | 4.661948 | 2.092595 | 2.692829 |
| C | 4.656216 | 4.124234 | 4.434976 | C | 4.36109 | 3.065943 | 4.531172 |
| H | 5.059108 | 5.103453 | 4.717981 | H | 4.518962 | 4.042621 | 4.99519 |
| H | 5.094351 | 3.390516 | 5.116739 | H | 4.934426 | 2.336591 | 5.106509 |
| C | 3.128751 | 4.149625 | 4.604973 | C | 2.876277 | 2.730722 | 4.542059 |
| H | 2.735926 | 3.137107 | 4.445557 | H | 2.746782 | 1.714438 | 4.154011 |
| H | 2.879271 | 4.420375 | 5.639854 | H | 2.494562 | 2.737162 | 5.567962 |
| C | 2.459491 | 5.124762 | 3.628263 | C | 2.083655 | 3.71108 | 3.684239 |
| H | 1.366757 | 5.0618 | 3.717534 | H | 1.023968 | 3.434601 | 3.668332 |
| H | 2.732048 | 6.156286 | 3.898228 | H | 2.146764 | 4.710438 | 4.1347 |
| C | 2.884535 | 4.855583 | 2.178703 | C | 2.630949 | 3.776486 | 2.262461 |
| H | 2.461438 | 5.619262 | 1.512041 | H | 2.078351 | 4.519555 | 1.676965 |
| H | 2.468572 | 3.892388 | 1.850594 | H | 2.482127 | 2.805272 | 1.775405 |
| C | 4.416647 | 4.822826 | 2.017604 | C | 4.120952 | 4.106785 | 2.257058 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | 4.661409 | 4.602776 | 0.973522 | H | 4.500327 | 4.130114 | 1.23288 |
| H | 4.812176 | 5.822809 | 2.230852 | H | 4.265425 | 5.104077 | 2.679903 |
| C | 6.941911 | 2.692791 | 0.94908 | C | 7.123511 | 2.735106 | 1.259412 |
| H | 6.614138 | 3.550695 | 0.348023 | H | 6.642256 | 3.497929 | 0.639942 |
| C | 6.00719 | 1.50776 | 0.626435 | C | 6.62233 | 1.362666 | 0.827932 |
| H | 6.284821 | 0.654413 | 1.254344 | H | 7.062815 | 0.620364 | 1.495164 |
| H | 4.968186 | 1.743104 | 0.871199 | H | 5.542158 | 1.287973 | 0.950898 |
| C | 6.092596 | 1.100709 | -0.85423 | C | 7.014904 | 1.054485 | -0.61051 |
| H | 5.694598 | 1.912708 | -1.481 | H | 6.527793 | 1.771482 | -1.28368 |
| H | 5.441928 | 0.232924 | -1.02625 | H | 6.649456 | 0.05923 | -0.88626 |
| C | 7.527702 | 0.78273 | -1.28817 | C | 8.523393 | 1.138955 | -0.79746 |
| H | 7.869795 | -0.12658 | -0.77315 | H | 9.002736 | 0.363471 | -0.1869 |
| H | 7.562177 | 0.562747 | -2.36342 | H | 8.79408 | 0.941117 | -1.84 |
| C | 8.472923 | 1.939077 | -0.94862 | C | 9.041208 | 2.502726 | -0.36187 |
| H | 8.228357 | 2.807615 | -1.57845 | H | 8.631333 | 3.271427 | -1.0295 |
| H | 9.509776 | 1.667191 | -1.18739 | H | 10.13165 | 2.546979 | -0.45535 |
| C | 8.384727 | 2.335423 | 0.53281 | C | 8.637812 | 2.819281 | 1.072016 |
| H | 9.070929 | 3.16458 | 0.720045 | H | 9.009369 | 3.80441 | 1.352713 |
| H | 8.739721 | 1.505108 | 1.151292 | H | 9.103173 | 2.106327 | 1.758451 |
| C | 7.985785 | 4.784614 | 2.789243 | C | 7.359574 | 4.792582 | 3.243279 |
| H | 8.969727 | 4.299198 | 2.751923 | H | 8.434725 | 4.606683 | 3.263581 |
| C | 7.91558 | 5.779489 | 1.609486 | C | 7.095931 | 5.822679 | 2.151392 |
| H | 6.948747 | 6.293802 | 1.607541 | H | 6.034326 | 6.071509 | 2.115854 |
| H | 7.996262 | 5.264056 | 0.649469 | H | 7.366812 | 5.427085 | 1.171761 |
| C | 9.034657 | 6.83328 | 1.69886 | C | 7.901629 | 7.088411 | 2.433971 |
| H | 10.00864 | 6.339027 | 1.572136 | H | 8.97002 | 6.847102 | 2.377589 |
| H | 8.936319 | 7.53953 | 0.863533 | H | 7.700684 | 7.839642 | 1.662297 |
| C | 9.017683 | 7.585992 | 3.033916 | C | 7.591826 | 7.653995 | 3.8155 |
| H | 9.868101 | 8.277944 | 3.091116 | H | 8.206892 | 8.539283 | 4.008698 |
| H | 8.110336 | 8.205076 | 3.091916 | H | 6.543791 | 7.979573 | 3.841216 |
| C | 9.044813 | 6.611981 | 4.217482 | C | 7.812083 | 6.606588 | 4.900914 |
| H | 8.952062 | 7.161684 | 5.163764 | H | 7.548766 | 7.013193 | 5.883571 |
| H | 10.0209 | 6.108612 | 4.24543 | H | 8.874617 | 6.340403 | 4.932695 |
| C | 7.925165 | 5.56215 | 4.120479 | C | 7.00167 | 5.350201 | 4.614399 |
| H | 7.980911 | 4.869734 | 4.963363 | H | 7.184332 | 4.583846 | 5.364159 |
| H | 6.963632 | 6.080581 | 4.201837 | H | 5.936872 | 5.595432 | 4.642759 |
| C | 7.44114 | -1.04948 | 9.678276 | C | 7.215144 | -1.223 | 9.352335 |
| N | 6.379823 | -1.15109 | 10.55471 | N | 6.398575 | -0.69103 | 10.31478 |
| C | 6.782514 | -1.53851 | 11.82498 | C | 6.694081 | -1.19048 | 11.57466 |
| H | 6.081404 | -1.67977 | 12.63393 | H | 6.15059 | -0.89034 | 12.45505 |
| C | 8.125169 | -1.69834 | 11.77556 | C | 7.717582 | -2.07204 | 11.41039 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | 8.826095 | -2.01966 | 12.53095 | H | 8.258239 | -2.67389 | 12.12169 |
| N | 8.516226 | -1.40592 | 10.47315 | N | 8.021979 | -2.0714 | 10.05561 |
| C | 4.976465 | -0.95756 | 10.26371 | C | 5.47309 | 0.34955 | 10.01802 |
| C | 4.236632 | -2.00159 | 9.709909 | C | 4.7336 | 0.271044 | 8.841409 |
| H | 4.728214 | -2.933 | 9.442366 | H | 4.745249 | -0.63341 | 8.25246 |
| C | 2.866673 | -1.84443 | 9.510408 | C | 4.004805 | 1.373257 | 8.418546 |
| H | 2.30054 | -2.66413 | 9.071713 | H | 3.462656 | 1.313273 | 7.480974 |
| C | 2.209756 | -0.65786 | 9.863685 | C | 3.977358 | 2.553477 | 9.168791 |
| C | 2.973372 | 0.368388 | 10.43683 | C | 4.672856 | 2.582429 | 10.38074 |
| H | 2.492992 | 1.302277 | 10.7219 | H | 4.662617 | 3.487077 | 10.98115 |
| C | 4.345002 | 0.227293 | 10.63879 | C | 5.42996 | 1.494305 | 10.80617 |
| H | 4.923516 | 1.036747 | 11.07712 | H | 6.03478 | 1.561503 | 11.7037 |
| C | 0.736195 | -0.47562 | 9.59432 | C | 3.250756 | 3.762113 | 8.658393 |
| H | 0.270654 | 0.187067 | 10.33036 | H | 3.159159 | 4.528175 | 9.431012 |
| H | 0.202597 | -1.43102 | 9.606188 | H | 2.250018 | 3.500073 | 8.303975 |
| H | 0.583201 | -0.02607 | 8.604296 | H | 3.78927 | 4.196552 | 7.80912 |
| C | 9.899915 | -1.5294 | 10.0903 | C | 9.083616 | -2.79838 | 9.445588 |
| C | 10.28308 | -2.35805 | 9.034553 | C | 9.273123 | -4.14462 | 9.746444 |
| H | 9.530149 | -2.87446 | 8.447916 | H | 8.609483 | -4.64271 | 10.44536 |
| C | 11.63484 | -2.52185 | 8.741994 | C | 10.294 | -4.84643 | 9.114581 |
| H | 11.91502 | -3.15635 | 7.904189 | H | 10.43307 | -5.90013 | 9.34009 |
| C | 12.63245 | -1.88677 | 9.496861 | C | 11.13107 | -4.22404 | 8.181324 |
| C | 12.22416 | -1.06464 | 10.55508 | C | 10.923 | -2.87116 | 7.904522 |
| H | 12.96916 | -0.54459 | 11.15439 | H | 11.56392 | -2.35884 | 7.196799 |
| C | 10.87433 | -0.87878 | 10.85088 | C | 9.90898 | -2.15335 | 8.528969 |
| H | 10.58189 | -0.21728 | 11.66266 | H | 9.757121 | -1.10612 | 8.300864 |
| C | 14.09312 | -2.08338 | 9.171162 | C | 12.22027 | -4.99607 | 7.496837 |
| H | 14.40424 | -3.11714 | 9.367808 | H | 12.94701 | -5.37492 | 8.223505 |
| H | 14.72984 | -1.42409 | 9.76802 | H | 12.7505 | -4.37236 | 6.774844 |
| H | 14.29191 | -1.88252 | 8.112331 | H | 11.80915 | -5.8619 | 6.967281 |

