Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

1. General Information

If not stated otherwise, all reactions were carried out under a dry argon atmosphere using standard Schlenk techniques or in a dinitrogen-filled glove box (MBraun, LABstar). The applied solvents were dried with an MBraun Solvent Purification System, degassed by three freeze-pump-thaw cycles and stored over molecular sieves prior to their use. The ligand L1 was synthesized according to the literature.[S1] 2,3,7,8-tetraaminodibenzo-[1,4]-dioxine-tetrahydrochloride was synthesized accordint to the literature.[S2] The reagents manganese(II) chloride, iron(II) chloride, Cobalt(II) chloride, nickel(II) chloride, copper(II) chloride, zinc(II) chloride, iron(II) acetate, cobalt(II) acetylacetonate were purchased from Sigma Aldrich, abcr or TCI and used without further purification. Elemental analysis was performed at the Microanalytical Laboratory of the University of Heidelberg using the vario EL and vario MICRO cube devices from Elementar Analysensysteme GmbH. NMR spectra were recorded on a Bruker Avance II 400 spectrometer or Bruker Avance III 600 spectrometer at a temperature of 298 K. Solvent resonances were taken as references for all ^{1}H NMR or ^{13}C NMR spectra if not stated otherwise, NMR spectra were recorded at 298 K. UV-vis spectra were measured on a VARIAN Cary 5000 UVVis-NIR spectrophotometer. CV measurements were carried out with a Metrohm Autolab PGSTAT 204 potentiostate/galvanostate and an Ag/AgCl reference electrode, Pt rod counter electrode and glassy carbon working electrode. The curves were recorded at room temperature with different scan rates (50, 100, 200 $mV \cdot s^{-1}$). CH_2Cl_2 was used as solvent for the individual compounds ($c = 10^{-3}$ M), whereas $^{n}Bu_4N(PF_6)$ was employed as supporting electrolyte (c = 0.1 M). X-band EPR spectra were measured with a Bruker Elexsys E500 EPR with an ER 4116DM CW dual mode resonator. The samples for solid-state measurements and the samples for room temperature measurements in solution were prepared in thin glass tubes (Ø ≈ 1 mm). As temperature system a ER 4112HV-CF58nc In-Cavaty Cryogen Free VT was used. The dc-SQUID measurements were taken with a MPMS-XL apparatus from LOT Quantum Design.

2. Experimental Section

L3: A solution of 3.38 g (19.74 mmol) 2-chloro-1,3-dimethylimidazolinium chloride in 20 mL CH_3CN was added under ice cooling to a suspension of 2,3,7,8-tetraaminodibenzo-[1,4]-dioxine (1.4 g, 3.59 mmol) in 20 mL CH_3CN. After dropwise addition of NEt_3 (10 mL, 71.78 mmol) to the suspension, the ice cooling was removed and the reaction mixture stirred at room temperature for 72 h. After solvent removal under vacuum, the remaining pale brown solid residue was dissolved in 10% HCl. Upon addition of 25% NaOH solution, a pale-brown solid precipitated, that was extracted with CH_2Cl_2. The CH_2Cl_2 solution was dried over Na_2SO_4 before the solvent was removed under vacuum. Then, the pale-brown solid was washed with CH_3CN. Yield of crude product: 1.25 g (1.96 mmol, 55%). Elemental analysis for $C_{32}H_{52}N_{12}O_2$ (636.85): calcd C 60.35, H 8.23, N 26.39; found C 60.26, H 7.94, N 26.03. ^{1}H NMR (400.13 MHz, CH_2Cl_2): δ (ppm) = 5.94 (s, 4 H, H_{ar}), 2.66 (s, 48 H, Me). ^{13}C NMR (150.92 MHz, CH_2Cl_2): δ (ppm) = 158.71 ($C_{guanidine}$), 139.18 (C_{ar}), 135.50 (C_{ar}), 108,36 ($C_{ar\text{-}H}$), 39.26 (Me). MS (ESI$^+$): m/z = 637.44 u ([L3 + H]$^+$, 100.0%), 638.44 u ([L3 + 2H]$^{2+}$, 29.5%), 1273.87 ([2xL3 + H]$^+$, 10.7%). UV-vis (CH_2Cl_2, c = $1.57\cdot10^{-4}$ mol l^{-1} , d = 0.5 cm): λ_{max} (nm (ε, in L mol^{-1} cm^{-1})) = 264 ($7.5602\cdot10^4$), 341 ($6.6349\cdot10^4$). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): $E_{1/2}(1)$ = -0.302 V, $E_{1/2}(2)$ = -0.144 V, $E_{1/2}(3)$ = 0.094 V, $E_{1/2}(4)$ = 0.302 V.

L4: A solution of 1.75 g (10.25 mmol) 2-chloro-1,3-dimethylimidazolinium chloride in 10 mL CH_3CN was added under ice cooling to a suspension of 2,3,7,8-tetraaminodibenzo-[1,4]-dioxine (0.80 g, 2.51 mmol) in 20 mL CH_3CN. After dropwise adding of NEt_3 (8 mL, 53.2 mmol) to the suspension, the ice cooling was removed and the reaction mixture stirred at room temperature for at least 36 h. After removal of the solvent under vacuum, the brown solid was dissolved in destilled water. Upon addition of 25% NaOH solution, a pale-brown solid precipitated, which was extracted with CH_2Cl_2. The CH_2Cl_2 solution was dried over Na_2SO_4 before the solvent was removed under vacuum. Then, the pale-brown solid was washed with CH_3CN. Yield of crude product: 1.15 g (1.83 mmol, 74%). Yellow colored crystals were grown by diffusion of Et_2O into a CH_2Cl_2 solution at room temperature. Elemental analysis for $C_{32}H_{44}N_{12}O_2$ (632.85): calcd C 61.13, H 7.05, N 26.73; found C 60.85, H 7.11, N 26.98. ^{1}H NMR (600.13 MHz, CH_2Cl_2): δ (ppm) = 6.24 (s, 4 H, H_{ar}), 3.22 (s, 16 H, Et), 2.67 (s, 24 H,

Me). ^{13}C NMR (150.92 MHz, CH_2Cl_2): δ (ppm) = 153.87 ($C_{guanidine}$), 137.42 (C_{ar}), 135.39 (C_{ar}), 109,07 (C_{ar}-H), 48.45 (Et), 34.47 (Me). MS (ESI$^+$): m/z = 629.37 u ([L4 + H]$^+$, 100.0%), 630.38 u ([L4 + 2H]$^{2+}$, 17.5%). UV-vis (CH_2Cl_2, c = $3.42\cdot10^{-5}$ mol l^{-1} , d = 0.5 cm): λ_{max} (nm (ε, in L mol^{-1} cm^{-1})) = 252 ($5.8362\cdot10^4$), 343 ($8.971\cdot10^3$) . CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): $E_{1/2}(1)$ = -0.363 V, $E_{1/2}(2)$ = -0.242 V, $E_{1/2}(3)$ = 0.045 V, $E_{1/2}(4)$ = 0.085 V. Crystal data for $C_{32}H_{44}N_{12}O_2$: *Mr* = 628.79, 0.30·0.15·0.15 mm^3, monoclinic, space group $P2_1/c$, *a* = 7.7374(11), *b* = 13.3856(17), *c* = 15.6864(19) Å, α = 90°, β = 97.574(5)°, γ = 90°, V = 1610.50 Å^3, *Z* = 2, d_{calc} = 1.297 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073A, *T* = 133 K, θ_{range} = 2.30 – 30.05°, reflections measured: 20467, indep: 4080, R_{int} = 0.0918, final *R* indices [I > 2σ(I)]: R_1 = 0.0577, wR_2 = 0.1308.

L5: Diisopropylcarbodiimide (0.80 mL, 5.13 mmol) was added dropwise to a suspension of 2,3,7,8-tetraaminobenzo-[1,4]-dioxine tetrahydrochloride (200 mg, 513 µmol) and zinktriflate (10.0 mg, 25.6 µmol) in 10 mL abs. THF. The suspension was stirred at room temperature for 14 d. Afterwards the solvent was removed by filtration and the light pink solid washed with diethyl ether (3 x 5 mL). NaOMe in methanol (4.0 mL, 5.4 M) was added and the solvent removed under vacuo. The light pink solid was washed with water (3x15 mL) and *n*-hexane (10 mL) to yield a light-brown solid. Yield of the crude product: 160 mg, 213 µmol, 41%. Elemental analysis for $C_{40}H_{68}N_{12}O_2$ (749.05): calcd. C 64.14, H 9.15, N 22.44; found C 64.35, H 9.53, N 22.37. ^{1}H NMR (400.13 MHz, C_3D_7NO): δ (ppm) = 6.26(s, 4 H, H_{ar}), 3.70, (br, 8 H, H_{iPr}), 1.13(d, 48 H, Me_{iPr}). ^{13}C NMR (150.92 MHz, C_3D_7NO): δ (ppm) = 149.79 ($C_{guanidine}$), 133.50 ($C_{ar\text{-}q}$), 131.18 ($C_{ar\text{-}q}$), 102.90 ($C_{ar\text{-}H}$), 42.56 (CH), 22.89 (CH_3). MS (ESI$^+$): m/z = 749.5663 u ([L5 + H]$^+$, 100.0%), 375.2865 u ([L5 + 2H]$^{2+}$, 35.0%), 1498.1276 ([2xL5 + H]$^+$, 23.4%). UV-vis (CH_2Cl_2, c = $8.01\cdot10^{-5}$ mol l^{-1} , d = 0.5 cm): λ_{max} (nm (ε, in L mol^{-1} cm^{-1})) = 250 ($1.9680\cdot10^4$), 328 ($1.1658\cdot10^4$).

Preliminary results for $L4(SbCl_6)_4$: $SbCl_5$ (60.9 µL, 4.83 mmol) was added dropwise to a solution of L4 (2,3,7,8-tetrakis(*N*,*N*'-dimethylethylenguanidino)dibenzo-[1,4]-dioxine (30.0 mg, 48.3 µmol) in CH_2Cl_2, forming a deep blue precipitate. The solvent was removed by filtration and the precipitate washed with CH_2Cl_2 (2 x 3 mL). Yield of the product: 35.2 mg (35.8 µmol, 75%). Elemental analyses for $C_{32}H_{44}N_{12}O_2Sb_4Cl_4$

(1289.8): calcd. C 29.62, H 3.42, N 12.95, O 2.47, Sb 18.77, Cl 32.78; found C 30.02, H 3.33, N 13.12.

2.1 Complexes with L3

[$(MnCl_2)_2$(L3)]: $MnCl_2$ (19.8 mg, 157 µmol) and L3 (50.0 mg, 78.5 µmol) were suspended in 5 mL CH_2Cl_2 and the reaction mixture stirred at room temperature for 36 h, leading to precipitation of a brown solid. The solution was removed by filtration and the product washed with Et_2O. Then, the solid was dissolved in DMF and layered wit Et_2O to give colourless crystals (62.0 mg, 69.8 µmol, 74%). Elemental analysis for $C_{32}H_{52}N_{12}O_2Mn_2Cl_4$ (880.46): calcd. C 43.26, H 5.90, N 18.92; found C 42.82, H 5.90, N 18.92. UV-vis (CH_2Cl_2, c = $5.04 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 233 (49504), 271 (29782), 300 (19130), 353 (9992). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): $E_{1/2}$ = 0.085 V, E_{Ox} = 0.367 V. Crystal data for $C_{32}H_{44}N_{12}O_2Mn_2Cl_4$: *Mr* = 888.53, 0.202·0.131·0.055 mm^3, monoclinic, space group *P-2₁/c*, *a* = 14.6765(13), *b* = 10.1217(8), *c* = 15.2133(14) Å, α = 90°, β = 105.469(4)°, γ = 90°, *V* = 2178.1(3) $Å^3$, *Z* = 2, d_{calc} = 1.355 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 100 K, θ_{range} = 2.54 – 26.771°, reflections measured: 22463, indep: 5605, R_{int} = 0.0483, final *R* indices [I > 2σ(I)]: R_1 = 0.0356, wR_2 = 0.0724.

[$(FeCl_2)_2$(L3)]: $FeCl_2$ (19.9 mg, 157 µmol) was added to a suspension of L3 (50.0 mg, 78.5 µmol) in CH_3CN and the reaction mixture stirred at room temperature for 16 h leading to precipitation of a dark green solid. The solution was removed by filtration, the solid dissolved in CH_2Cl_2 and overlayered with *n*-pentane and stored at room temperature for another 16 h to form dark green crystals (58.0 mg, 65.1 µmol, 83%). Elemental analysis for $C_{32}H_{52}N_{12}O_2Fe_2Cl_4$ (890.34): calcd. C 43.17, H 5.89, N 18.88; found C 42.63, H 5.98, N 18.51. UV-vis (CH_2Cl_2, c = $5.04 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 241 (37470), 269 (29054), 304 (15227), 354 (12773), 753 (2511). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): E_{Ox}(1) = -0.103 V, E_{Ox}(2) = 0.028 V, E_{Ox}(3) = -0.219 V, E_{Ox}(4) = 0.805 V, E_{Red}(1) = -1.095 V, E_{Red}(2) = -0.142 V, E_{Red}(3) = -0.118 V. Crystal data for $C_{32}H_{44}N_{12}O_2Fe_2Cl_4$: *Mr* = 890.35, 0.287·0.124·0.09 mm^3, monoclinic, space group *P-2₁/m*, *a* = 13.1832(11), *b* = 12.1023(9), *c* = 14.4602(13) Å, α = 90°, β = 92.807(4)°, γ = 90°, *V* = 2304.3(3) A^3,

Z = 2, d_{calc} = 1.283 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), T = 100 K, θ_{range} = 2.04 – 29.00°, reflections measured: 109563, indep: 6403, R_{int} = 0.0404, final R indices [I > 2σ(I)]: R_1 = 0.0404, wR_2 = 0.1141.

[(CoCl$_2$)$_2$(L3)]: $CoCl_2$ (20.1 mg, 157 µmol) was added to a suspension of L3 (50.0 mg, 78.5 µmol) in CH_3CN and the reaction mixture stirred at room temperature for 16 h, leading to a blue solution. The solvent was removed under vacuo and the turquoise solid residue dissolved in CH_2Cl_2. Then, the solution was layered with *n*-pentane and stored over night to form turquoise crystals. Yield: 68.0 mg, 75.8 µmol, 96%. Elemental analysis for $C_{32}H_{52}N_{12}O_2Co_2Cl_4$ (896.52): calcd. C 42.87, H 5.85, N 18.75; found C 42.46, H 5.84, N 18.55. UV-vis (CH_2Cl_2, c = 1.23·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (ε in M^{-1} cm^{-1}) = 240 (17144), 270 (12261), 348 (6465), 548 (26),566 (25), 623 (26), 661 (29) nm. CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc$^+$/Fc): $E_{1/2}$(1) = 0.030 V, $E_{1/2}$(2) = 0.267 V, E_{Red}(1) = 0.426 V, E_{Ox}(1) = 0.645 V. Crystal data for $C_{32}H_{44}N_{12}O_2Co_2Cl_4$: Mr = 618.11, 0.523·0.405·0.39 mm^3, monoclinic, space group $P2_1/n$, a = 9.3647(8), b = 26.564(2), c = 11.1128(10) Å, α = 90°, β = 94.674(4)°, γ = 90°, V = 2755.3(4) A^3, Z = 4, d_{calc} = 1.490 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), T = 100 K, $2\theta_{range}$ = 3.984 – 60.000°, reflections measured: 135091, indep: 8035, R_{int} = 0.0305, final R indices [I > 2σ(I)]: R_1 = 0.0305, wR_2 = 0.0687.

[(NiCl$_2$)$_2$(L3)]: $NiCl_2(dme)_2$ (48.7 mg, 157 µmol) was added to a suspension of L3 (50.0 mg, 78.5 µmol) in CH_3CN and the reaction mixture stirred at room temperature for 16 h, leading to a green-brown solid. The solution was removed by filtration, and the solid residue dissolved in CH_2Cl_2, layered with *n*-pentane and stored at room temperature for 16 h to give red crystals (54.0 mg, 65.3 µmol, 77%). ^{1}H NMR (200 MHz, CD_2Cl_2 7.06 (s, CH_{ar}), 41.01 (s, CH_3) ppm. Elemental analysis for $C_{32}H_{52}N_{12}O_2Ni_2Cl_4$ (890.34): calcd. C 42.89, H 5.85, N 18.76; found C 42.37, H 5.89, N 18.97. UV-vis (CH_2Cl_2, c = 7.01·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 255 (28079), 271 (28302), 301 (21587), 348 (17482), 461 (996), 583 (272). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc$^+$/Fc): E_{Ox}(1) = -0.153 V, E_{Ox}(2) = 0.256 V, E_{Ox}(3) = 0.622 V, E_{Ox}(4) = 0.837 V, E_{Red}(1) = 0.322 V, E_{Red}(2) = -0.023 V, E_{Red}(1) = -0.203 V. Crystal data for $C_{32}H_{44}N_{12}O_2Ni_2Cl_4$: Mr = 1065.92, 0.457·0.41·0.19 mm^3, monoclinic, space group $P\text{-}1$, a = 8.45596(7), b = 11.5717(9),

c = 15.0481(12) Å, α = 72.379(3)°, β = 86.528(4)°, γ = 71.530(3)°, V = 1330.63(19) Å^3, Z = 1, d_{calc} = 1.330 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), T = 100 K, $2\theta_{range}$ = 3.89 – 55.124°, reflections measured: 44577, indep: 6123, R_{int} = 0.0487, final R indices [I>2σ(I)]: R_1 = 0.0374, wR_2 = 0.1145.

[(CuCl$_2$)$_2$(L3)]: $CuCl_2$ (8.00 mg, 59.7 µmol) was added to a solution of L_3 (20.0 mg, 31.4 µmol) in CH_2Cl_2 and the reaction mixture stirred at room temperature for 16 h. The dark green solution was layered with *n*-pentane and stored at 4 °C for 48 h to give dark-green crystals (24.0 mg, 26.5 µmol, 84%). Elemental analysis for $C_{32}H_{52}N_{12}O_2Cu_2Cl_4$ (905.74): calcd. C 42.44, H 5.79, N 18.56; found C 42.66, H 5.85, N 18.43. UV-vis (CH_2Cl_2, c = 1.34·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 236 (49631), 275 (60238), 316 (33388), 359 (31387), 737 (710). UV-vis (MeCN, c = 1.29·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 234(11673), 273 (71312), 311 (40598), 357 (36380) 735 (702). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc$^+$/Fc): $E_{1/2}$(1) = -0.023 V, $E_{1/2}$(2) = 0.2420 V, E_{Red}(1) = -1144 V, E_{Red}(2) = 0.323 V, E_{ox}(1) = 0.821 V. Crystal data for $C_{32}H_{44}N_{12}O_2Cu_2Cl_4$: Mr = 1237.40 , 0.27·0.202·0.108 mm^3, monoclinic, space group *P-1 21/c, a* = 12.7604(10), *b* = 13.84841(13), *c* = 16.4023(14) Å, α = 90°, β = 109.778(3)°, γ = 90°, V = 2727.4(4) A^3, Z = 4, d_{calc} = 1.517 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), T = 100 K, θ_{range} = 3.952 – 58.812°, reflections measured: 145247, indep: 7517, R_{int} = 0.0701, final R indices [I > 2σ(I)]: R_1 = 0.0400, wR_2 = 0.1065.

[(ZnCl$_2$)$_2$(L3)]: $ZnCl_2$ (21.4 mg, 157 µmol) was added to a suspension of L3 (50.0 mg, 78.5 µmol) in CH_3CN and the reaction mixture stirred at room temperature for 16 h, leading to a colourless suspension. The solution was removed by filtration, and the remaining solid residue dissolved in DMF, layered with Et_2O and stored at room temperature for 16 h to give colourless crystals (54.0 mg, 65.3 µmol, 77%). ^{1}H NMR (200 MHz, CD_2Cl_2): δ (ppm) = 6.06 (s, CH_{ar}), 2.93 (s, CH_3) ppm. ^{13}C NMR (400 MHz, CD_2Cl_2): δ (ppm) = 163.92 ($C_{q\ guanidine}$), 136.68 (C_{ar}), 135, 07 (C_{ar}), 106,79 (C_{ar}), 40.29 (C_{Me}). Elemental analysis for $C_{32}H_{52}N_{12}O_2Zn_2Cl_4$ (890.34): calcd. C 42.26, H 5.76, N 18.48; found C 42.63, H 5.89, N 18.49. UV-vis (CH_2Cl_2, c = 1.03·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 240 (32505), 273 (31487), 298 (19061), 353 (16229). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc$^+$/Fc): $E_{1/2}$(1)

= 0.118 V, $E_{1/2}(2)$ = 0.293 V, $E_{Red}(1)$ = 0.456 V, $E_{Ox}(1)$ = 0.588 V, $E_{ox}(2)$ = 0.780 V. Crystal data for $C_{32}H_{44}N_{12}O_2Zn_2Cl_4$: *Mr* =1110.41, 0.293·0.22·0.2 mm^3, monoclinic, space group *P-1,* *a* = 12.298(4), *b* = 16.001(5), *c* = 17.105(6) Å, α = 64.787(15)°, β = 87.964(15)°, γ = 67.988(13)°, *V* = 2782.2(18) Å^3, *Z* = 2, d_{calc} = 1.321 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 100 K, θ_{range} = 2.30 – 26.073°, reflections measured: 10945, indep: 10945 R_{int} = 0.0873, final *R* indices [I > 2σ(I)]: R_1 = 0.0804, wR_2 = 0.2421.

2.2 Complexes with L4

[(CuCl$_2$)$_2$(L4)]: $CuCl_2$ (20.9 mg, 166.1 µmol) was added to a solution of L4 (50.0 mg, 79.5 µmol) in CH_2Cl_2 and the reaction mixture stirred at room temperature for 2 h. The solvent was removed under reduced pressure leaving a dark green solid residue, that was washed with THF (3 x 3 mL) and Et_2O (2 x 3 mL). Yield of tthe crude product: 48.3 mg (53.8 µmol, 69%). Green crystals were obtained by diffusion of *n*-pentante into the CH_2Cl_2 solution at room temperature. Elemental analysis for $C_{32}H_{44}N_{12}O_2Cu_2Cl_4$ (897.68): calcd C 42.82, H 4.94, N 18.72; found C 42.49, H 5.12, N 18.33. UV-vis (CH_3CN, c = 1.48·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 228 (52619), 264 (46601), 347 (25154), 862 (2474). UV-vis (CH_2Cl_2, c = 1.33·10^{-5} mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 227 (72548), 265 (61165), 347 (27991), 868 (5899). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc$^+$/Fc): $E_{1/2}(1)$ = -0.139 V, $E_{1/2}(2)$ = 0.116 V, $E_{Red}(1)$ = -0.687 V, $E_{Red}(2)$ = 0.320 V, $E_{Ox}(1)$ = 0.816 V. Crystal data for $C_{32}H_{44}N_{12}O_2Cu_2Cl_4$: *Mr* = 1237.40, 0.30·0.15·0.15 mm^3, monoclinic, space group *P-1,* *a* = 9.7437(15), *b* = 1.8254(18), *c* = 12.179(2) Å, α = 69.555(6)°, β = 78.281(6)°, γ = 85.484(6)°, *V* = 287.5 Å^3, *Z* = 2, d_{calc} = 1.596 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 133 K, $2\theta_{range}$ = 4.063 – 52.146°, reflections measured: 16479, indep: 8346, R_{int} = 0.0612, final *R* indices [I > 2σ(I)]: R_1 = 0.038, wR_2 = 0.1694.

[(CuBr$_2$)$_2$(L4)]: L4 (100 mg, 159 µmol, 0.56 eq) and $CuBr_2$ (63.9 mg, 286 µmol, 1.00 eq) are suspended in anhydrous THF (5 ml). The reaction mixture was stirred at r. t. for 16 h. The formed precipitate was separated by filtration, washed three times with toluene, THF and Et_2O and dried under vacuum to yield a dark brown powder

(130 mg, 121 µmol, 76%). Elemental analysis for $C_{32}H_{44}N_{12}O_2Cu_2Br_4 \cdot 0.25CH_2Cl_2$ (1075.49, %): calcd. C 35.74, H 4.12, N 15.63; found C 35.32, H 4.09, N 15.33. IR (KBr): $\tilde{\nu}$ (cm^{-1}) = 2921, 2876, 1559, 1540, 1474, 1411, 1379, 1296, 1273, 1173, 1023, 972, 940, 856, 813. UV-vis (CH_3CN, c = $1.02 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 214 (74906), 222 (82018), 255 (62082), 356 (16381), 842 (3012). UV-vis (CH_2Cl_2, c = $2.18 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 241 (42741), 267 (40044), 350 (19095), 846 (3008). Crystal Data for $C_{32}H_{44}N_{12}O_2Cu_2Br_4$: *Mr* = 1415.20, 0.437·0.107·0.101 mm^3, monoclinic, space group *P-1, a* = 9.8593(9), *b* = 11.7388(10), *c* = 12.3720(11) Å, α = 70.057(3)°, β = 78.366(4)°, γ = 85.877(3)°, *V* = 1318.4 A^3, *Z* = 1, d_{calc} = 1.783 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 100 K, $2\theta_{range}$ = 4.188–55.998°, reflections measured: 49178 indep: 6337, R_{int} = 0.0812, final *R* indices [I>2σ(I)]: R_1 = 0.0453, wR_2 = 0.1112.

$[(CuCl(MeCN))_2(L4)](SbF_6)_2$: L4 (100 mg, 159 µmol, 0.56 eq.) and CuCl (41.1 mg, 286 µmol, 1.00 eq.) were suspended together in anhydrous CH_3CN (5 ml). The grey reaction mixture was stirred at room temperature for a period of 1 h. $NOSbF_6$ (84.5 mg, 318 µmol, 1.10 eq.) was added, and the black reaction mixture stirred at room temperature for 16 h. Then, the reaction mixture was layered with anhydrous Et_2O (10 ml) and stored at 4 °C for 24 h. The precipitate was separated by filtration, washed three times with toluene, THF and Et_2O and dried under vacuum to yield a black powder (158 mg, 114 µmol, 72%). Elemental analysis ($C_{36}H_{50}Cl_2Cu_2N_{14}O_2F_{12}Sb_2$, MW: 1469.29, %): calcd. C 31.32, H 3.65, N 14.21; found C 31.20, H 3.82, N 13.78. IR (KBr): $\tilde{\nu}$ (cm^{-1}) = 2934, 2887, 1540, 1480, 1413, 1379, 1295, 1271, 1237, 1172, 1026, 973, 936, 815, 658. UV-vis (CH_3CN, c = $1.26 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 206 (78515), 254 (56867), 353 (21210). UV-vis (CH_2Cl_2, c = $1.40 \cdot 10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 226 (54653), 274 (21648), 358 (5207).

2.3 Complexes with L1

$([(MnCl_2)_2(L1)])_n$: $MnCl_2$ (23.7 mg, 188µmol) was added to a solution of L1 (50.0 mg, 94.2 µmol) in CH_3CN. The solution was stirred at room temperature for 16 h, leading to a yellow solid. The solvent was removed by filtration and the yellow solid washed first with CH_3CN, then with THF and finally with Et_2O. Yellow crystals were obtained by

overlayering a solution in CH_2Cl_2 with *n*-pentane. (Yield: 64.3 mg, 87%). Elemental analysis for $C_{26}H_{50}N_{12}Mn_2Cl_4$ (784.26): calcd. C 39.80, H 6.43, N 21.43; found C 39.88, H 6.45, N 21.25. UV-vis (CH_2Cl_2, c = $4.02\cdot10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 280 (17188), 324 (10552), 369 (6162), 575 (494). $C_{52}H_{100}N_{24}Mn_4Cl_8$: *Mr* = 733.95, $0.4\cdot0.3\cdot0.3$ mm^3, monoclinic, space group *P21/n,* *a* = 16.5412(11), *b* = 17.5177(11), *c* = 19.2787(13) Å, α = 90°, β = 111.374(3)°, γ = 90°, *V* = 2169.3(2) $Å^3$, *Z* = 6, d_{calc} = 1.406 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 101 K, $2\theta_{range}$ = 4.064 – 55.022°, reflections measured: 209703, indep: 11951, R_{int} = 0.1028, final *R* indices [I > 2σ(I)]: R_1 = 0.0421, wR_2 = 0.1104.

[$(FeCl_2)_2$(L1)]: To a solution of L1 (50.0 mg, 94.2µmol) in CH_3CN $FeCl_2$ (23.88 mg, 188µmol) were added. The solution was stirred at rt for 16 h, leading to a yellow solid. The solvent was removed by filtration and the yellow solid was washed with CH_3CN and Et_2O. Yellow crystals could be obtained by overlayering a solution in CH_2Cl_2 with *n*-pentane. (Yield: 68.0 mg, 92%). ^{1}H NMR (200 MHz, CD_2Cl_2): δ (ppm) = 9.98 (s, CH_{ar}), 20.1 (s, CH_3) ppm. Elemental analysis for $C_{26}H_{50}N_{12}Fe_2Cl_4$ (784.26): calcd. C 39.8, H 6.43, N 21.43; found C 39.88, H 6.45, N 21.25. UV-vis (CH_2Cl_2, c = $1.03\cdot10^{-5}$ mol l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 233 (24231), 282 (14578), 346 (12079). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): $E_{1/2}$(1) = -0.233 V, E_{Red}(1) = -0.478 V, E_{Red}(2) = -0.557 V, E_{Ox}(1) = -0.478 V, E_{ox}(2) = 0.662 V. Crystal data for $C_{26}H_{50}N_{12}Fe_2Cl_4$: *Mr* = 954.13 , $0.46\cdot0.415\cdot0.408$ mm^3, monoclinic, space group *P-1 21/c1,* *a* = 10.8239(7), *b* = 13.4918(7), *c* = 14.9161(9) Å, α = 90°, β = 95.205(2)°, γ = 90°, *V* = 2169.3(2) $Å^3$, *Z* = 2, d_{calc} = 1.461 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 100 K, $2\theta_{range}$ = 3.778 – 61.996°, reflections measured: 69828, indep: 6897, R_{int} = 0.0542 final *R* indices [I > 2σ(I)]: R_1 = 0.0228, wR_2 = 0.0560.

[$(CoCl_2)_2$(L1)]: $CoCl_2$ (24.5mg, 188µmol) was added to a solution of L1 (50.0 mg, 94.2 µmol) in CH_3CN. The solution was stirred at rt for 16 h, leading to a blue solid. The solvent was removed by filtration and the blue solid was washed with CH_3CN, THF and Et_2O. Blue crystals could be obtained by layering a solution in CH_2Cl_2 with *n*-pentane. Yield: 67.6 mg, 91%. Elemental analysis for $C_{26}H_{50}N_{12}Co_2Cl_4$ (790.44): calcd. C 39.51, H 6.38, N 21.26; found C 39.72, H 6.65, N 21.44. UV-vis (CH_2Cl_2, c = $2.03\cdot10^{-5}$ mol

l^{-1}, d = 1 cm): λ_{max} (nm (ε in M^{-1} cm^{-1})) = 240 (13539), 284 (8285), 335 (7486), 550 (233), 566 (224), 625 (250), 663 (282). CV (CH_2Cl_2, Ag/AgCl, NBu_4PF_6, potentials given rel. to Fc^+/Fc): $E_{1/2}(1)$ = -0.168 V, $E_{Red}(1)$ = -0.580 V, $E_{Ox}(1)$ = 0.128 V. Crystal data for $C_{26}H_{50}N_{12}Co_2Cl_4$: *Mr* = 960.29, 0.31·0.25·0.13 mm^3, triclinic, space group *P-1*, *a* = 10.578(6), *b* = 12.864(7), *c* = 16.726(7) Å, α = 89.34(2)°, β = 78.74(2)°, γ = 88.76(2)°, *V* = 2232.3(2) $Å^3$, *Z* = 2, d_{calc} = 1.429 g dm^{-3}, $Mo_{K\alpha}$ radiation (graphite monochromated, λ = 0.71073 Å), *T* = 103 K, θ_{range} = 2.00 – 27.551°, reflections measured: 10199, indep: 10199, R_{int} = 0.1627, final *R* indices [I > 2σ(I)]: R_1 = 0.1073, wR_2 = 0.2043.

3. Analytical data

3.1 NMR spectra (all measured at room temperature if not stated otherwise)

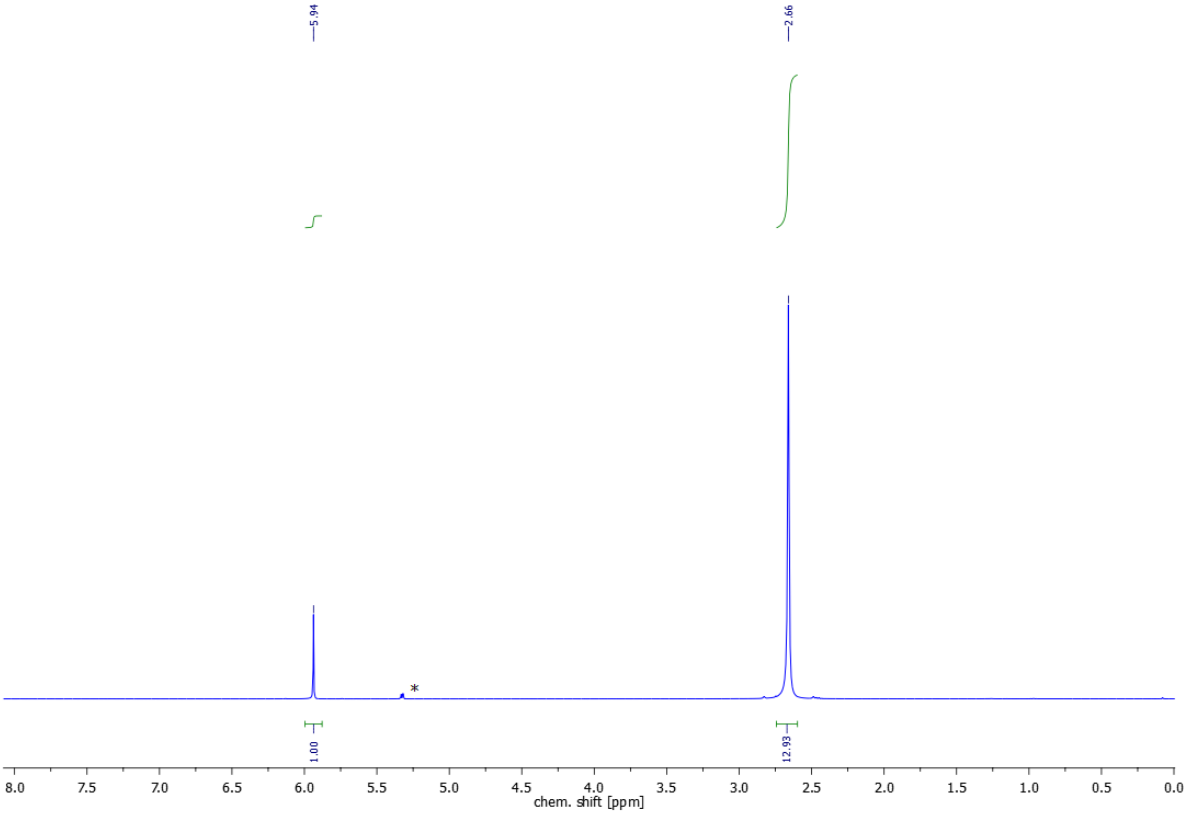

Figure S1: ^{1}H NMR spectrum (400 MHz, CD_2Cl_2) of L3.

