# Supporting Information



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## Experimental Procedures

### Materials

All general reagents and chemicals were used as purchased from Sigma-Aldrich, Fluka and Merck chemical companies without further purification unless otherwise stated. The ligand precursor ([2,2'-bipyridine]-6,6'-dicarboxylic acid) and 5-amino-*m*-xylol-4-sulfonic acid were prepared according to the experimental procedure reported in the literature.[1,2] Air and moisture sensitive reactions were carried out under $N_2$ or Ar in oven-dried (120 °C) glassware. Evaporation of solvents *in vacuo* was done with a *Büchi Rotevapor R-200* at 40 °C.

### Instrumentation and measurements

NMR spectra were measured on a *Bruker AV-500, Bruker AV-400,* and *Bruker 300 MHz* spectrometers. All NMR experiments were performed at room temperature in corresponding deuterated solvents and using solvent signals as reference. UV-Vis spectra were measured on a *Cary 50 UV-vis* spectrometer by *Varian Inc*. Electrospray ionization mass spectra (ESI-MS) were performed on an *Agilent Technologies 6130-Quadrupole LC/MS* connected to an *Agilent Technologies HPLC-1200 series*. Samples were dissolved in MeOH or $H_2O$ and injected directly with an auto-sampler. HRMS samples were measured on a Bruker HPLC-QqTOF Maxis impact device. Elemental Analysis of the samples was carried out in a Thermo Finnigan elemental analyzer Flash 1112 model. Electron Paramagnetic Resonance was performed in an EMX Micro X-band EPR spectrometer (Bruker) at 77 K using a liquid N2 finger dewar. Data acquisition: perpendicular mode, modulation frequency of 100 KHz, microwave frequency of 9.38 GHz, modulation amplitude of 4 G, a 0.01 ms time constant and 4.12 ms conversion time with a microwave power of 0.556 mW.

### Electrochemical measurements

Differential pulse voltammetry (DPV) and cyclic voltammetry (CV) were measured on a CHI660D potentiostat using a three-electrode cell. Glassy carbon (GC), Carbon paper (C-paper, SGL Carbon, Sigracet 39 AA) or boron-doped diamond (BDD) (d = 3 mm) working electrodes were employed while a Pt rod/mesh was used as counter electrode and a $Hg/HgSO_4$ ($K_2SO_4$ sat.) or Ag/AgCl (KCl sat.) electrode were used as a reference electrode. Working electrodes were polished with 1 and 0.05 micron alumina paste, washed with distilled water and acetone, and sonicated in acetone for 5 minutes before each measurement. DMF employed for electrochemical measurements was prepared containing the necessary amount of *n*-$Bu_4NPF_6$ ($TBAPF_6$) as supporting electrolyte to yield a solution of 0.1 M ionic strength. CVs were typically recorded at different scan rates from 25 to 1000 mV/s. DPVs were recorded with the following parameters: amplitude = 50 mV, step height = 4 mV, pulse width = 0.05 s. All redox potentials in the present work are reported versus NHE by adding 0.648 V to the measured potential.

# SUPPORTING INFORMATION

### $O_2$ evolution experiments

Controlled Potential Electrolysis (CPE) experiments were performed at different potentials and different pH values to catalyze the water oxidation reaction by the complexes by using a two-compartment cell closed with a septum. As working electrode large surface BDD electrodes (rectangular shape with 1.5 $cm^2$ surface) were used together with a silver/silver chloride (KCl sat.) as a reference electrode. These ones were placed in one of the compartments that was filled with a 1.5 mM solution of the complex (phosphate buffer pH 7, borate buffer pH 9 or phosphate buffer pH 11.6, of 0.1 M ionic strength). In the other compartment, containing only the buffer solution, a mesh platinum counter electrode was used.
The oxygen evolution was monitored with an OXNP type Clark electrode in gas phase (from Unisense Company). The CPE was carried out using an IJ-Cambria CHI-660 potentiostat and was started as soon as the oxygen sensor signal was stable under air atmosphere. During the experiment, solutions of both compartments were vigorously stirred. Calibration of the oxygen sensor was performed after each experiment by adding known amounts of pure oxygen into the cell using a Hamilton syringe. The results of the water oxidation catalysis with the complexes were compared with blank experiments under the same conditions but in the absence of the complex. The Faradaic efficiency was determined according to the total charge passed during the CPE and the total amount of generated oxygen by considering that water oxidation is a $4e^-$ oxidation process.