$\{(\text{CO})_2\text{CpMn}\}_2\text{B}\{\text{Cu}(\text{IMe})\}\{\text{Pt}(\text{PCy}_3)\}$
without dispersion

| | | | |
|----|----------|----------|----------|
| Mn | 6.159797 | 5.970676 | 6.99574 |
| Mn | 6.479844 | 8.27701 | 3.933296 |
| B | 6.676617 | 6.879546 | 5.348187 |
| O | 7.503287 | 3.331486 | 7.245825 |
| C | 7.217832 | 4.454655 | 6.953754 |
| O | 4.049808 | 4.72665 | 5.39964 |
| C | 4.939845 | 5.21273 | 6.006055 |

$\{(\text{CO})_2\text{CpMn}\}_2\text{B}\{\text{Cu}(\text{IMe})\}\{\text{Pt}(\text{PCy}_3)\}$
without dispersion

| | | | |
|----|----------|----------|----------|
| Mn | 6.031203 | 5.869388 | 6.79264 |
| Mn | 6.926799 | 8.275812 | 4.025692 |
| B | 6.872041 | 6.855541 | 5.36074 |
| O | 7.283299 | 3.241026 | 7.347481 |
| C | 6.995769 | 4.338905 | 6.975803 |
| O | 4.276722 | 4.863038 | 4.682668 |
| C | 5.012149 | 5.238089 | 5.529358 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| O | 8.867432 | 8.122442 | 2.224085 | O | 9.299553 | 7.980039 | 2.315969 |
| C | 7.919655 | 8.072953 | 2.931212 | C | 8.382452 | 8.015539 | 3.064331 |
| O | 8.081735 | 9.740849 | 5.895353 | O | 8.197353 | 9.563702 | 6.320414 |
| C | 7.457629 | 9.110336 | 5.124103 | C | 7.740197 | 9.015075 | 5.384715 |
| C | 6.54784 | 6.107317 | 9.151655 | C | 6.151588 | 6.049058 | 8.917999 |
| H | 7.236812 | 5.45845 | 9.678412 | H | 6.742958 | 5.381227 | 9.527733 |
| C | 6.869387 | 7.360969 | 8.558034 | C | 6.611273 | 7.257294 | 8.326605 |
| H | 7.838122 | 7.842277 | 8.559888 | H | 7.602256 | 7.675349 | 8.402815 |
| C | 5.690904 | 7.872898 | 7.94484 | C | 5.547206 | 7.795362 | 7.550145 |
| H | 5.604611 | 8.821397 | 7.43586 | H | 5.588642 | 8.704521 | 6.976819 |
| C | 4.64472 | 6.930101 | 8.156951 | C | 4.434696 | 6.916745 | 7.665346 |
| H | 3.617249 | 7.030859 | 7.828232 | H | 3.474026 | 7.039537 | 7.185834 |
| C | 5.174351 | 5.833268 | 8.91081 | C | 4.804684 | 5.83192 | 8.517983 |
| H | 4.62975 | 4.952981 | 9.229402 | H | 4.185985 | 4.987891 | 8.785148 |
| C | 4.593645 | 7.783927 | 2.927926 | C | 5.14893 | 7.729442 | 2.952328 |
| H | 4.303946 | 6.80636 | 2.566302 | H | 4.904983 | 6.728841 | 2.633078 |
| C | 5.27797 | 8.794159 | 2.187515 | C | 5.874171 | 8.712865 | 2.218177 |
| H | 5.63194 | 8.70629 | 1.167425 | H | 6.304849 | 8.578979 | 1.237001 |
| C | 5.431007 | 9.937159 | 3.019187 | C | 5.974325 | 9.888857 | 3.010831 |
| H | 5.917442 | 10.86641 | 2.749048 | H | 6.485933 | 10.80054 | 2.73926 |
| C | 4.838251 | 9.629225 | 4.282162 | C | 5.315483 | 9.624858 | 4.245942 |
| H | 4.785865 | 10.29703 | 5.133612 | H | 5.2333 | 10.3132 | 5.074791 |
| C | 4.317995 | 8.305861 | 4.224107 | C | 4.803738 | 8.298258 | 4.20803 |
| H | 3.801285 | 7.785407 | 5.016601 | H | 4.279518 | 7.790124 | 4.998052 |
| Pt | 8.447159 | 5.698677 | 5.809988 | Pt | 8.424318 | 5.555958 | 5.948004 |
| P | 10.74388 | 5.197049 | 5.595271 | P | 10.64419 | 5.240117 | 5.549882 |
| C | 11.95926 | 6.648804 | 5.322642 | C | 11.67617 | 6.7583 | 5.283414 |
| H | 12.78736 | 6.413638 | 6.002516 | H | 12.52256 | 6.654773 | 5.968501 |
| C | 11.33721 | 7.983786 | 5.780571 | C | 10.85508 | 7.974633 | 5.699109 |
| H | 10.51395 | 8.240732 | 5.108059 | H | 9.999822 | 8.038278 | 5.030363 |
| H | 10.89447 | 7.891977 | 6.774974 | H | 10.44228 | 7.835415 | 6.69771 |
| C | 12.36724 | 9.123489 | 5.779206 | C | 11.67114 | 9.256482 | 5.619904 |
| H | 13.13354 | 8.928053 | 6.544279 | H | 12.48834 | 9.213704 | 6.352327 |
| H | 11.87032 | 10.05739 | 6.070789 | H | 11.0382 | 10.10634 | 5.889894 |
| C | 13.04119 | 9.285823 | 4.412996 | C | 12.25728 | 9.445366 | 4.225845 |
| H | 12.30142 | 9.648898 | 3.685804 | H | 11.4381 | 9.57625 | 3.510219 |
| H | 13.82868 | 10.04915 | 4.463484 | H | 12.87293 | 10.35039 | 4.187833 |
| C | 13.62359 | 7.957385 | 3.919821 | C | 13.07956 | 8.228488 | 3.815905 |
| H | 14.47245 | 7.669523 | 4.557707 | H | 13.9438 | 8.130215 | 4.485789 |
| H | 14.02668 | 8.072315 | 2.904774 | H | 13.47162 | 8.357372 | 2.800977 |