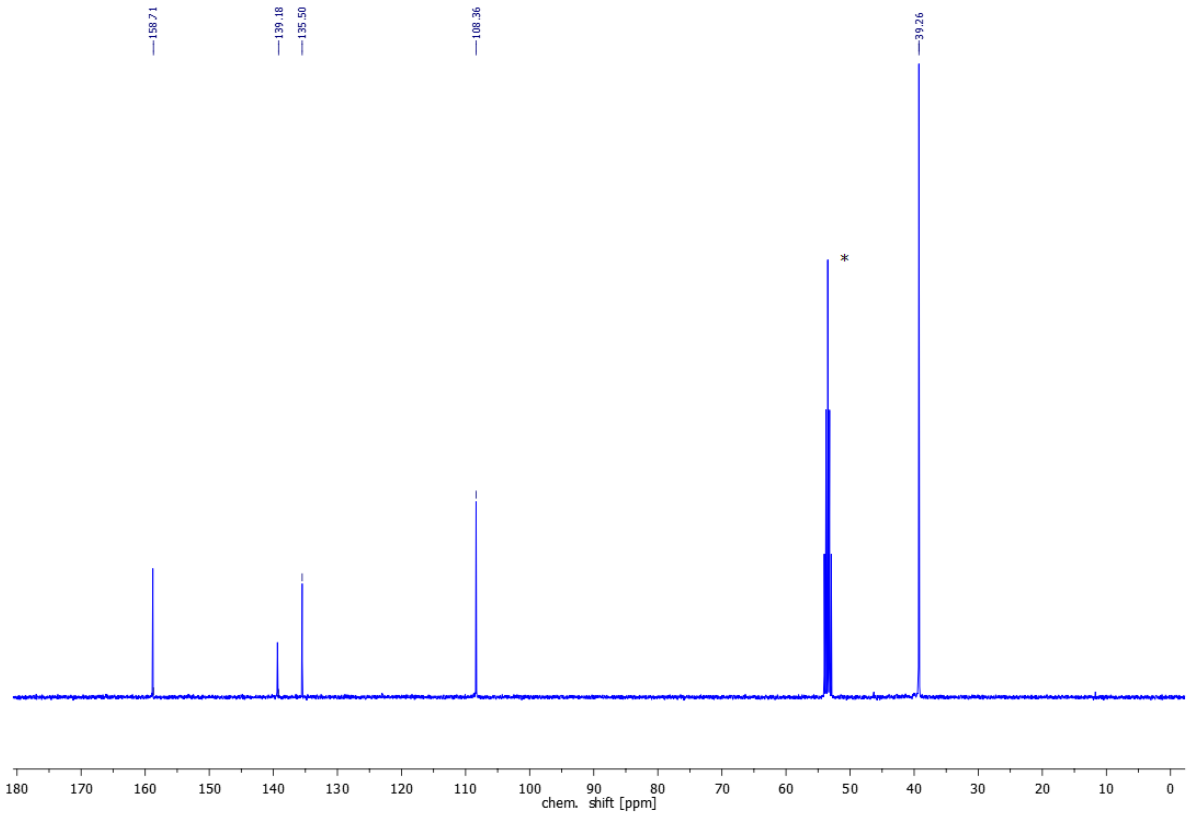

Figure S2: ^{13}C NMR spectrum (400 MHZ, CD_2Cl_2) of L3.

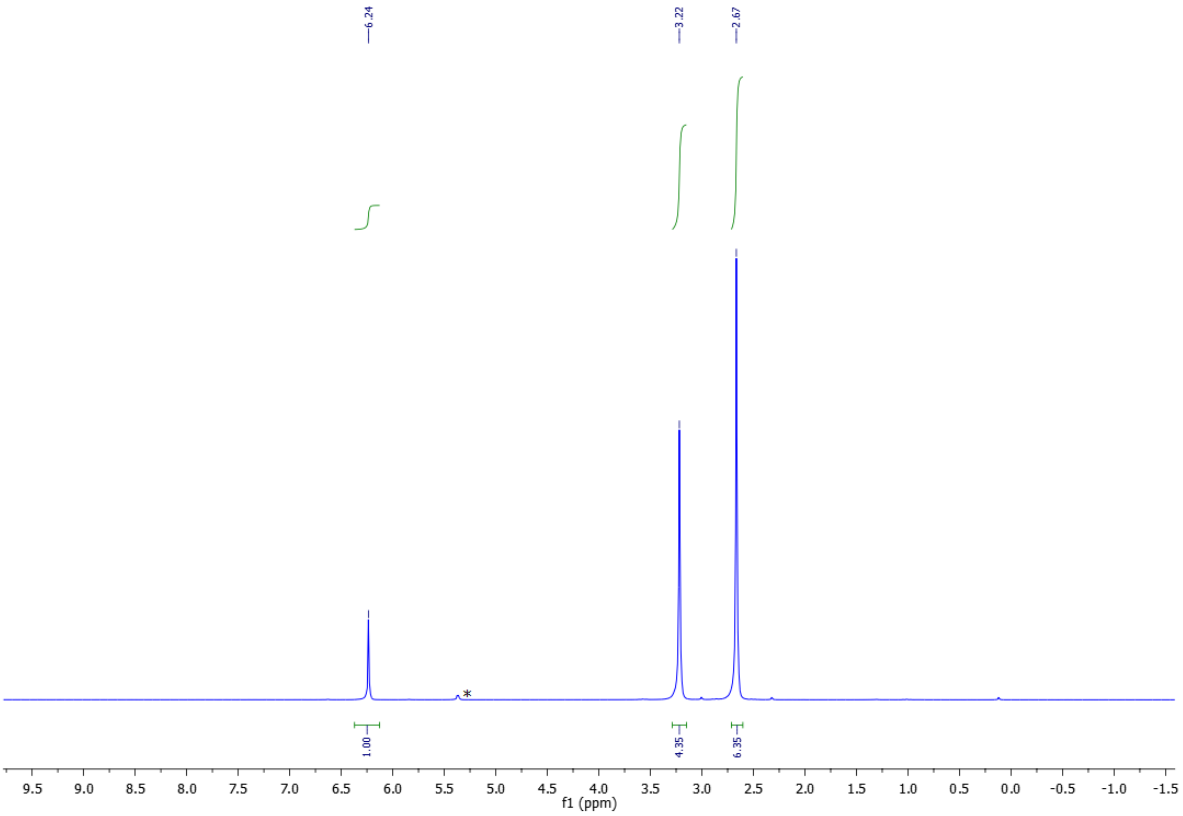

Figure S3: ^{1}H NMR spectrum of L4 (400 MHz, CD_2Cl_2).

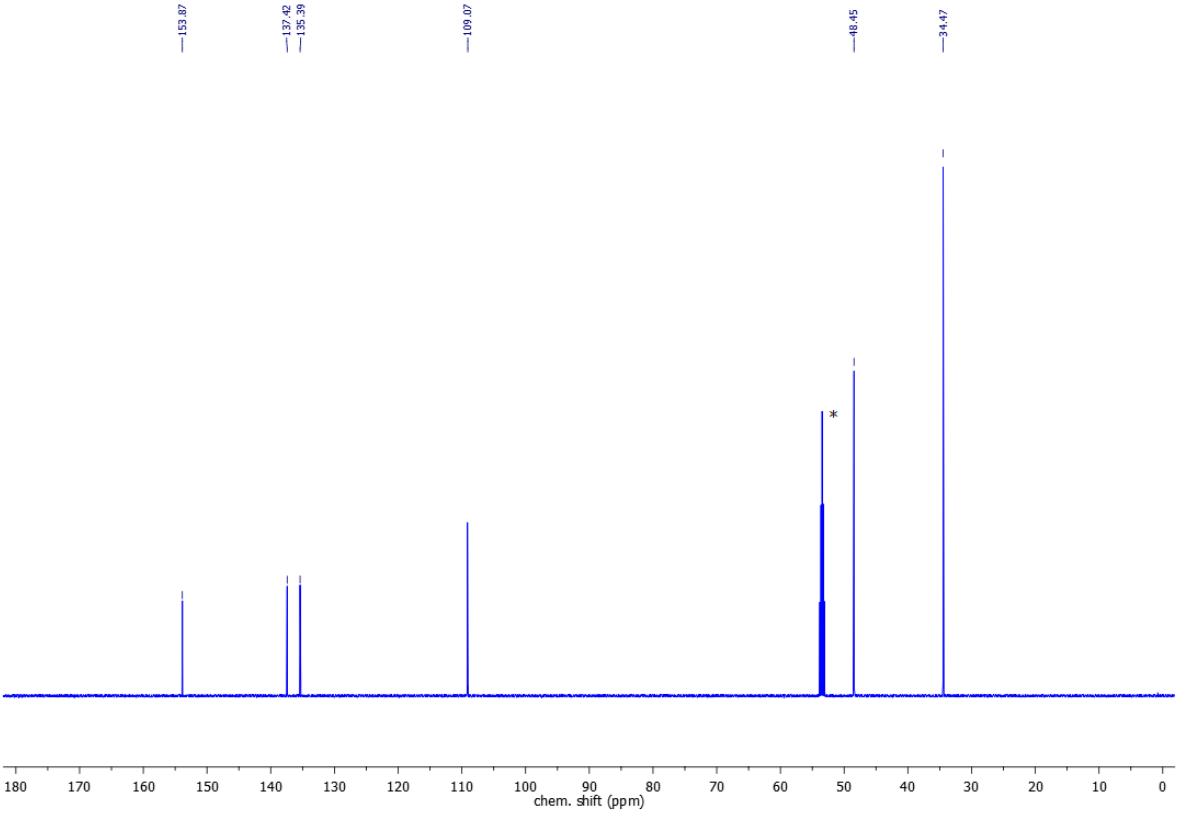

Figure S4: ^{13}C NMR spectrum of L4 (400 MHz, CD_2Cl_2).

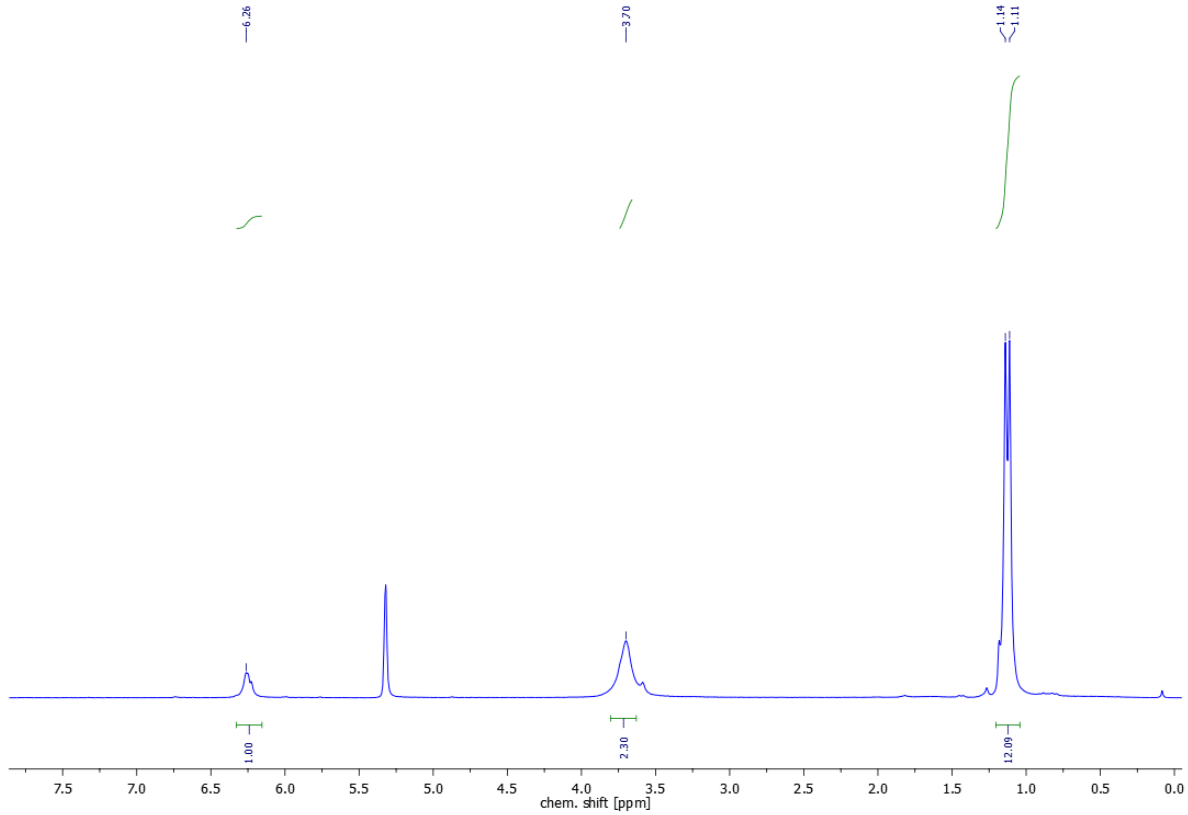

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Figure S5: ^{1}H NMR spectrum of L5 (400 MHz, CD_2Cl_2).

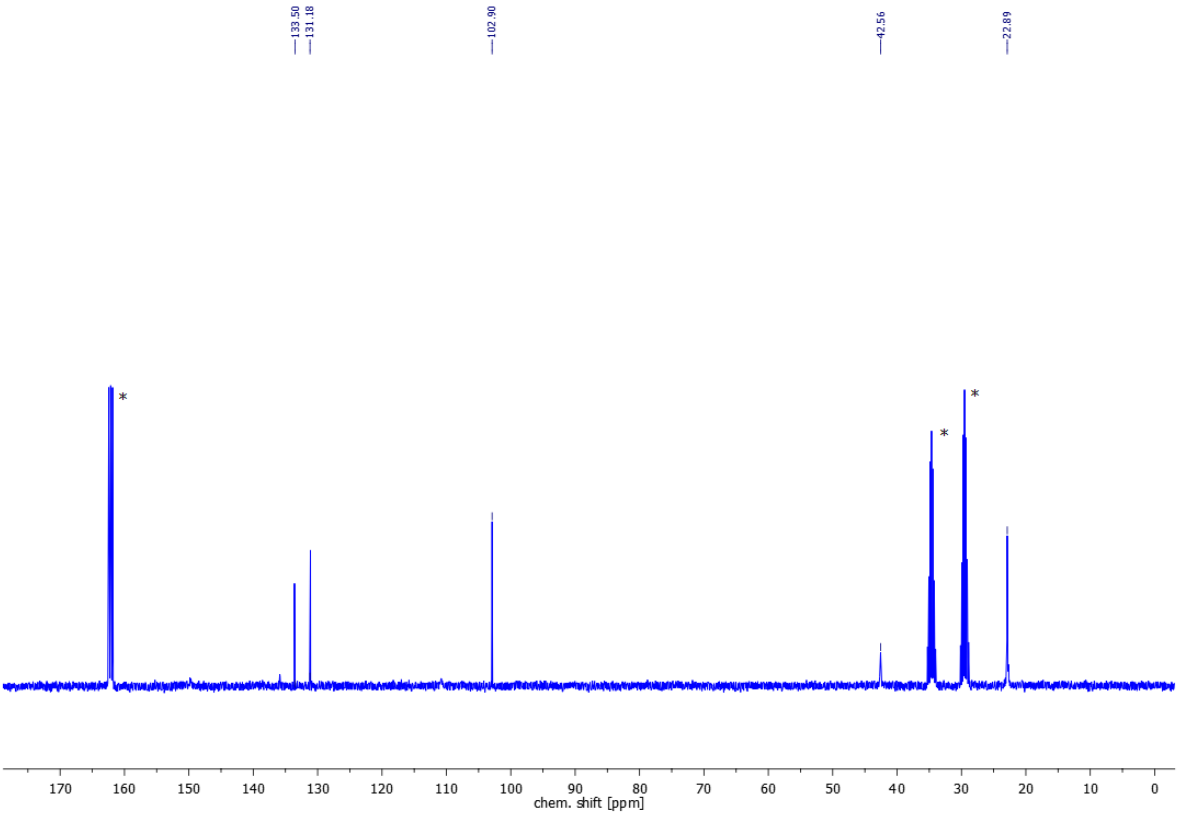


Figure S6:^{13}C NMR spectrum of L5 (400 MHz, CD_2Cl_2).

3.2 UV-vis spectra (measured at room temperature if not stated otherwise)

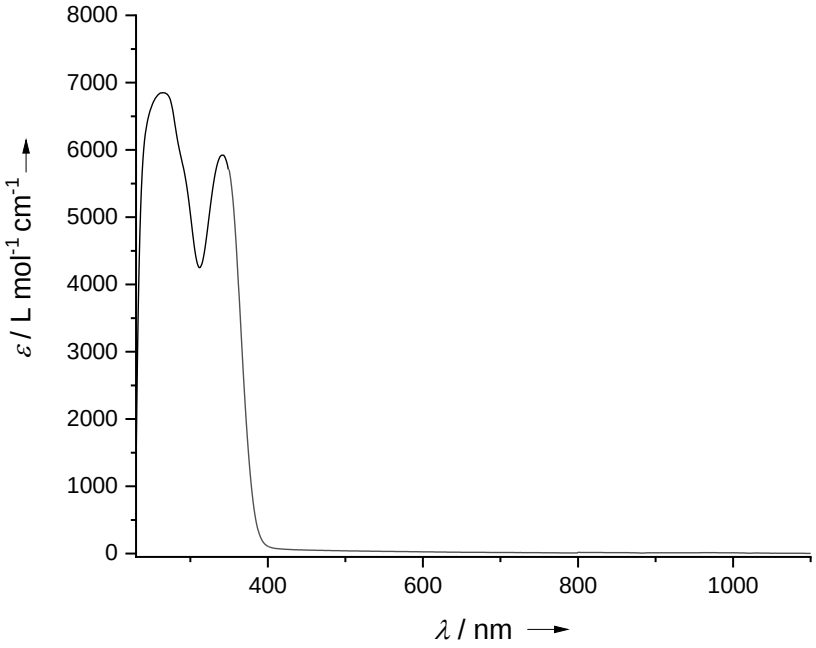
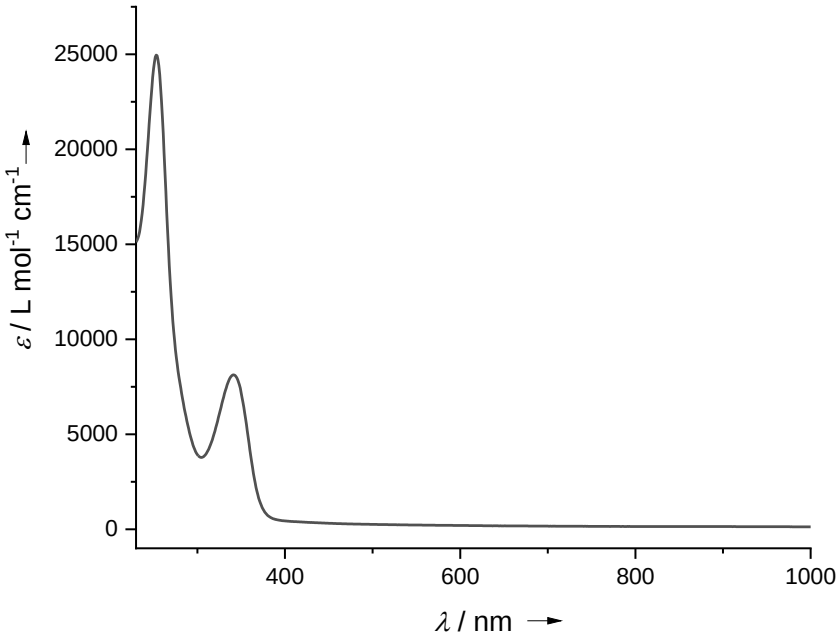


Figure S7: UV-vis spectrum of L3 in CH_2Cl_2 solution.

a)



b)

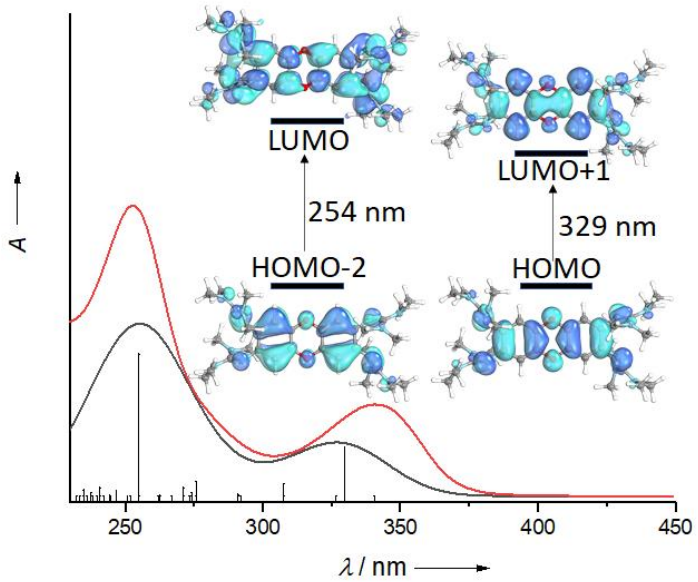


Figure S8: a) UV-vis spectrum of L4 in CH_2Cl_2 solution. b) Comparison between the experimentally observed UV-vis spectrum of L4 and a simulation based on a TD-DFT calculation (B3LYP/def2-TZVP).

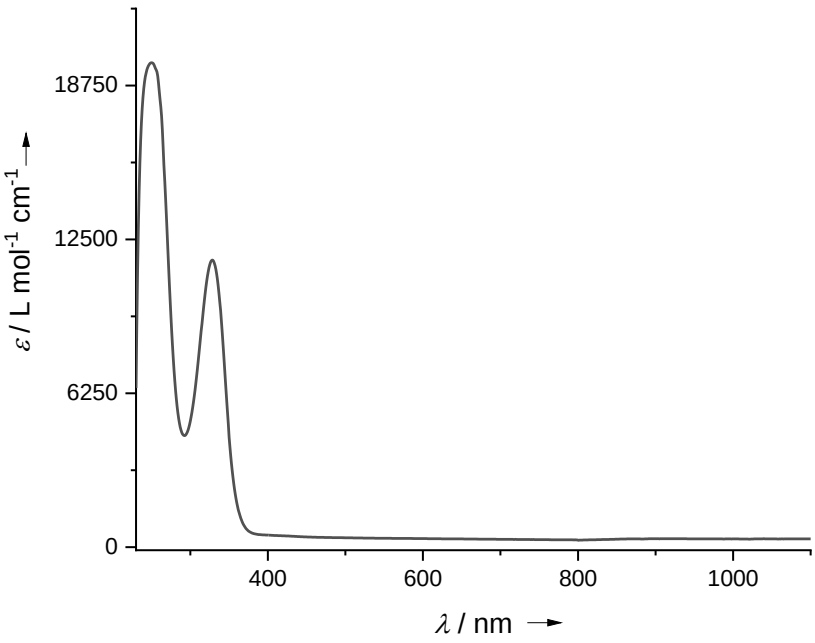


Figure S9: UV-vis spectrum of L5 in CH_2Cl_2 solution.

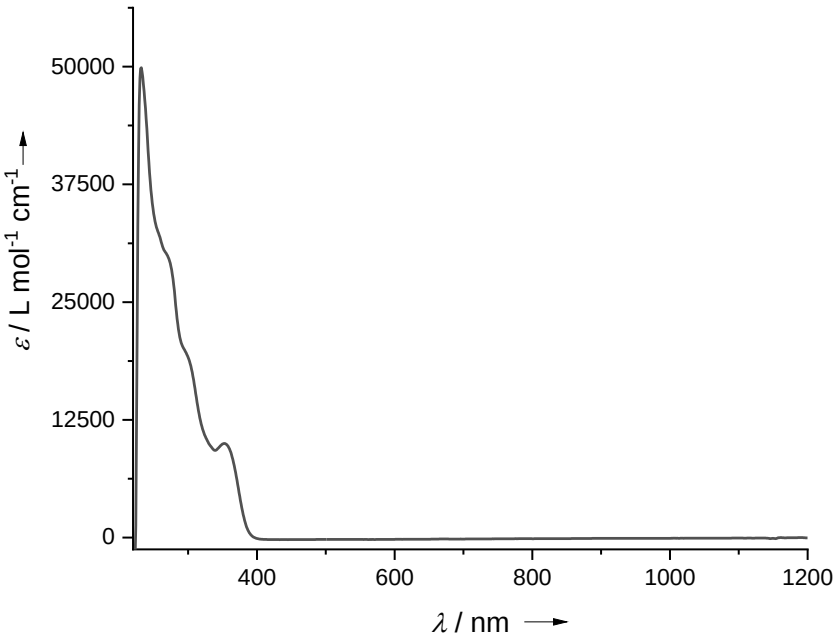


Figure S10: UV-vis spectrum of $[(MnCl_2)_2(L3)]$ in CH_2Cl_2 solution.

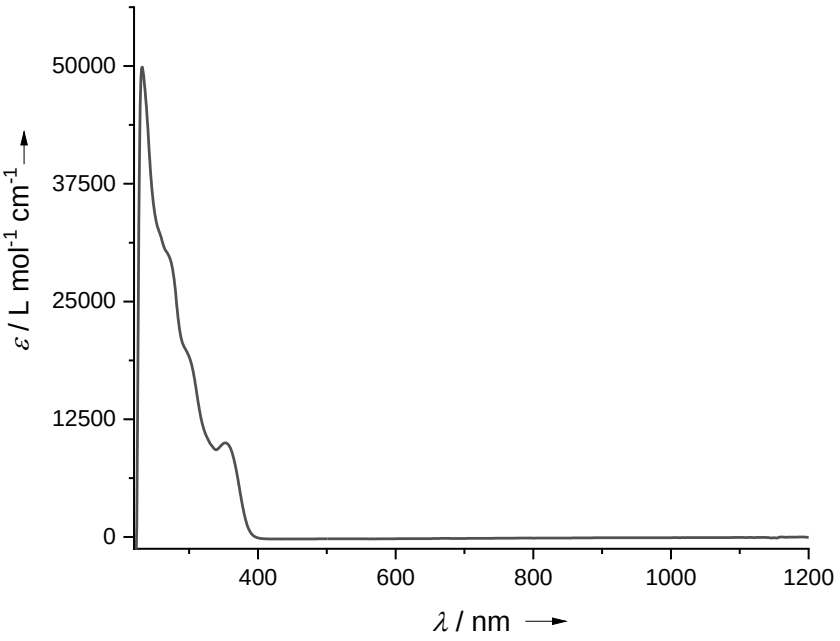


Figure S11: UV-vis spectrum of $[(MnCl_2)_2(L3)]$ in CH_2Cl_2 solution.

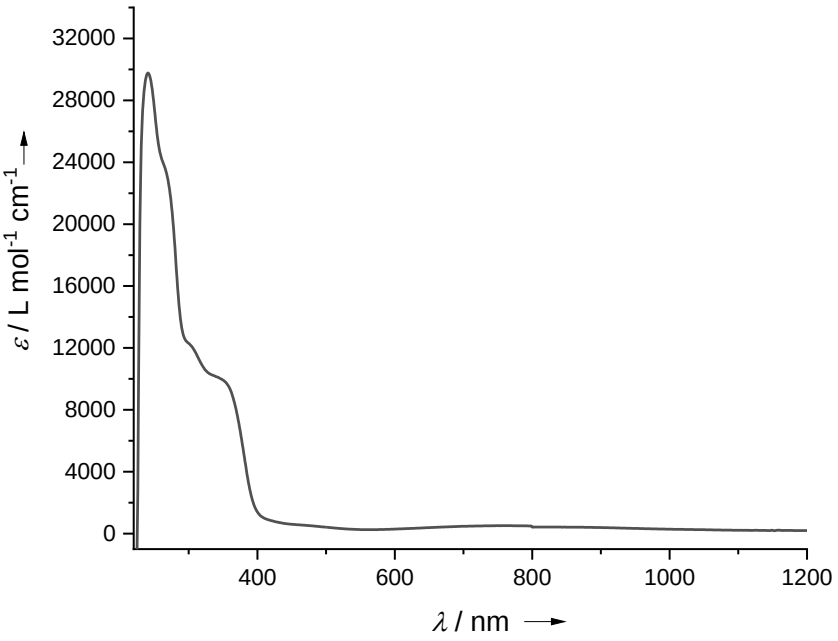


Figure S12: UV-vis spectrum of $[(FeCl_2)_2(L3)]$ in CH_2Cl_2 solution.

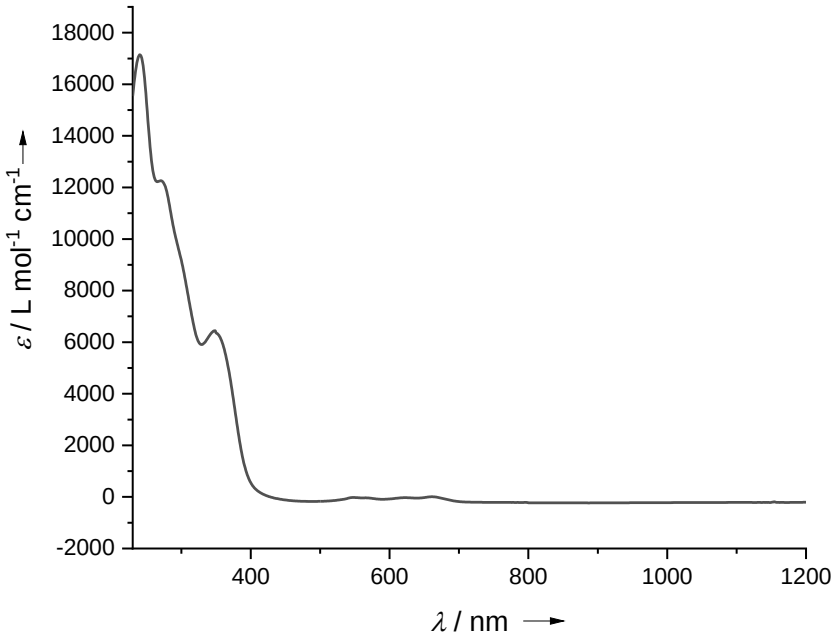


Figure S13: UV-vis spectrum of $[(CoCl_2)_2(L3)]$ in CH_2Cl_2 solution.

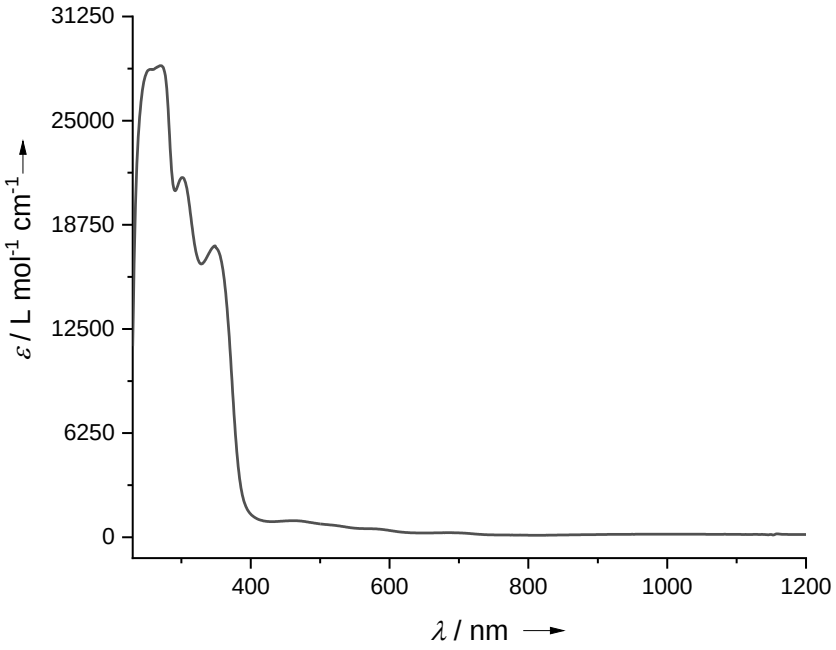


Figure S14: UV-vis spectrum of $[(NiCl_2)_2(L3)]$ in CH_2Cl_2 solution.

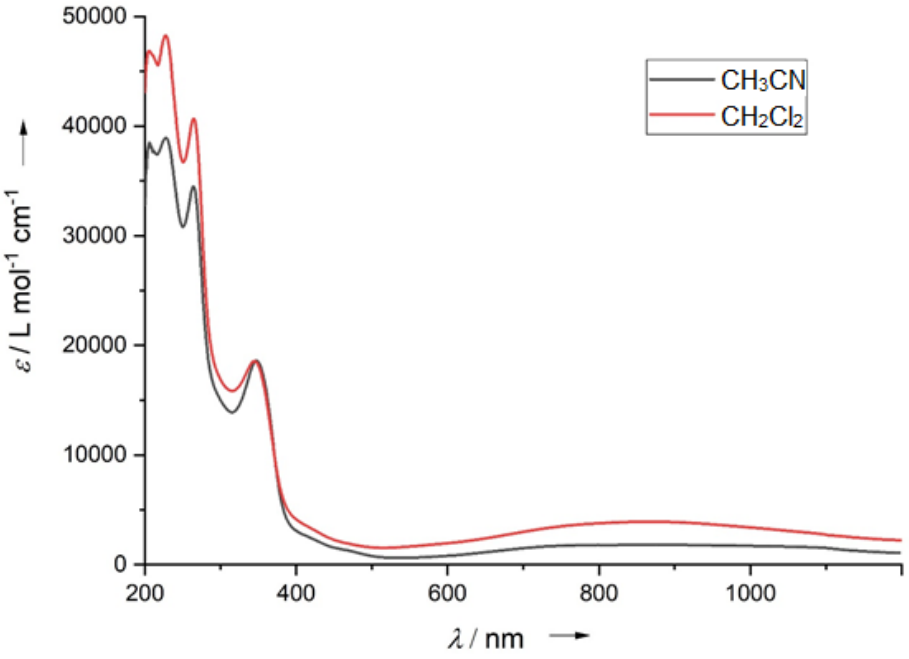


Figure S15: UV-vis spectrum of $[(CuCl_2)_2(L3)]$ in CH_2Cl_2 (red) and CH_3CN (black) solution.

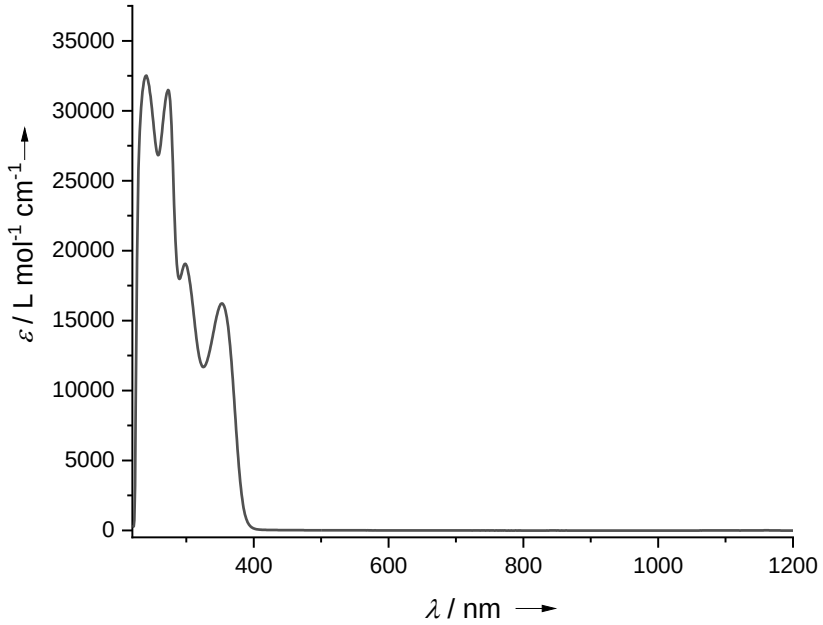


Figure S16: UV-vis spectrum of $[(ZnCl_2)_2(L3)]$ in CH_2Cl_2 solution.