### Foot of the Wave Analysis (FOWA). $k_{obs}$ Calculation

Under catalytic conditions FOWA equation is operative.

$$\frac{i}{i_p} = \frac{n \cdot 2.24 \cdot \sqrt{\frac{R \cdot T}{F \cdot v} k_{obs}}}{1+\exp[\frac{F}{RT}(E^o{}_{cat} - E)]} \qquad \text{Equation (1)}$$

where $k_{obs}$ is the apparent WNA pseudo-rate constant ($k[H_2O]$), $E^0_{cat}$ corresponds to the standard potential for the catalytic wave ($E^0_{cat}$ according to the DPVs shown in Figure S46), $i$ is the current in the presence of substrate, $i_p$ corresponds to the peak current of one-electron redox process of the catalyst (extracted from the $Cu^{II}/Cu^{I}$ couple when available), $F$ is the faradaic constant (96485 C $mol^{-1}$), T is the temperature (298 K), $v$ is the scan rate (100 mV $s^{-1}$) and $R$ is 8.314 J $mol^{-1}$ $K^{-1}$.[3]

### TON Calculation

The total TON values can be obtained from the oxygen evolution experiment taking in account the total amount of catalyst present in the solution by using equation (2). However, since only the catalyst present in the layer of the solution in contact with the electrode is involved in the water oxidation reaction, this TON value is underestimated. Lin and co-workers adapted it to the formula (3) based on the previous methodology developed by Savéant and co-workers, which gives a more realistic TON value based on the amount catalyst in contact with the electrode.[4]

$$TON = \frac{\mu mol\ produced\ O_2}{\mu mol\ cat.} \qquad \text{Equation (2)}$$

$$TON = \frac{k_{obs} t}{1+\exp[\frac{F}{RT}(E^o{}_{cat} - E)]} \qquad \text{Equation (3)}$$

### Synthesis of the ligands

The general procedure for the synthesis of ligands, $[H_2L1]$, $[H_2L3]$, $[H_2L4]^{2-}$ and $[H_2L5]^{2-}$ was adapted from the literature[5] as follows: 500 mg (2.05 mmol) of [2,2'-bipyridine]-6,6'-dicarboxylic acid were suspended in 20 mL of $SOCl_2$ and the mixture was refluxed at 85 °C under a nitrogen atmosphere during 6 hours. After complete dissolution of the reactant, $SOCl_2$ was completely removed under vacuum, yielding a white powder corresponding to the acyl chloride derivative. The white solid was re-suspended in 40 mL of dry DCM and the temperature was decreased until 0 °C using an ice bath. Then, 4 eq. of $NEt_3$ were added dropwise and stirred for 10 minutes. Finally, a previously prepared dispersion of the corresponding phenylamine or naphthylamine (4.1 mmol, 2.0 eq.) in 40 mL of dry DCM were added dropwise to the reaction volume and the mixture was vigorous stirred for 72 h at room temperature. The appearing solid consisted in the corresponding ligand ($[H_2L1]$, $[H_2L3]$, $[H_2L4]^{2-}$ and $[H_2L5]^{2-}$), which was filtered and washed with DCM and $Et_2O$, yielding the desired product without further purification.
In case of ligands $[H_2L2]$, $[H_2L6]^{2-}$, $[H_2L7]^{2-}$ and $[H_2L8]^{2-}$, the general procedure was adapted as follows. The acyl chloride derivative was re-dissolved in 20 mL of dry DMA and added dropwise to a dispersion of the corresponding amine (4 mmol, 2 eq.) in 8 mL of dry DMA containing 4 eq. of $Et_3N$. This solution was stirred under a nitrogen atmosphere for 15 h at 50 °C. The appearing solid consisted in the corresponding ligand ($[H_2L6]^{2-}$, $[H_2L7]^{2-}$ and $[H_2L8]^{2-}$) which was filtered and washed with acetone and $Et_2O$, yielding the desired product

without further purification. In case of [$H_2$L2], the reaction mixture showed no precipitate after 4 days of reaction. The clean solution was mixed with 0.1 M $Na_2CO_3$ solution, extracted with DCM, dried over $MgSO_4$, and evaporated to yield [$H_2$L2] as a white powder.