| C | 12.5798 | 6.826774 | 3.923527 | C | 12.23832 | 6.956441 | 3.879956 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| H | 11.79613 | 7.071583 | 3.197571 | H | 11.41259 | 7.062678 | 3.179029 |
| H | 13.06089 | 5.904334 | 3.584709 | H | 12.83054 | 6.090528 | 3.574636 |
| C | 11.24015 | 3.827972 | 4.375743 | C | 11.04741 | 3.987154 | 4.259259 |
| H | 12.33849 | 3.817749 | 4.355038 | H | 12.13231 | 3.947023 | 4.120761 |
| C | 10.72575 | 4.107048 | 2.948667 | C | 10.36326 | 4.367349 | 2.949139 |
| H | 11.0623 | 5.079608 | 2.587724 | H | 10.72424 | 5.323633 | 2.581522 |
| H | 9.632729 | 4.15486 | 2.978095 | H | 9.300305 | 4.501506 | 3.167259 |
| C | 11.16809 | 3.02149 | 1.955135 | C | 10.52168 | 3.297814 | 1.878252 |
| H | 10.75678 | 3.248529 | 0.962497 | H | 9.988088 | 3.609289 | 0.974264 |
| H | 12.26236 | 3.047678 | 1.84563 | H | 11.58114 | 3.198695 | 1.608945 |
| C | 10.73532 | 1.621236 | 2.399621 | C | 9.99585 | 1.955077 | 2.365028 |
| H | 11.13584 | 0.861389 | 1.715602 | H | 10.14236 | 1.183339 | 1.601739 |
| H | 9.640692 | 1.545771 | 2.341412 | H | 8.920725 | 2.042549 | 2.533614 |
| C | 11.18761 | 1.333789 | 3.834217 | C | 10.68146 | 1.552788 | 3.664079 |
| H | 12.28322 | 1.238665 | 3.856832 | H | 11.748 | 1.383457 | 3.468853 |
| H | 10.78976 | 0.367774 | 4.172506 | H | 10.27232 | 0.60721 | 4.037652 |
| C | 10.75417 | 2.430977 | 4.820379 | C | 10.53524 | 2.626948 | 4.73646 |
| H | 9.661291 | 2.440669 | 4.905319 | H | 9.482883 | 2.744164 | 5.009458 |
| H | 11.13447 | 2.173486 | 5.811134 | H | 11.06256 | 2.31484 | 5.638263 |
| C | 11.32751 | 4.499085 | 7.268569 | C | 11.34931 | 4.545692 | 7.108262 |
| H | 10.65964 | 3.636735 | 7.388486 | H | 10.74239 | 3.655193 | 7.297562 |
| C | 12.78274 | 3.993768 | 7.35263 | C | 12.81608 | 4.139272 | 7.033031 |
| H | 13.4793 | 4.835016 | 7.245961 | H | 13.4258 | 5.017992 | 6.800764 |
| H | 13.01375 | 3.298083 | 6.541024 | H | 12.97271 | 3.420601 | 6.225833 |
| C | 13.05818 | 3.300982 | 8.69934 | C | 13.28418 | 3.548625 | 8.361006 |
| H | 12.46137 | 2.379667 | 8.760054 | H | 12.73952 | 2.614238 | 8.546289 |
| H | 14.11063 | 2.990076 | 8.740065 | H | 14.34815 | 3.294703 | 8.299945 |
| C | 12.72445 | 4.201023 | 9.893809 | C | 13.03047 | 4.508687 | 9.51851 |
| H | 12.85947 | 3.648272 | 10.83256 | H | 13.34736 | 4.055077 | 10.46334 |
| H | 13.43416 | 5.040884 | 9.925009 | H | 13.63845 | 5.411596 | 9.375841 |
| C | 11.29608 | 4.748307 | 9.799169 | C | 11.56022 | 4.90673 | 9.584827 |
| H | 11.10705 | 5.455419 | 10.61759 | H | 11.39348 | 5.618492 | 10.40054 |
| H | 10.57873 | 3.925517 | 9.92821 | H | 10.95312 | 4.018958 | 9.800854 |
| C | 11.03305 | 5.441745 | 8.453491 | C | 11.10008 | 5.512604 | 8.265359 |
| H | 9.996391 | 5.786037 | 8.405871 | H | 10.03665 | 5.767474 | 8.294321 |
| H | 11.6677 | 6.33418 | 8.389636 | H | 11.64975 | 6.441399 | 8.086779 |
| Cu | 7.063243 | 5.875888 | 3.437445 | Cu | 7.375975 | 5.886192 | 3.567193 |
| C | 6.831644 | 4.42796 | 2.145261 | C | 6.959173 | 4.441965 | 2.417343 |
| N | 6.388015 | 3.144765 | 2.365682 | N | 6.585005 | 3.175645 | 2.769968 |
| C | 6.202401 | 2.45144 | 1.177043 | C | 6.203124 | 2.42528 | 1.667005 |
| C | 6.545957 | 3.297427 | 0.172234 | C | 6.349616 | 3.227308 | 0.579471 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| N | 6.930955 | 4.490607 | 0.771384 | N | 6.813883 | 4.449999 | 1.054979 |
| C | 7.366944 | 5.660281 | 0.008556 | C | 7.116272 | 5.610234 | 0.22924 |
| C | 6.127446 | 2.557939 | 3.682968 | C | 6.62037 | 2.687355 | 4.142048 |
| H | 7.872308 | 6.354577 | 0.674284 | H | 7.598277 | 6.348643 | 0.865567 |
| H | 6.507087 | 6.156216 | -0.45423 | H | 6.196392 | 6.026212 | -0.19073 |
| H | 8.062711 | 5.344931 | -0.77395 | H | 7.792545 | 5.322741 | -0.57875 |
| H | 6.557223 | 3.150979 | -0.89797 | H | 6.171881 | 3.041326 | -0.46757 |
| H | 5.856644 | 1.428611 | 1.147812 | H | 5.87464 | 1.402472 | 1.753672 |
| H | 6.508212 | 1.533619 | 3.701289 | H | 7.14409 | 1.731759 | 4.175263 |
| H | 5.056259 | 2.559201 | 3.896762 | H | 5.610487 | 2.586409 | 4.535896 |
| H | 6.64324 | 3.145619 | 4.437165 | H | 7.163439 | 3.42585 | 4.725542 |