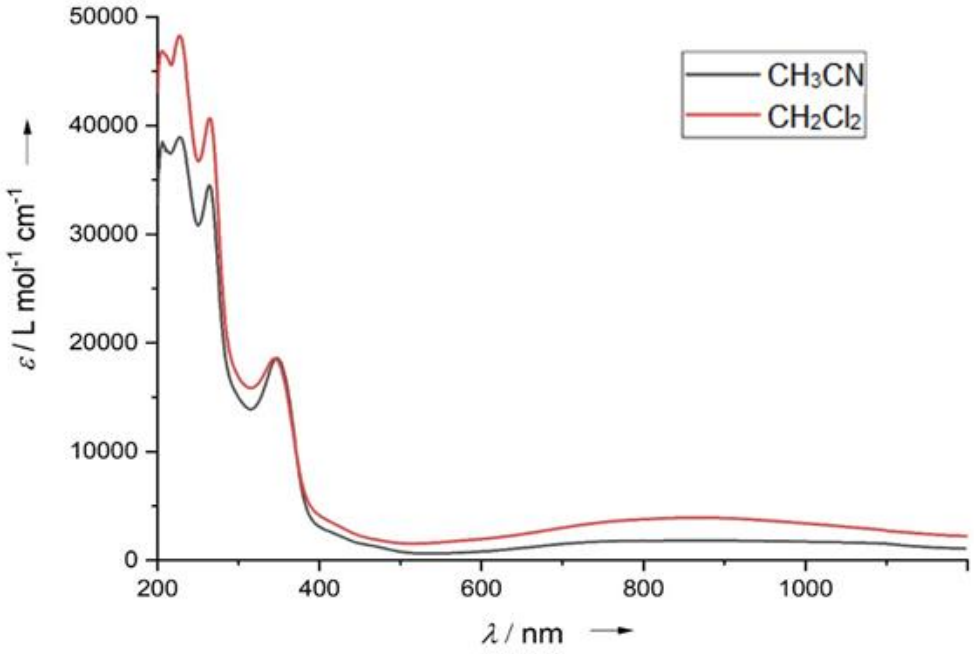


Figure S17: UV-vis spectra of $[(CuCl_2)_2(L4)]$ in CH_3CN (black) and CH_2Cl_2 (red) solution.

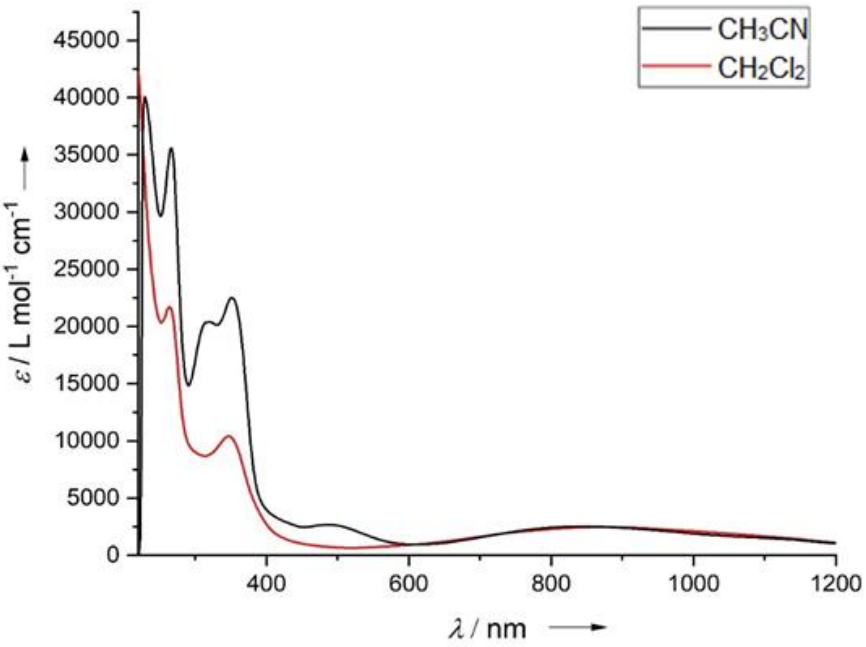


Figure S18: UV-vis spectra of $[(CuBr_2)_2(L4)]$ in CH_3CN (red) and CH_2Cl_2 (black) solution.

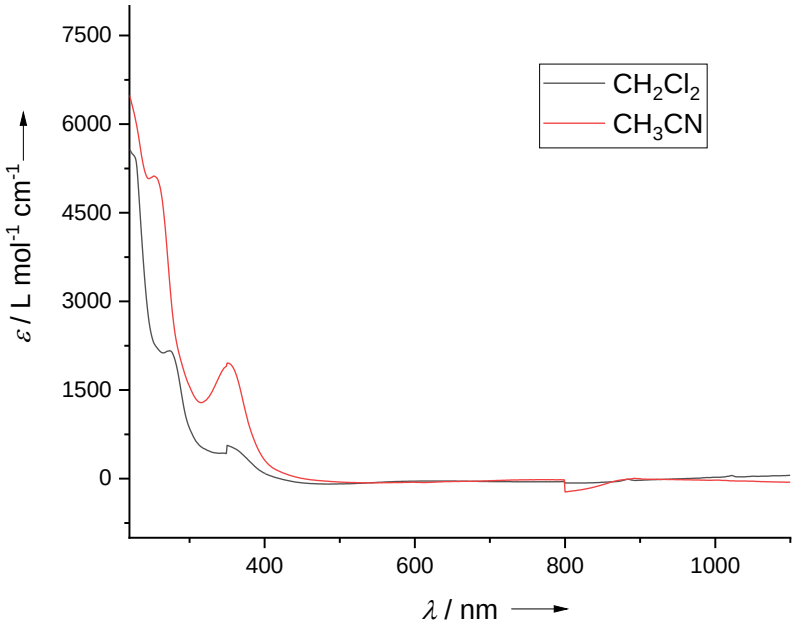


Figure S19: UV-vis spectra of $[(CuCl(CH_3CN))_2(L4)](SbF_6)_2$ in CH_3CN (red) and CH_2Cl_2 (black) solution.

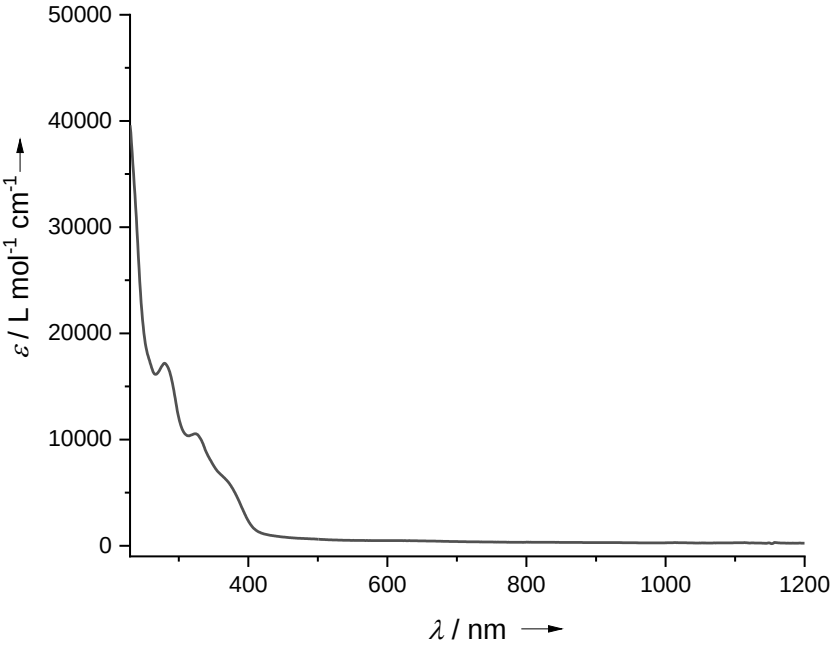


Figure S20: UV-vis spectrum of [$(MnCl_2)_2$(L1)] in CH_2Cl_2 solution.

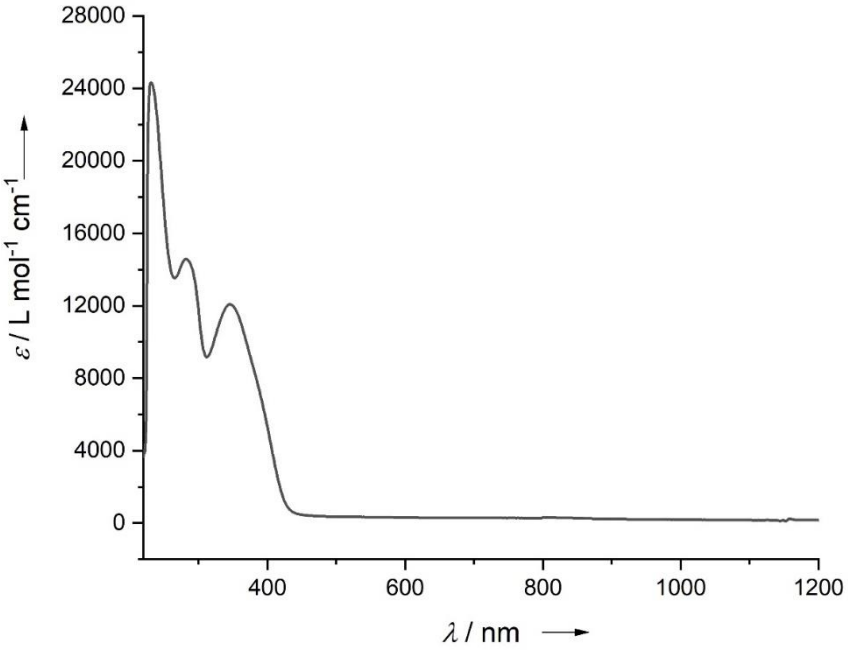


Figure S21: UV-vis spectrum of [$(FeCl_2)_2$(L1)] in CH_2Cl_2 solution.

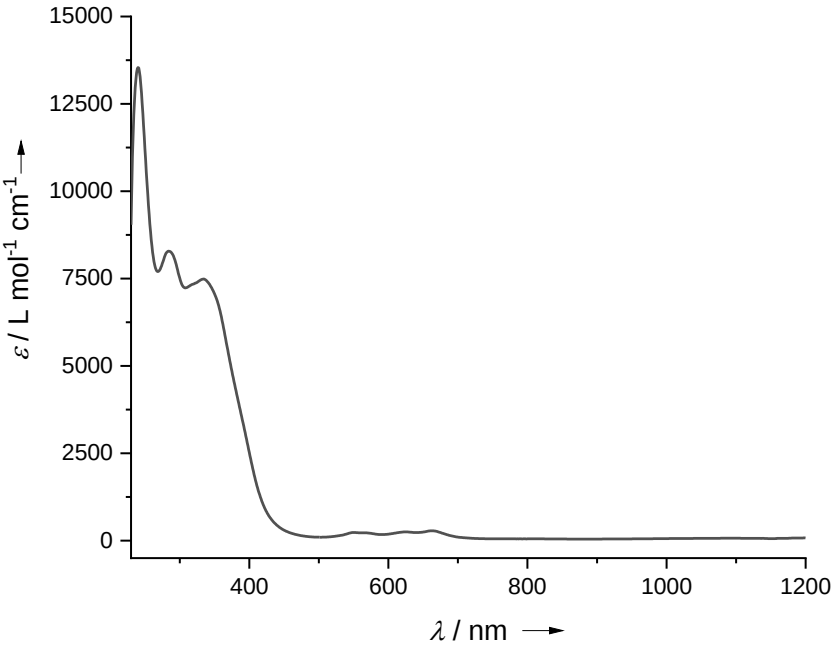


Figure S22: UV-vis spectrum of $[(CoCl_2)_2(L1)]$ in CH_2Cl_2 solution.

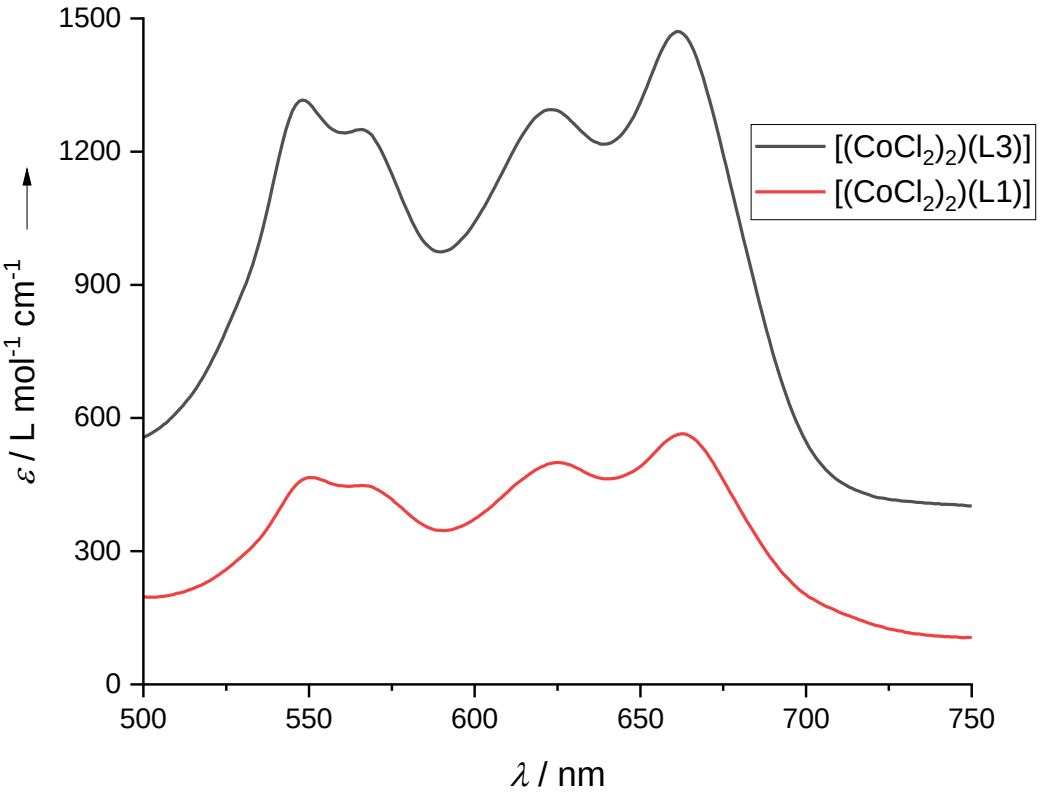


Figure S23: Comparison of the charge transfer bands of the UV-vis spectra of the complexes $[(CoCl_2)_2(L1)]$ (black) and $[(CoCl_2)_2(L3)]$ red.

3.3 Cyclic voltammetry (CV) measurements (All measurements were taken at room temperature with a Ag/AgCl reference electrode, 0.1 M N(*n*Bu)$_4$(PF$_6$) as supporting electrolyte, and a scan rate of 100 mV s^{-1}, potentials are given vs. the Fc$^+$/Fc redox couple if not stated otherwise.)

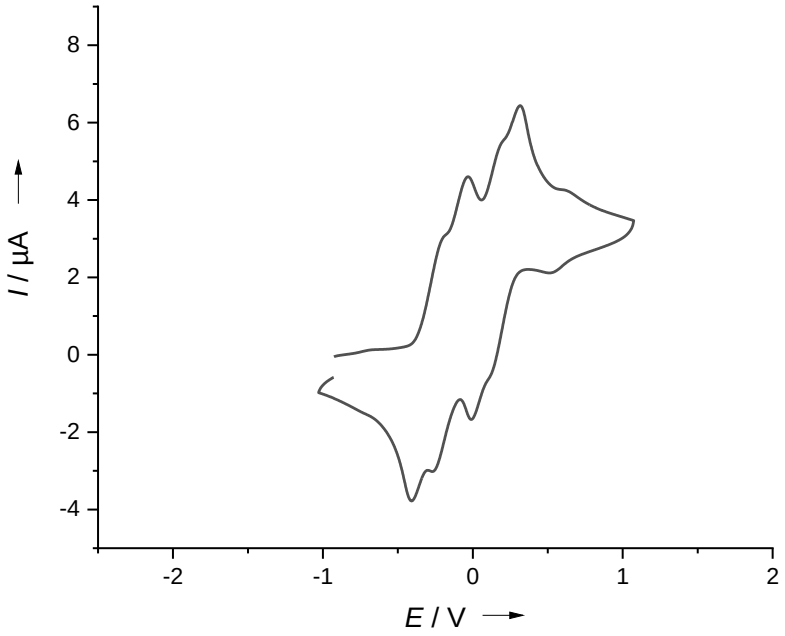


Figure S24: Cyclic voltammogram for L3 in CH_2Cl_2 solution.

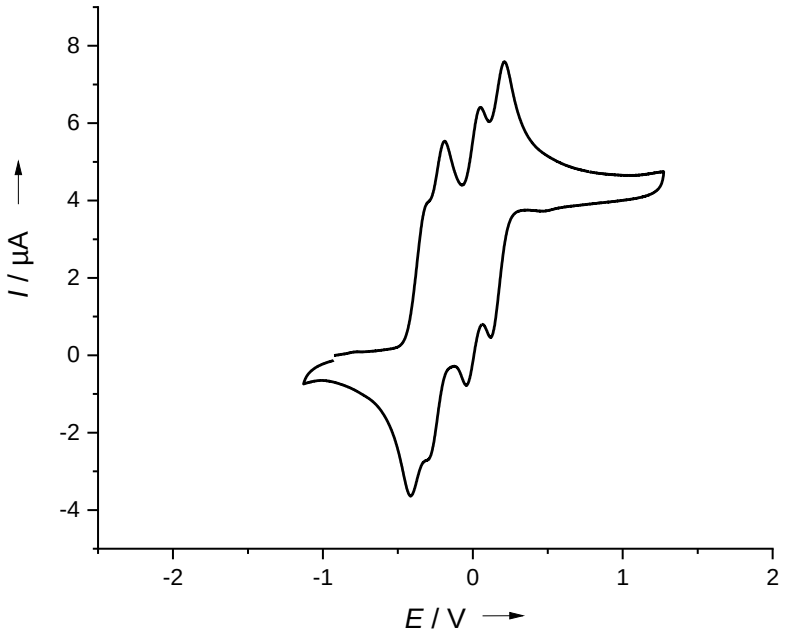


Figure S25: Cyclic voltammogram for L4 in CH_2Cl_2 solution.

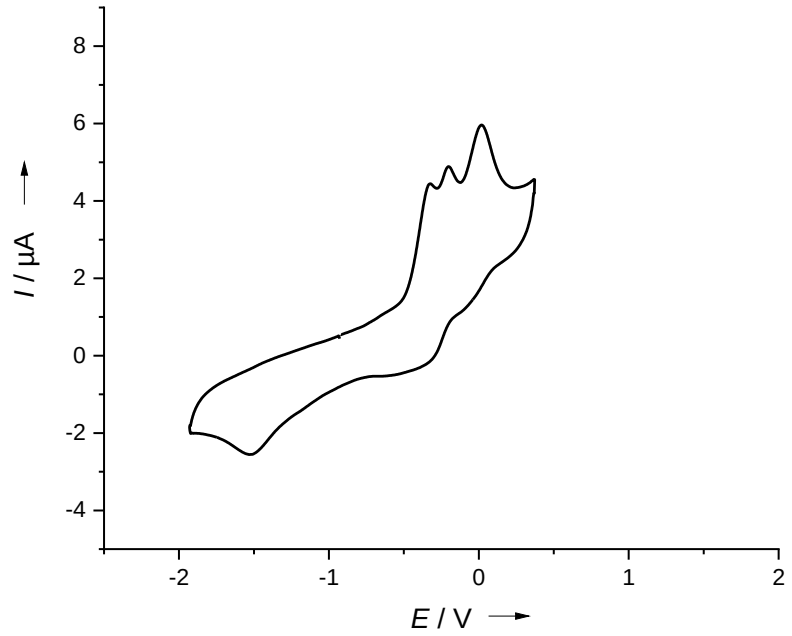


Figure S26: Cyclic voltammogram for L5 in CH_2Cl_2 solution.

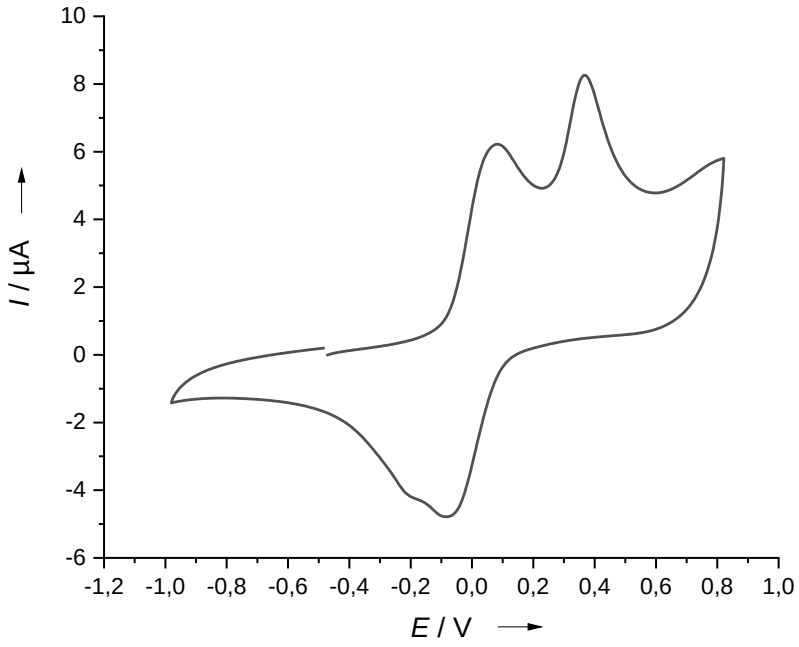


Figure S27: Cyclic voltammogram for $[(MnCl_2)_2(L3)]$ in CH_2Cl_2.

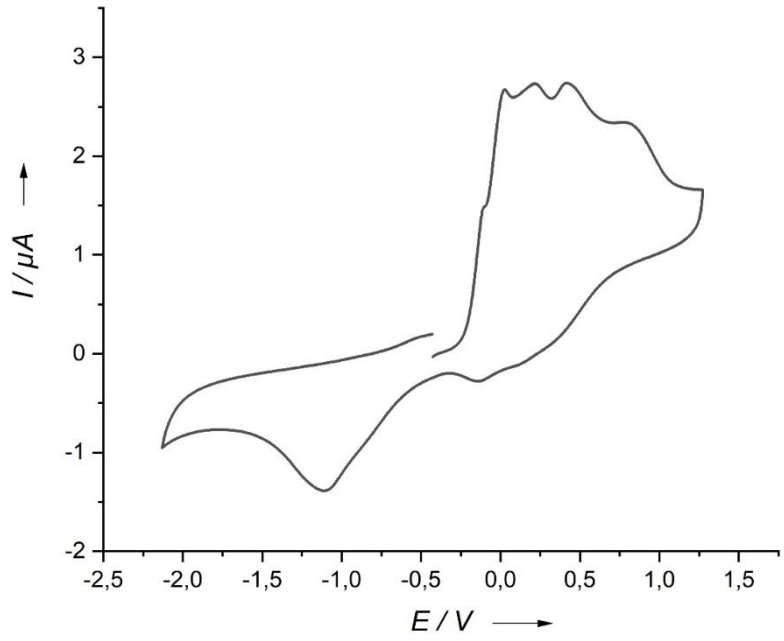


Figure S28: Cyclic voltammogram for $[(FeCl_2)_2(L3)]$ in CH_2Cl_2.

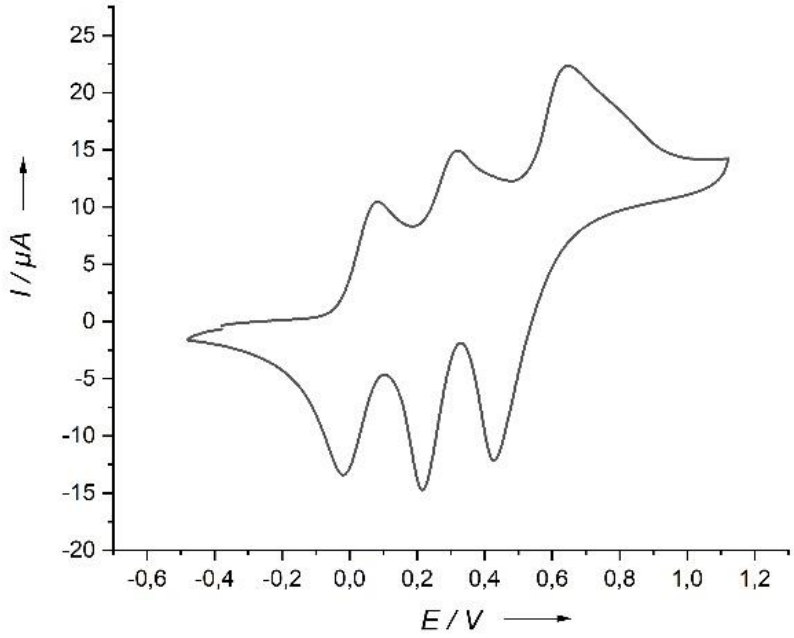


Figure S29: Cyclic voltammogram for $[(CoCl_2)_2(L3)]$ in CH_2Cl_2.

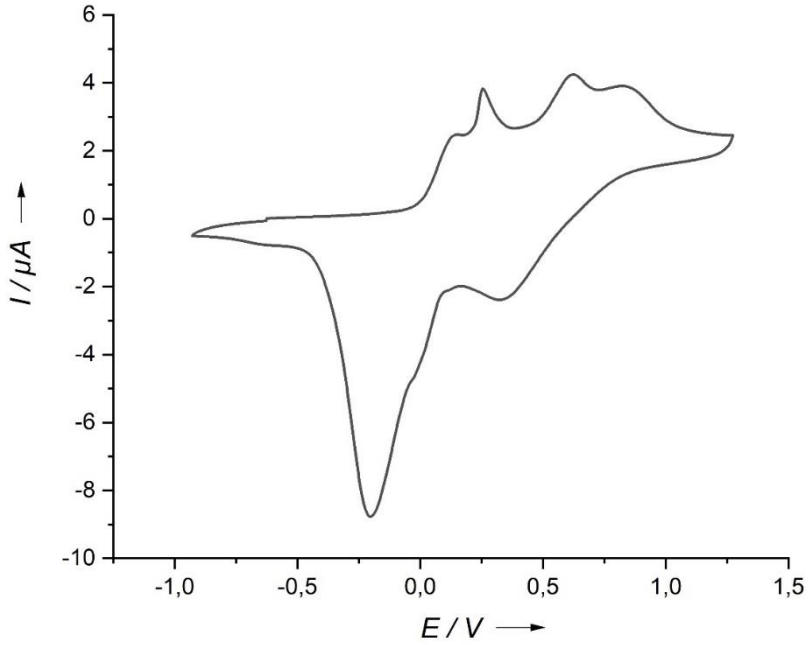


Figure S30: Cyclic voltammogram for $[(NiCl_2)_2(L3)]$ in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M $N(nBu)_4(PF_6)$ as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

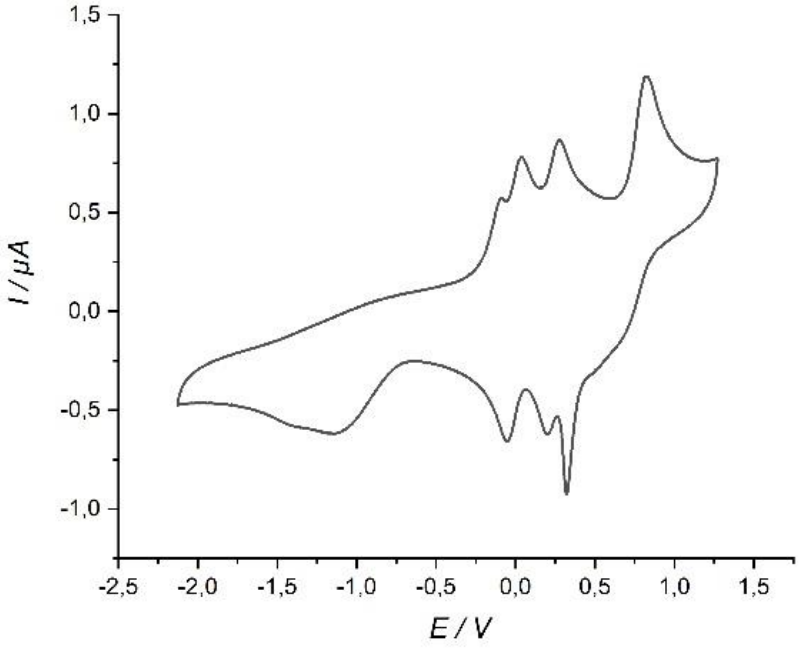


Figure S31: Cyclic voltammogram for $[(CuCl_2)_2(L3)]$ in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M $N(nBu)_4(PF_6)$ as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

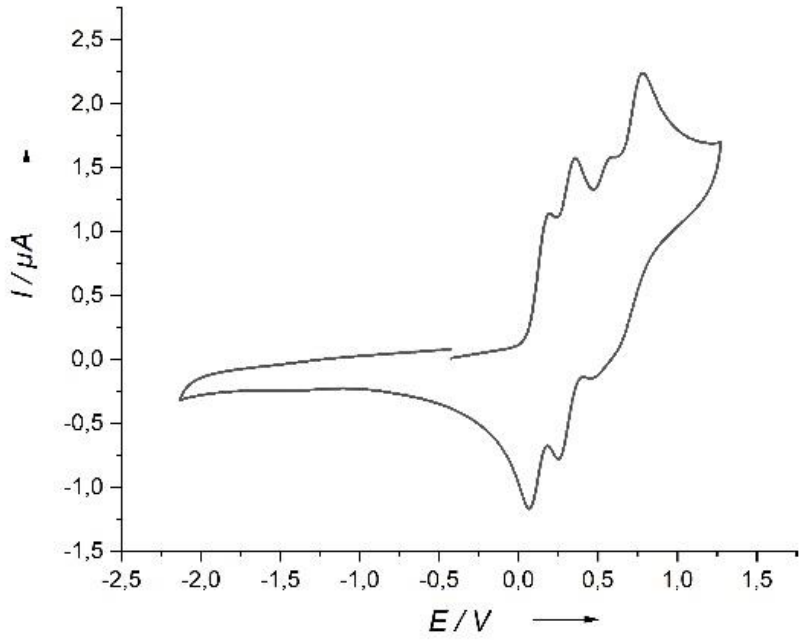


Figure S32: Cyclic voltammogram for $[(ZnCl_2)_2(L3)]$ in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M $N(nBu)_4(PF_6)$ as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

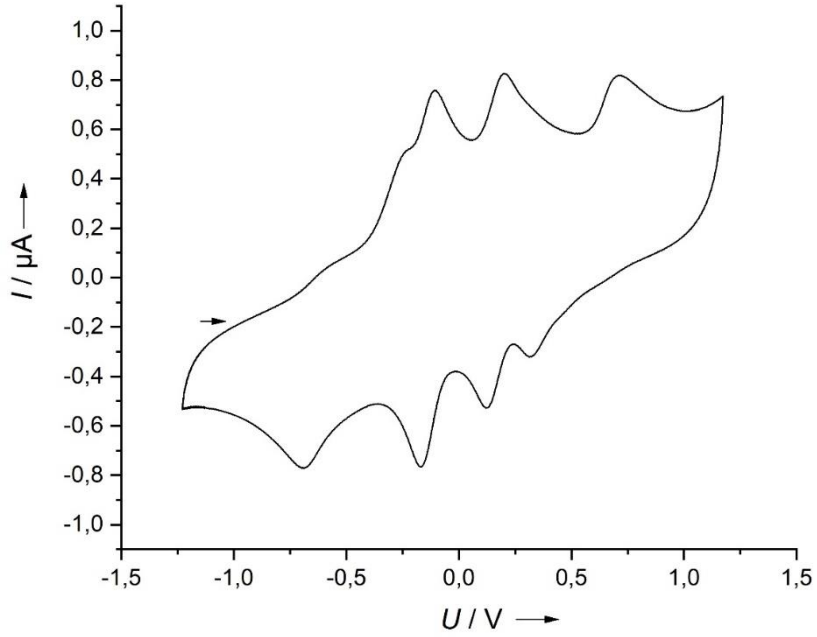


Figure S33: Cyclic voltammogram for $[(CuCl_2)_2(L4)]$ in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M $N(nBu)_4(PF_6)$ as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

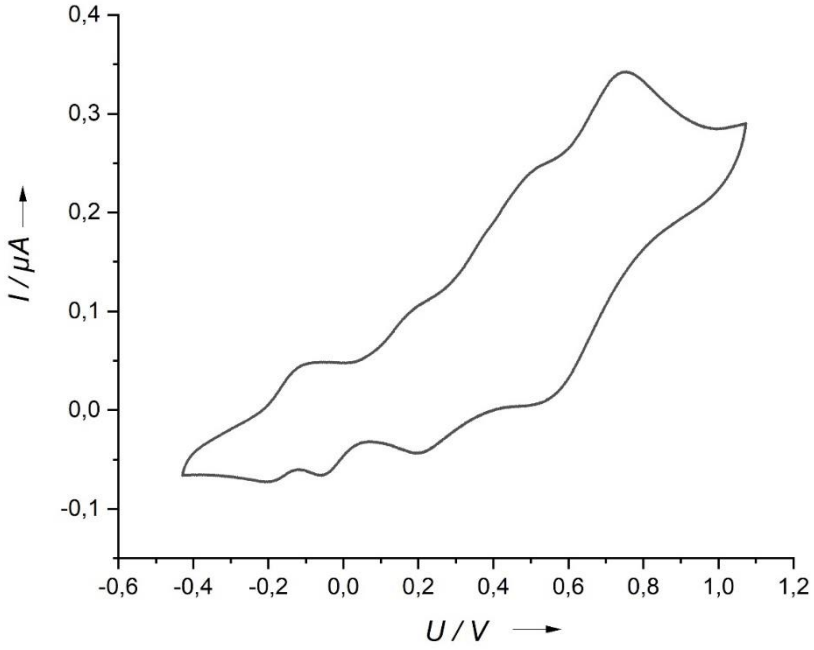


Figure S34: Cyclic voltammogram for [$(CuBr_2)_2$(L4)] in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M N(*n*Bu)$_4$(PF_6) as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

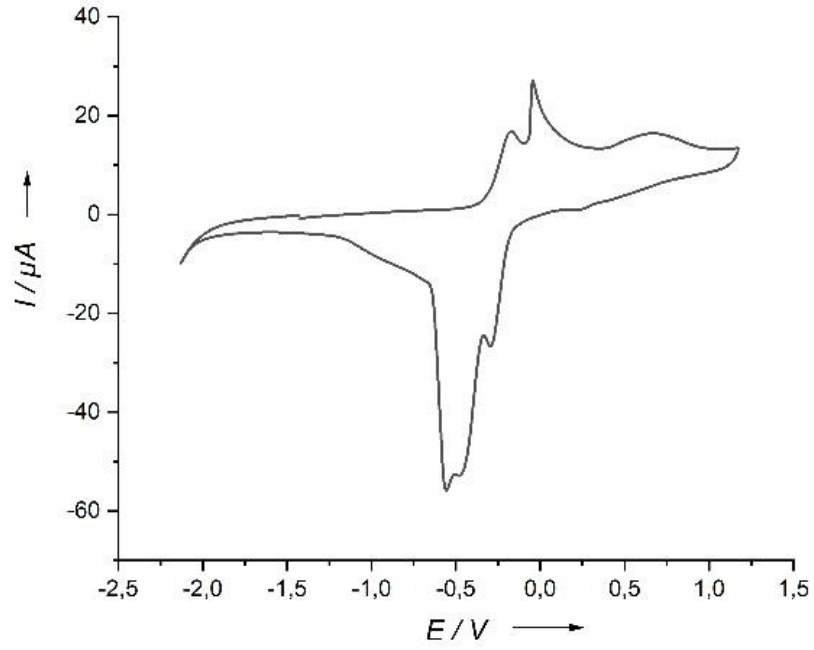


Figure S35: Cyclic voltammogram for [$(FeCl_2)_2$(L1)] in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M N(*n*Bu)$_4$(PF_6) as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

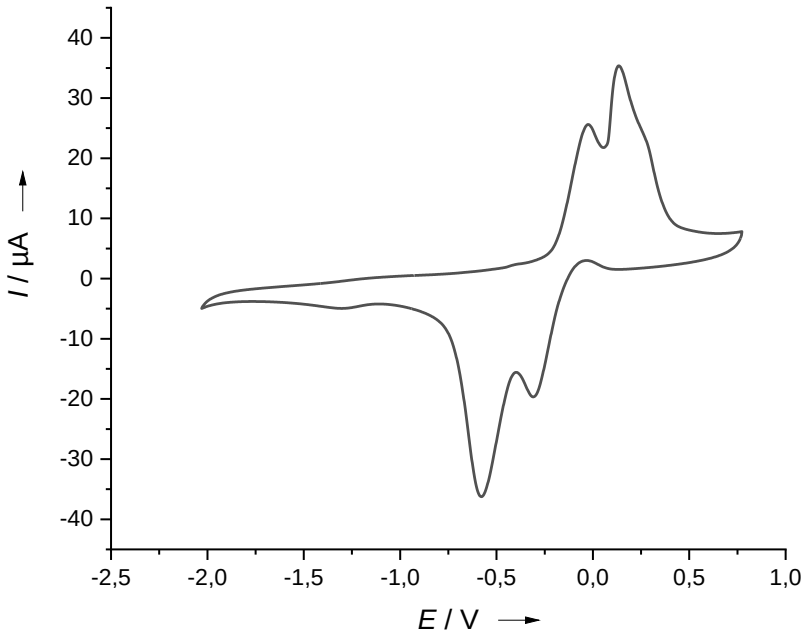


Figure S36: Cyclic voltammogram for $[(CoCl_2)_2(L1)]$ in CH_2Cl_2 (Ag/AgCl reference electrode, 0.1 M $N(n\text{Bu})_4(PF_6)$ as supporting electrolyte, scan rate 100 mV s^{-1}). Potentials given vs. the Fc^+/Fc redox couple.