***[$H_2$L1]**·0.8 $H_2O$*

Yield: 695 mg, 1.75 mmol, 86 %. $^1$H NMR (DMSO-$d_6$): $\delta$ [ppm] = 10.66 ($H_4$, s, 2H), 9.22 ($H_1$, dd, $J$ = 6.9, 2.1 Hz, 2H), 8.29 ($H_{2\text{-}3}$, m, 4H), 7.93 ($H_5$, dd, $J$ = 8.71, 1.2 Hz, 4H), 7.4 ($H_6$, dd, $J$ = 8.7 Hz, 4H), 7.16 ($H_7$, tt, $J$ = 7.4, 1.2 Hz, 2H). $^{13}$C NMR (DMSO-$d_6$): 162.9 ($C_6$), 153.9 ($C_5$), 150.2 ($C_1$), 139.7 ($C_4$), 138.6 ($C_7$), 129.1 ($C_9$), 125.3 ($C_2$), 124.7 ($C_{10}$), 123.6 ($C_3$), 121.6 ($C_8$). ESI-MS (MeOH) m/z positive mode: 417.0 [$H_2$L1+$Na^+$]$^+$. Elemental analysis (% found): C, 70.36; H, 4.86; N, 13.79. Calcd. for $C_{24}H_{18}N_4O_2$·0.8 $H_2O$: C, 70.51; H, 4.83; N, 13.70. IR ($\tilde{\nu}$ / cm$^{-1}$): 3421m, 3347s, 1663m, 1598m, 1530s, 1498w, 1448m, 14312m, 1325m, 1244w, 1077m, 994w, 756m, 687m, 664m, 494w.

***[$H_2$L2]**·0.3 $H_2O$*

Yield: 453 mg, 1.00 mmol, 49%. $^1$H NMR (500 MHz, $CDCl_3$): $\delta$ [ppm] = 9.92 ($H_4$, s, 2H), 8.62 ($H_1$, dd, $J$ = 7.9, 1.0 Hz, 2H), 8.42 ($H_3$, d, $J$ = 7.7, 1.0 Hz, 2H), 8.16 ($H_2$, t, $J$ = 7.8 Hz, 2H), 7.46 ($H_5$, s, 4H), 6.84 ($H_7$, s, 2H), 2.38 ($H_6$, s, 12H). $^{13}$C NMR (126 MHz, $CDCl_3$): $\delta$ [ppm] = 161.7 ($C_6$), 153.7 ($C_1$), 149.9 ($C_5$), 139.1 ($C_3$, $C_9$), 137.5 ($C_7$), 126.6 ($C_{11}$), 123.9 ($C_2$), 123.2 ($C_4$), 117.8 ($C_8$), 21.6 ($C_{10}$). ESI-HRMS ($CHCl_3$/MeOH) m/z positive mode: calcd for [$H_2$L2-$H^+$]$^-$, ($C_{28}H_{25}N_4O_2$) :449.1983, found: 449.1981. Elemental analysis (% found): C, 73.39; H, 5.54; N, 12.55. Calcd for $C_{28}H_{26}N_4O_2$·0.3 $H_2O$: C: 73.76; H: 5.88; N: 12.29. IR ($\tilde{\nu}$ / cm$^{-1}$): 3352s, 3095w, 3015w, 2914m, 2856w, 1683s, 1611m, 1581m, 1553s, 1417s, 1237w, 1178w, 1075w, 996w, 834m, 758m, 685m, 633m.