Table S7. Optimized structures used for thermochemical calculations. For the methods employed see the **Computational Details**. Columns are multi-page.

| [[{(CO) ₂ CpMn} ₂ B{Au(DMS)}}] | | | | [[{(CO) ₂ CpMn} ₂ BAu] | | | |
|--|----------|----------|----------|--|----------|----------|----------|
| Au | 1.310159 | 0.404629 | 0.015781 | Au | 0.697373 | -1.64932 | 0.232982 |
| Mn | -1.39012 | -1.8947 | 0.175498 | Mn | -2.19912 | 0.4204 | 0.123489 |
| Mn | -0.85343 | 1.861174 | -0.19675 | Mn | 1.638314 | 0.698406 | -0.25715 |
| B | -0.85278 | -0.12673 | -0.0041 | B | -0.37321 | 0.256609 | -0.03355 |
| O | 0.187027 | -2.12518 | 2.636472 | O | -1.84157 | 0.196267 | 3.025933 |
| C | -0.44671 | -2.02368 | 1.667473 | C | -1.98528 | 0.287482 | 1.880287 |
| O | -3.73551 | -0.81656 | 1.553252 | O | -1.78712 | 3.318419 | 0.155053 |
| C | -2.80114 | -1.25173 | 1.02108 | C | -1.95934 | 2.172563 | 0.151649 |
| O | -2.65761 | 0.975282 | -2.32181 | O | 0.334679 | 1.747112 | -2.66297 |
| C | -1.92438 | 1.290046 | -1.48856 | C | 0.80496 | 1.302281 | -1.71312 |
| O | 0.945982 | 2.943533 | -2.27709 | O | 3.380793 | -0.89185 | -2.06241 |
| C | 0.290314 | 2.466237 | -1.45812 | C | 2.677847 | -0.32406 | -1.35808 |
| C | -0.96511 | -2.23425 | -1.93643 | C | -2.53224 | -0.84163 | -1.62616 |
| H | -0.54772 | -1.49612 | -2.60328 | H | -1.75424 | -1.18207 | -2.29141 |
| C | -0.23149 | -3.17992 | -1.16736 | C | -3.01122 | -1.52882 | -0.47459 |
| H | 0.841774 | -3.28671 | -1.14767 | H | -2.66115 | -2.48109 | -0.10773 |
| C | -1.16891 | -3.99952 | -0.46665 | C | -4.06797 | -0.75136 | 0.087373 |
| H | -0.9261 | -4.80467 | 0.209624 | H | -4.63033 | -0.99899 | 0.974677 |
| C | -2.46942 | -3.55609 | -0.79772 | C | -4.24386 | 0.403188 | -0.71071 |
| H | -3.39308 | -3.96138 | -0.41424 | H | -4.95827 | 1.192931 | -0.53776 |
| C | -2.3499 | -2.45824 | -1.70383 | C | -3.28291 | 0.356801 | -1.76705 |
| H | -3.16183 | -1.90132 | -2.14399 | H | -3.16054 | 1.092707 | -2.54655 |
| C | -0.35394 | 2.758278 | 1.758848 | C | 2.423855 | 0.869905 | 1.809074 |
| C | -1.47947 | 1.892422 | 1.888624 | C | 1.324256 | 1.755479 | 1.618725 |
| C | -2.51924 | 2.39785 | 1.06276 | C | 1.674632 | 2.671218 | 0.584724 |
| C | -2.03457 | 3.569473 | 0.407308 | C | 2.976915 | 2.335434 | 0.118085 |