3.4 EPR spectra

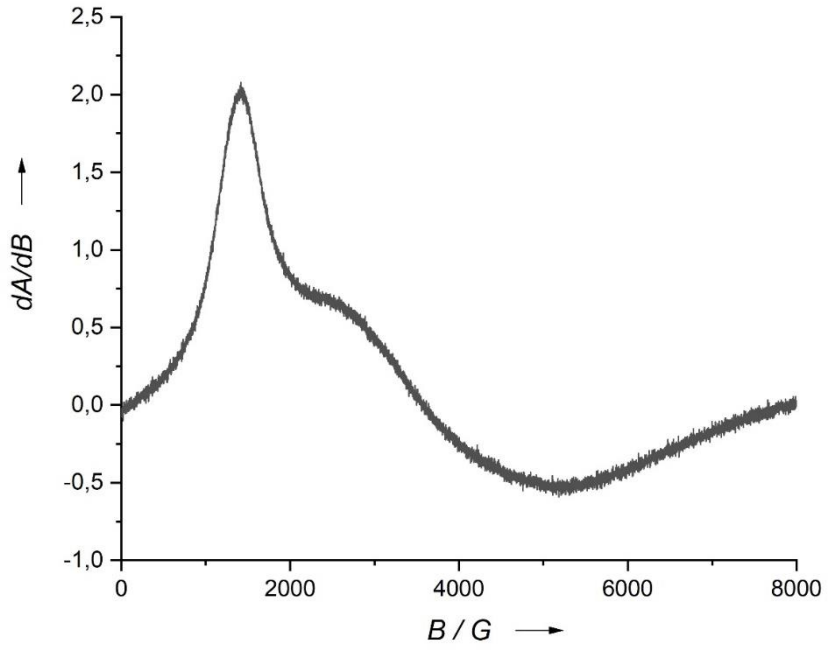


Figure S37: EPR spectrum (CH_2Cl_2) of [$(CoCl_2)_2$(L3)] at 6.8 K with $g_\perp$= 4.85 and $g_\parallel$ = 1.31.

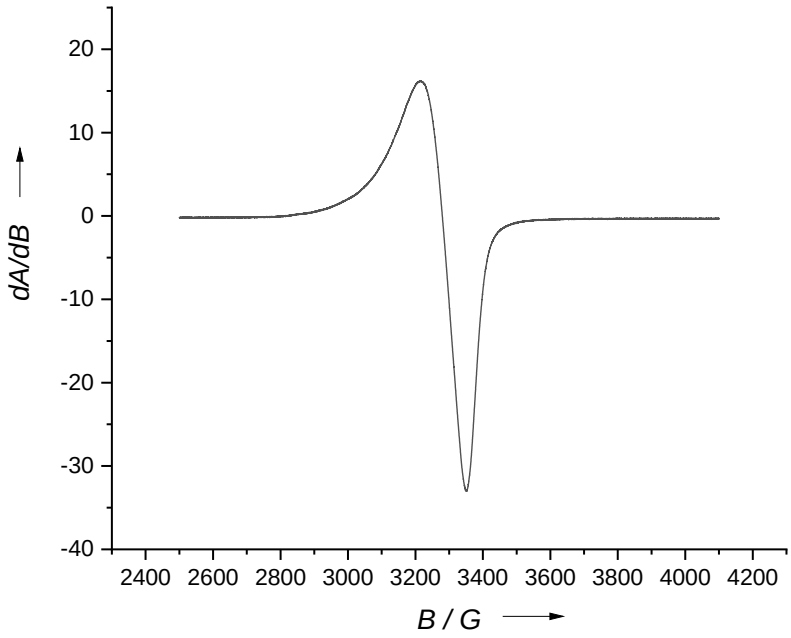


Figure S38: EPR spectrum (CH_2Cl_2) of [$(CuCl_2)_2$(L3)] at 5.0 K with g = 2.07.

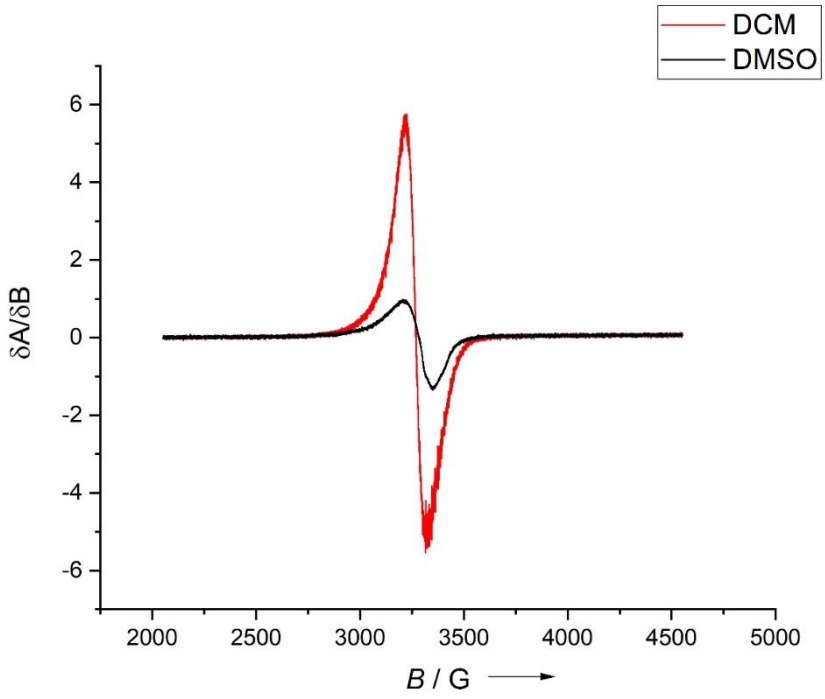


Figure S39: EPR spectrum (CH_2Cl_2) of [$(CuBr_2)_2$(L4)] at 6.0 K with g = 2.08.

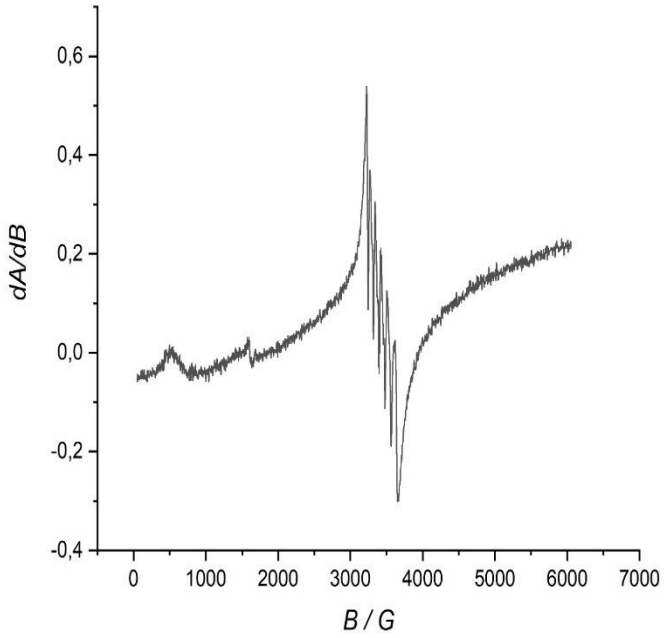


Figure S40: EPR spectrum (CH_2Cl_2) of [$(FeCl_2)_2$(L1)] at 6.8 K.

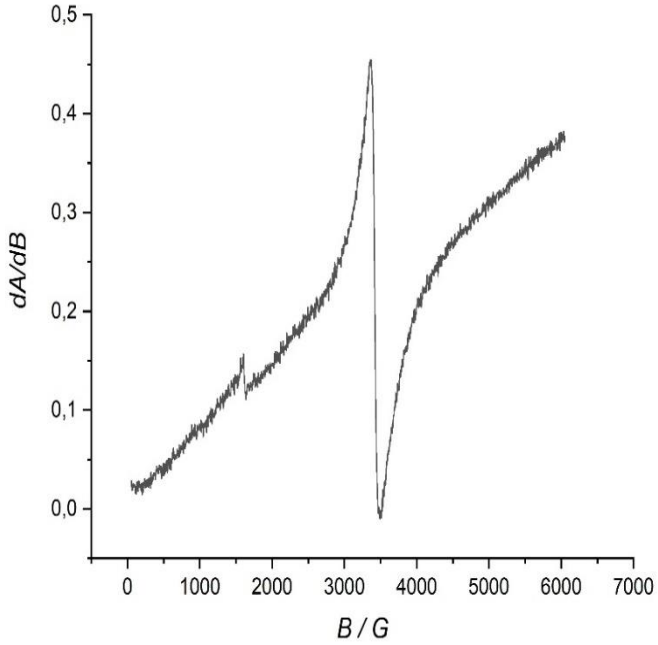


Figure S41: EPR spectrum of the solid state of $[(FeCl_2)_2(L1)]$ at room temperature with g = 2.01.

3.5 SQUID-spectra

a) **b)**

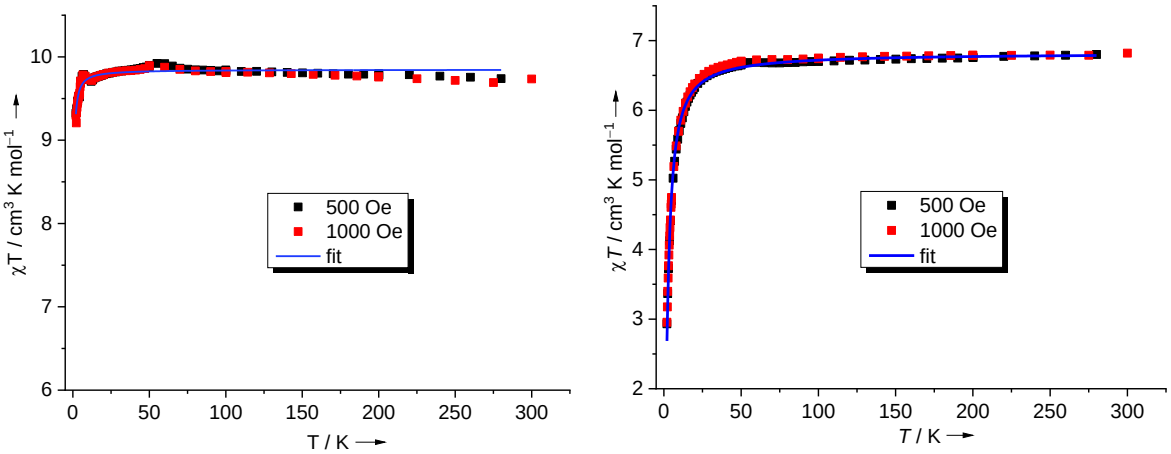


Figure S42. Magnetometric (SQUID) data recorded at a field of 500 and 1000 Oe for a) $[(MnCl_2)_2(L1)]_n$ (fit with g = 2.12 and J = -0.03 cm^{-1}) and b) $[(FeCl_2)_2(L1)]$ (fit with g = 2.13 and J = -0.76 cm^{-1}).

4. Crystallographic data

4.1 Details of the structural characterizations.

Suitable crystals for single-crystal structure determination were taken directly from the mother liquor, immersed in perfluorinated polyether oil and fixed on a cryo loop. Full shells of intensity data for all compounds were collected at low temperature with a Nonius Kappa CCD diffractometer an Bruker D8 Venture, dual source (Mo- or Cu-Kα radiation, microfocus X-ray tube, Photon III detector. Data were processed with the standard Nonius and Bruker (SAINT, APEX3) software package.[S3] Multiscan absorption correction was applied using the SADABS program.[S4] The structures were solved by intrinsic phasing [S5] and refined using the SHELXTL software package (Version 2014/6 and 2018/3).[S6] Graphical handling of the structural data during solution and refinement were performed with OLEX2.[S7] All non-hydrogen atoms were given anisotropic 28 displacement parameters. Hydrogen atoms bound to carbon were input at calculated positions and refined with a riding model. Hydrogen atoms bound to nitrogen were located in difference Fourier syntheses and refined, either fully or with appropriate distance and/or symmetry. CCDC No. 2045934-2045940 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/data_request/cif.

Figure S43: Illustration of the structure of L4 in the solid state. Color code: N pale blue, O red, C dark grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

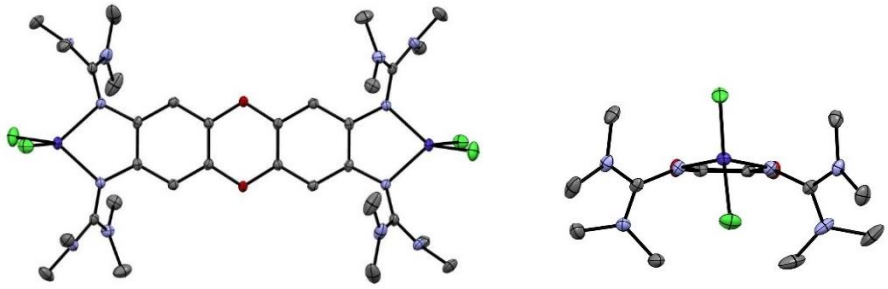


Figure S44: Illustration of the structure of [$(CoCl_2)_2$(L3)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

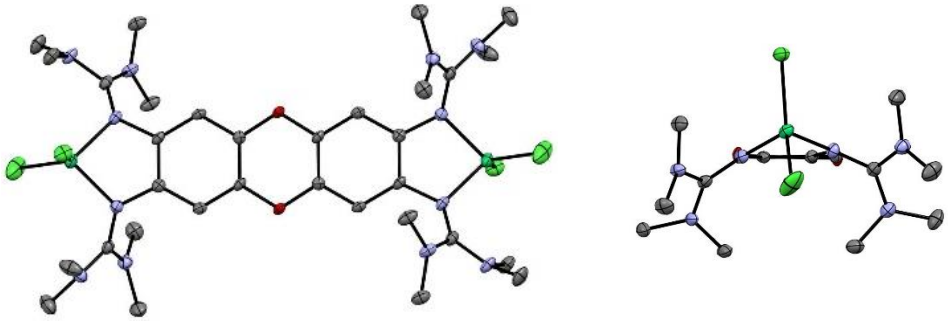


Figure S45: Illustration of the structure of [$(NiCl_2)_2$(L3)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

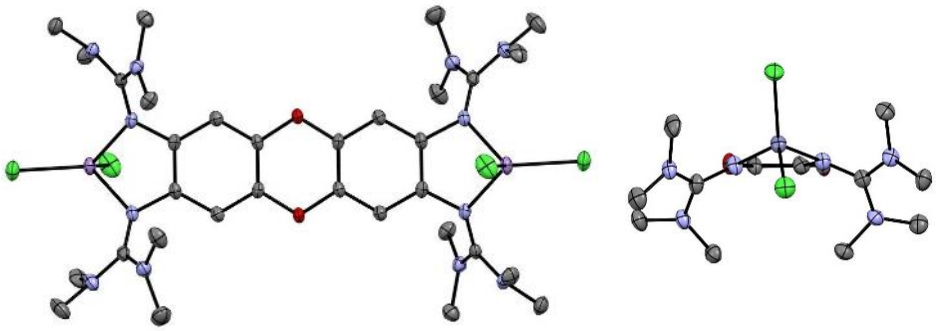


Figure S46: Illustration of the structure of [$(ZnCl_2)_2$(L3)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

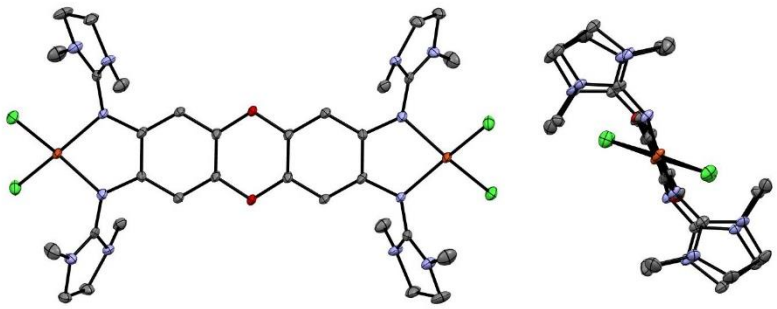


Figure S47: Illustration of the structure of [$(CuCl_2)_2$(L4)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

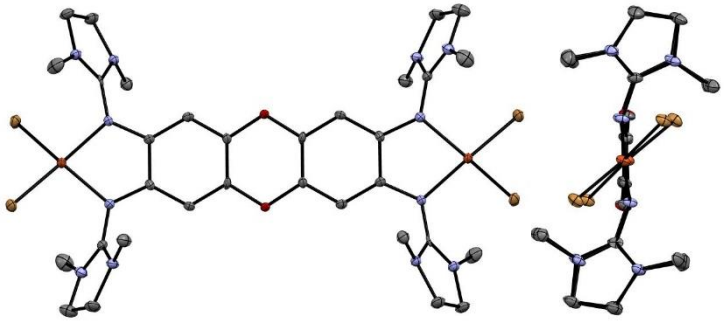


Figure S48: Illustration of the structure of [$(CuBr_2)_2$(L4)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

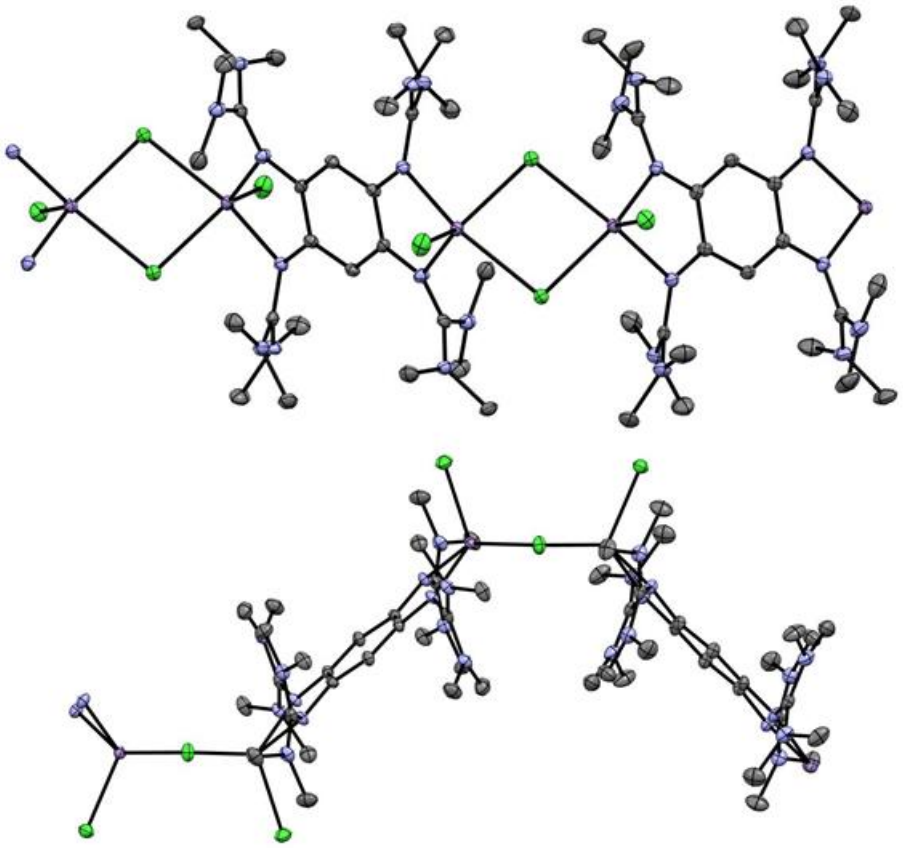


Figure S49: Illustration of the structure of [$(MnCl_2)_2$(L1)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

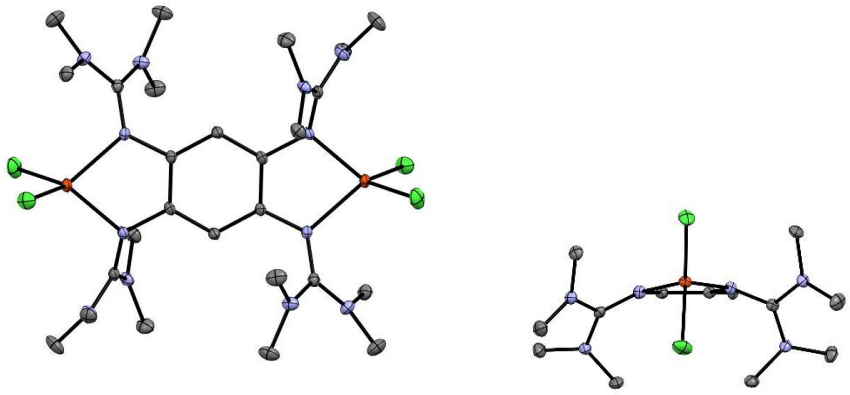


Figure 50 Illustration of the structure of [$(FeCl_2)_2$(L1)] in the solid state. Color code: N pale blue, O red, C dark grey, H pale grey. Displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms bound to carbon omitted.

Table S1: Comparison of structure parameters (bond lengths in Å, angles in °) for the different copper complexes with ligand L4.

L4		[$(CuBr_2)_2$(L4)]		[$(CuCl_2)_2$(L4)]	
N1-C1	1.396(2)	N1-C1	1.395(5)	N1-C1	1.408(5)
C2-N4	1.402(2)	C2-N4	1.404(5)	C2-N4	1.401(5)
C1-C2	1.421(2)	C1-C2	1.423(6)	C1-C2	1.417(6)
C1-C6	1.403(2)	C1-C6	1.392(6)	C1-C6	1.394(5)
C6-C5	1.376(3)	C6-C5	1.381(5)	C6-C5	1.388(5)
C4-C5	1.388(2)	C4-C5	1.391(6)	C4-C5	1.389(6)
C5-O1	1.393(2)	C5-O1	1.390(4)	C5-O1	1.394(4)
C4-O1	1.386(2)	C4-C3	1.383(6)	C4-C3	1.392(5)
C4-C3	1.377(2)	C3-C2	1.391(5)	C3-C2	1.392(5)
C3-C2	1.396(3)	N1-C7	1.349(5)	N1-C7	1.348(5)
N1-C7	1.283(3)	C7-N2	1.340(5)	C7-N2	1.325(5)
C7-N2	1.387(3)	C7-N3	1.330(6)	C7-N3	1.348(4)
C7-N3	1.378(3)	N4-C12	1.345(5)	N4-C12	1.347(5)
N4-C12	1.291(2)	C12-N6	1.331(6)	C12-N6	1.336(6)
C12-N6	1.375(3)	C12-N5	1.348(4)	C12-N5	1.338(5)
C12-N5	1.384(2)	Cu-Br1	2.3797(5)	Cu-Cl1	2.249(1)
		Cu-Br2	2.3799(6)	Cu-Cl2	2.238(1)
		Cu-N1	1.967(4)	Cu-N1	1.973(4)
		Cu-N4	1.974(4)	Cu-N4	1.970(3)
		N1-Cu-N4	82.9(1)	N1-Cu-N4	83.0(1)
		Br1-Cu-Br2	101.83(2)	Cl1-Cu-Cl2	102.46(4)
		dihedral	53.12	dihedral	52.07

Table S2: Comparison of the structure parameters (bond lengths in Å, angles in °) for the different chlorido complexes $[(MCl_2)_2(L3)]$. The atom numbering follows the numbers in the Lewis structure below.

	MnCl2	$FeCl_2$	$CoCl_2$	$NiCl_2$	$CuCl_2$	$ZnCl_2$
N1-C1	1.415(2)	1.411(2)	1.414(2)	1.415(2)	1.408(2)	1.404(7)
C2-N4	1.418(2)	1.411(2)	1.412(2)	1.409(3)	1.408(2)	1.411(1)
C1-C2	1.410(3)	1.410(2)	1.407(2)	1.411(3)	1.411(3)	1.423(1)
C1-C6	1.399(2)	1.399(2)	1.396(2)	1.397(3)	1.394(3)	1.400(1)
C6-C5	1.378(3)	1.385(2)	1.382(2)	1.386(3)	1.383(2)	1.384(8)
C4-C5	1.388(3)	1.383(2)	1.389(2)	1.388(3)	1.389(6)	1.386(1)
C5-O1	1.390(2)	1.392(2)	1.389(2)	1.390(2)	1.386(3)	1.401(1)
C4-C3	1.379(2)	1.385(2)	1.383(2)	1.383(3)	1.385(3)	1.396(1)
C3-C2	1.395(2)	1.399(2)	1.397(2)	1.396(3)	1.393(2)	1.393(9)
N1-C7	1.327(2)	1.331(2)	1.335(2)	1.325(3)	1.346(3)	1.339(1)
C7-N2	1.362(3)	1.361(2)	1.350(2)	1.360(2)	1.349(3)	1.350(9)
C7-N3	1.353(2)	1.344(3)	1.351(2)	1.357(3)	1.338(3)	1.370(1)
N4-C12	1.316(3)	1.332(3)	1.337(2)	1.330(3)	1.342(3)	1.330(1)
C12-N6	1.354(2)	1.434(4)	1.346(2)	1.353(3)	1.349(3)	1.374(1)
C12-N5	1.369(3)	1.354(2)	1.355(2)	1.350(3)	1.341(3)	1.343(1)
M-Cl1	2.147(1)	2.2527	2.2496(5)	2.2419(6)	2.242(2)	2.228(3)
M-Cl2	2.3294(6)	2.2552	2.2607(7)	2.2352(7)	2.230(1)	2.249(3)
M-N1	2.147(1)	2.066(1)	2.024(1)	1.9985(18)	1.977(4)	2.060(6)
M-N4	2.140(2)	2.070(1)	2.016(1)	1.9938(17)	1.973(1)	2.007(6)
N1-M-N4	78.05(6)	80.31(7)	82.9(5)	83.29(7)	84.42(1)	82.0(3)
Cl1-M-Cl2	119.67(2)	121.99(4)	110.19(2)	126.92(3)	105.13(4)	117.4(1)
Diederwinkel	89.46	90	85,03	88.97	41.78	89.03

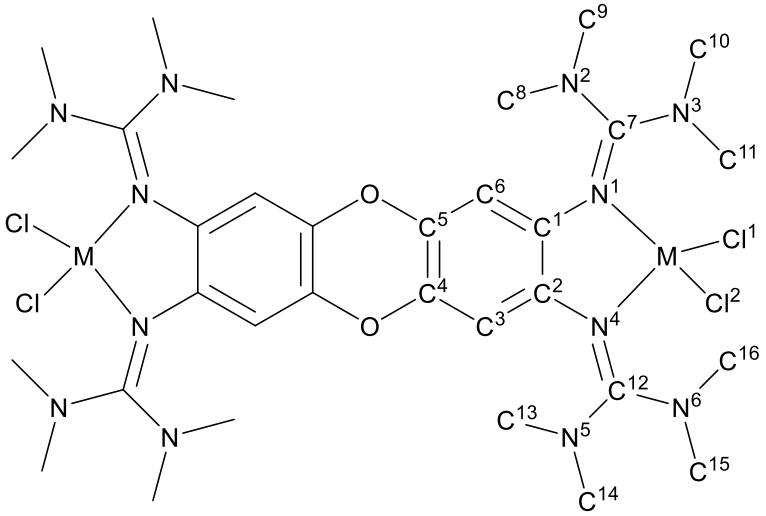
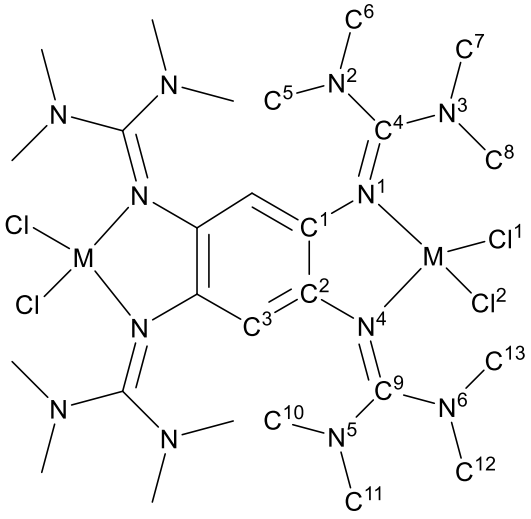
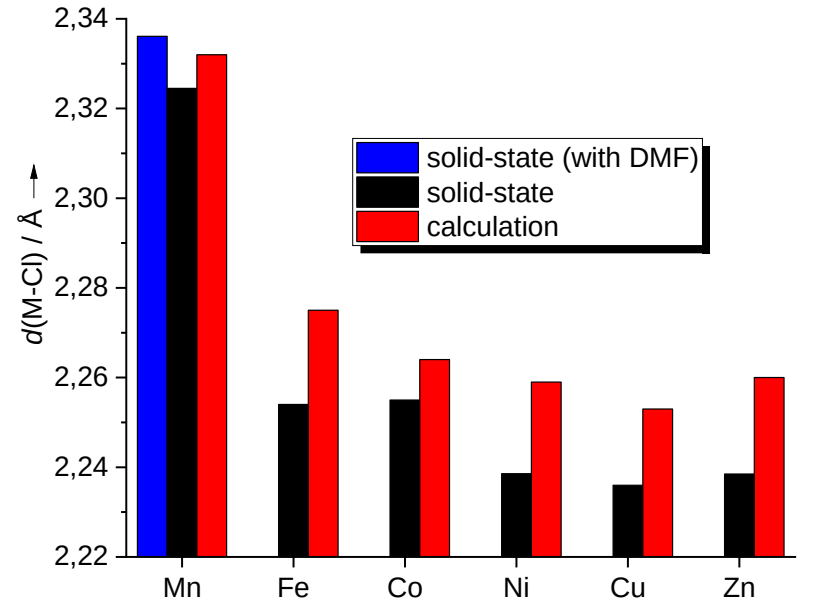


Table S3: Comparison of the structure parameters (bond lengths in Å, angles in °) for the different chlorido complexes $[(MCl_2)_2(L1)]$. The atom numbering follows the numbers in the Lewis structure below.

parameters	$[(MnCl_2)_2(L1)]_n$	$[(FeCl_2)_2(L1)]$	$[(CoCl_2)_2(L1)]$
C1-C2	1.401(4)	1.408(1)	1.408(6)
C2-C3	1.395(3)	1.397(1)	1.395(6)
C3-C1	1.396(4)	1.398(1)	1.415(7)
C1-N1	1.420(3)	1.416(1)	1.419(5)
C2-N4	1.417(3)	1.418(1)	1.420(6)
N1-C4	1.337(4)	1.338(1)	1.345(6)
C4-N2	1.364(4)	1.356(1)	1.353(6)
C4-N3	1.341(3)	1.354(1)	1.340(6)
N4-C9	1.336(3)	1.331(1)	1.333(6)
C9-N6	1.363(3)	1.368(1)	1.358(6)
C9-N5	1.349(3)	1.351(1)	1.357(6)
N1-M1	2.169(2)	2.0658(8)	2.008(4)
N4-M1	2.220(2)	2.0835(8)	2.036(3)
M1-Cl1	2.6134(8)	2.2688(4)	2.270(1)
M1-Cl2	2.4746(7)	2.2724(4)	2.256(7)
M1-Cl3	2.3746(9)	-	-
Cl1-M2	2.4719(6)	-	-
Cl2-M2	2.5821(8)	-	-
		-	-
N1-M-N4	76.91(8)	80.41(3)	82.8(2)
Cl1-M-Cl2	82.24(2)	113.74(1)	109.4(2)
Cl3-M-Cl1	100.73(3)	-	
Cl3-M-Cl1	108.23(3)	-	
dihedral	-	85.54	87.18



a)



b)

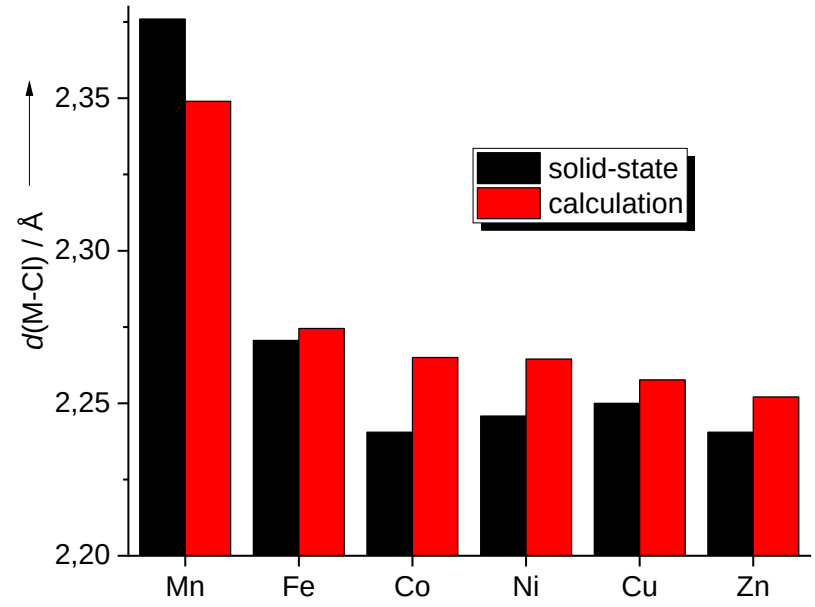


Figure S51. Comparison between average calculated (B3LYP/def2-TZVP) and experimental M-Cl bond lengths in complexes a) $[(MCl_2)_2(L3)]$ and b) $[(MCl_2)_2(L1)]$. Two different crystal structures were obtained for the complex $[(MnCl_2)_2(L3)]$, one containing solvent (DMF/Et_2O) molecules (blue) and one without (black). In the case of the complex $[(MnCl_2)_2(L1)]_n$, only the terminal Mn-Cl bond was considered. Please note that the solid-state value for $[(MnCl_2)_2(L1)]_n$ is of limited significance due to its special polymeric structure.