***[$H_2$L3]**·0.5 $H_2O$*

Yield: 1.40 g, 1.42 mmol, 71%. $^1$H NMR (400MHz, $CDCl_3$): $\delta$ [ppm] = 10.74 ($H_4$, s, 2H), 8.78 ($H_1$, dd, $J$ = 7.9, 1.0 Hz, 2H), 8.52 ($H_3$, dd, $J$ = 7.7, 1.0 Hz, 2H), 8.40 (d, $J$ = 6.8 Hz, 2H), 8.23 ($H_2$, t, $J$ = 7.8 Hz, 2H), 8.13 (d, $J$ = 8.5 Hz, 2H), 7.95 (d, $J$ = 8.7 Hz, 2H), 7.77 (d, $J$ = 8.2 Hz, 2H), 7.66 – 7.53 ($H_{6,9,10}$, m, 6H). HRMS-ESI: Calcd for [$H_2$L3+$Na^+$]$^+$, ($C_{32}H_{22}N_4O_2Na$): 517.1635, found: 517.1625. Elemental analysis (% found): C, 76.2; H, 4.5; N, 11.1. Calcd for $C_{32}H_{22}N_4O_2$·0.5 $H_2O$: C, 76.3; H, 4.6; N, 11.1. IR ($\tilde{\nu}$ / cm$^{-1}$): 3370s, 3356s, 3055m, 3012w, 1685s, 1584m, 1536s, 1496s, 1430m, 1405m, 1344m, 1255m, 1133m, 1068m, 996w, 792m, 770m, 735m, 631m.

***[$H_2$L4]**($Et_3NH)_2$·2 $H_2O$*

Yield: 931 mg, 1.68 mmol, 61%. $^1$H NMR (DMSO-$d_6$): $\delta$ [ppm] = 10.70 ($H_4$, s, 2H), 9.24 ($H_1$, dd, $J$ = 7.3, 1.6 Hz, 2H), 8.30 ($H_{2\text{-}3}$, m, 4H), 7.90 ($H_5$, d, $J$ = 8.7 Hz, 4H), 7.65 ($H_6$, d, $J$ = 8.7 Hz, 4H). $^{13}$C NMR (DMSO-$d_6$): 162.9 ($C_6$), 153.9 ($C_5$), 150.0 ($C_1$), 144.7 ($C_{10}$), 139.8 ($C_4$), 138.6 ($C_7$), 126.5 ($C_9$), 125.3 ($C_2$), 123.7 ($C_3$), 120.4 ($C_8$). ESI-MS (MeOH) m/z negative mode: 553.0 [$H_2$L4+$H^+$]$^-$, 276.1 [$H_2$L4]$^{2-}$. Elemental analysis (% found): C, 54.6; H, 6.7; N, 10.6. Calcd for $C_{24}H_{16}N_4O_8S_2^{2-}$·2 $Et_3NH^+$·2 $H_2O$: C, 54.5; H, 6.6; N, 10.6. IR ($\tilde{\nu}$ / cm$^{-1}$): 3333m, 3316m, 3055w, 2933w, 1690s, 1583m, 1522s, 1434m, 1398m, 1275m, 1230w, 1166m, 1126m, 1073m, 893w, 826m, 681m, 548m.

***[$H_2$L5]**($Et_3NH)_2$·1.3 $H_2O$*

Yield: 965 mg, 1.74 mmol, 64%. $^1$H NMR (DMSO-$d_6$): $\delta$ [ppm] = 12.55 ($H_4$, s, 2H), 9.51 ($H_1$, dd, $J$ = 7.3, 1.7 Hz, 2H), 8.67 ($H_5$, dd, $J$ = 8.2, 1.1 Hz, 2H), 8.26 ($H_{2\text{-}3}$, m, 4H), 7.82 ($H_8$, dd, $J$ = 7.7, 1.7 Hz, 2H), 7.43 ($H_6$, t, $J$ = 1.2 Hz, 2H), 7.14 ($H_7$, td, $J$ = 7.5, 1.2 Hz, 2H). $^{13}$C NMR (DMSO-$d_6$): 162,4 ($C_6$), 153.9 ($C_5$), 149.6 ($C_1$), 139.9 ($C_4$), 136.8 ($C_{12}$), 135.3 ($C_7$), 130.1 ($C_9$), 127.6 ($C_8$), 125.4 ($C_2$), 123.2 ($C_{1\text{-}2}$), 120.2 ($C_{3\text{-}7}$). ESI-MS (MeOH) m/z negative mode: 553.0 [$H_2$L5+$H^+$]$^-$, 276.1 [$H_2$L5]$^{2-}$. Elemental analysis (% found): C, 55.3; H, 6.0; N, 10.6. Calcd for $C_{24}H_{16}N_4O_8S_2^{2-}$·2 $Et_3NH^+$·1.3 $H_2O$: C, 55.4; H, 6.5; N, 10.8. IR ($\tilde{\nu}$ / cm$^{-1}$): 3422m, 3344m, 3276m, 3001m, 2702m, 2502w, 1682m, 1580s, 1524s, 1425s, 1398w, 1245s, 1222m, 1165s, 1149m, 1124m, 1008m, 904w, 785w, 613m.