| | | | |
|---|----------|----------|----------|
| C | -0.70148 | 3.790258 | 0.848953 |
| H | 0.590585 | 2.651829 | 2.267571 |
| H | -1.5439 | 1.026627 | 2.527491 |
| H | -3.49924 | 1.960213 | 0.953927 |
| H | -2.58694 | 4.187954 | -0.28261 |
| H | -0.05567 | 4.59436 | 0.530008 |
| S | 3.640085 | -0.40889 | 0.391438 |
| C | 4.28934 | -0.86756 | -1.25571 |
| H | 5.267249 | -1.33489 | -1.13613 |
| H | 3.602199 | -1.53929 | -1.76807 |
| H | 4.393312 | 0.055196 | -1.82484 |
| C | 3.448155 | -2.06083 | 1.153671 |
| H | 4.436203 | -2.48648 | 1.330828 |
| H | 2.925568 | -1.91984 | 2.098431 |
| H | 2.854729 | -2.71019 | 0.512314 |

| | | | |
|---|----------|----------|----------|
| C | 3.43639 | 1.222807 | 0.885434 |
| H | 2.465374 | 0.05866 | 2.518211 |
| H | 0.416087 | 1.767694 | 2.19858 |
| H | 1.049876 | 3.471894 | 0.219918 |
| H | 3.52766 | 2.84689 | -0.65564 |
| H | 4.388756 | 0.727106 | 0.772739 |

[[{(CO)₂CpMn₂B{Cu(DMS)}}]

| | | | |
|----|----------|----------|----------|
| Mn | -2.03727 | 0.414627 | 0.193204 |
| Mn | 1.673493 | 1.153044 | -0.15148 |
| B | -0.19549 | 0.850112 | 0.029993 |
| O | -2.12076 | -1.98538 | 1.90811 |
| C | -1.98482 | -1.06517 | 1.206433 |
| O | -1.80232 | 2.112914 | 2.574148 |
| C | -1.89227 | 1.432536 | 1.640392 |
| O | 0.752321 | 2.974405 | -2.25896 |
| C | 1.115625 | 2.244446 | -1.43579 |
| O | 2.542813 | -0.78609 | -2.20095 |
| C | 2.118736 | -0.08445 | -1.37316 |
| C | -2.33527 | 1.228914 | -1.80944 |
| H | -1.58273 | 1.729482 | -2.39801 |
| C | -2.64293 | -0.16062 | -1.84072 |
| H | -2.15734 | -0.90504 | -2.45262 |
| C | -3.73177 | -0.38657 | -0.94946 |
| H | -4.19414 | -1.34112 | -0.74736 |
| C | -4.10149 | 0.85368 | -0.37212 |
| H | -4.89167 | 1.011998 | 0.345369 |
| C | -3.23288 | 1.853842 | -0.90096 |
| H | -3.25731 | 2.906275 | -0.66251 |
| C | 2.565741 | 0.545951 | 1.76311 |
| C | 1.727458 | 1.678229 | 1.966312 |
| C | 2.250424 | 2.751318 | 1.194804 |
| C | 3.416789 | 2.286551 | 0.516691 |
| C | 3.606347 | 0.927251 | 0.866082 |

[[{(CO)₂CpMn₂BCu]

| | | | |
|----|----------|----------|----------|
| Mn | -1.89094 | 0.187028 | 0.194542 |
| Mn | 1.891049 | 0.187011 | -0.1946 |
| B | 0.000052 | 0.42345 | -7.8E-05 |
| O | -2.37136 | -2.51904 | 1.314895 |
| C | -2.05004 | -1.49698 | 0.84827 |
| O | -1.44546 | 1.304423 | 2.876125 |
| C | -1.61917 | 0.845358 | 1.828788 |
| O | 1.445467 | 1.305646 | -2.87565 |
| C | 1.619233 | 0.846069 | -1.82854 |
| O | 2.371213 | -2.51862 | -1.31606 |
| C | 2.050091 | -1.49672 | -0.84898 |
| C | -2.08899 | 1.231911 | -1.70515 |
| H | -1.27238 | 1.572703 | -2.32262 |
| C | -2.74982 | -0.02138 | -1.81317 |
| H | -2.50769 | -0.80793 | -2.51112 |
| C | -3.80374 | -0.04795 | -0.85131 |
| H | -4.48645 | -0.86735 | -0.68463 |
| C | -3.79593 | 1.183301 | -0.15287 |
| H | -4.46924 | 1.467802 | 0.641034 |
| C | -2.73155 | 1.977157 | -0.67471 |
| H | -2.46923 | 2.97453 | -0.35687 |
| C | 2.749747 | -0.02209 | 1.813123 |
| C | 2.088757 | 1.231158 | 1.705592 |
| C | 2.731269 | 1.976944 | 0.675539 |
| C | 3.795827 | 1.183476 | 0.153456 |
| C | 3.803783 | -0.04806 | 0.851377 |

| | | | |
|----|----------|----------|----------|
| H | 2.451765 | -0.41881 | 2.232698 |
| H | 0.869437 | 1.729278 | 2.617964 |
| H | 1.839633 | 3.747978 | 1.141751 |
| H | 4.038359 | 2.865267 | -0.14891 |
| H | 4.4012 | 0.288588 | 0.511003 |
| Cu | 0.178625 | -1.10397 | -0.11544 |
| S | 0.517704 | -3.36462 | -0.43324 |
| C | 0.143258 | -4.2519 | 1.122068 |
| H | 0.297003 | -5.31949 | 0.963494 |
| H | 0.77717 | -3.89218 | 1.932213 |
| H | -0.89836 | -4.05448 | 1.366002 |
| C | 2.307572 | -3.71143 | -0.5813 |
| H | 2.841104 | -3.36451 | 0.303506 |
| H | 2.450271 | -4.78391 | -0.7166 |
| H | 2.66456 | -3.1747 | -1.45803 |

| | | | |
|----|----------|----------|----------|
| H | 2.507767 | -0.80891 | 2.51081 |
| H | 1.271949 | 1.571495 | 2.323039 |
| H | 2.468864 | 2.974436 | 0.358149 |
| H | 4.469217 | 1.468448 | -0.64021 |
| H | 4.486606 | -0.8673 | 0.684389 |
| Cu | 0.000066 | -1.54409 | -0.00011 |