5 DFT calculations

DFT calculations were carried out with the TURBOMOLE program package.[S8] The B3LYP functional [S9] in combination with the def2-TZVP basis set [S10] was used in all calculations. Structural optimizations were performed at the RI-DFT [S11] level of theory with multipole accelerated RI-approximation (MARI-J) [S12] . The solvent effect was simulated with the conductor-like screening model (COSMO). For all structures calculated at $\varepsilon_r = 1$ (without COSMO), a vibrational analysis was carried out to confirm that the optimized structures are energy minima on the potential energy hypersurface. The deviation between the experimentally derived and calculated structures are analysed with the program aRMSD.[S12]

5.1 Calculated electronic transitions for L4

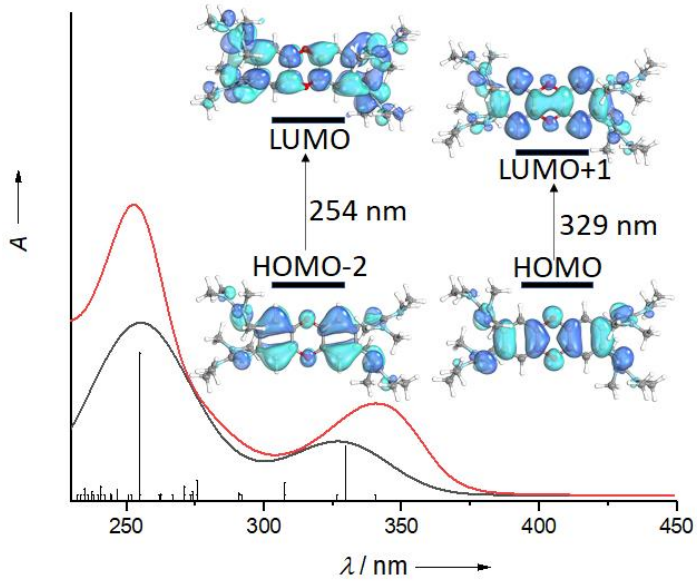


Figure S52: Comparison between the exerimental (red curve) UV-vis spectrum and the simulated spectrum (black curve) on the basis of TD-DFT calculations for L4.

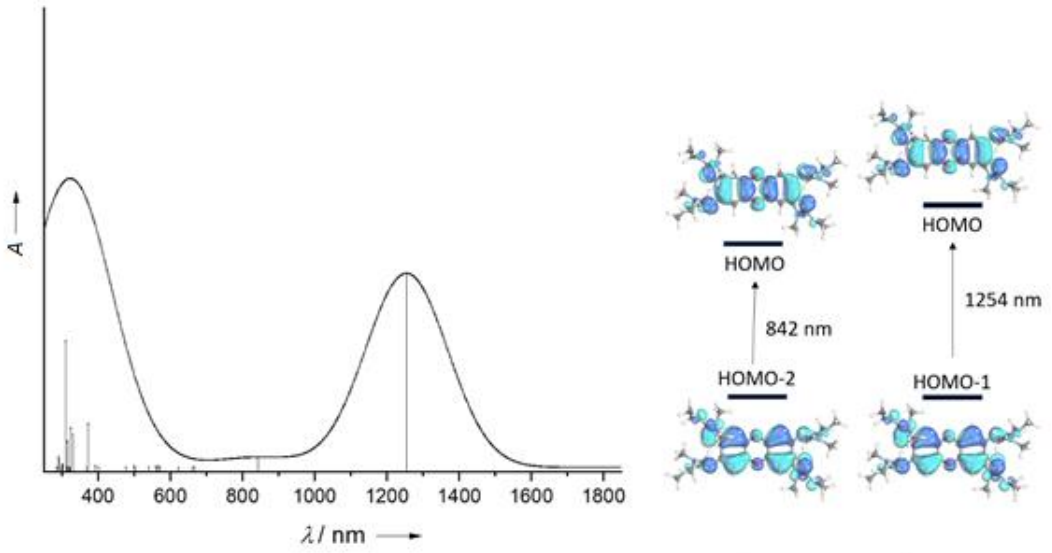


Figure S53: Simulated UV-vis spectrum on the basis of TD-DFT calculations for $L4^{+}$.

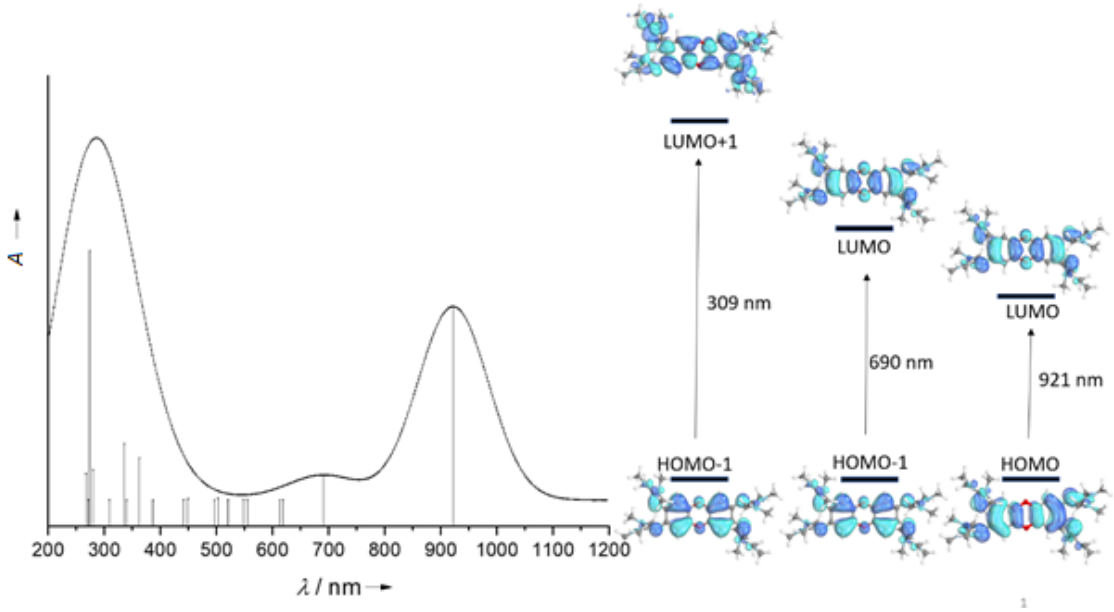


Figure S54: Simulated UV-vis spectrum on the basis of TD-DFT calculations for $L4^{2+}$.

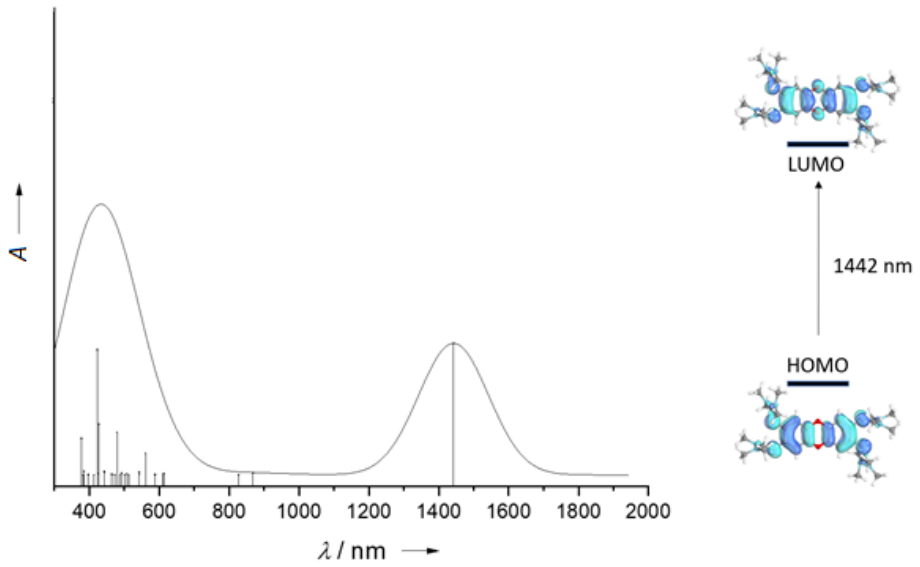


Figure S55: Simulated UV-vis spectrum on the basis of TD-DFT calculations for $L4^{3+}$.

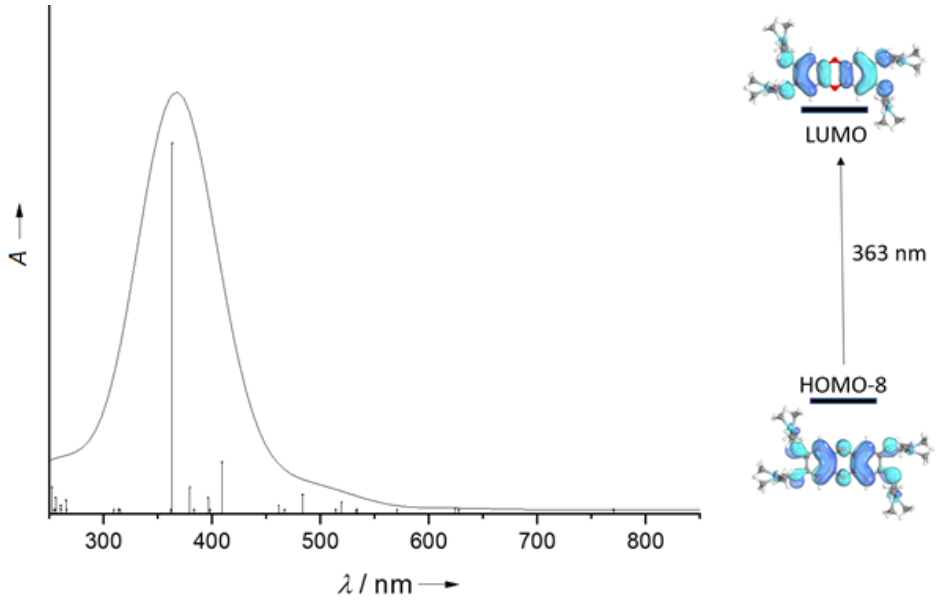


Figure S56: Simulated UV-vis spectrum on the basis of TD-DFT calculations for $L4^{4+}$.

5.2 aRMSD-Plots

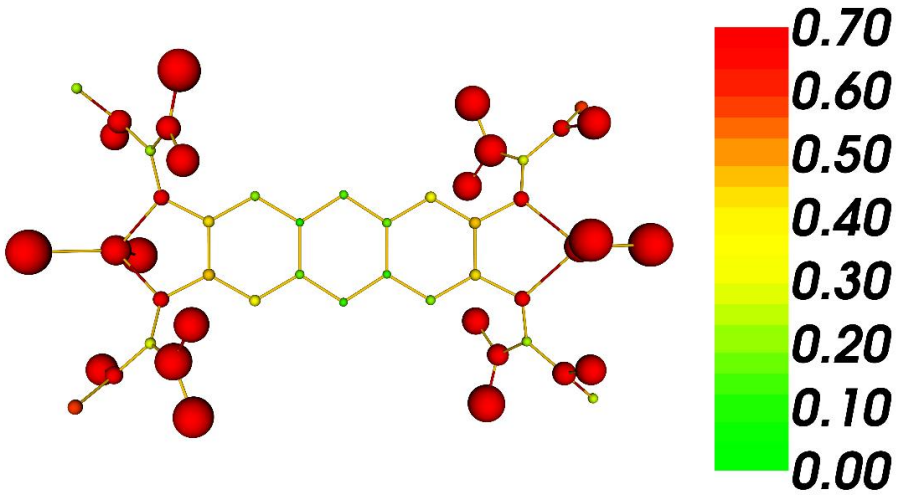


Figure S57: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(MnCl_2)_2$(L1)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

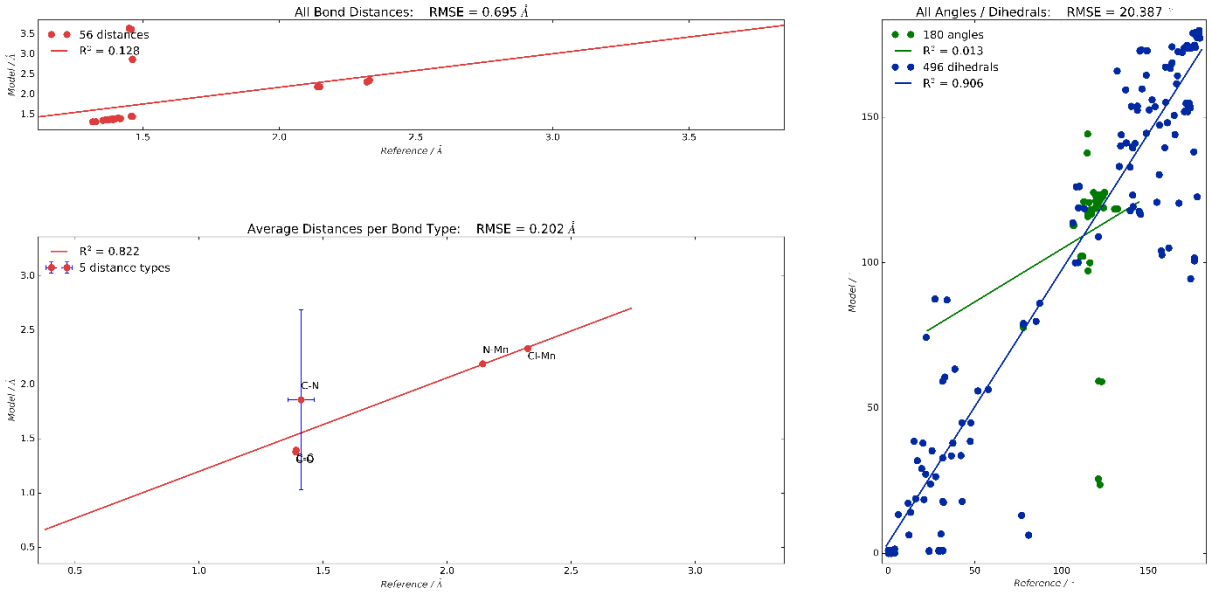


Figure S58: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(MnCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

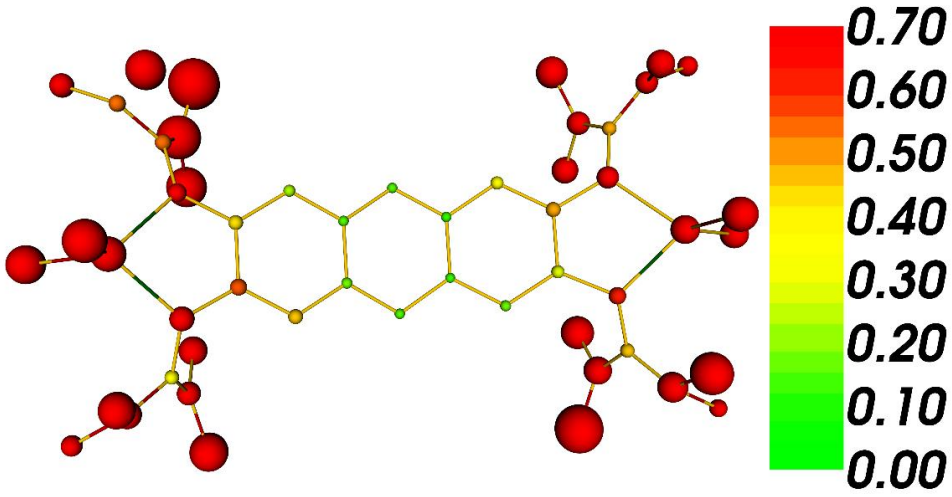


Figure S59: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(FeCl_2)_2$(L3)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

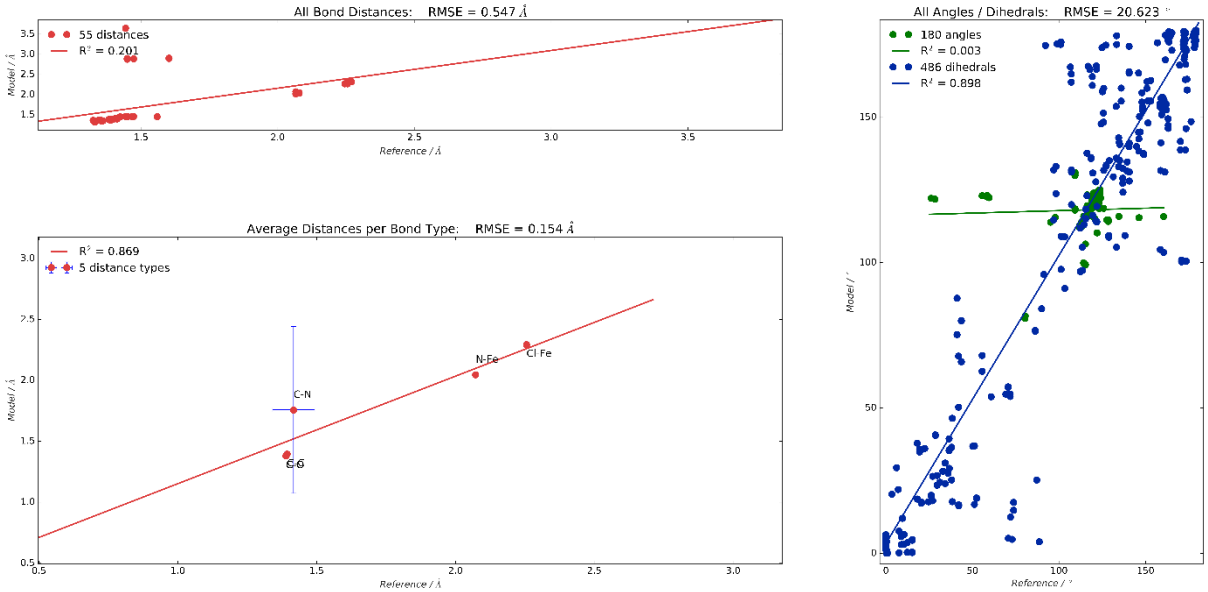


Figure S60: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(FeCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

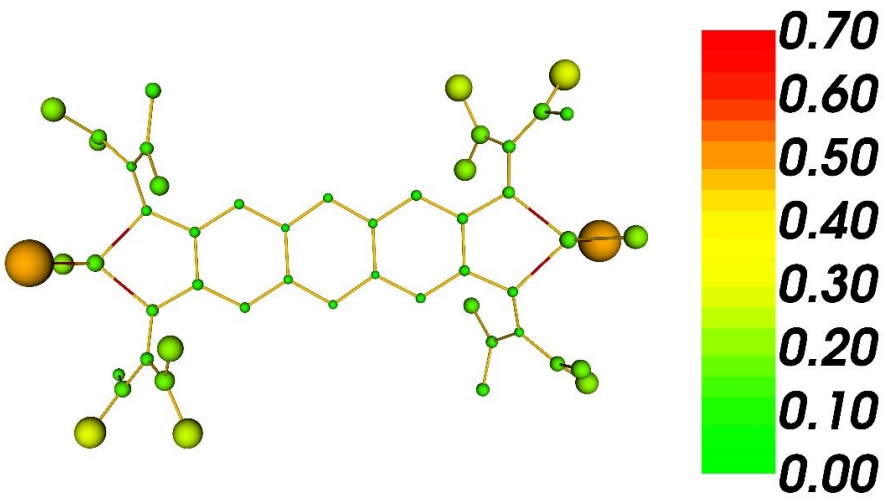


Figure S61: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(CoCl_2)_2$(L3)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

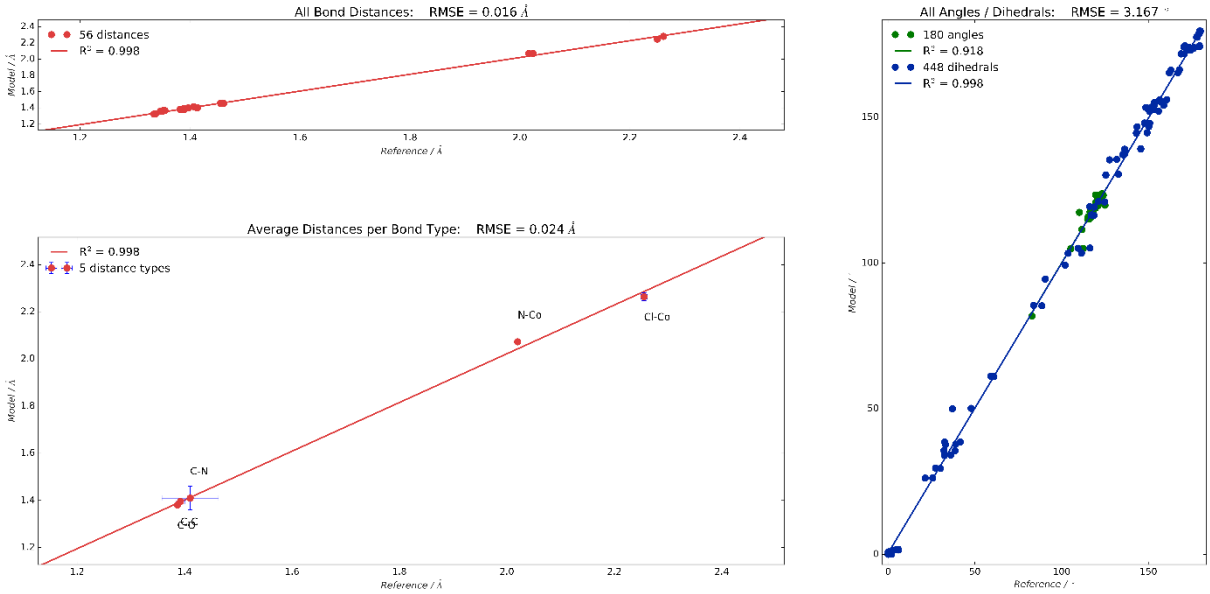


Figure S62: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(CoCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

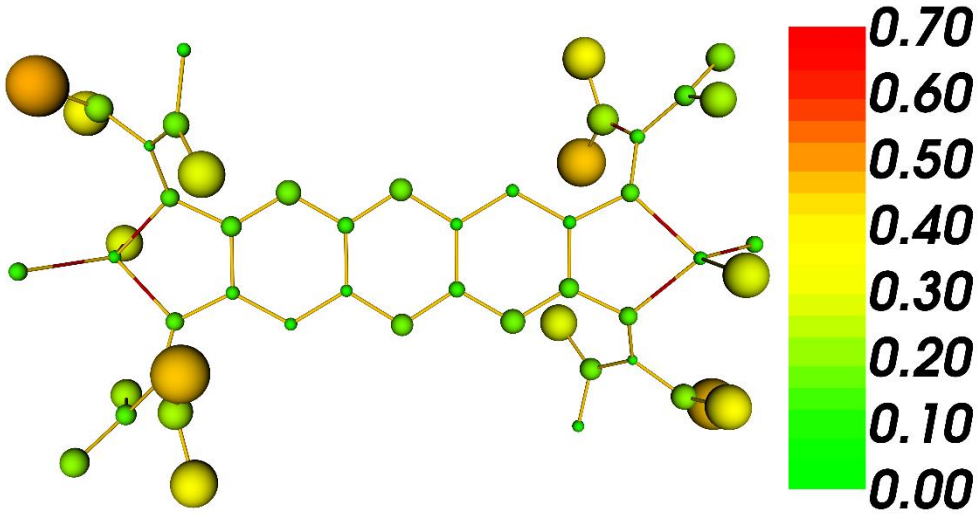


Figure S63: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(MnCl_2)_2$(L1)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

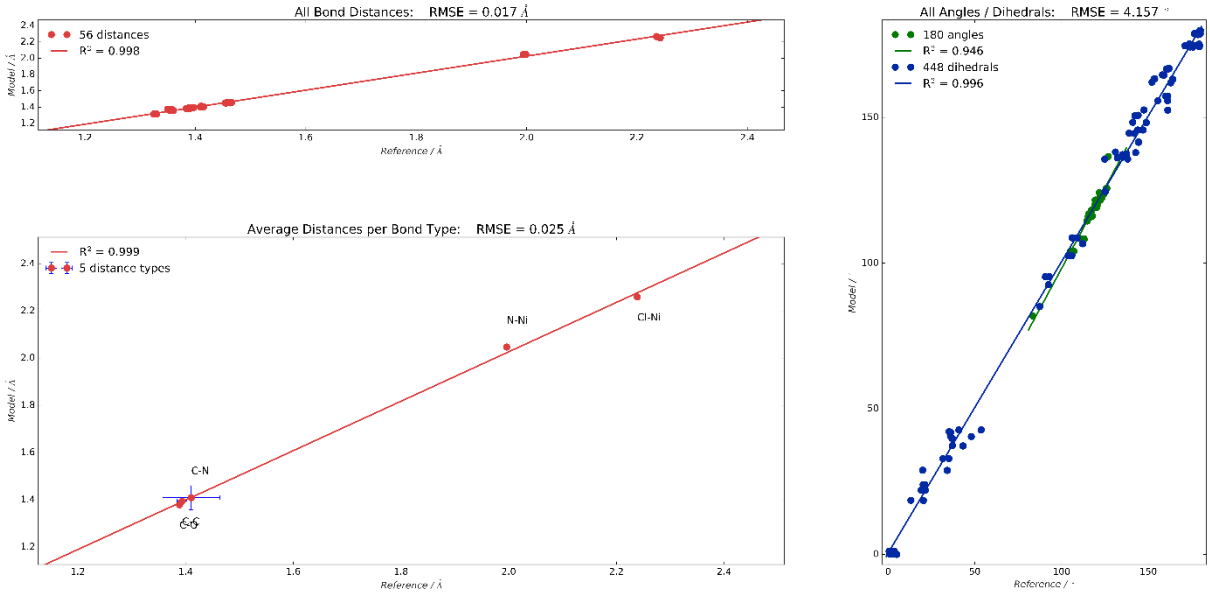


Figure S64: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(NiCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

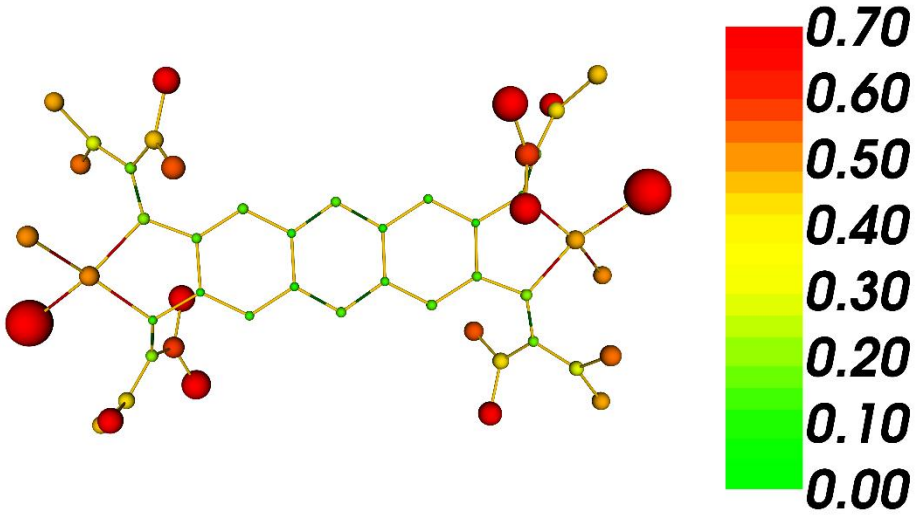


Figure S65: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(MnCl_2)_2$(L1)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

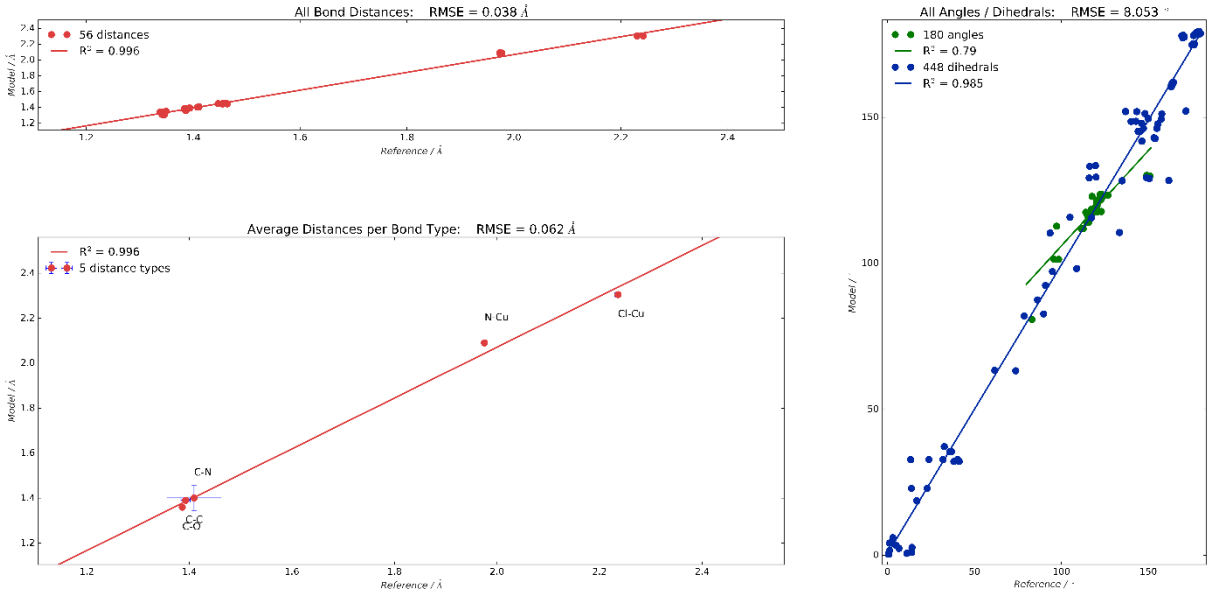


Figure S66: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(CuCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

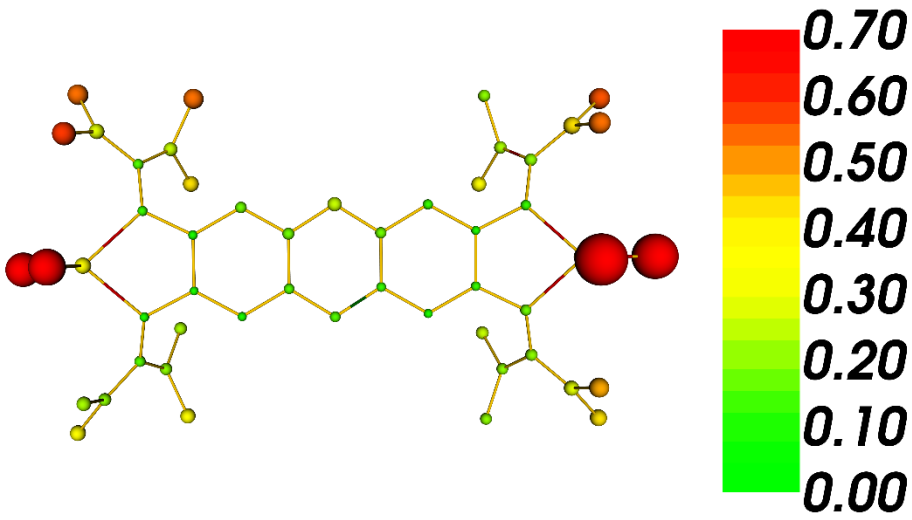


Figure S67: Superposition with Root-Mean-Square-Deviation (RMSD) for the experimentally determined and calculated structures of [$(MnCl_2)_2$(L1)]. The sphere dimensions reflect the relative RMSD distribution and the color code the absolute deviation (small for green color and large for red color).

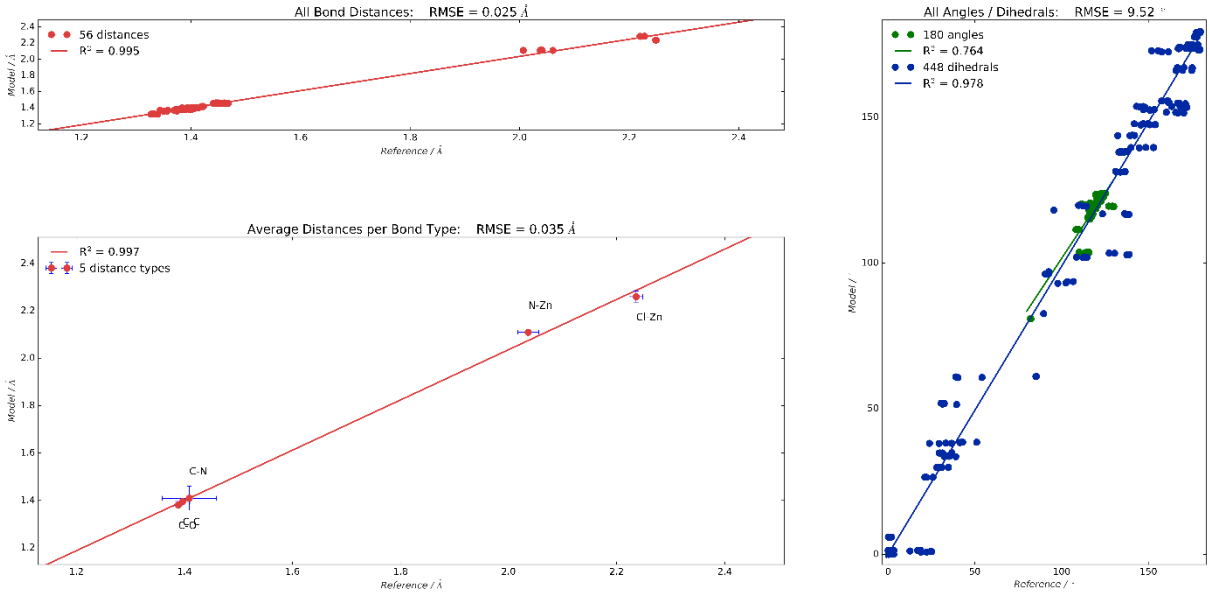


Figure S68: Detailed analysis of the Root-Mean-Square-Error (RMSE) for bonds and angles for the experimentally determined structure of [$(ZnCl_2)_2$(L3)] (Model) and the calculated structure (Reference).