***[$H_2$L6]**($Et_3NH)_2$*

Yield: 1.29 g, 1.48 mmol, 74 %. $^1$H NMR (DMSO-$d_6$): $\delta$ [ppm] = 10.48 ($H_4$, s, 2H), 9.21 ($H_1$, d, $J$ = 7.9, 1.0 Hz, 2H), 8.87 (($CH_3CH_2)_3NH$, s, 2H), 8.25-8.32 ($H_{2\text{-}3}$, m, 4H), 7.56 ($H_5$, s, 4H), 3.09 (($CH_3CH_2)_3NH$, q, $J$ = 6.9 Hz, 12H), 2.60 ($H_6$, s, 12H), 1.17 (($CH_3CH_2)_3NH$, tr, $J$ = 7.2 Hz, 18H). $^{13}$C NMR (DMSO-$d_6$): 162.4 ($C_6$), 153.9 ($C_5$), 149.6 ($C_1$), 139.9 ($C_4$), 136.8 ($C_{12}$), 135.3 ($C_7$), 130.1 ($C_9$), 127.6 ($C_8$), 125.4 ($C_2$), 123.2 ($C_{1\text{-}2}$), 120.2 ($C_{3\text{-}7}$), 62.0 (($CH_3CH_2)_3NH$), 25.5 (($CH_3CH_2)_3NH$). HRMS-ESI(MeOH): calcd for [$H_2$L6]$^{2-}$, ($C_{28}H_{24}N_4O_8S_2$): 304.0523, found 304.0535. Elemental analysis (% found): C, 57.8; H, 6.3; N, 10.2. Calcd for $C_{24}H_{26}N_4O_8S_2^{2-}$·2$Et_3NH^+$: C, 58.1; H, 7.0; N, 10.2. IR ($\tilde{\nu}$ / cm$^{-1}$): 3441br, 3330w, 3084w, 2984m, 1681s, 1644m, 1581m, 1530s, 1436m, 1399m, 1169s, 1082s, 1011s, 681m.

***[H$_2$L7]***(*Et$_3$NH)$_2$·2 H$_2$O*

Yield: 500 mg, 0.58 mmol, 29 %. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ [ppm] = 11.13 (H$_4$, s, 2H), 9.37 (H$_1$, dd, *J* = 7.1, 1.8 Hz, 2H), 8.95 (H$_7$, m, 2H, *H*12), 8.30 (H$_{2,3}$, m, 4H), 8.05 (H$_{6,10}$, m, 4H), 7.72 (H$_5$, d, *J* = 7.7 Hz, 2H), 7.59 (H$_{8,9}$, m, 4H, *H*13, *H*14), 3.09 ((CH$_3$CH$_2$)$_3$NH, q, 7.3 Hz, 12H), 1.17 ((CH$_3$CH$_2$)$_3$NH, tr, *J* = 7.2 Hz, 18H). $^{13}$C NMR (101 MHz, DMSO-d$_6$): $\delta$ [ppm] = 163.3 (C$_6$), 153.7(C$_1$), 149.5 (C$_5$), 142.4 (C$_{10}$), 139.3 (C$_3$), 134.5 (C$_{11}$), 129.8 (C$_7$), 129.3 (C$_{16}$), 128.1 (C$_{12}$), 125.8 (C$_{13+14}$), 124.8 (C$_2$), 124.2 (C$_9$), 123.2 (C$_4$), 122.8 (C$_{15}$), 121.8 (C$_8$), 62.0 ((CH$_3$CH$_2$)$_3$NH), 25.5 ((CH$_3$CH$_2$)$_3$NH). HRMS-ESI (MeOH): Calcd. for [H$_2$L7]$^{2-}$, (C$_{32}$H$_{22}$N$_4$O$_8$S$_2$): 326.0367, found 326.0373. Elemental analysis (% found): C, 59.25; H, 6.72; N, 9.47. Calcd for C$_{32}$H$_{22}$N$_4$O$_8$S$_2^{2-}$·2Et$_3$NH$^+$·2H$_2$O: C, 59.18; H, 6.32; N, 9.41. IR ($\tilde{\nu}$ / cm$^{-1}$): 3398s, 3206s, 3088s, 1685s, 1610m, 1532s, 1508s, 1438w, 1147s, 1041s, 750m, 681m.