[[{(CO)₂CpMn]₂BCu]₂

| | | | |
|----|----------|----------|----------|
| Cu | -0.02108 | -1.25342 | -0.16194 |
| O | 0.02318 | 2.507538 | -2.6709 |
| C | 0.843999 | 2.052551 | -1.98758 |
| Mn | 2.313749 | 1.483257 | -1.10499 |
| B | 1.880055 | -0.11265 | -0.0755 |
| Cu | 0.08203 | 1.255015 | 0.022697 |
| O | 2.803881 | -0.51014 | -3.20875 |
| C | 2.580211 | 0.250525 | -2.37372 |
| Mn | 2.146958 | -1.71739 | 1.015725 |
| B | -1.82891 | 0.09286 | 0.004424 |
| Mn | -2.12593 | 1.652499 | 1.168141 |
| O | 4.610758 | -1.80128 | -0.57272 |
| C | 3.617836 | -1.76559 | 0.015231 |
| C | -0.98922 | -1.73572 | -2.26851 |
| O | -0.25195 | -1.99014 | -3.12055 |
| C | -2.45418 | 0.338653 | 2.313983 |
| O | -2.68193 | -0.50296 | 3.077564 |
| C | -0.61587 | 2.039829 | 2.058251 |
| O | 0.241661 | 2.392771 | 2.762693 |
| Mn | -2.33615 | -1.43119 | -1.10097 |
| O | 1.118192 | -4.06209 | -0.45934 |
| C | 1.456263 | -3.08251 | 0.060111 |
| C | -2.87966 | -0.1048 | -2.15255 |
| O | -3.28168 | 0.720381 | -2.85458 |
| C | 3.030887 | 3.560268 | -1.0259 |
| H | 2.50131 | 4.393384 | -1.46345 |

[[{(CO)₂CpMn]₂BAu]₂

| | | | |
|----|----------|----------|----------|
| Au | 0.005918 | -1.44773 | -0.01653 |
| O | 4.655676 | -1.75058 | 0.605636 |
| C | 3.741195 | -1.64214 | -0.08997 |
| B | 1.958012 | 0.000036 | 0.000006 |
| O | 1.601178 | -4.219 | -0.34094 |
| Mn | -2.37033 | -1.48084 | 1.229949 |
| B | -1.81966 | 0 | 0.000006 |
| C | 1.810075 | -3.11587 | -0.61831 |
| Mn | 2.383232 | -1.50545 | -1.21643 |
| C | -1.02385 | -1.97941 | 2.314519 |
| O | -0.28188 | -2.3451 | 3.120283 |
| O | -2.70711 | 0.875829 | 2.923718 |
| C | -2.56018 | -0.04083 | 2.233061 |
| C | 1.378646 | -1.01797 | -3.11914 |
| H | 0.317734 | -0.88743 | -3.25536 |
| C | 2.093156 | -2.23667 | -3.26471 |
| H | 1.6604 | -3.19582 | -3.50582 |
| C | 3.470586 | -1.98135 | -3.0266 |
| H | 4.267974 | -2.70716 | -3.06315 |
| C | 3.609377 | -0.59353 | -2.73032 |
| H | 4.52964 | -0.07701 | -2.50839 |
| C | 2.317279 | 0.000493 | -2.78294 |
| H | 2.091447 | 1.046207 | -2.65135 |
| C | -3.1938 | -2.86557 | -0.28102 |
| H | -2.75295 | -3.03913 | -1.24893 |
| C | -4.16028 | -1.86853 | 0.02411 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 2.868022 | 3.075685 | 0.302494 | H | -4.59719 | -1.17757 | -0.67654 |
| H | 2.225107 | 3.491756 | 1.062406 | C | -4.47434 | -1.97156 | 1.409083 |
| C | 4.433112 | 1.759149 | -0.75861 | H | -5.18437 | -1.36232 | 1.947586 |
| H | 5.161999 | 0.987621 | -0.95356 | C | -3.70925 | -3.03292 | 1.959792 |
| C | 3.742552 | 1.963018 | 0.465083 | H | -3.72089 | -3.359 | 2.988202 |
| H | 3.878721 | 1.394003 | 1.369726 | C | -2.91138 | -3.58064 | 0.911822 |
| C | 1.013679 | -1.49699 | 2.896873 | H | -2.20768 | -4.39316 | 1.008701 |
| H | -0.04193 | -1.30065 | 2.996719 | Au | 0.00588 | 1.44776 | 0.01655 |
| C | 3.988834 | 2.750162 | -1.68481 | O | 4.655573 | 1.750254 | -0.60581 |
| H | 4.322422 | 2.861143 | -2.70501 | C | 3.741166 | 1.642245 | 0.089955 |
| C | 3.030223 | -2.60758 | 2.799998 | O | 1.601196 | 4.21902 | 0.340724 |
| H | 3.769243 | -3.39302 | 2.766005 | Mn | -2.37037 | 1.480816 | -1.22995 |
| C | 3.290679 | -1.20465 | 2.781951 | C | 1.809999 | 3.11593 | 0.618331 |
| H | 4.268416 | -0.74803 | 2.746113 | Mn | 2.383215 | 1.50553 | 1.216435 |
| C | 2.048292 | -0.51958 | 2.842884 | C | -1.02391 | 1.979399 | -2.31453 |
| H | 1.906522 | 0.548237 | 2.884692 | O | -0.28228 | 2.345067 | -3.12062 |
| C | -2.93849 | 2.889283 | -0.45692 | O | -2.70728 | -0.87624 | -2.92316 |
| H | -2.62507 | 2.833884 | -1.48689 | C | -2.56019 | 0.040779 | -2.23302 |
| C | -2.38901 | 3.735577 | 0.540689 | C | 1.37866 | 1.01803 | 3.119153 |
| H | -1.57689 | 4.432594 | 0.399734 | H | 0.317752 | 0.887456 | 3.255384 |
| C | -3.10197 | 3.517794 | 1.757151 | C | 2.093137 | 2.236751 | 3.264713 |
| H | -2.91932 | 4.011204 | 2.699381 | H | 1.660359 | 3.195893 | 3.505823 |
| C | -4.08666 | 2.530075 | 1.506984 | C | 3.470573 | 1.981464 | 3.0266 |
| H | -4.7916 | 2.144616 | 2.228225 | H | 4.267941 | 2.7073 | 3.063138 |
| C | -3.99061 | 2.139608 | 0.140925 | C | 3.609397 | 0.593654 | 2.730322 |
| H | -4.62222 | 1.425105 | -0.36119 | H | 4.52967 | 0.077155 | 2.50838 |
| C | -4.32588 | -2.30836 | -1.16654 | C | 2.317316 | -0.00041 | 2.782948 |
| H | -5.13291 | -1.90153 | -1.75727 | H | 2.091509 | -1.04613 | 2.651352 |
| C | -4.02223 | -1.96447 | 0.181871 | C | -3.19388 | 2.865551 | 0.280998 |
| H | -4.56789 | -1.27175 | 0.802002 | H | -2.75303 | 3.039137 | 1.248903 |
| C | -2.89258 | -2.73206 | 0.581176 | C | -4.16033 | 1.868473 | -0.02411 |
| H | -2.43918 | -2.71717 | 1.559042 | H | -4.59721 | 1.177519 | 0.676559 |
| C | -2.49938 | -3.54069 | -0.5189 | C | -4.4744 | 1.971475 | -1.40908 |
| H | -1.66949 | -4.23089 | -0.53531 | H | -5.18441 | 1.362204 | -1.94758 |
| C | -3.39224 | -3.28342 | -1.59932 | C | -3.70934 | 3.032846 | -1.95981 |
| H | -3.3558 | -3.74077 | -2.57606 | H | -3.72099 | 3.358911 | -2.98823 |
| C | 1.625885 | -2.781 | 2.872112 | C | -2.91148 | 3.580602 | -0.91186 |
| H | 1.107418 | -3.7278 | 2.896883 | H | -2.2078 | 4.393141 | -1.00876 |