5.3 Cartesian coordinates (in Å) for all complexes, calculated with B3LYP/def2-TZVP

[$(MnCl_2)_2$(L3)]
104
Energy = -6200.542850 hartree

Mn	9.507429	0.409030	9.163090
Cl	10.137379	0.738818	11.404840
Cl	10.304428	-1.337216	7.875210
O	6.398899	5.887607	6.922525
N	9.469925	2.458360	8.388335
N	11.717885	2.806310	7.980164
N	10.579052	4.362191	9.279710
N	3.245375	9.240384	5.456021
N	4.700087	9.247161	3.576249
N	4.112423	11.224717	4.648878
C	8.170264	2.982351	8.297953
C	3.527896	7.956792	5.950224
C	4.833398	7.498169	6.160369
H	5.680610	8.112669	5.886606
C	5.084900	6.271192	6.746928
C	6.594366	4.661502	7.525130
C	7.892093	4.214588	7.695420
H	8.695658	4.837459	7.325857
C	10.545253	3.210667	8.541483
C	12.996687	2.941881	8.666174
H	12.848973	3.350916	9.661357
H	13.687509	3.582578	8.109628
H	13.453247	1.954317	8.769780
C	11.734660	1.944939	6.801769
H	11.889624	0.895152	7.062521
H	12.545248	2.270943	6.144485
H	10.788734	2.025993	6.274276
C	9.703607	4.551238	10.425858
H	8.825194	5.155879	10.179243
H	10.267322	5.058809	11.212196
H	9.389416	3.583268	10.807327
C	11.373769	5.517369	8.896375
H	12.139599	5.750465	9.642798
H	10.722094	6.391936	8.797350
H	11.858615	5.340950	7.939845
C	4.017218	9.868078	4.586190
C	6.018717	9.676677	3.140464
H	6.375963	10.490852	3.765541
H	6.014747	10.007978	2.097327
H	6.721440	8.841127	3.226292
C	4.203552	8.021725	2.969981
H	4.696941	7.132005	3.373721
H	4.390589	8.066981	1.894501
H	3.129855	7.949415	3.122491
C	3.892185	11.941279	5.901577
H	2.880692	12.349125	5.968783
H	4.611427	12.762416	5.963266
H	4.041570	11.267987	6.740568
C	4.137073	12.059408	3.454314
H	5.065966	12.633320	3.381748

H	3.301688	12.762993	3.492823
H	4.021640	11.447417	2.564532
O	4.218112	4.253684	7.772879
N	1.145510	7.666002	6.271709
N	-1.103493	7.315160	6.671179
N	0.045172	5.753785	5.386966
N	7.370022	0.884851	9.205333
N	5.925959	0.872812	11.093072
N	6.500409	-1.100933	10.006305
C	2.446087	7.145905	6.371201
C	7.088439	2.171805	8.719397
C	5.783120	2.634527	8.517477
H	4.935709	2.020372	8.791407
C	5.531940	3.865563	7.939321
C	4.022502	5.475206	7.161091
C	2.724514	5.917814	6.982028
H	1.920769	5.295088	7.351449
C	0.072758	6.909999	6.118019
C	-2.378673	7.172316	5.979926
H	-2.225179	6.757732	4.987912
H	-3.070607	6.533226	6.536943
H	-2.837164	8.158106	5.868283
C	-1.127856	8.183872	7.844064
H	-1.283762	9.231645	7.575918
H	-1.940904	7.860153	8.499437
H	-0.184293	8.108156	8.376579
C	0.926688	5.559262	4.246360
H	1.805105	4.958082	4.501252
H	0.367918	5.045448	3.460551
H	1.240708	6.525398	3.860118
C	-0.748877	4.599281	5.773759
H	-1.510652	4.359846	5.025201
H	-0.095758	3.726809	5.881287
H	-1.238596	4.780579	6.726885
C	6.600836	0.254945	10.075853
C	4.607874	0.446338	11.533465
H	4.243991	-0.362931	10.905848
H	4.615957	0.109293	12.574737
H	3.908146	1.285206	11.455890
C	6.430770	2.092871	11.703279
H	5.938979	2.986826	11.307002
H	6.249286	2.042580	12.779488
H	7.503908	2.161579	11.545293
C	6.710922	-1.811445	8.748506
H	7.720250	-2.223289	8.673690
H	5.987810	-2.629119	8.686027
H	6.560124	-1.132864	7.914053
C	6.478790	-1.942091	11.196372
H	5.547913	-2.512532	11.270878
H	7.310997	-2.648915	11.149399
H	6.601634	-1.335512	12.088860
Mn	1.105839	9.708334	5.479205
Cl	0.494510	9.358044	3.235143
Cl	0.292958	11.461366	6.747915

[$(FeCl_2)_2$(L3)]

104

Energy = -6425.933800 hartree

Fe	12.823945	2.996991	1.887443
Fe	4.925810	2.956821	12.117713
Cl	11.984527	2.998857	-0.210378
Cl	15.071544	3.001677	2.325163
Cl	2.682563	2.950890	11.848324
Cl	5.927942	2.956321	14.176630
O	9.343797	4.403444	7.369978
N	12.013244	4.344723	3.333692
N	13.180792	6.035363	4.526667
N	12.452289	6.394651	2.350366
N	6.109619	4.314733	10.969312
N	7.548941	6.010308	11.804715
C	11.402701	3.695414	4.417216
C	10.690977	4.366963	5.416809
H	10.632461	5.447242	5.420519
C	10.017621	3.676359	6.409186
C	8.586184	3.669156	8.260327
C	7.792611	4.352387	9.165137
H	7.777477	5.432906	9.112932
C	7.006954	3.673301	10.102387
C	12.526421	5.560873	3.421569
C	13.081542	7.417592	4.964892
H	14.051792	7.923759	4.939745
H	12.712024	7.447818	5.995453
H	12.384852	7.963825	4.334607
C	13.897274	5.142062	5.422494
H	13.310798	4.893336	6.312817
H	14.820465	5.633919	5.738343
H	14.163591	4.231562	4.892568
C	6.317263	5.530251	11.448554
C	8.601693	5.121253	12.268674
H	8.161371	4.206675	12.656380
H	9.137073	5.613157	13.084441
H	9.316846	4.880030	11.475725
C	7.939879	7.395836	11.604417
H	8.843542	7.434147	10.986694
H	8.157720	7.898746	12.551931
H	7.150961	7.939937	11.092058
H	13.277963	8.310871	1.973634
C	4.027042	6.210585	10.879344
H	4.233059	5.673260	9.958452
H	3.646369	7.207591	10.640852
H	3.264200	5.657547	11.431113
C	5.149235	7.210046	12.826938
H	4.241747	6.947219	13.376587

H	5.999143	7.054731	13.485059
C	11.396496	6.251753	1.353425
H	11.740035	5.705652	0.472436
H	11.066736	7.249726	1.051769
H	10.558850	5.708808	1.780991
C	13.560776	7.253941	1.955442
H	14.411673	7.098048	2.612037
H	13.865901	6.998027	0.937504
H	5.090982	8.268076	12.553855
N	5.257020	6.356947	11.650623
O	9.351809	1.551711	7.365070
N	12.020488	1.639466	3.328783
N	13.197145	-0.049213	4.515472
N	12.470515	-0.404404	2.337837
N	6.117501	1.609872	10.964944
N	7.566634	-0.080381	11.794220
C	11.406537	2.281495	4.414673
C	10.698636	1.602499	5.411957
H	10.646144	0.521899	5.411900
C	10.021521	2.285877	6.406775
C	8.590123	2.278665	8.257959
C	7.800476	1.587878	9.160461
H	7.791506	0.507472	9.104602
C	7.011026	2.259305	10.100040
C	12.540271	0.425830	3.412118
C	13.105461	-1.433597	4.948498
H	14.078509	-1.934261	4.921741
H	12.735843	-1.469727	5.978844
H	12.411971	-1.981319	4.315997
C	13.908609	0.844643	5.414732
H	13.320597	1.086946	6.305812
H	14.834355	0.356594	5.729009
H	14.170165	1.758483	4.888203
C	6.332163	0.393851	11.439928
C	8.614361	0.813091	12.261080
H	8.168842	1.723580	12.652457
H	9.153004	0.321242	13.074721
H	9.327706	1.061539	11.468737
C	7.965482	-1.462885	11.588686
H	8.869535	-1.493657	10.971115
H	8.185861	-1.968299	12.534283
H	7.179840	-2.009449	11.073923
C	11.413923	-0.263378	1.341476
H	11.089611	-1.261950	1.035916
H	13.306829	-2.314512	1.953545
H	3.279573	0.248048	11.422636
C	5.174387	-1.297875	12.812319
H	5.124013	-2.355318	12.535423
H	4.264614	-1.043657	13.362219

H	11.754387	0.288082	0.462628
H	10.573298	0.273224	1.771206
C	13.583740	-1.255957	1.939449
H	14.433861	-1.097882	2.596530
H	13.887297	-0.994372	0.922482
C	4.045880	-0.297866	10.868569
H	4.248502	0.244623	9.949966
H	3.671489	-1.296247	10.625888
H	6.022719	-1.138774	13.471581
N	5.276712	-0.439548	11.639335

[$(CoCl_2)_2$(L1)]

104

Energy = -6664.041070 hartree

Co	1.572001	17.615202	6.922019
Cl	-0.347162	17.550622	5.754376
Cl	2.922141	19.429164	6.623249
O	4.444619	12.603289	10.012956
N	1.579662	17.274653	8.966393
N	0.144227	18.914595	9.739802
N	2.252809	18.747598	10.702072
N	2.856327	15.987664	6.946183
N	5.103681	15.867121	6.191002
N	3.328769	15.702434	4.700234
C	2.367095	16.161957	9.300361
C	3.032328	15.490459	8.246941
C	3.713011	14.301335	8.527982
H	4.200184	13.746122	7.737616
C	3.761028	13.785006	9.810657
C	3.107582	14.445237	10.846081
C	2.413620	15.613559	10.586236
H	1.884676	16.083713	11.404490
C	1.340589	18.275309	9.800020
C	-1.050103	18.240918	9.238457
H	-1.244778	18.483416	8.191904
H	-1.903491	18.552442	9.846885
H	-0.924699	17.165038	9.316812
C	0.030871	20.362550	9.862777
H	1.015017	20.810760	9.962222
H	-0.586923	20.647521	10.719738
H	-0.432293	20.760487	8.956625
C	1.875565	19.238281	12.017340
H	2.109708	20.300519	12.139146
H	2.424399	18.681764	12.784233
H	0.811311	19.092619	12.182605
C	3.682077	18.672571	10.442403
H	4.150896	17.827500	10.956164
H	4.147170	19.596696	10.793671

H	3.852863	18.594537	9.372056
C	3.752684	15.840935	5.982650
C	6.030579	15.035814	5.440806
H	5.486000	14.365128	4.781364
H	6.622498	14.432019	6.136546
H	6.722886	15.635272	4.841330
C	5.687389	16.646448	7.271581
H	5.000466	17.437174	7.560975
H	6.606068	17.111701	6.906431
H	5.929961	16.028405	8.141657
C	2.009821	15.156955	4.393009
H	1.652534	14.566601	5.231561
H	2.097345	14.518116	3.510004
H	1.279125	15.944470	4.198050
C	4.001194	16.357645	3.585299
H	4.821596	16.970360	3.947047
H	3.289123	17.011648	3.076138
H	4.381715	15.631446	2.860678
O	3.104186	13.958014	12.137308
N	5.973417	9.289531	13.184660
N	7.410028	7.650701	12.411004
N	5.300364	7.814744	11.450553
N	4.696976	10.576615	15.204975
N	2.450114	10.694976	15.961922
N	4.226114	10.862912	17.451081
C	5.184449	10.401083	12.850523
C	4.519374	11.072672	13.903992
C	3.837588	12.261100	13.622683
H	3.350714	12.816527	14.413080
C	3.788231	12.776574	12.339716
C	4.441517	12.116248	11.304257
C	5.136440	10.948546	11.564306
H	5.664745	10.477993	10.745870
C	6.212847	8.288523	12.351550
C	8.604110	8.326168	12.910534
H	8.800162	8.084786	13.957084
H	9.457212	8.015100	12.301472
H	8.477400	9.401837	12.831390
C	7.524997	6.202794	12.288928
H	6.541293	5.753321	12.190846
H	8.142229	5.917967	11.431517
H	7.989593	5.806051	13.194872
C	5.677001	7.323651	10.135262
H	5.443988	6.261066	10.014319
H	5.126839	7.879054	9.368519
H	6.740940	7.470450	9.968960
C	3.871235	7.888608	11.711337
H	3.401231	8.732968	11.197486
H	3.406708	6.963866	11.360955

H	3.701234	7.967097	12.781778
C	3.801245	10.723064	16.169132
C	1.522741	11.525690	16.712192
H	2.066990	12.197739	17.370519
H	0.929378	12.128022	16.016418
H	0.831790	10.925847	17.312846
C	1.866542	9.914055	14.882412
H	2.554201	9.123922	14.593142
H	0.948689	9.448013	15.248625
H	1.622593	10.531091	14.012007
C	5.544821	11.409869	17.756708
H	5.900684	12.000133	16.917488
H	5.457531	12.049091	18.639458
H	6.276496	10.623185	17.951355
C	3.555568	10.207458	18.567004
H	2.735545	9.593581	18.206372
H	4.268915	9.554559	19.075796
H	3.174890	10.933566	19.291632
Co	5.983066	8.950452	15.229297
Cl	7.902954	9.018344	16.395490
Cl	4.635126	7.135187	15.530435

[$(NiCl_2)_2$(L3)]

104

Energy = -6915.110730 hartree

Ni	8.491373	12.607663	3.959835
Cl	9.908550	14.079107	4.905160
Cl	6.827308	12.676742	2.421520
O	9.798987	7.977131	8.200813
N	7.762053	11.381132	5.428306
N	5.915945	12.578494	6.158756
N	5.793710	10.260807	6.133835
N	11.951032	4.550361	10.856245
N	11.754173	6.227542	12.521920
N	11.193976	4.022817	12.983274
C	8.675028	10.333360	5.632949
C	11.882515	5.379773	9.724674
C	10.881522	6.332136	9.520265
H	10.123416	6.506116	10.271902
C	10.812863	7.052399	8.340725
C	9.756646	8.654533	6.999974
C	8.772374	9.611126	6.824447
H	8.094505	9.805353	7.644633
C	6.534192	11.394492	5.900418
C	6.674662	13.792585	6.428793
H	7.679798	13.549041	6.757329
H	6.160192	14.358197	7.210583
H	6.751644	14.425618	5.540792

C	4.517533	12.803365	5.814307
H	4.458013	13.569624	5.036793
H	3.947127	13.142121	6.684101
H	4.070208	11.894207	5.424810
C	5.932534	9.074837	5.309509
H	6.406979	9.338602	4.368853
H	4.937228	8.677194	5.092481
H	6.520388	8.292041	5.799321
C	4.914829	10.127102	7.283198
H	4.984004	11.010502	7.912410
H	5.211967	9.254550	7.875142
H	3.870749	9.990089	6.983126
C	11.636866	4.933629	12.074808
C	10.778284	6.836941	13.409330
H	9.963318	6.144312	13.601814
H	10.366062	7.737598	12.941349
H	11.224631	7.129156	14.365548
C	12.801632	7.109384	12.041824
H	13.595193	6.520755	11.591034
H	13.219822	7.656106	12.891544
H	12.433989	7.834488	11.308804
C	11.646162	4.041941	14.369025
H	12.279087	4.904825	14.551329
H	12.235443	3.142551	14.566726
H	10.798187	4.064208	15.059653
C	10.570283	2.773136	12.568674
H	10.186265	2.855671	11.557095
H	9.749428	2.548974	13.255439
H	11.278505	1.940709	12.596268
O	11.694369	7.491323	6.126998
N	13.736718	4.093446	8.903016
N	15.586243	2.899534	8.175566
N	15.703407	5.217506	8.198808
N	9.545693	10.921661	3.473564
N	9.737549	9.244020	1.807762
N	10.301729	11.447600	1.345806
C	12.821912	5.139407	8.697229
C	9.613591	10.091999	4.604976
C	10.613453	9.138286	4.808619
H	11.371181	8.963885	4.056695
C	10.681482	8.417231	5.987709
C	11.737986	6.815434	7.328638
C	12.723776	5.860587	7.505177
H	13.402239	5.666817	6.685368
C	14.965123	4.082409	8.432359
C	14.830421	1.683560	7.905887
H	13.825186	1.924605	7.575796
H	15.347075	1.118204	7.125360
H	14.753744	1.051309	8.794489

C	16.984630	2.677883	8.522261
H	17.044579	1.913045	9.301147
H	17.556784	2.338793	7.653752
H	17.429737	3.588537	8.910798
C	15.561060	6.403982	9.021796
H	15.085389	6.140326	9.961853
H	16.555273	6.803620	9.240197
H	14.972665	7.185253	8.530210
C	16.583424	5.352068	7.050409
H	16.517020	4.467914	6.421967
H	16.285078	6.223392	6.457263
H	17.626815	5.491712	7.351668
C	9.857914	10.537686	2.254702
C	10.711337	8.632558	0.919462
H	11.527540	9.323491	0.726130
H	11.122156	7.731102	1.387131
H	10.263462	8.341188	-0.036299
C	8.688788	8.364332	2.288984
H	7.896868	8.954611	2.740495
H	8.268651	7.818397	1.439720
H	9.055715	7.638550	3.021685
C	9.848537	11.429110	-0.039615
H	9.213156	10.567851	-0.221077
H	9.261508	12.329978	-0.237254
H	10.695923	11.404310	-0.730884
C	10.928344	12.696025	1.759781
H	11.312937	12.612760	2.771079
H	11.749139	12.918401	1.072360
H	10.221860	13.529934	1.732724
Ni	13.007335	2.865500	10.370211
Cl	11.592328	1.394069	9.421580
Cl	14.669393	2.796358	11.910681

[$(CuCl_2)_2$(L3)]

104

Energy = -7179.422740 hartree

O	2.199661	7.074737	7.920513
N	1.470691	5.555753	3.374315
N	-0.297872	4.457921	4.512735
N	-0.686161	5.645269	2.550552
N	4.104844	5.264918	2.996572
N	5.888224	4.482277	1.753523
N	6.017564	6.625130	2.649437
C	2.301507	5.846335	4.465833
C	3.696083	5.756133	4.244514
C	4.566812	6.058426	5.296464
H	5.635894	5.946895	5.179703
C	4.091718	6.489487	6.523270

C	2.723744	6.628071	6.723648
C	1.843589	6.308731	5.703824
H	0.786693	6.442683	5.888247
C	0.189343	5.225894	3.493402
C	0.520551	3.429431	5.135122
H	1.367154	3.197129	4.495575
H	-0.081580	2.524645	5.250187
H	0.884343	3.737034	6.120299
C	-1.610347	4.659760	5.102239
H	-2.075400	5.551028	4.689119
H	-1.504352	4.793223	6.184032
H	-2.272228	3.804912	4.931854
C	-0.341069	6.744340	1.655599
H	0.337789	7.430743	2.152608
H	-1.259360	7.271858	1.388643
H	0.134339	6.378615	0.741351
C	-1.778391	4.803151	2.071294
H	-1.782054	3.853031	2.594241
H	-1.618971	4.593305	1.012083
H	-2.743840	5.300638	2.199724
C	5.316558	5.463732	2.489262
C	5.394422	3.112049	1.835234
H	4.983360	2.922126	2.822130
H	6.230773	2.433531	1.653783
H	4.618504	2.923474	1.088161
C	6.678970	4.763756	0.558776
H	6.747454	5.833339	0.392766
H	6.172705	4.330193	-0.305560
H	7.682274	4.336355	0.641524
C	7.462645	6.667677	2.793770
H	7.864031	5.659814	2.859546
H	7.718532	7.203985	3.713685
H	7.943145	7.185257	1.957684
C	5.334493	7.903271	2.771595
H	4.310441	7.806802	2.422748
H	5.844960	8.634814	2.140214
H	5.333386	8.269304	3.802929
Cu	2.526593	4.928893	1.732912
Cl	3.400518	5.757847	-0.175303
Cl	1.189744	3.243198	1.051881
O	5.010431	6.773352	7.514206
N	5.739506	8.292847	12.060334
N	7.507696	9.391067	10.921717
N	7.896445	8.203852	12.883927
N	3.105285	8.583066	12.438073
N	1.321876	9.364996	13.681486
N	1.193070	7.222186	12.785379
C	4.908781	8.001963	10.968789
C	3.514205	8.091947	11.190173

C	2.643348	7.789106	10.138491
H	1.574216	7.899804	10.255628
C	3.118372	7.358559	8.911480
C	4.486348	7.220080	8.711033
C	5.366583	7.539605	9.730733
H	6.423491	7.406088	9.546067
C	7.020760	8.623065	11.941174
C	6.689032	10.419407	10.299403
H	5.842618	10.651781	10.939168
H	7.291087	11.324198	10.183997
H	6.324954	10.111617	9.314390
C	8.819968	9.189179	10.331771
H	9.285187	8.297964	10.744818
H	8.713598	9.055597	9.250029
H	9.481895	10.044054	10.501830
C	7.551679	7.104631	13.778825
H	6.872921	6.418119	13.281829
H	8.470109	6.577295	14.045659
H	7.076275	7.470198	14.693138
C	8.988401	9.046273	13.363289
H	8.991684	9.996505	12.840547
H	8.828968	9.255832	14.422553
H	9.954027	8.549167	13.234697
C	1.893657	8.383856	12.945417
C	1.815407	10.735330	13.599992
H	2.226073	10.925601	12.612997
H	0.979002	11.413647	13.781938
H	2.591566	10.923838	14.346832
C	0.531795	9.083012	14.876550
H	0.463652	8.013367	15.042310
H	1.038388	9.516467	15.740749
H	-0.471654	9.510192	14.794416
C	-0.252024	7.179055	12.641397
H	-0.653833	8.186752	12.575686
H	-0.507915	6.642615	11.721560
H	-0.732114	6.661302	13.477614
C	1.876616	5.944313	12.663083
H	2.900737	6.041207	13.011607
H	1.366639	5.212590	13.294654
H	1.877552	5.578233	11.631766
Cu	4.683558	8.919425	13.701732
Cl	3.809919	8.090537	15.610068
Cl	6.020035	10.605546	14.382540

[$(ZnCl_2)_2$(L3)]

104

Energy = -7457.246380 hartree

Zn	9.492645	17.297944	0.815078

Zn	9.962397	5.881786	6.575957
Cl	9.604380	17.500303	-1.409574
Cl	9.840448	5.814201	8.854503
Cl	9.286521	19.149473	2.135154
Cl	10.158563	3.996591	5.388560
O	11.093630	11.985919	4.369344
O	8.253873	11.789218	4.211036
N	11.244465	7.512837	6.191179
N	8.518892	7.323590	6.038473
N	8.166451	15.912354	1.691961
N	6.555109	6.116392	6.211331
N	10.891960	16.101946	1.845659
N	12.440053	16.762131	3.520269
N	12.891760	17.106473	1.266828
C	7.288504	7.221108	6.509063
N	13.323292	6.585945	6.594752
N	12.771053	8.570857	7.669696
N	6.705353	8.148089	7.329499
C	8.223347	13.837261	3.013286
H	7.152119	13.711695	2.930114
N	6.125074	16.636783	0.885257
N	6.364959	16.341452	3.177709
C	13.819229	16.592421	3.945943
H	13.870592	15.814511	4.715206
H	14.231003	17.513642	4.370039
H	14.437762	16.285930	3.106530
C	8.853334	14.951034	2.446898
C	11.147992	9.805794	5.304161
H	12.226317	9.891930	5.308992
C	10.328716	12.949534	3.743628
C	5.295675	8.492072	7.248039
H	5.192064	9.568519	7.074536
H	4.762416	8.246562	8.171858
H	4.826327	7.964823	6.421699
C	10.527105	8.641078	5.768893
C	7.174047	16.657601	4.343997
H	7.443484	15.762529	4.913755
H	6.601887	17.325469	4.992533
H	8.074067	17.180318	4.031255
C	5.695684	5.465436	7.191637
H	6.017044	4.428150	7.314113
H	4.648566	5.465708	6.873678
H	5.780070	5.960160	8.154742
C	9.029122	10.768128	4.722412
C	10.264149	15.049083	2.526256
C	9.116308	8.543254	5.690197
C	8.943601	12.853496	3.666191
C	12.872662	16.587263	-0.097328
H	12.411291	15.604294	-0.109173

H	13.903569	16.509084	-0.453507
H	12.308097	17.234482	-0.771279
C	6.916369	16.269964	1.927540
C	12.046930	16.625899	2.216747
C	11.778075	9.249039	8.487226
H	11.492630	10.219690	8.069144
H	12.198294	9.407760	9.483357
H	10.898615	8.618736	8.588328
C	10.414305	10.864021	4.799464
C	7.498402	8.948697	8.248568
H	8.438833	8.443479	8.452254
H	6.951323	9.040091	9.190033
H	7.693666	9.952651	7.858302
C	11.469818	16.954828	4.586192
H	11.262902	16.026490	5.128058
H	10.547623	17.352590	4.170980
H	11.869192	17.688805	5.290309
C	13.319315	5.794576	5.368192
H	12.821167	4.832942	5.505677
H	14.355066	5.622346	5.062738
H	12.797009	6.335170	4.584505
C	12.416394	7.577593	6.797842
C	14.147715	6.053043	7.671695
H	13.958043	4.981226	7.768752
H	13.890080	6.527313	8.614099
H	15.214067	6.196940	7.472290
C	13.646335	18.339779	1.448644
H	14.725452	18.162022	1.410075
H	13.390869	18.801799	2.397708
H	13.384734	19.038470	0.650161
C	8.396464	9.615285	5.150976
H	7.322666	9.552516	5.035965
C	10.974651	14.028259	3.167495
H	12.055496	14.051965	3.204821
C	14.120457	9.105531	7.743253
H	14.094566	10.186912	7.571381
H	14.747586	8.652008	6.980220
H	14.574970	8.930716	8.723508
C	4.982880	15.982073	3.447565
H	4.952240	15.199845	4.213471
H	4.510332	15.598981	2.546960
H	4.404052	16.835709	3.814166
C	5.194237	17.754679	0.970981
H	5.276591	18.240719	1.938656
H	4.160505	17.432011	0.813384
H	5.446278	18.487960	0.200934
C	6.367722	16.134709	-0.463806
H	6.911442	16.857275	-1.075441
H	5.403608	15.919864	-0.932920

H	6.956464	15.223466	-0.415565
C	6.805059	5.345183	4.997390
H	7.333147	5.959889	4.274499
H	5.843514	5.036194	4.578183
H	7.411524	4.459343	5.195415

[$(MnCl_2)_2$(L1)]

94

Energy = -5820.322850 hartree

Mn	9.620263	10.563065	3.493325
Cl	8.430230	9.764949	5.354996
Cl	11.302404	12.146850	3.611594
N	8.044934	10.752190	1.983694
N	5.689930	10.818897	2.303010
N	7.008911	12.689403	2.707258
N	6.631043	8.766351	-2.296691
N	6.804229	11.038401	-2.975477
N	4.916362	9.778048	-3.474587
C	8.107528	9.736865	1.010432
C	7.339937	9.756124	-0.155492
H	6.606555	10.542535	-0.277752
C	7.475522	8.807555	-1.170741
C	6.934750	11.389618	2.301655
C	4.493624	11.542658	1.908590
H	4.752358	12.543108	1.571798
H	3.776267	11.623073	2.731517
H	4.001099	11.015280	1.084410
C	5.509269	9.402040	2.573940
H	5.402086	8.813791	1.657280
H	4.607932	9.276576	3.178473
H	6.354754	9.033580	3.148135
C	6.212901	13.201356	3.816135
H	5.563584	14.023356	3.499525
H	6.881547	13.572754	4.596918
H	5.607214	12.407767	4.243407
C	8.111840	13.548840	2.291443
H	8.893919	13.615410	3.051846
H	7.719537	14.551667	2.100819
H	8.560860	13.157795	1.383116
C	6.140905	9.844099	-2.878395
C	8.255769	11.092536	-3.036527
H	8.705113	11.311837	-2.062982
H	8.544376	11.876564	-3.740554
H	8.637081	10.146236	-3.410009
C	6.128876	12.321618	-2.885797
H	5.071346	12.177438	-2.680438
H	6.232113	12.901685	-3.808352
H	6.564044	12.908714	-2.069737

C	4.643121	10.415437	-4.756884
H	4.339039	9.653595	-5.479206
H	5.538532	10.898863	-5.136034
H	3.838879	11.153220	-4.676420
C	3.916685	8.807212	-3.042958
H	3.901233	7.918926	-3.679368
H	2.932219	9.282135	-3.076607
H	4.129106	8.487189	-2.027097
N	8.496168	6.765007	-1.983727
N	10.851145	6.698591	-2.303380
N	9.532348	4.827964	-2.707524
N	9.910280	8.751144	2.296518
N	9.737219	6.479370	2.976343
N	11.625172	7.740013	3.474495
C	8.433491	7.780231	-1.010355
C	9.200967	7.760898	0.155627
H	9.934362	6.974482	0.277810
C	9.065529	8.709608	1.170808
C	9.606402	6.127724	-2.301868
C	12.047630	5.974843	-1.909451
H	11.788974	4.974579	-1.572033
H	12.764457	5.893938	-2.732787
H	12.540726	6.502565	-1.085845
C	11.031651	8.115450	-2.574386
H	11.138617	8.703784	-1.657758
H	11.933044	8.240974	-3.178805
H	10.186206	8.483732	-3.148761
C	10.327797	4.316397	-3.817003
H	10.977257	3.494284	-3.501010
H	9.658730	3.945315	-4.597577
H	10.933245	5.110134	-4.244329
C	8.429396	3.968513	-2.291763
H	7.646977	3.902574	-3.051872
H	8.821581	2.965496	-2.101949
H	7.980843	4.359065	-1.382991
C	10.400525	7.673614	2.878526
C	8.285684	6.425301	3.037818
H	7.836074	6.205463	2.064513
H	7.997250	5.641645	3.742338
H	7.904521	7.371795	3.410941
C	10.412505	5.196092	2.887151
H	11.470083	5.340117	2.681953
H	10.309034	4.616352	3.809889
H	9.977478	4.608723	2.071204
C	11.898528	7.103465	4.757183
H	12.202420	7.865813	5.479053
H	11.003215	6.620057	5.136588
H	12.702951	6.365818	4.677201
C	12.624588	8.710879	3.042351

H	12.639948	9.599401	3.678442
H	13.609167	8.236178	3.076008
H	12.411911	9.030473	2.026410
Mn	6.920728	6.954229	-3.493272
Cl	8.111168	7.751981	-5.355051
Cl	5.238579	5.370624	-3.610889

[$(FeCl_2)_2$(L1)]

94

Energy = -6045.714170 hartree

Fe	7.716661	7.455540	4.186166
Cl	5.791401	8.561554	4.734757
Cl	8.252319	6.804989	2.087449
N	9.230985	8.413368	5.349295
N	9.143476	10.518303	6.448685
N	9.524607	10.382941	4.162245
N	7.976251	6.047299	5.772990
N	6.374828	4.463835	5.223243
N	6.384650	5.320491	7.381267
C	9.675859	7.625591	6.426721
C	9.022742	6.393640	6.647184
C	9.510443	5.544318	7.642092
H	9.009493	4.599842	7.810780
C	9.309469	9.731573	5.339001
C	8.295868	10.098512	7.552042
H	7.563474	9.381393	7.192640
H	7.759824	10.972067	7.930842
H	8.870015	9.656067	8.372189
C	9.903854	11.736343	6.669543
H	10.445000	11.663656	7.619278
H	9.256297	12.617583	6.719250
H	10.626961	11.879220	5.870818
C	8.816159	11.608186	3.815005
H	8.132702	11.887690	4.611134
H	8.228744	11.438921	2.908748
H	9.509434	12.433658	3.626312
C	10.201431	9.728695	3.049055
H	10.790555	8.893603	3.416043
H	10.860106	10.456055	2.565761
H	9.495968	9.341712	2.310806
C	6.952740	5.295355	6.134382
C	7.124864	3.958895	4.079754
H	6.930959	4.537392	3.174021
H	6.836587	2.918135	3.906243
H	8.189753	4.010626	4.286127
C	4.928901	4.310136	5.124861
H	4.431961	4.932411	5.863063
H	4.625148	3.268279	5.265732

H	4.599697	4.633399	4.133849
C	5.862740	4.130723	8.031248
H	6.040863	3.254775	7.413080
H	4.788517	4.211030	8.226140
H	6.368061	3.986304	8.992528
C	6.402071	6.524160	8.195485
H	7.205861	6.511949	8.938135
H	5.444822	6.605847	8.716018
H	6.513448	7.393275	7.553579
N	11.063505	5.078341	9.505442
N	11.151559	2.973370	8.406183
N	10.770142	3.108793	10.692578
N	12.318314	7.444384	9.081583
N	13.919866	9.027918	9.630947
N	13.909804	8.170908	7.473084
C	10.618713	5.866020	8.427894
C	11.271865	7.097937	8.207368
C	10.784153	7.947276	7.212498
H	11.285019	8.891810	7.043880
C	10.985164	3.760143	9.515799
C	11.999439	3.393228	7.303070
H	12.731684	4.110391	7.662701
H	12.535632	2.519707	6.924408
H	11.425522	3.835666	6.482756
C	10.391342	1.755262	8.185148
H	9.850312	1.827920	7.235341
H	11.039011	0.874102	8.135492
H	9.668141	1.612252	8.983766
C	11.478850	1.883731	11.039917
H	12.162320	1.604269	10.243787
H	12.066266	2.053213	11.946133
H	10.785737	1.058151	11.228734
C	10.093223	3.762962	11.805753
H	9.504034	4.598011	11.438779
H	9.434619	3.035537	12.289048
H	10.798641	4.150005	12.544012
C	13.341904	8.196144	8.720069
C	13.169905	9.533464	10.774212
H	13.363908	8.955487	11.680253
H	13.458164	10.574328	10.947135
H	12.105000	9.481579	10.567978
C	15.365779	9.181896	9.729046
H	15.862709	8.559455	8.990981
H	15.669313	10.223759	9.587765
H	15.695193	8.859033	10.720117
C	14.431461	9.360668	6.822885
H	14.253535	10.236629	7.441094
H	15.505622	9.280374	6.627643
H	13.925818	9.505064	5.861768

C	13.892293	6.967160	6.658997
H	13.088364	6.979220	5.916494
H	14.849450	6.885477	6.138294
H	13.781072	6.098110	7.301023
Fe	12.576880	6.036900	10.669206
Cl	14.502504	4.930927	10.122287
Cl	12.039180	6.688288	12.767175

[$(CoCl_2)_2$(L1)]

94

Energy = -6283.821260 hartree

Co	4.630664	9.935592	9.009522
Cl	2.632614	10.034983	7.916382
Cl	4.976002	8.215839	10.417316
N	5.016511	11.877566	9.624154
N	3.560337	13.751583	9.704233
N	3.511280	12.127803	11.364597
N	6.053903	10.416922	7.581279
N	5.837065	10.543248	5.219943
N	6.088084	8.496622	6.289488
C	6.071904	12.445897	8.886717
C	6.611158	11.686382	7.823403
C	7.721842	12.183554	7.139915
C	4.067262	12.585964	10.211068
C	3.142317	14.858937	10.546864
C	3.517611	13.997641	8.272038
C	4.246503	11.239871	12.258994
C	2.076837	12.201862	11.613905
C	6.008485	9.850794	6.387702
C	5.084955	11.786795	5.182178
C	6.478487	10.156047	3.975145
C	5.243472	7.737256	5.375399
C	6.756872	7.701143	7.313620
N	9.377947	13.968773	6.730406
N	10.828961	12.091044	6.640087
N	10.878310	13.721135	4.985719
N	8.342155	15.427762	8.775102
N	8.552546	15.299648	11.137025
N	8.305799	17.347111	10.067792
C	8.321675	13.400716	7.466645
C	7.782784	14.159882	8.530518
C	6.671253	13.663290	9.213107
C	10.324109	13.259748	6.138842
C	11.243590	10.986252	5.792408
C	10.873432	11.839089	8.071387
C	10.142864	14.614763	4.097080
C	12.311947	13.644695	4.732323
C	8.384638	15.992938	9.969526