***[H$_2$L8]***(*Et$_3$NH)$_2$·1.5H$_2$O*

Yield: 774 mg, 1.81 mmol, 88%. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ [ppm] = 10.88 (H$_4$, s, 2H), 9.29 (H$_1$, dd, *J* = 6.3, 2.7 Hz, 2H), 8.54 (H$_{10}$, s, 2H), 8.40 – 8.29 (H$_{2,3}$, m, 4H), 8.14 (H$_7$, s, 2H), 8.04 (H$_{5,6}$, m, 4H), 7.86 (H$_9$, d, *J* = 8.7 Hz, 2H), 7.72 (H$_8$, dd, *J* = 8.5, 1.5 Hz, 2H), 3.09 ((CH$_3$CH$_2$)$_3$NH, m, 12H), 1.17 ((CH$_3$CH$_2$)$_3$NH, tr, *J* = 7.2 Hz, 18H). $^{13}$C NMR (101 MHz, DMSO) $\delta$ 162.7 (C$_6$), 153.5 (C$_1$), 149.6 (C$_5$), 144.7 (C$_{12}$), 139.4 (C$_3$), 136.3 (C$_7$), 133.1 (C$_{15}$), 129.3 (C$_{10}$), 128.9 (C$_9$), 127.0 (C$_{14}$), 124.9 (C$_2$), 124.5 (C$_{13}$), 123.9 (C$_{11}$), 123.2 (C$_4$), 121.9 (C$_8$), 117.3 (C$_{16}$), 62.0 ((CH$_3$CH$_2$)$_3$NH), 25.5 ((CH$_3$CH$_2$)$_3$NH). HRMS-ESI (MeOH): calcd for [H$_2$L8]$^{2-}$, (C$_{32}$H$_{22}$N$_4$O$_8$S$_2$): 326.0367, found 326.0362. Elemental analysis (% found): C, 59.6; H, 5.9; N, 9.5. Calcd. for C$_{32}$H$_{22}$N$_4$O$_8$S$_2^{2-}$·2Et$_3$NH$^+$·1.5H$_2$O: C, 59.8; H, 6.3; N, 9.5. IR ($\tilde{\nu}$ / cm$^{-1}$): 3310s, 3021s, 2860s,2776s, 2501m, 1682s, 1580m, 1536s, 1493m,1438m, 1393m, 1340w, 1241s, 1159s, 1090s, 1019s, 823m, 670m.