[[{(CO)₂CpMn₂B{Cu(I Me)}}]

| | | | |
|----|----------|----------|----------|
| Mn | 1.127906 | -1.88531 | -0.23013 |
| Mn | 1.127495 | 1.885727 | 0.229984 |
| B | 1.141249 | 0.000241 | -0.00011 |

[[{(CO)₂CpMn₂B{Au(I Me)}}]

| | | | |
|----|----------|----------|----------|
| Au | -1.0216 | -0.42012 | 0.006794 |
| Mn | 1.61275 | 1.963204 | 0.041152 |
| Mn | 1.255705 | -1.8104 | -0.09095 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| O | -1.15163 | -2.43392 | -2.02446 | B | 1.169991 | 0.158705 | -0.02803 |
| C | -0.30261 | -2.123 | -1.29092 | O | 0.390114 | 2.095362 | 2.698847 |
| O | 2.812914 | -1.185 | -2.52675 | C | 0.884178 | 2.040948 | 1.645443 |
| C | 2.134831 | -1.45908 | -1.6262 | O | 4.186181 | 1.062852 | 1.102689 |
| O | 2.816413 | 1.185553 | 2.523748 | C | 3.163408 | 1.425836 | 0.692276 |
| C | 2.136765 | 1.459555 | 1.624356 | O | 2.982274 | -1.0383 | -2.32246 |
| O | -1.15009 | 2.431328 | 2.027659 | C | 2.283141 | -1.31506 | -1.44647 |
| C | -0.30167 | 2.121779 | 1.292862 | O | -0.59244 | -3.02513 | -2.04243 |
| C | 1.642718 | -2.09625 | 1.878994 | C | 0.084024 | -2.49159 | -1.26883 |
| H | 1.695104 | -1.28675 | 2.589586 | C | 0.928862 | 2.216231 | -2.01572 |
| C | 0.508708 | -2.91012 | 1.607791 | H | 0.520284 | 1.422806 | -2.62175 |
| H | -0.4648 | -2.81965 | 2.06425 | C | 0.188849 | 3.097761 | -1.17844 |
| C | 0.890728 | -3.89026 | 0.643679 | H | -0.87974 | 3.085751 | -1.03208 |
| H | 0.248705 | -4.6515 | 0.226858 | C | 1.109003 | 4.019556 | -0.59213 |
| C | 2.250945 | -3.67995 | 0.317348 | H | 0.860546 | 4.808124 | 0.101489 |
| H | 2.830262 | -4.25342 | -0.38999 | C | 2.405312 | 3.704521 | -1.06028 |
| C | 2.720342 | -2.56821 | 1.079815 | H | -3.31914 | 4.207853 | -0.78465 |
| H | 3.719313 | -2.16054 | 1.063312 | C | 2.300226 | 2.581666 | -1.93799 |
| C | 0.506231 | 2.90847 | -1.60849 | H | 3.11374 | 2.099562 | -2.4571 |
| C | 1.642383 | 2.097326 | -1.87907 | C | 0.781329 | -2.61081 | 1.906324 |
| C | 2.718532 | 2.572224 | -1.07969 | C | 1.858486 | -1.68134 | 1.998265 |
| C | 2.246154 | 3.683067 | -0.31773 | C | 2.936685 | -2.17867 | 1.218279 |
| C | 0.885499 | 3.889817 | -0.64455 | C | 2.525708 | -3.41456 | 0.633157 |
| H | -0.46681 | 2.815583 | -2.06547 | C | 1.199802 | -3.67839 | 1.067077 |
| H | 1.696973 | 1.287726 | -2.58937 | H | -0.17457 | -2.5261 | 2.397659 |
| H | 3.718491 | 2.166998 | -1.06264 | H | 1.863904 | -0.7743 | 2.581323 |
| H | 2.823794 | 4.25822 | 0.389613 | H | 3.892013 | -1.69418 | 1.090519 |
| H | 0.241446 | 4.649577 | -0.22816 | H | 3.119834 | -4.0408 | -0.01376 |
| Cu | -0.86379 | -0.00043 | -0.00027 | H | 0.603436 | -4.53419 | 0.788973 |
| C | -2.83581 | -0.0004 | 0.000157 | C | -5.19743 | 0.475571 | -0.40649 |
| N | -3.67484 | 0.068857 | -1.06994 | C | -4.96554 | 1.110787 | 0.767753 |
| C | -5.00248 | -0.04228 | 0.67672 | C | -3.01779 | 0.176037 | 0.109375 |
| C | -5.00289 | 0.041707 | -0.67512 | N | -3.9961 | -0.09379 | -0.79466 |
| H | -5.81761 | -0.08232 | 1.379022 | H | -6.09779 | 0.380481 | -0.98901 |
| H | -5.81843 | 0.081777 | -1.37693 | H | -5.62634 | 1.671726 | 1.406332 |
| N | -3.67422 | -0.06958 | 1.070756 | N | -3.62748 | 0.918214 | 1.068694 |
| C | -3.24295 | 0.119131 | -2.46325 | C | -2.98307 | 1.435231 | 2.275953 |
| H | -2.17424 | 0.317918 | -2.48812 | H | -3.12669 | 2.514917 | 2.336968 |
| H | -3.43078 | -0.83513 | -2.95737 | H | -3.41148 | 0.959222 | 3.160027 |
| H | -3.77203 | 0.919169 | -2.98429 | H | -1.91816 | 1.224746 | 2.230812 |
| C | -3.24147 | -0.1202 | 2.463815 | C | -3.81445 | -0.85133 | -2.03181 |
| H | -2.17345 | -0.32282 | 2.488092 | H | -4.6284 | -1.56925 | -2.14109 |
| H | -3.42555 | 0.835079 | 2.95737 | H | -3.80375 | -0.17761 | -2.89091 |