C	9.302569	14.054631	11.175551
C	7.908818	15.686941	12.380644
C	9.147551	18.105754	10.985132
C	7.640008	18.143155	9.042066
Co	9.781176	15.902232	7.360946
Cl	11.770194	15.771173	8.468072
Cl	9.473107	17.639016	5.965667
H	8.134632	11.602301	6.325559
H	3.365940	14.644346	11.588582
H	2.070998	15.062376	10.451768
H	3.683484	15.765140	10.254389
H	2.578682	14.503197	8.034301
H	4.349179	14.623132	7.933232
H	3.534359	13.049368	7.742312
H	4.017009	11.519981	13.290921
H	5.313379	11.343233	12.084373
H	3.981965	10.191854	12.104491
H	1.685689	11.190524	11.749643
H	1.854586	12.782382	12.514459
H	1.568374	12.646079	10.763441
H	4.402997	11.821700	6.027036
H	5.735832	12.666488	5.197795
H	4.491192	11.806057	4.265254
H	7.146848	9.315358	4.141945
H	7.065841	10.996436	3.589912
H	5.748048	9.877919	3.208834
H	5.840236	7.160027	4.662650
H	4.627510	7.043053	5.952362
H	4.578919	8.403596	4.833755
H	7.455826	8.323463	7.864481
H	6.049953	7.277092	8.029594
H	7.300386	6.889585	6.821713
H	6.258416	14.244254	10.027659
H	12.314822	10.780921	5.884363
H	10.701860	10.079776	6.082906
H	11.017851	11.204920	4.751982
H	10.859510	12.785188	8.605152
H	11.811803	11.330819	8.305422
H	10.041275	11.213560	8.408599
H	9.076124	14.511559	4.272795
H	10.409182	15.661563	4.256869
H	10.370403	14.339623	3.063407
H	12.821641	13.196301	5.579844
H	12.705016	14.655614	4.599004
H	12.530438	13.066879	3.829121
H	9.893583	14.033646	12.094181
H	9.987153	14.019518	10.332780
H	8.650048	13.176235	11.157407
H	7.320379	14.846661	12.764406

H	8.637845	15.964528	13.148457
H	7.241080	16.527916	12.212738
H	9.812587	17.439184	11.525941
H	8.548908	18.680196	11.698564
H	9.762927	18.802553	10.410706
H	7.096083	18.955195	9.532706
H	6.941633	17.521249	8.489960
H	8.349129	18.566241	8.327679

[$(NiCl_2)_2$(L1)]

94

Energy = -6534.895990 hartree

Ni	-2.820360	0.697758	12.289913
Cl	-3.070902	-1.518389	11.896185
Cl	-3.939349	2.610462	11.838453
N	-2.194575	0.817767	14.232108
N	-2.244289	2.093738	16.231213
N	-4.192400	1.185930	15.350735
N	-0.842284	1.074410	11.941866
N	-0.883454	1.814966	9.744736
N	0.740793	2.664052	11.171524
C	-0.838141	0.444003	14.255729
C	-0.123644	0.580089	13.045971
C	1.194295	0.132943	12.981988
H	1.741776	0.237441	12.054916
C	-2.842076	1.345975	15.245338
C	-2.646661	2.008018	17.624597
H	-3.422257	1.256391	17.745457
H	-3.024538	2.965372	17.998320
H	-1.785677	1.725436	18.240283
C	-1.085615	2.929239	15.967828
H	-1.217590	3.885115	16.482124
H	-1.010520	3.122391	14.902161
H	-0.151045	2.475427	16.310533
C	-4.879424	0.082763	14.692511
H	-4.193311	-0.737036	14.502768
H	-5.316850	0.394926	13.739545
H	-5.687976	-0.262338	15.342900
C	-5.062392	2.295071	15.724751
H	-4.474164	3.155806	16.027690
H	-5.729059	2.010295	16.543771
H	-5.668875	2.584659	14.862040
C	-0.331774	1.824178	10.992055
C	-1.679500	0.688622	9.275773
H	-1.427275	-0.213460	9.824915
H	-1.475864	0.536372	8.212207
H	-2.750457	0.877729	9.395129
C	-1.096513	3.050093	8.998967

H	-0.630732	3.888205	9.508104
H	-2.169636	3.248861	8.929249
H	-0.686400	2.972066	7.988013
C	1.759867	2.853214	10.153508
H	2.742725	2.595800	10.563401
H	1.803298	3.891923	9.809624
H	1.560319	2.211592	9.299415
C	0.995764	3.326910	12.438615
H	1.795291	2.848517	13.011974
H	0.089921	3.329998	13.037066
H	1.281143	4.363886	12.241477
N	3.181761	-0.818325	14.105475
N	3.233238	-2.093844	12.106144
N	5.180325	-1.184733	12.987581
N	1.829301	-1.075395	16.395316
N	1.870654	-1.815352	18.592681
N	0.247158	-2.665807	17.165841
C	1.825098	-0.445284	14.081411
C	1.110498	-0.581637	15.291056
C	-0.207435	-0.134516	15.355062
H	-0.754837	-0.238813	16.282205
C	3.830071	-1.345874	13.092457
C	3.636120	-2.007441	10.712943
H	4.411318	-1.255316	10.592648
H	4.014724	-2.964455	10.339084
H	2.775228	-1.725174	10.096986
C	2.074989	-2.930134	12.368805
H	2.207767	-3.885784	11.854291
H	1.999526	-3.123626	13.434395
H	1.140287	-2.476793	12.025827
C	5.866203	-0.081088	13.646188
H	5.179395	0.738229	13.835546
H	6.303371	-0.393000	14.599357
H	6.674828	0.264645	12.996222
C	6.051348	-2.293161	12.613879
H	5.463915	-3.154274	12.310462
H	6.718251	-2.007759	11.795272
H	6.657574	-2.582427	13.476882
C	1.319185	-1.825230	17.345250
C	2.665719	-0.688286	19.061584
H	2.412723	0.213531	18.512346
H	2.461861	-0.536068	20.125113
H	3.736836	-0.876541	18.942327
C	2.084521	-3.050163	19.338732
H	1.619375	-3.888704	18.829712
H	3.157779	-3.248143	19.408607
H	1.674238	-2.972228	20.349624
C	-0.771959	-2.855326	18.183760
H	-1.754889	-2.598378	17.773747

H	-0.814950	-3.894027	18.527721
H	-0.572780	-2.213544	19.037815
C	-0.007328	-3.328909	15.898797
H	-0.806987	-2.850923	15.325277
H	0.898600	-3.331648	15.300452
H	-0.292275	-4.365993	16.095997
Ni	3.806856	-0.695411	16.047718
Cl	4.052865	1.521666	16.439513
Cl	4.929120	-2.605729	16.501052

[$(CuCl_2)_2$(L1)]

94

Energy = -6799.202030 hartree

Cu	3.281621	10.725537	3.523112
Cl	2.305032	9.341879	2.030143
N	1.939780	12.274547	3.492676
N	-0.079466	11.155287	3.620662
N	0.216568	12.718602	1.923280
C	2.576283	13.528586	3.487353
C	1.903765	14.752161	3.524264
H	0.822704	14.751874	3.524492
C	0.718689	12.069707	3.017265
C	0.220063	10.687591	4.969212
H	0.859865	9.801003	4.950932
H	-0.720590	10.432711	5.462619
H	0.723685	11.468292	5.531420
C	-0.956703	10.267163	2.862795
H	-0.896552	10.488303	1.802764
H	-1.992931	10.356952	3.201247
H	-0.619582	9.238379	3.001977
C	-1.176363	13.109733	1.800465
H	-1.710582	12.893847	2.722069
H	-1.676328	12.592717	0.975380
H	-1.236155	14.186287	1.606532
C	1.087333	13.143487	0.839248
H	1.277394	14.220853	0.864965
H	0.610510	12.892892	-0.111766
H	2.032299	12.611157	0.898424
N	1.938731	17.229727	3.556067
N	-0.080835	18.348366	3.427919
N	0.215657	16.785112	5.125336
C	2.575718	15.976039	3.561276
C	0.717566	17.434247	4.031389
C	0.218470	18.815998	2.079297
H	0.857863	19.702882	2.097483
H	-0.722305	19.070387	1.585867
H	0.722444	18.035458	1.517190
C	-0.958220	19.236448	4.185637

H	-0.898046	19.015532	5.245709
H	-1.994434	19.146419	3.847202
H	-0.621280	20.265263	4.046243
C	-1.177051	16.393180	5.248045
H	-1.711426	16.609069	4.326538
H	-1.677267	16.909635	6.073330
H	-1.236265	15.316523	5.441624
C	1.086683	16.360361	6.209214
H	1.277134	15.283073	6.183328
H	0.609911	16.610653	7.160336
H	2.031478	16.893001	6.149986
N	4.622740	12.275209	3.555676
N	6.642798	11.157430	3.428151
N	6.344925	12.720224	5.125840
C	3.985533	13.528916	3.561071
C	4.657471	14.752798	3.524267
H	5.738556	14.753091	3.524470
C	5.843820	12.071052	4.031506
C	6.344230	10.690148	2.079244
H	5.705083	9.803087	2.096957
H	7.285279	10.436188	1.586109
H	5.840239	11.470714	1.517190
C	7.520069	10.269374	4.185994
H	7.459027	10.489672	5.246147
H	8.556493	10.360062	3.848384
H	7.183725	9.240477	4.045757
C	7.737281	13.113195	5.249112
H	8.272128	12.897862	4.327744
H	8.237611	12.596983	6.074482
H	7.795605	14.189864	5.442847
C	5.473229	13.143932	6.209602
H	5.281773	14.221059	6.183909
H	5.950033	12.893919	7.160778
H	4.528947	12.610415	6.150037
N	4.621679	17.230415	3.493071
N	6.641378	18.348894	3.620488
N	6.344068	16.786081	1.922814
C	3.984971	15.976361	3.487578
C	5.842691	17.434924	3.017200
C	6.342561	18.816282	4.969303
H	5.703046	19.703079	4.951468
H	7.283485	19.070700	5.462438
H	5.838874	18.035589	5.531464
C	7.518608	19.236900	2.862509
H	7.457694	19.016278	1.802411
H	8.555007	19.146449	3.200256
H	7.182092	20.265785	3.002403
C	7.736723	16.394182	1.799384
H	8.271402	16.609591	2.720835

H	8.236666	16.911082	0.974211
H	7.795828	15.317631	1.605258
C	5.472681	16.362126	0.838907
H	5.281789	15.284891	0.864389
H	5.949479	16.612564	-0.112157
H	4.528137	16.895175	0.898459
Cu	3.279849	18.779411	3.525131
Cl	4.256364	20.165112	2.033987
Cl	2.302854	20.163121	5.017742

[$(ZnCl_2)_2$(L1)]

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Energy = -7077.029300 hartree

Zn	7.341579	9.368774	1.052998
Cl	8.516958	10.195430	2.789510
Cl	5.343738	10.133602	0.355224
N	8.624673	8.982677	-0.585137
N	8.832035	9.054324	-2.950777
N	8.559328	11.002988	-1.718524
N	7.376594	7.253224	1.085623
N	6.110988	5.281447	0.692506
N	5.507041	6.771174	2.367549
C	9.246493	7.741605	-0.354926
C	8.595261	6.839269	0.517107
C	9.234322	5.646134	0.850836
H	8.735717	4.955726	1.518387
C	8.681088	9.644519	-1.718155
C	8.313974	7.728326	-3.236350
H	9.091489	6.958977	-3.216045
H	7.856951	7.735384	-4.229658
H	7.549071	7.471440	-2.510089
C	9.638508	9.646095	-4.004802
H	10.106356	10.560954	-3.651080
H	9.041115	9.877883	-4.892648
H	10.424842	8.944698	-4.304826
C	8.852825	11.791576	-0.528712
H	7.943917	12.030040	0.030524
H	9.321224	12.729532	-0.839233
H	9.526855	11.252293	0.129541
C	7.749164	11.697630	-2.712604
H	7.385860	11.001495	-3.462398
H	8.322821	12.487783	-3.205697
H	6.883985	12.149618	-2.219894
C	6.376544	6.449695	1.367317
C	6.429629	5.117787	-0.714545
H	6.549905	6.092658	-1.176857
H	5.599005	4.603960	-1.206096
H	7.342590	4.536703	-0.875031

C	5.631316	4.085362	1.363967
H	5.563834	4.257345	2.434857
H	6.327698	3.258511	1.185946
H	4.647156	3.778657	0.994953
C	4.067778	6.589690	2.217350
H	3.842532	6.085542	1.282527
H	3.581093	7.568729	2.202156
H	3.655556	6.007470	3.046607
C	5.886756	7.681828	3.439950
H	6.965827	7.705735	3.555786
H	5.428984	7.334634	4.370250
H	5.539316	8.700179	3.245105
N	11.115006	4.070587	0.584605
N	10.908037	3.999309	2.950287
N	11.180132	2.050416	1.718228
N	12.363463	5.800245	-1.085839
N	13.628647	7.772298	-0.692593
N	14.233564	6.282255	-2.366988
C	10.493377	5.311743	0.354427
C	11.144657	6.214107	-0.517547
C	10.505558	7.407237	-0.851300
H	11.004177	8.097655	-1.518832
C	11.058574	3.408880	1.717721
C	11.426676	5.325173	3.235506
H	10.649548	6.094904	3.214823
H	11.883545	5.318215	4.228882
H	12.191850	5.581408	2.509288
C	10.101481	3.408047	4.004529
H	9.633294	2.493266	3.651055
H	10.698892	3.176255	4.892360
H	9.315416	4.109779	4.304481
C	10.886838	1.261848	0.528351
H	11.795810	1.023465	-0.030811
H	10.418480	0.323851	0.838790
H	10.212864	1.801115	-0.129969
C	11.990157	1.355745	2.712418
H	12.353475	2.051879	3.462204
H	11.416378	0.565671	3.205492
H	12.855342	0.903655	2.219810
C	13.363500	6.603904	-1.367278
C	13.309663	7.936199	0.714365
H	13.189128	6.961432	1.176823
H	14.140232	8.449996	1.206043
H	12.396746	8.517435	0.874530
C	14.108476	8.968289	-1.364116
H	14.176021	8.796217	-2.434987
H	13.412129	9.795187	-1.186200
H	15.092628	9.274980	-0.995060
C	15.672743	6.463716	-2.215957

H	15.897434	6.968321	-1.281248
H	16.159352	5.484653	-2.199944
H	16.085508	7.045496	-3.045249
C	13.854514	5.371297	-3.439352
H	12.775510	5.347239	-3.555729
H	14.312734	5.718300	-4.369508
H	14.201942	4.353029	-3.244076
Zn	12.399375	3.684735	-1.052560
Cl	11.226244	2.856448	-2.789807
Cl	14.396896	2.921022	-0.352558

[$(CuBr_2)_2$)(L4)] – triplet

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Energy = -15630,2063053679 hartree

Cu	3.049341	12.298899	2.510908
O	5.627415	6.920562	5.256918
N	3.065125	10.269048	2.876860
N	1.201119	9.447870	1.715862
N	1.197312	9.144426	3.906914
N	8.389406	3.670850	7.549591
N	6.258753	2.865522	8.341570
N	7.658217	1.450210	7.376479
C	4.122291	9.882066	3.707531
C	8.075959	4.982213	7.176291
C	6.952459	5.336673	6.423697
H	6.223043	4.591409	6.134937
C	6.757445	6.640546	5.998873
C	5.469611	8.236238	4.869758
C	4.343676	8.569678	4.135130
H	3.650327	7.779996	3.876997
C	1.895881	9.641836	2.856728
C	-0.172995	9.058321	2.005523
H	-0.504518	8.275844	1.322177
H	-0.837096	9.923125	1.907999
C	-0.069914	8.568850	3.458843
H	-0.889457	8.934924	4.077824
H	-0.048060	7.476058	3.526306
C	1.577240	9.958730	0.415295
H	1.103959	10.925639	0.222782
H	1.272386	9.244516	-0.352040
H	2.655756	10.086806	0.379589
C	1.440249	9.450273	5.300543
H	1.829458	8.585714	5.845665
H	0.504801	9.771307	5.762771
H	2.155184	10.264107	5.379346
C	7.468387	2.735331	7.743129
C	5.566563	1.578587	8.393376
H	4.723587	1.560065	7.694568

H	5.183839	1.397164	9.398072
C	6.668063	0.581510	7.999946
H	7.102427	0.081970	8.871844
H	6.318033	-0.173052	7.294815
C	5.839652	3.984774	9.157989
H	5.462156	3.608682	10.110782
H	5.057008	4.573679	8.671371
H	6.688889	4.630995	9.360211
C	8.883845	0.914847	6.824229
H	9.425331	1.709716	6.318433
H	8.640252	0.129579	6.105957
H	9.521546	0.503962	7.611905
O	7.536529	8.934524	5.925714
N	10.083560	5.592112	8.330678
N	11.944279	6.415418	9.495469
N	11.957613	6.708527	7.303058
N	4.759401	12.189737	3.659122
N	6.885291	13.001560	2.861000
N	5.488148	14.410690	3.838403
C	9.030439	5.977248	7.494002
C	5.076462	10.877286	4.025560
C	6.203459	10.521532	4.772304
H	6.932694	11.266819	5.061479
C	6.402406	9.216145	5.190641
C	7.690379	7.620368	6.319587
C	8.812735	7.288252	7.060293
H	9.506190	8.077948	7.318116
C	11.253819	6.217381	8.352681
C	13.320261	6.801196	9.209633
H	13.650326	7.586367	9.890590
H	13.982428	5.935717	9.314062
C	13.224081	7.283849	7.753567
H	14.045456	6.913253	7.139724
H	13.204602	8.376347	7.680750
C	11.562025	5.911070	10.796788
H	12.032961	4.944299	10.995627
H	11.864873	6.628291	11.562112
H	10.483166	5.784877	10.828640
C	11.719504	6.397141	5.909829
H	11.334264	7.260142	5.359440
H	12.656081	6.072149	5.452684
H	11.003160	5.584477	5.831752
C	5.678199	13.127407	3.465434
C	7.575461	14.289673	2.811722
H	8.421484	14.306350	3.506895
H	7.953516	14.475982	1.806154
C	6.474324	15.283474	3.214323
H	6.035404	15.786138	2.346511
H	6.826413	16.035485	3.921148

C	7.302617	11.886273	2.038278
H	7.675333	12.266799	1.085362
H	8.088339	11.296703	2.519097
H	6.453544	11.239479	1.837195
C	4.264110	14.941911	4.398134
H	3.725963	14.144116	4.902881
H	4.509644	15.724493	5.118672
H	3.622438	15.355171	3.614938
Cu	10.094083	3.563961	8.705942
Br	0.707527	12.797274	2.819349
Br	3.768823	13.814804	0.775302
Br	9.363962	2.056879	10.444830
Br	12.436271	3.059977	8.410522

[$(CuBr_2)_2$(L4)]- singlet

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Energy = -15630.2063053679 hartree

Cu	3.023832	12.354140	2.399895
O	5.588777	6.965611	5.359163
N	3.117467	10.247088	2.855202
N	1.287121	9.469645	1.617563
N	1.131793	9.295621	3.820752
N	8.349525	3.710768	7.579734
N	6.313558	2.752408	8.454613
N	7.765381	1.460624	7.380926
C	4.121901	9.869833	3.689921
C	8.030477	4.980225	7.223350
C	6.878199	5.353638	6.513538
H	6.115171	4.623177	6.280563
C	6.718767	6.646700	6.059042
C	5.439965	8.246309	4.905499
C	4.306565	8.571697	4.188765
H	3.583152	7.794520	3.982156
C	1.921224	9.670960	2.788177
C	-0.131596	9.207021	1.836196
H	-0.473167	8.384101	1.206984
H	-0.715222	10.102115	1.601342
C	-0.181227	8.866545	3.335334
H	-0.966538	9.417534	3.853859
H	-0.328908	7.797465	3.515586
C	1.770285	9.916144	0.326005
H	1.343611	10.888731	0.066288
H	1.494399	9.182762	-0.434147
H	2.851183	10.015828	0.357678
C	1.319730	9.671619	5.206741
H	1.489489	8.794311	5.837523
H	0.433706	10.203722	5.557202
H	2.166435	10.344489	5.295737

C	7.494819	2.711899	7.776194
C	5.896405	1.381481	8.781165
H	4.830555	1.246256	8.593145
H	6.100691	1.185876	9.837000
C	6.778912	0.510914	7.873759
H	7.266322	-0.297151	8.422379
H	6.222159	0.075680	7.037569
C	5.990502	3.788789	9.426802
H	6.551501	3.633395	10.352693
H	4.919803	3.744945	9.629607
H	6.219691	4.771775	9.027296
C	8.913285	1.035828	6.609755
H	9.506942	1.903107	6.336852
H	8.585979	0.513846	5.705957
H	9.538647	0.367607	7.205304
O	7.558567	8.895337	5.850852
N	10.029830	5.614099	8.354915
N	11.858847	6.392033	9.594192
N	12.015035	6.568368	7.391241
N	4.799509	12.149938	3.628015
N	6.836058	13.104522	2.750384
N	5.386594	14.399685	3.823237
C	9.025588	5.991244	7.519972
C	5.117691	10.880489	3.985446
C	6.269802	10.507028	4.695463
H	7.033125	11.237328	4.928034
C	6.428794	9.214138	5.150586
C	7.707342	7.614683	6.304552
C	8.840570	7.289484	7.021612
H	9.563608	8.066860	7.228711
C	11.225525	6.191253	8.423071
C	13.277305	6.656828	9.376533
H	13.617274	7.479925	10.006377
H	13.862114	5.762514	9.611334
C	13.327464	6.998150	7.877577
H	14.113422	6.447963	7.359192
H	13.474525	8.067407	7.697953
C	11.375996	5.942715	10.884907
H	11.803769	4.970169	11.142895
H	11.650961	6.675042	11.646389
H	10.295238	5.841856	10.852955
C	11.827567	6.194331	6.004657
H	11.654315	7.072123	5.375509
H	12.715309	5.666123	5.652730
H	10.983304	5.518500	5.914924
C	5.655241	13.147500	3.429501
C	7.254870	14.474458	2.421835
H	8.321045	14.608433	2.608955
H	7.050129	14.669061	1.365886

C	6.374200	15.347360	3.328762
H	5.887716	16.155580	2.779527
H	6.932098	15.782662	4.164170
C	7.156965	12.066549	1.779174
H	6.595301	12.221501	0.853593
H	8.227536	12.108850	1.575335
H	6.926962	11.084321	2.180105
C	4.239663	14.827077	4.594412
H	3.645008	13.960946	4.868883
H	4.568125	15.349925	5.497300
H	3.614865	15.495279	3.998217
Cu	10.124568	3.506707	8.808483
Br	0.777179	12.906253	3.153253
Br	3.878246	13.540752	0.459482
Br	9.270196	2.317367	10.747201
Br	12.371959	2.957036	8.055492

[(CuBrMeCN)$_2$(L1)] - singlet

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Energy = -10668.4462659084 hartree

Cu	2.948955	12.348644	2.565665
O	5.578897	6.983674	5.414873
N	2.923409	10.308621	3.184470
N	1.347301	9.285722	1.763389
N	1.019184	9.053891	3.943577
N	8.407394	3.694823	7.473933
N	6.400296	2.804867	8.468776
N	7.684599	1.473970	7.249059
C	3.993934	9.906832	3.898581
C	8.112658	4.948212	7.088487
C	6.916372	5.340783	6.460153
H	6.126588	4.622706	6.287344
C	6.740517	6.636435	6.031167
C	5.393409	8.259858	4.986285
C	4.213483	8.595865	4.360776
H	3.471455	7.824082	4.210341
C	1.828220	9.559134	2.980952
C	0.151951	8.444359	1.850341
H	0.397209	7.422932	1.544492
H	-0.634334	8.817218	1.194528
C	-0.213916	8.533643	3.337749
H	-1.034196	9.236160	3.516803
H	-0.487077	7.571143	3.768800
C	2.052747	9.454413	0.501301
H	1.349814	9.806551	-0.252969
H	2.478825	8.502616	0.171225
H	2.836620	10.199445	0.608915
C	0.997703	9.499088	5.325789

H	0.827344	8.646337	5.983780
H	0.195415	10.226852	5.482783
H	1.945950	9.958446	5.585969
C	7.507987	2.722335	7.701345
C	5.903317	1.449227	8.755800
H	4.817188	1.410849	8.683275
H	6.201451	1.167787	9.769303
C	6.607486	0.592057	7.696955
H	7.009088	-0.335754	8.104328
H	5.953569	0.345769	6.854560
C	6.137365	3.847848	9.453156
H	6.665979	3.633815	10.384801
H	5.062732	3.885334	9.632331
H	6.457723	4.814571	9.078623
C	8.636104	1.058951	6.240402
H	9.338302	1.867149	6.056179
H	8.124752	0.805199	5.307215
H	9.182388	0.180966	6.588424ü

[(CuBrMeCN)$_2$(L1)] – triplet

100

Energy = -10668.4543639583 hartree

Cu	3.005477	12.343906	2.627502
O	5.571975	6.957648	5.385528
N	2.930688	10.311095	3.139227
N	1.234801	9.417882	1.782671
N	1.078302	8.998915	3.955303
N	8.437697	3.672831	7.434957
N	6.409068	2.856584	8.444752
N	7.604617	1.487378	7.190505
C	4.003322	9.910371	3.896277
C	8.130750	4.958224	7.076566
C	6.938303	5.343057	6.440042
H	6.161443	4.617446	6.240578
C	6.747843	6.640139	6.018918
C	5.403552	8.256920	4.979336
C	4.228109	8.597784	4.344597
H	3.497188	7.819803	4.172773
C	1.815427	9.589808	2.981886
C	0.063747	8.546937	1.887022
H	0.300267	7.561929	1.473022
H	-0.779986	8.955148	1.330845
C	-0.183663	8.494735	3.399696
H	-1.004436	9.152221	3.703759
H	-0.400207	7.490056	3.761690
C	1.861594	9.653553	0.491266
H	1.131222	10.093867	-0.187320
H	2.218863	8.712873	0.061809

H	2.691846	10.344788	0.601617
C	1.133000	9.345751	5.365174
H	1.110673	8.440775	5.973984
H	0.273528	9.967337	5.634391
H	2.044930	9.891282	5.583494
C	7.497601	2.733389	7.669239
C	5.702911	1.574593	8.560741
H	4.706411	1.645854	8.118854
H	5.596061	1.307981	9.612292
C	6.618190	0.596010	7.801512
H	7.115705	-0.110974	8.470134
H	6.086758	0.032964	7.033886
C	6.108205	3.947325	9.352586
H	5.978419	3.547826	10.359058
H	5.195653	4.466431	9.049369
H	6.933439	4.650903	9.375222
C	8.672261	0.978997	6.357189
H	9.236894	1.812365	5.949056
H	8.252789	0.393827	5.536958
H	9.341655	0.338753	6.938517
O	7.575683	8.904108	5.826377
N	10.218317	5.549861	8.069739
N	11.914256	6.443748	9.425933
N	12.070223	6.862233	7.253185
N	4.710946	12.188373	3.774114
N	6.740055	13.002637	2.763462
N	5.544834	14.373820	4.015844
C	9.145236	5.950855	7.313831
C	5.017738	10.902922	4.133324
C	6.209914	10.518352	4.770383
H	6.986837	11.243952	4.969636
C	6.400071	9.221426	5.192294
C	7.744379	7.604750	6.232069
C	8.919936	7.263755	6.866453
H	9.650722	8.041787	7.038637
C	11.333408	6.271501	8.226936
C	13.085336	7.314608	9.321089
H	12.849033	8.299709	9.734977
H	13.929179	6.906410	9.877105
C	13.332358	7.366490	7.808323
H	14.153031	6.708928	7.504165
H	13.548823	8.371095	7.446073
C	11.288032	6.207916	10.717603
H	12.018983	5.768288	11.395997
H	10.930288	7.148451	11.146976
H	10.458269	5.516016	10.607775
C	12.014677	6.515694	5.843292
H	12.035936	7.420808	5.234638
H	12.874331	5.894716	5.573279

H	11.102932	5.969600	5.625588
C	5.651424	13.127212	3.538656
C	7.446816	14.284203	2.646331
H	8.442675	14.213313	3.089745
H	7.555224	14.549102	1.594513
C	6.530805	15.264252	3.402704
H	6.032860	15.969003	2.732028
H	7.061696	15.829718	4.168904
C	7.040247	11.911074	1.856414
H	7.168613	12.309512	0.849317
H	7.953416	11.392725	2.159053
H	6.215401	11.206980	1.835713
C	4.476613	14.883832	4.847444
H	3.912934	14.051245	5.258504
H	4.895558	15.472223	5.665617
H	3.806486	15.521359	4.263948
Cu	10.143249	3.516807	8.582581
Br	3.742786	13.351481	0.587981
Br	9.405188	2.516887	10.625606
N	11.927621	2.597880	8.329903
C	12.842546	1.920252	8.435670
H	13.689392	1.276877	8.551308
N	1.218450	13.258867	2.879006
C	0.302951	13.935675	2.773150
H	-0.544418	14.578382	2.657570

[$(CuCl_2)_2$(L4)]

96

Energy = -7174.624360 hartree

Cu	2.993643	12.402802	2.440457
Cl	3.878934	13.346786	0.561835
Cl	0.936076	12.920252	3.280361
O	5.585105	6.971596	5.367752
N	3.105770	10.264524	2.896525
N	1.284371	9.587313	1.608410
N	1.079046	9.321684	3.805017
N	8.357966	3.700999	7.539040
N	6.357026	2.728011	8.472931
N	7.800102	1.443207	7.375229
C	4.107119	9.882125	3.719577
C	8.039089	4.968571	7.194821
C	6.879022	5.349193	6.500880
H	6.111626	4.621527	6.273363
C	6.719542	6.644515	6.054044
C	5.433240	8.251821	4.917324
C	4.292562	8.581244	4.215088
H	3.560573	7.809343	4.018728
C	1.902064	9.718371	2.791855

C	-0.079067	9.104822	1.766002
H	-0.163460	8.076077	1.397830
H	-0.776840	9.729715	1.206283
C	-0.289844	9.204764	3.281909
H	-0.851298	10.106224	3.543381
H	-0.793084	8.332862	3.700461
C	1.869100	9.831974	0.307916
H	1.257516	10.549540	-0.241709
H	1.933761	8.901847	-0.265697
H	2.860805	10.258033	0.431030
C	1.220658	9.817240	5.169778
H	2.244547	9.700967	5.512823
H	0.576570	9.219435	5.815226
H	0.933882	10.871140	5.224688
C	7.520921	2.697147	7.761487
C	5.994781	1.352406	8.843881
H	4.919277	1.196437	8.756617
H	6.304259	1.166543	9.876325
C	6.805849	0.498845	7.861241
H	7.286366	-0.352118	8.346607
H	6.197668	0.125206	7.029640
C	6.063172	3.770468	9.450273
H	6.708665	3.664771	10.326728
H	5.016903	3.675185	9.741964
H	6.203514	4.754145	9.011863
C	8.905375	1.033672	6.536420
H	9.560889	1.882057	6.360926
H	8.539509	0.643998	5.581048
H	9.482848	0.257593	7.041702
O	7.563574	8.889540	5.840831
N	10.043066	5.596096	8.311650
N	11.864146	6.272118	9.600817
N	12.070141	6.539558	7.404477
N	4.790656	12.159865	3.669011
N	6.791744	13.133022	2.735538
N	5.348080	14.417705	3.832564
C	9.041717	5.978791	7.488709
C	5.109643	10.892389	4.013419
C	6.269694	10.511876	4.707432
H	7.037037	11.239587	4.934915
C	6.429166	9.216610	5.154474
C	7.715445	7.609318	6.291304
C	8.856157	7.279796	6.993487
H	9.588192	8.051674	7.189860
C	11.246727	6.142114	8.417061
C	13.227461	6.755177	9.443962
H	13.311269	7.783923	9.812329
H	13.925256	6.130478	10.003895
C	13.438897	6.655593	7.928146

H	13.999991	5.753891	7.666642
H	13.942767	7.527364	7.510062
C	11.279010	6.026550	10.900964
H	11.890881	5.309170	11.450541
H	11.213445	6.956389	11.474984
H	10.287640	5.599813	10.777262
C	11.928771	6.045317	6.039202
H	10.905119	6.162750	5.695767
H	12.573669	6.643182	5.394609
H	12.214707	4.991211	5.983469
C	5.627647	13.163806	3.446615
C	7.154024	14.508587	2.364439
H	8.229338	14.664962	2.453253
H	6.846122	14.693749	1.331430
C	6.341210	15.362602	3.345323
H	5.859638	16.211978	2.858234
H	6.948388	15.738625	4.176538
C	7.086085	12.090513	1.758412
H	6.441036	12.196180	0.881651
H	8.132487	12.185786	1.467226
H	6.945550	11.106864	2.196767
C	4.241731	14.827361	4.669876
H	3.589333	13.977531	4.849657
H	4.606919	15.222573	5.623185
H	3.661203	15.599097	4.161453
Cu	10.155078	3.457362	8.767237
Cl	9.270549	2.514532	10.646673
Cl	12.211677	2.939553	7.925171

[$(CuCl_2)_2$(L4)]- triplet

96

Energy = -7174.662020 hartree

Cu	3.040317	12.302932	2.525348
Cl	3.718641	13.834616	1.005169
Cl	0.818083	12.665658	2.744652
O	5.654031	6.910524	5.212009
N	3.071247	10.271450	2.867657
N	1.195221	9.470055	1.711948
N	1.205628	9.147026	3.900537
N	8.395657	3.670028	7.545795
N	6.266319	2.868081	8.342664
N	7.670942	1.445515	7.395220
C	4.132718	9.878950	3.692346
C	8.082990	4.980426	7.164036
C	6.968407	5.330510	6.397317
H	6.244213	4.582987	6.100976
C	6.775707	6.634176	5.968683
C	5.489219	8.229590	4.837814

C	4.361210	8.563787	4.105525
H	3.671808	7.773063	3.839781
C	1.899742	9.650928	2.849893
C	-0.183513	9.107318	2.014249
H	-0.545703	8.348841	1.319725
H	-0.826015	9.991383	1.948211
C	-0.067414	8.583594	3.453877
H	-0.879866	8.935491	4.090089
H	-0.046501	7.489276	3.494320
C	1.559160	10.009548	0.419374
H	1.106136	10.992796	0.265187
H	1.223787	9.323960	-0.361069
H	2.639960	10.111762	0.366839
C	1.460747	9.440379	5.294418
H	1.860797	8.573744	5.828310
H	0.527965	9.750844	5.769261
H	2.171876	10.257702	5.373915
C	7.477844	2.734909	7.747577
C	5.580064	1.578693	8.407348
H	4.748295	1.542059	7.695681
H	5.182755	1.412419	9.408956
C	6.693738	0.583421	8.047587
H	7.136402	0.121823	8.936227
H	6.353787	-0.199525	7.369165
C	5.843397	3.996124	9.144345
H	5.456365	3.630395	10.097459
H	5.066607	4.583422	8.646480
H	6.692821	4.642261	9.346993
C	8.907228	0.908240	6.868819
H	9.439043	1.692515	6.336480
H	8.677708	0.095277	6.177386
H	9.545870	0.536595	7.674883
O	7.551984	8.929543	5.901139
N	10.077344	5.591069	8.338207
N	11.940184	6.401639	9.509056
N	11.966691	6.684158	7.315116
N	4.755033	12.189636	3.662165
N	6.865277	13.014478	2.838841
N	5.472797	14.414941	3.835608
C	9.031534	5.976435	7.490394
C	5.080956	10.875290	4.018569
C	6.209049	10.520267	4.762943
H	6.933374	11.267546	5.059632
C	6.415724	9.211373	5.168644
C	7.702309	7.615867	6.299551
C	8.816601	7.286652	7.054776
H	9.505877	8.077606	7.320220
C	11.252525	6.204325	8.363566
C	13.325884	6.750069	9.222146