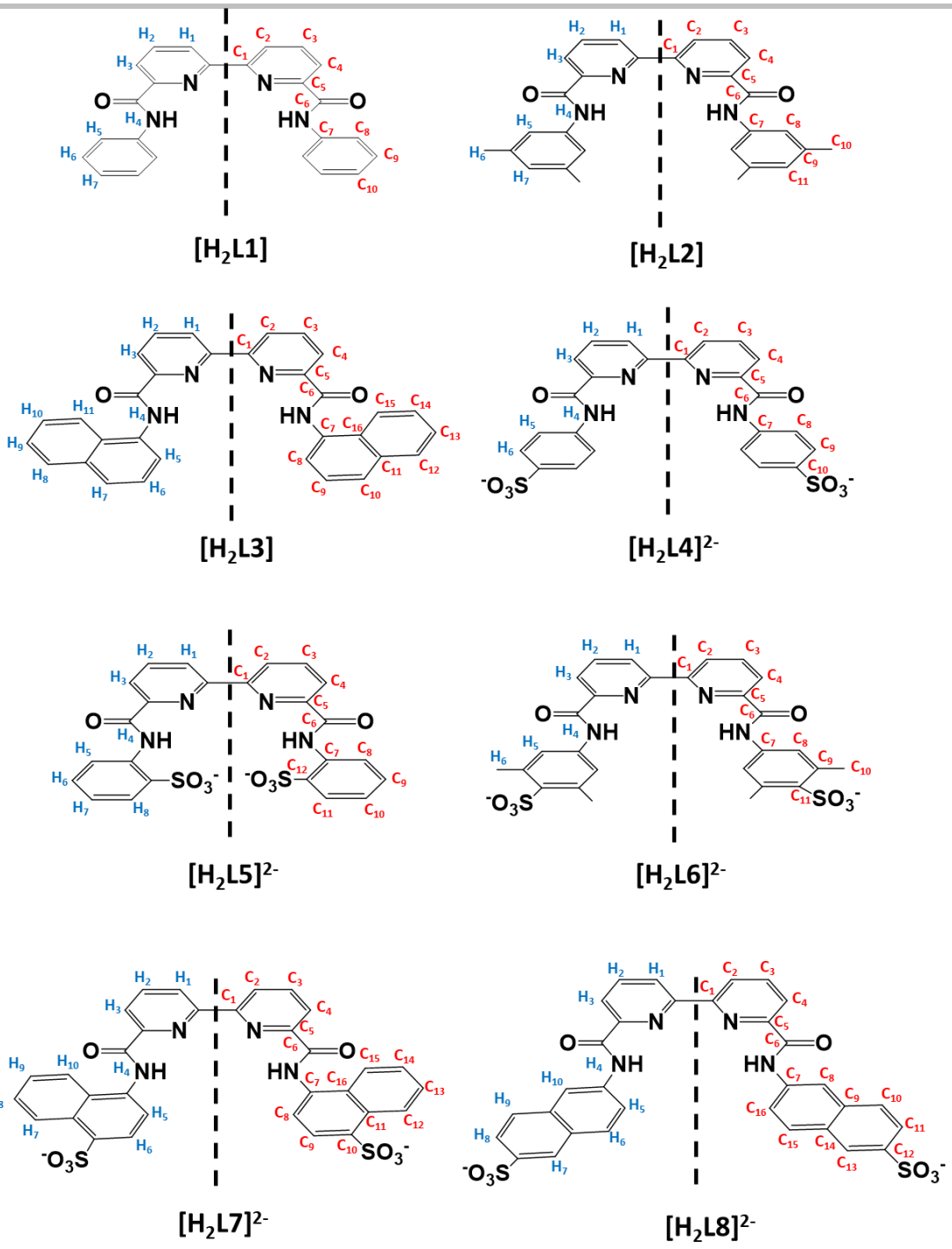



**Figure S1**. Schematic drawing of the ligands synthetized in this work and their $^{1}H$ NMR and $^{13}C$ NMR assignments.

# SUPPORTING INFORMATION

**Synthesis of Cu-complexes**

The general procedure for the synthesis of the copper complexes was adapted from a previous published work.[6] Typically, 0.2 mmol of the corresponding ligand were suspended in 8 mL of MeOH and stirred during 15 minutes. Afterwards, 7.2 mL (4 eq.) of 0.1 M $NaOH_{aq.}$ were added to the reaction mixture and vigorously stirred during 30 minutes at room temperature. After complete dissolution of the ligand, 0.2 mmol of copper perchlorate hexahydrate dissolved in 8 mL of MeOH were added dropwise to the mixture, which were allowed to react overnight (16 h) at room temperature. Then, the reaction mixture was filtrated and MeOH was evaporated under vacuum, and the remaining solution was diffused with the corresponding solvent (further details about crystallization are explained in Table S1), yielding the corresponding pure copper complexes.

***[(L1)Cu]**·1.5 $H_2O$·MeOH*

Yield: 38 mg, 0.08 mmol, 42% ESI-MS (MeOH) m/z positive mode: 456.0 $[(L1)Cu+H]^-$, 494.1 $[(L1)Cu+K]^-$. Elemental analysis (% found): C, 54.6; H, 3.2; N, 10.5. Calcd. for $C_{24}H_{16}CuN_4O_2$·1.5 $H_2O$ ·MeOH: C, 54.8; H, 3.3; N, 10.6. IR ($\tilde{\nu}$ / $cm^{-1}$): 3396s, 3055w, 2922w, 2837w, 1625m, 1614m, 1577s, 1487m, 1468m, 1354m, 1337m, 1283m, 1142m, 1028m, 747m, 689m, 485w.