H -3.773 -0.91801 2.985754

H -2.86902 -1.38639 -1.98125

[[{(CO)₂CpMn]₂B{Cu(PCy₃)}}]

| | | | |
|----|----------|----------|----------|
| Mn | -1.97774 | 0.720931 | 0.217721 |
| Mn | 1.772668 | 1.170961 | -0.19843 |
| B | -0.10795 | 1.010621 | 0.014186 |
| O | -2.31674 | -1.78589 | 1.740306 |
| C | -2.06111 | -0.83376 | 1.116383 |
| O | -1.55696 | 2.226113 | 2.700728 |
| C | -1.71887 | 1.618542 | 1.726881 |
| O | 0.970986 | 3.004877 | -2.34236 |
| C | 1.285404 | 2.268885 | -1.50375 |
| O | 2.42731 | -0.88759 | -2.21235 |
| C | 2.09008 | -0.13204 | -1.39394 |
| C | -2.23227 | 1.623602 | -1.75264 |
| H | -1.44151 | 2.033821 | -2.36036 |
| C | -2.7275 | 0.290738 | -1.80359 |
| H | -2.36653 | -0.49557 | -2.44833 |
| C | -3.80573 | 0.189104 | -0.87689 |
| H | -4.38743 | -0.69858 | -0.6784 |
| C | -3.98071 | 1.450553 | -0.25661 |
| H | -4.71511 | 1.693291 | 0.495761 |
| C | -3.00325 | 2.339054 | -0.79536 |
| H | -2.87675 | 3.378229 | -0.5327 |
| C | 2.594451 | 0.574895 | 1.75154 |
| C | 1.906476 | 1.814561 | 1.883826 |
| C | 2.55627 | 2.763212 | 1.048682 |
| C | 3.650681 | 2.115533 | 0.40236 |
| C | 3.667994 | 0.766025 | 0.834283 |
| H | 2.363281 | -0.33652 | 2.280422 |
| H | 1.065448 | 2.011199 | 2.529814 |
| H | 2.273959 | 3.798552 | 0.932527 |
| H | 4.335962 | 2.569568 | -0.29653 |
| H | 4.373453 | 0.011621 | 0.519553 |
| Cu | 0.117137 | -0.98381 | -0.0462 |
| P | 0.387492 | -3.2545 | -0.03784 |
| C | -0.9293 | -4.18331 | -0.93547 |
| H | -0.76944 | -5.26279 | -0.86782 |
| H | -1.89989 | -3.93603 | -0.50233 |
| H | -0.93399 | -3.88937 | -1.98688 |
| C | 1.939656 | -3.93494 | -0.76261 |
| H | 1.944133 | -5.02786 | -0.73272 |
| H | 2.043422 | -3.5938 | -1.79345 |

[[{(CO)₂CpMn]₂B{Au(PCy₃)}}]

| | | | |
|----|----------|----------|----------|
| Au | -1.21703 | 0.320054 | 0.155464 |
| Mn | 1.615402 | -1.80285 | -0.24082 |
| Mn | 0.901955 | 1.908981 | 0.166509 |
| B | 1.025848 | -0.05425 | -0.02661 |
| O | -0.39535 | -2.32056 | -2.31067 |
| C | 0.408197 | -2.09698 | -1.49905 |
| O | 3.540097 | -0.66427 | -2.12846 |
| C | 2.771018 | -1.12336 | -1.39073 |
| O | 2.981813 | 1.225049 | 2.103917 |
| C | 2.143144 | 1.462167 | 1.346572 |
| O | -0.79564 | 2.784202 | 2.417532 |
| C | -0.18026 | 2.374519 | 1.530088 |
| C | 1.593268 | -2.05549 | 1.924536 |
| H | 1.224395 | -1.32238 | 2.624443 |
| C | 0.835205 | -3.10376 | 1.333811 |
| H | -0.21213 | -3.30016 | 1.500924 |
| C | 1.71564 | -3.87667 | 0.515454 |
| H | 1.441235 | -4.73717 | -0.07513 |
| C | 3.003302 | -3.29869 | 0.593708 |
| H | 3.883526 | -3.64102 | 0.071609 |
| C | 2.933976 | -2.16722 | 1.462511 |
| H | 3.751117 | -1.51798 | 1.73408 |
| C | 0.089102 | 2.831865 | -1.66392 |
| C | 1.202899 | 2.004628 | -1.99054 |
| C | 2.344783 | 2.520964 | -1.32257 |
| C | 1.937184 | 3.666149 | -0.57187 |
| C | 0.548772 | 3.856885 | -0.79257 |
| H | -0.91834 | 2.714652 | -2.02928 |
| H | 1.189767 | 1.152987 | -2.65142 |
| H | 3.340877 | 2.110802 | -1.37794 |
| H | 2.573835 | 4.284018 | 0.041888 |
| H | -0.05891 | 4.634916 | -0.35595 |
| P | -3.32842 | -0.76094 | -0.09893 |
| C | -3.40324 | -2.47203 | 0.568006 |
| H | -2.64087 | -3.07894 | 0.077484 |
| H | -3.20128 | -2.45777 | 1.640344 |
| H | -4.38681 | -2.91596 | 0.392192 |
| C | -4.7739 | 0.076534 | 0.671272 |
| H | -4.61308 | 0.162397 | 1.747297 |
| H | -4.87216 | 1.082999 | 0.261076 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | 2.796436 | -3.55761 | -0.20116 | H | -5.69649 | -0.48044 | 0.486563 |
| C | 0.343311 | -4.01269 | 1.641835 | C | -3.80063 | -0.95913 | -1.86279 |
| H | -0.59373 | -3.74163 | 2.130544 | H | -3.88465 | 0.02415 | -2.32905 |
| H | 0.42582 | -5.10128 | 1.584364 | H | -3.0166 | -1.51812 | -2.37689 |
| H | 1.16946 | -3.6256 | 2.241679 | H | -4.7533 | -1.48686 | -1.95935 |

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