H	13.682105	7.518776	9.908462
H	13.961413	5.863328	9.314439
C	13.235944	7.248124	7.771572
H	14.056178	6.879882	7.154863
H	13.222498	8.341642	7.710886
C	11.552230	5.888903	10.805530
H	11.997162	4.906403	10.985682
H	11.878637	6.587541	11.578181
H	10.470165	5.793400	10.842211
C	11.730592	6.369442	5.922608
H	11.346436	7.230316	5.368083
H	12.667836	6.043107	5.467562
H	11.013550	5.557063	5.845781
C	5.664660	13.132338	3.458700
C	7.545246	14.307536	2.783346
H	8.389373	14.336002	3.480733
H	7.924070	14.492050	1.777772
C	6.434074	15.291825	3.179257
H	5.973139	15.765369	2.306334
H	6.783048	16.065481	3.863710
C	7.279743	11.899983	2.014199
H	7.652183	12.281394	1.061434
H	8.065130	11.307291	2.491787
H	6.429142	11.254602	1.813849
C	4.244737	14.938086	4.394509
H	3.726185	14.142629	4.923319
H	4.484367	15.740042	5.095318
H	3.589473	15.320696	3.607174
Cu	10.086630	3.566253	8.718609
Cl	9.363902	2.068785	10.252748
Cl	12.309768	3.182651	8.551707

[(CuClMeCN)$_2$(L4)] singlet

100

Energy = -6440.441870 hartree

Cu	2.958717	12.407588	2.656795
O	5.579099	6.984935	5.397612
N	2.892641	10.372190	3.249897
N	1.284717	9.442889	1.789137
N	1.001790	9.062217	3.962638
N	8.442906	3.633498	7.356067
N	6.454952	2.815163	8.438594
N	7.676930	1.406621	7.230736
C	3.968111	9.950893	3.958384
C	8.136697	4.904892	7.009357
C	6.929517	5.309530	6.396698
H	6.136895	4.587473	6.197371
C	6.743200	6.623726	5.998648

C	5.385362	8.269103	5.000045
C	4.193334	8.622059	4.386855
H	3.448364	7.843437	4.221034
C	1.793343	9.638105	3.019091
C	0.109450	8.571103	1.843654
H	0.365746	7.573280	1.444295
H	-0.712175	8.976144	1.233300
C	-0.220088	8.531611	3.346507
H	-1.076938	9.180960	3.603472
H	-0.444403	7.517630	3.710975
C	1.947617	9.733371	0.525747
H	1.194908	10.076555	-0.199524
H	2.436534	8.829340	0.121555
H	2.688884	10.535395	0.651790
C	1.029407	9.366653	5.381331
H	1.126201	8.446903	5.980541
H	0.096186	9.876963	5.677455
H	1.874483	10.027109	5.607997
C	7.536712	2.682351	7.642960
C	5.783225	1.519346	8.609947
H	4.798097	1.522704	8.111805
H	5.627530	1.313888	9.679116
C	6.766725	0.523953	7.962114
H	7.330163	-0.055329	8.715503
H	6.270926	-0.182580	7.279484
C	6.181680	3.951630	9.303580
H	5.676541	3.584950	10.207818
H	5.535752	4.701374	8.816601
H	7.131572	4.402619	9.622847
C	8.787436	0.891786	6.460101
H	9.298975	1.724370	5.961869
H	8.422641	0.184730	5.698450
H	9.509502	0.367175	7.111177
O	7.568971	8.875873	5.811071
N	10.255962	5.488400	7.957809
N	11.864968	6.417548	9.417496
N	12.146667	6.797873	7.243768
N	4.705090	12.227277	3.852737
N	6.693446	13.046584	2.771703
N	5.470441	14.454270	3.979511
C	9.180224	5.909771	7.249742
C	5.011402	10.955892	4.199290
C	6.218491	10.551313	4.812166
H	7.011009	11.273409	5.011722
C	6.404865	9.237087	5.210058
C	7.762787	7.591657	6.208461
C	8.954971	7.238613	6.821308
H	9.700052	8.017191	6.986881
C	11.355553	6.222280	8.187869

C	13.040378	7.289085	9.362156
H	12.784535	8.287011	9.761560
H	13.862299	6.883945	9.972053
C	13.369011	7.328339	7.859095
H	14.225591	6.678805	7.601688
H	13.593275	8.342239	7.494361
C	11.202760	6.127368	10.681321
H	11.955854	5.784228	11.406219
H	10.714166	7.031523	11.085642
H	10.461320	5.325406	10.555833
C	12.118169	6.493215	5.825138
H	12.021312	7.412905	5.225840
H	13.051073	5.982572	5.528569
H	11.272762	5.832976	5.599052
C	5.611200	13.178772	3.566767
C	7.365040	14.342607	2.601414
H	8.349924	14.339125	3.100030
H	7.521239	14.548696	1.532442
C	6.381073	15.337488	3.249334
H	5.818094	15.917314	2.496028
H	6.876405	16.043542	3.932795
C	6.967512	11.910579	1.906360
H	7.473019	12.277806	1.002554
H	7.613403	11.160815	2.393348
H	6.017923	11.459466	1.586382
C	4.359438	14.968515	4.749818
H	3.847493	14.135529	5.246945
H	4.723725	15.674881	5.512349
H	3.637885	15.493742	4.098685
Cu	10.189860	3.453072	8.551195
Cl	3.868095	12.931629	0.645518
Cl	9.281466	2.929196	10.562968
N	11.846910	2.389405	8.292913
C	12.764229	1.692780	8.375050
H	13.616595	1.032322	8.467680
N	1.301501	13.471100	2.914376
C	0.384144	14.167624	2.831865
H	-0.468254	14.827987	2.738885

[(CuClMeCN)$_2$(L4)] triplet

100

Energy = -6440.681820 hartree

Cu	3.068371	12.319580	2.598499
O	5.575921	6.953374	5.361715
N	2.957717	10.325843	3.088145
N	1.177331	9.515286	1.793501
N	1.123757	9.013637	3.953974
N	8.433139	3.656955	7.429299

N	6.385867	2.858680	8.426731
N	7.591166	1.474499	7.199800
C	4.027690	9.917759	3.875623
C	8.119507	4.957688	7.079332
C	6.937298	5.338186	6.428884
H	6.166434	4.610815	6.212681
C	6.747092	6.639450	6.010377
C	5.414677	8.259149	4.964638
C	4.246091	8.605013	4.313168
H	3.522563	7.825139	4.119817
C	1.821474	9.634251	2.970897
C	0.003044	8.652561	1.919344
H	0.200897	7.691764	1.434436
H	-0.868604	9.099170	1.440474
C	-0.155421	8.511620	3.439022
H	-0.970784	9.130712	3.825715
H	-0.332373	7.483246	3.753833
C	1.751465	9.771463	0.483215
H	1.035678	10.318755	-0.130689
H	1.994153	8.829327	-0.017325
H	2.653199	10.367300	0.585461
C	1.238679	9.309366	5.372435
H	1.356846	8.388774	5.946266
H	0.335554	9.820916	5.717496
H	2.096563	9.947504	5.555853
C	7.486604	2.724158	7.669500
C	5.660150	1.585791	8.517783
H	4.698248	1.657093	8.003863
H	5.475906	1.337851	9.562789
C	6.617803	0.589819	7.840966
H	7.123603	-0.055890	8.563816
H	6.120435	-0.034641	7.099278
C	6.088655	3.948106	9.335766
H	5.955787	3.547562	10.342005
H	5.178488	4.472694	9.035342
H	6.914375	4.651493	9.355413
C	8.697464	0.946282	6.431232
H	9.233662	1.767035	5.963367
H	8.316985	0.278677	5.657050
H	9.381003	0.386897	7.076658
O	7.573043	8.907077	5.845611
N	10.191221	5.534746	8.119319
N	11.972535	6.345314	9.412678
N	12.025386	6.845596	7.251864
N	4.714925	12.203812	3.779681
N	6.762267	13.003972	2.783873
N	5.555626	14.386507	4.011332
C	9.121115	5.942765	7.332028
C	5.028971	10.902998	4.128982

C	6.211236	10.522487	4.779308
H	6.981959	11.249914	4.995817
C	6.401707	9.221081	5.197276
C	7.734245	7.601332	6.242786
C	8.902871	7.255436	6.894154
H	9.626559	8.035234	7.087220
C	11.327816	6.225910	8.235641
C	13.147130	7.207463	9.285767
H	12.949843	8.168716	9.770006
H	14.018763	6.760861	9.764668
C	13.305096	7.347165	7.765934
H	14.119901	6.727239	7.379393
H	13.482594	8.375183	7.450272
C	11.398827	6.090236	10.723368
H	12.114728	5.543233	11.337394
H	11.156537	7.032790	11.223314
H	10.496927	5.494517	10.621897
C	11.909740	6.549004	5.833643
H	11.792586	7.469367	5.259240
H	12.812128	6.036081	5.488678
H	11.050998	5.911842	5.650872
C	5.661085	13.137297	3.540659
C	7.487328	14.277333	2.694154
H	8.449105	14.206110	3.208311
H	7.671768	14.526260	1.649414
C	6.528913	15.272227	3.371504
H	6.023197	15.918455	2.649062
H	7.025656	15.896158	4.114061
C	7.060415	11.915527	1.873972
H	7.193147	12.316995	0.868081
H	7.970929	11.391377	2.174111
H	6.235232	11.211529	1.853633
C	4.448758	14.913496	4.779921
H	3.912727	14.092059	5.246774
H	4.828596	15.580538	5.554905
H	3.765257	15.473182	4.134718
Cu	10.080107	3.541231	8.610027
Cl	3.767518	13.660064	0.956755
Cl	9.380931	2.202486	10.253181
N	12.017347	2.818857	8.514196
C	12.941905	2.166483	8.673220
H	13.797805	1.544791	8.834348
N	1.130624	13.040858	2.693881
C	0.205783	13.692854	2.534960
H	-0.650386	14.314204	2.373935

[$(CuBr_2)_2$(L1)] – singlet

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Energy = -15254,7245564361 hartree

Cu	3.279396	10.567416	3.526515
Br	2.740316	9.413193	1.461799
N	1.971093	12.321153	3.594298
N	-0.028673	11.257031	4.081404
N	0.203870	12.364650	2.040527
C	2.539871	13.529871	3.522840
C	1.865145	14.752803	3.523709
H	0.782998	14.752916	3.523273
C	0.711730	12.014204	3.245321
C	0.321777	11.195837	5.501843
H	1.063590	10.417602	5.698832
H	-0.588666	10.987265	6.066527
H	0.725591	12.150627	5.827723
C	-0.814944	10.119725	3.596390
H	-0.660056	9.979671	2.531016
H	-1.879588	10.243625	3.809786
H	-0.457042	9.219266	4.098527
C	-1.225881	12.470341	1.786486
H	-1.779260	12.456050	2.721439
H	-1.588642	11.664351	1.143299
H	-1.419416	13.420197	1.281321
C	1.067981	12.716931	0.917470
H	1.185923	13.801230	0.828910
H	0.613827	12.333377	0.003584
H	2.033893	12.232996	1.031651
N	1.971991	17.184611	3.454923
N	-0.026578	18.250378	2.967145
N	0.202343	17.138622	5.006168
C	2.540201	15.975509	3.525749
C	0.712242	17.491276	3.802835
C	0.326131	18.314717	1.547417
H	1.067435	19.094142	1.353260
H	-0.583601	18.523405	0.981610
H	0.731584	17.361036	1.220367
C	-0.814103	19.386327	3.453150
H	-0.661620	19.523854	4.519199
H	-1.878264	19.262688	3.237197
H	-0.455385	20.288059	2.953874
C	-1.227832	17.031956	5.257412
H	-1.779512	17.047462	4.321476
H	-1.592140	17.836772	5.901200
H	-1.421908	16.081238	5.760751
C	1.064429	16.784979	6.130353
H	1.181691	15.700549	6.218182
H	0.608907	17.167965	7.043810
H	2.030768	17.268561	6.018269
N	4.589196	12.320509	3.455282
N	6.588047	11.254912	2.968109

N	6.358503	12.367125	5.006833
C	4.020900	13.529577	3.525878
C	4.695940	14.752270	3.524639
H	5.778088	14.752154	3.525030
C	5.848884	12.014020	3.803497
C	6.235487	11.189933	1.548374
H	5.494588	10.410078	1.354421
H	7.145352	10.981493	0.982695
H	5.829558	12.143284	1.220965
C	7.375970	10.119417	3.454557
H	7.223729	9.982386	4.520695
H	8.440044	10.243277	3.238314
H	7.017407	9.217318	2.955832
C	7.788574	12.475061	5.258112
H	8.340351	12.459124	4.322243
H	8.153422	11.671092	5.902651
H	7.981918	13.426379	5.760617
C	5.496015	12.720657	6.130736
H	5.377489	13.805016	6.217749
H	5.951968	12.338911	7.044496
H	4.530221	12.235891	6.018975
N	4.590042	17.183928	3.594120
N	6.590336	18.247224	4.080991
N	6.356771	17.140062	2.039951
C	4.021217	15.975210	3.523116
C	5.849497	17.490435	3.245018
C	6.240198	18.308623	5.501489
H	5.499578	19.087928	5.698722
H	7.151026	18.515664	6.066122
H	5.834890	17.354408	5.827185
C	7.377728	19.383690	3.595928
H	7.222528	19.524162	2.530648
H	8.442337	19.258526	3.808794
H	7.021133	20.284431	4.098482
C	7.786342	17.032884	1.785560
H	8.339994	17.046518	2.720359
H	8.149788	17.838539	1.142337
H	7.978788	16.082853	1.280299
C	5.491948	16.788797	0.917109
H	5.372520	15.704653	0.828655
H	5.946469	17.171623	0.003099
H	4.526721	17.274074	1.031479
Cu	3.282004	18.937630	3.527052
Br	3.820180	20.092585	1.462661
Br	2.745094	20.085264	5.595829
Br	3.817607	9.418977	5.594663

[$(CuBr_2)_2$(L1)]

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Energy = -15254.7448838898 hartree

Cu	3.280711	10.727936	3.524229
Br	2.358112	9.252342	1.858056
N	1.935388	12.275897	3.490954
N	-0.094613	11.176457	3.619298
N	0.217612	12.731380	1.917123
C	2.575875	13.528092	3.486611
C	1.904673	14.752405	3.524162
H	0.823659	14.752403	3.523775
C	0.711982	12.081552	3.013417
C	0.186956	10.720831	4.976114
H	0.801998	9.816946	4.974635
H	-0.762055	10.499821	5.470053
H	0.711622	11.494800	5.527928
C	-0.997511	10.307301	2.870324
H	-0.919640	10.505542	1.806846
H	-2.033147	10.439412	3.196929
H	-0.701475	9.269282	3.033077
C	-1.171249	13.137413	1.792413
H	-1.708760	12.931426	2.714320
H	-1.676214	12.623569	0.968573
H	-1.218014	14.213881	1.594928
C	1.093642	13.152658	0.835263
H	1.288739	14.228988	0.863666
H	0.617181	12.905793	-0.116719
H	2.035289	12.614666	0.894967
N	1.935327	17.229048	3.557578
N	-0.094784	18.328294	3.429106
N	0.217637	16.773648	5.131513
C	2.575749	15.976782	3.561995
C	0.711927	17.423388	4.035126
C	0.186601	18.783627	2.072152
H	0.801595	19.687541	2.073356
H	-0.762478	19.004462	1.578267
H	0.711247	18.009559	1.520456
C	-0.997835	19.197423	4.177923
H	-0.919731	18.999551	5.241454
H	-2.033488	19.064902	3.851540
H	-0.702124	20.235468	4.014770
C	-1.171171	16.367442	5.256259
H	-1.708682	16.573272	4.334311
H	-1.676252	16.881302	6.080019
H	-1.217776	15.290991	5.453839
C	1.093854	16.352214	6.213162
H	1.289001	15.275897	6.184543
H	0.617528	16.598886	7.165262
H	2.035469	16.890265	6.153383

N	4.625833	12.275958	3.557782
N	6.656011	11.176826	3.429158
N	6.343636	12.731500	5.131533
C	3.985297	13.528151	3.562163
C	4.656392	14.752509	3.524518
H	5.737409	14.752541	3.524722
C	5.849279	12.081705	4.035226
C	6.374493	10.721420	2.072267
H	5.759597	9.817434	2.073542
H	7.323524	10.500682	1.578241
H	5.849695	11.495419	1.520614
C	7.559114	10.307732	4.177955
H	7.481148	10.505749	5.241468
H	8.594726	10.440176	3.851410
H	7.263334	9.269683	4.014961
C	7.732474	13.137665	5.256186
H	8.269927	12.931769	4.334224
H	8.237550	12.623800	6.079943
H	7.779115	14.214115	5.453751
C	5.467527	13.152928	6.213269
H	5.272382	14.229247	6.184671
H	5.943938	12.906230	7.165318
H	4.525907	12.614878	6.153584
N	4.625743	17.228950	3.490910
N	6.655734	18.328360	3.619623
N	6.343820	16.773409	1.917422
C	3.985176	15.976796	3.486545
C	5.849246	17.423224	3.013625
C	6.373782	18.784094	4.976311
H	5.758681	19.687942	4.974625
H	7.322645	19.005202	5.470495
H	5.849037	18.010130	5.528064
C	7.558593	19.197623	2.870727
H	7.480944	18.999235	1.807261
H	8.594190	19.065738	3.197545
H	7.262317	20.235596	3.033319
C	7.732744	16.367490	1.792914
H	8.270071	16.573436	2.714933
H	8.237790	16.881477	0.969217
H	7.779615	15.291053	1.595298
C	5.468032	16.352286	0.835307
H	5.272821	15.275974	0.863574
H	5.944758	16.599199	-0.116528
H	4.526422	16.890372	0.894807
Cu	3.280613	18.776996	3.523796
Br	4.203423	20.251615	1.856876
Br	2.357745	20.253712	5.188823
Br	4.203378	9.252228	5.190253

[(CuBrMeCN)$_2$(L1)] - singlet

98

Energy = -10292.9760705747 hartree

Cu	5.782936	9.742386	4.369438
N	4.520019	8.031814	4.733628
N	2.415217	8.039421	3.675230
N	2.671629	8.926154	5.819182
N	7.052539	8.056933	4.048274
N	9.268748	8.247860	4.778066
N	8.706517	8.750228	2.559673
N	7.053587	3.212536	3.702177
N	8.895620	2.322262	2.603002
N	9.164624	3.202376	4.748290
N	4.523381	3.186917	4.395130
N	2.304604	2.992401	3.673764
N	2.874845	2.497548	5.891781
C	5.055573	6.835619	4.483216
C	6.514216	6.853625	4.145047
C	7.171994	5.637178	3.897514
H	8.220238	5.659882	3.629216
C	6.519158	4.408492	3.955663
C	5.061081	4.390347	4.296287
C	4.403076	5.606891	4.542899
H	3.354799	5.584355	4.811107
C	3.188164	8.300095	4.746820
C	2.986272	7.843052	2.341562
H	3.923398	8.386265	2.251922
H	2.292482	8.257766	1.611217
H	3.131793	6.780330	2.127279
C	0.966476	7.863169	3.759446
H	0.654566	7.731921	4.791351
H	0.701218	6.964485	3.198626
H	0.425517	8.703842	3.321296
C	1.658774	9.982778	5.712854
H	1.514701	10.267668	4.675446
H	2.025369	10.857660	6.251870
H	0.706590	9.682109	6.152790
C	3.349557	8.857502	7.112109
H	3.948479	7.954627	7.179910
H	2.595225	8.840773	7.899577
H	3.994600	9.726197	7.264028
C	8.368091	8.321657	3.779138
C	8.850799	8.157307	6.177364
H	7.851080	8.561813	6.299018
H	9.545471	8.737904	6.784615
H	8.866665	7.122105	6.527620
C	10.708903	8.109258	4.557893
H	10.914197	7.840204	3.526458
H	11.075154	7.310394	5.205189

H	11.251770	9.022420	4.808392
C	9.704264	9.801451	2.318565
H	10.041035	10.235941	3.254118
H	9.221508	10.586108	1.734793
H	10.560431	9.423841	1.757740
C	7.833586	8.480916	1.406991
H	7.316533	7.534940	1.537074
H	8.465274	8.412182	0.521450
H	7.103601	9.283304	1.281982
C	8.385508	2.944672	3.680554
C	8.209078	2.394115	1.314759
H	7.562790	1.525941	1.165117
H	8.958207	2.412465	0.522387
H	7.610054	3.297338	1.252956
C	9.910060	1.266206	2.699090
H	10.858346	1.568548	2.251911
H	9.539778	0.392077	2.161352
H	10.063051	0.979394	3.734666
C	8.601301	3.395406	6.085774
H	8.458718	4.457718	6.304037
H	9.298578	2.977408	6.810901
H	7.663792	2.853479	6.179082
C	10.612844	3.379317	4.656230
H	11.156540	2.537703	5.089152
H	10.880946	4.276620	5.217890
H	10.918857	3.513424	3.622941
C	3.208692	2.922371	4.669798
C	0.865045	3.130184	3.898504
H	0.322319	2.215723	3.652553
H	0.495756	3.926810	3.250187
H	0.663060	3.402048	4.929852
C	2.717624	3.079587	2.272782
H	3.717370	2.675857	2.148763
H	2.699411	4.113821	1.919815
H	2.021472	2.496602	1.669530
C	1.879031	1.446072	6.139750
H	1.024546	1.824538	6.702563
H	2.364807	0.663742	6.724137
H	1.539264	1.008379	5.206789
C	3.751087	2.771683	7.040816
H	4.481595	1.969932	7.166727
H	3.121921	2.843822	7.927880
H	4.267488	3.717260	6.905482
Cu	5.789843	1.502926	4.069681
Br	5.132708	10.944043	2.407263
Br	6.441253	0.303645	6.034553
N	5.338603	0.146201	2.676365
C	5.154142	-0.856755	2.154276
H	4.989928	-1.805861	1.688755

N	6.234917	11.095274	5.768927
C	6.411998	12.096318	6.297190
H	6.569945	13.043709	6.768348

[(CuBrMeCN)$_2$(L1)] - triplet

98

Energy = -10292.9639489927 hartree

Cu	5.678032	9.628235	4.203638
N	4.494636	8.100546	4.684195
N	2.288905	7.862517	3.852631
N	2.702567	9.023178	5.828208
N	6.976407	8.163131	3.783096
N	9.286464	7.921499	4.278625
N	8.559578	9.323996	2.566783
N	7.079178	3.236301	3.730612
N	9.018172	2.247245	2.931755
N	9.054485	3.287795	5.020149
N	4.548949	3.184737	4.519930
N	2.370458	3.116379	3.632475
N	2.810562	2.308222	5.782366
C	5.065172	6.862961	4.396286
C	6.455953	6.889270	4.025807
C	7.127773	5.687409	3.835269
H	8.160984	5.697672	3.517650
C	6.492436	4.441670	3.976346
C	5.089520	4.415015	4.324242
C	4.422452	5.637756	4.531417
H	3.387033	5.614637	4.843322
C	3.157600	8.311461	4.784586
C	2.698161	7.664423	2.465833
H	3.610760	8.215584	2.263564
H	1.913461	8.050531	1.814116
H	2.853922	6.606308	2.243218
C	0.897991	7.527070	4.143533
H	0.738745	7.460465	5.215860
H	0.677878	6.554322	3.698720
H	0.202481	8.254740	3.720659
C	1.563301	9.941124	5.737112
H	1.260205	10.067845	4.703723
H	1.883594	10.914684	6.109649
H	0.719850	9.596968	6.338436
C	3.494016	9.166531	7.047635
H	4.193129	8.342526	7.145306
H	2.816605	9.167300	7.902596
H	4.043925	10.111468	7.044485
C	8.269970	8.440733	3.545405
C	9.099300	7.541938	5.673016
H	8.168331	7.952736	6.052142

H	9.928270	7.939337	6.262277
H	9.077975	6.457215	5.792130
C	10.608349	7.631770	3.726934
H	10.596471	7.722482	2.644811
H	10.876742	6.604373	3.983176
H	11.376975	8.291844	4.134933
C	9.690710	10.249185	2.625101
H	10.132974	10.248888	3.616821
H	9.325046	11.254296	2.407009
H	10.457333	10.002646	1.887667
C	7.656203	9.538039	1.433696
H	6.986108	8.691546	1.325377
H	8.255584	9.638954	0.527417
H	7.064577	10.447965	1.560133
C	8.384442	2.957243	3.889914
C	8.503224	2.233278	1.566162
H	7.855370	1.369501	1.395463
H	9.345552	2.175873	0.875035
H	7.939946	3.139589	1.365430
C	9.960442	1.167444	3.243395
H	10.970970	1.396452	2.899804
H	9.622627	0.261123	2.738079
H	9.967400	0.965730	4.309843
C	8.356713	3.482309	6.290841
H	8.169179	4.539938	6.493819
H	8.978898	3.077242	7.088798
H	7.421240	2.930097	6.289300
C	10.504794	3.444261	5.071940
H	10.991148	2.612981	5.586987
H	10.736712	4.357374	5.624869
H	10.914742	3.529963	4.069268
C	3.234296	2.901275	4.655754
C	0.929794	3.275831	3.812467
H	0.369777	2.409541	3.453603
H	0.603670	4.144228	3.236214
H	0.693036	3.444894	4.858781
C	2.843180	3.276587	2.260969
H	3.847265	2.875975	2.161207
H	2.849664	4.326921	1.959172
H	2.174683	2.731611	1.592649
C	1.806174	1.240510	5.807266
H	0.908438	1.540729	6.350620
H	2.244457	0.378672	6.312912
H	1.537769	0.941284	4.798974
C	3.583639	2.436115	7.023914
H	4.276095	1.600301	7.139151
H	2.881802	2.450171	7.858726
H	4.145727	3.365061	7.020081
Cu	5.819766	1.571610	4.137793

Br	4.162242	11.261008	3.422786
Br	6.506851	0.180642	5.954853
N	5.380143	0.202505	2.710740
C	5.206261	-0.791491	2.170759
H	5.052219	-1.732176	1.684942
N	6.975377	11.071481	5.035288
C	7.387936	12.032449	5.494900
H	7.758296	12.943372	5.919828

$[(CuZn_2)_2(L4)]^+$

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Energy = -7457.040280

Zn	9.456132	17.549591	1.197510
Zn	9.926946	6.035333	6.999754
Cl	9.534641	18.011194	-0.970084
Cl	9.778681	6.359711	9.231228
Cl	9.273348	19.133353	2.799083
Cl	10.117154	4.031530	6.068905
O	11.068666	11.989004	4.376591
O	8.277158	11.797350	4.222580
N	11.210155	7.604265	6.350698
N	8.521300	7.416064	6.195321
N	8.170702	15.992200	1.869730
N	6.585136	6.156408	6.097371
N	10.859848	16.175122	2.014891
N	12.594378	16.744054	3.525234
N	12.873147	16.994436	1.227793
C	7.224389	7.266265	6.513788
N	13.300702	6.627275	6.493811
N	12.911863	8.602707	7.662101
N	6.556703	8.151841	7.295817
C	8.199810	13.883614	3.110394
H	7.128345	13.760478	3.038868
N	6.159810	16.528656	0.862742
N	6.222540	16.310174	3.179584
C	14.010140	16.598144	3.844458
H	14.109935	15.896114	4.676655
H	14.461957	17.546077	4.146747
H	14.553494	16.201074	2.991589
C	8.826688	15.010698	2.565422
C	11.154505	9.855836	5.395374
H	12.231273	9.949348	5.407912
C	10.330515	12.978658	3.794240
C	5.124100	8.395358	7.169846
H	4.958711	9.473174	7.090998
H	4.568511	8.031338	8.037575
H	4.734912	7.920423	6.273631
C	10.532873	8.700238	5.883247
C	6.933364	16.647705	4.409031

H	7.154506	15.755330	5.002378
H	6.300101	17.310196	5.001311
H	7.850599	17.181133	4.173797
C	5.605044	5.449582	6.920233
H	5.904338	4.401883	6.982374
H	4.601900	5.496500	6.489749
H	5.589929	5.857777	7.926392
C	9.018264	10.791715	4.773449
C	10.271799	15.109097	2.643728
C	9.088411	8.599690	5.801013
C	8.932889	12.883064	3.717774
C	12.680254	16.434352	-0.111730
H	12.124624	15.504016	-0.047883
H	13.662649	16.238246	-0.546758
H	12.129286	17.124281	-0.752095
C	6.856294	16.250079	1.981201
C	12.106332	16.610129	2.266155
C	12.003747	9.327228	8.545635
H	11.764255	10.318789	8.149585
H	12.490872	9.448918	9.514497
H	11.094454	8.751488	8.696795
C	10.415623	10.888014	4.851162
C	7.247000	8.985959	8.274698
H	8.204521	8.541110	8.532501
H	6.639647	9.027495	9.180332
H	7.389126	10.005653	7.903988
C	11.717472	16.969074	4.670210
H	11.560250	16.049401	5.241895
H	10.765678	17.373123	4.335634
H	12.186542	17.707403	5.322600
C	13.129844	5.866935	5.253722
H	12.649593	4.906104	5.443030
H	14.115596	5.701572	4.813519
H	12.515702	6.428269	4.556510
C	12.469162	7.635602	6.819077
C	14.267527	6.062286	7.433584
H	14.112508	4.982753	7.474515
H	14.108237	6.465302	8.429282
H	15.297431	6.250988	7.121404
C	13.774064	18.144062	1.289883
H	14.822158	17.845095	1.213451
H	13.618688	18.698096	2.210840
H	13.542357	18.804332	0.452345
C	8.372069	9.663473	5.239362
H	7.297953	9.608497	5.131747
C	10.982715	14.073531	3.261989
H	12.062353	14.097226	3.307825
C	14.300947	9.046087	7.697477
H	14.321627	10.136728	7.623097

H	14.853662	8.632986	6.858329
H	14.798346	8.761961	8.628073
C	4.814595	15.968435	3.348038
H	4.724529	15.255214	4.171763
H	4.425237	15.504436	2.446204
H	4.206702	16.843272	3.591244
C	5.106070	17.540894	0.815347
H	5.082140	18.107040	1.741695
H	4.124320	17.098710	0.629790
H	5.332545	18.230699	0.000485
C	6.570865	16.005956	-0.442291
H	7.085621	16.768618	-1.027892
H	5.677483	15.676121	-0.977000
H	7.240676	15.162199	-0.309238
C	7.002370	5.443956	4.887605
H	7.609059	6.094295	4.265262
H	6.106718	5.150008	4.336019
H	7.586294	4.556432	5.134260

$[(CuCl_2)_2(L4)]$
104
Energy = -7179.208800

O	2.199726	7.075446	7.920383
N	1.470710	5.555299	3.374503
N	-0.298192	4.458068	4.513019
N	-0.685921	5.644657	2.550237
N	4.104889	5.264827	2.996791
N	5.888431	4.482674	1.753670
N	6.016952	6.625793	2.649081
C	2.301437	5.846276	4.465988
C	3.696014	5.756273	4.244604
C	4.566820	6.058968	5.296372
H	5.635920	5.947767	5.179436
C	4.091787	6.490016	6.523201
C	2.723809	6.628574	6.723602
C	1.843596	6.308840	5.703954
H	0.786688	6.442524	5.888508
C	0.189318	5.225578	3.493471
C	0.519960	3.429677	5.135929
H	1.366505	3.196836	4.496497
H	-0.082415	2.525110	5.251418
H	0.883823	3.737655	6.120964
C	-1.610684	4.660420	5.102316
H	-2.075527	5.551591	4.688754
H	-1.504757	4.794349	6.184059
H	-2.272708	3.805618	4.932258
C	-0.340453	6.743313	1.654922
H	0.338290	7.429885	2.151856
H	-1.258618	7.270781	1.387425

H	0.135241	6.377165	0.740989
C	-1.777963	4.802352	2.070877
H	-1.781851	3.852444	2.594203
H	-1.618110	4.592075	1.011815
H	-2.743460	5.299903	2.198707
C	5.316481	5.464012	2.489341
C	5.395206	3.112257	1.835708
H	4.984454	2.922321	2.822732
H	6.231798	2.434059	1.654169
H	4.619196	2.923244	1.088841
C	6.678688	4.764284	0.558631
H	6.746756	5.833871	0.392476
H	6.172277	4.330446	-0.305483
H	7.682166	4.337238	0.641110
C	7.462039	6.669094	2.793117
H	7.863921	5.661444	2.859139
H	7.717836	7.205829	3.712808
H	7.942133	7.186632	1.956770
C	5.333265	7.903631	2.770953
H	4.309200	7.806534	2.422312
H	5.843257	8.635231	2.139252
H	5.332145	8.269996	3.802170
Cu	2.526779	4.927599	1.733402
Cl	3.400253	5.756089	-0.175349
Cl	1.190222	3.241289	1.053360
O	5.010494	6.773953	7.514129
N	5.739516	8.292733	12.060363
N	7.508112	9.390501	10.921900
N	7.896361	8.203224	12.884145
N	3.105312	8.583215	12.438260
N	1.321858	9.365007	13.681726
N	1.193138	7.222265	12.785385
C	4.908684	8.002166	10.968856
C	3.514111	8.092202	11.190238
C	2.643344	7.789750	10.138359
H	1.574232	7.900812	10.255328
C	3.118423	7.359160	8.911384
C	4.486400	7.220554	8.711004
C	5.366573	7.539898	9.730802
H	6.423484	7.406200	9.546269
C	7.020863	8.622624	11.941296
C	6.689778	10.419042	10.299478
H	5.843338	10.651620	10.939143
H	7.292077	11.323684	10.184181
H	6.325756	10.111372	9.314407
C	8.820543	9.188491	10.332350
H	9.285577	8.297271	10.745593
H	8.714485	9.054853	9.250583
H	9.482470	10.043338	10.502559

C	7.551297	7.104106	13.779056
H	6.872352	6.417772	13.282071
H	8.469586	6.576523	14.045897
H	7.075988	7.469796	14.693373
C	8.988670	9.045271	13.363366
H	8.992381	9.995389	12.840418
H	8.829296	9.255127	14.422581
H	9.954082	8.547713	13.234907
C	1.893746	8.383886	12.945701
C	1.815147	10.735427	13.600130
H	2.225868	10.925670	12.613152
H	0.978595	11.413604	13.781926
H	2.591196	10.924158	14.347029
C	0.531596	9.083050	14.876684
H	0.463424	8.013414	15.042467
H	1.038069	9.516532	15.740940
H	-0.471840	9.510226	14.794372
C	-0.251932	7.179214	12.641134
H	-0.653685	8.186945	12.575585
H	-0.507666	6.642993	11.721124
H	-0.732205	6.661290	13.477140
C	1.876687	5.944427	12.662755
H	2.900776	6.041211	13.011412
H	1.366641	5.212510	13.294048
H	1.877730	5.578665	11.631324
Cu	4.683605	8.919807	13.701721
Cl	3.810389	8.090779	15.610320
Cl	6.020255	10.605916	14.382163

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