***[(L2)Cu]**·2 $H_2O$·MeOH*

Yield: 41 mg, 0.08 mmol, 42% ESI-MS (MeOH) m/z positive mode: 512.1 $[(L2)Cu+Na]^+$, 1023.0 $[2(L2)Cu+H]^+$. HRMS-ESI($CHCl_3$/MeOH): calcd for $[(L3)Cu+H]^+$, (C28H25N4O2Cu) : 512.1259, found 512.1268. Elemental analysis (% found): C, 58.5; H, 6.1; N, 9.5. Calcd for $C_{28}H_{24}CuN_4NO_2$·2 $H_2O$ ·MeOH: C, 58.2; H, 5.7; N, 9.4. IR ($\tilde{\nu}$ / $cm^{-1}$): 3355m, 3031w, 2999w, 2911m, 2860w, 1623m, 1570s, 169m, 1353s, 1262m, 1076m, 1027m, 826m, 767m, 688m, 579w.

***[(L3)Cu]**·1.5MeOH*

Yield: 45 mg, 0.08 mmol, 40% ESI-MS (MeOH) m/z positive mode: 556.1 $[(L3)Cu+H]^+$, 578.1 $[(L3)Cu+Na]^+$ 1111.1 $[2·(L3)Cu+H]^+$. HRMS-ESI(+ve): calcd for $[(L3)Cu+H]^+$, ($C_{32}H_{21}CuN_4O_2$): 556.0955, found: 556.0948. Elemental analysis (% found): C, 66.3; H, 3.9; N, 9.6. Calcd for $C_{32}H_{20}CuN_4Na_2O_8S_2$·1.5 MeOH: C, 66.6; H, 4.3; N, 9.3. IR ($\tilde{\nu}$ / $cm^{-1}$): 3655w, 3381m, 3192m, 3051m, 1624m, 1578s, 1565s, 1504m, 1472w, 1392m, 1338m, 1285m, 1037m, 790m, 763m, 705w.

***[(L4)Cu]**$Na_2$ ·3$H_2O$*

Yield: 19 mg, 0.03 mmol, 32% ESI-MS (MeOH) m/z negative mode: 636.0 $[(L4)Cu+Na^+]^-$, 614.0 $[(L4)Cu+H]^-$. Elemental analysis (% found): C, 40.2; H, 2.5; N, 7.7. Calcd for $C_{24.}H_{14}CuN_4Na_2O_8S_2$·3 $H_2O$: C, 40.4; H, 2.8; N, 7.8. IR ($\tilde{\nu}$ / $cm^{-1}$): 3585s, 3513s, 3460s, 3382m, 3227m, 1621m, 1597s, 1574m, 1497m, 1474m, 1358m, 1199m, 1120s, 1032s, 1007m, 820w, 693m, 570m.

***[(L5)Cu]**$Na_2$·4 $H_2O$·2 MeOH*

Yield: 15 mg, 0.02 mmol, 25%. ESI-MS (MeOH) m/z negative mode: 636.0 $[(L5)Cu+Na^+]^-$, 614.0 $[(L5)Cu+H]^-$. Elemental analysis (% found): C, 39.2; H, 3.9; N, 6.5. Calcd for $C_{24}H_{14}CuN_4Na_2O_8S_2$·4 $H_2O$ ·2 MeOH: C, 39.2; H, 3.8; N, 7.0. IR ($\tilde{\nu}$ / $cm^{-1}$): 3585s, 3513s, 3459m, 3417s, 3331m, 3226m, 3097w, 1620w, 1593m, 1574s, 1472m, 1388m, 1293w, 1177m, 1084s, 1013m, 761w, 161m, 569m.

***[(L6)Cu]**$Na_2$·2.4$H_2O$*

Yield: 42 mg, 0.06 mmol, 72% ESI-MS (MeOH) m/z negative mode: 609.0 $[(L6)Cu+H^+]^-$. Elemental analysis (% found): C, 44.4; H, 3.9; N, 7.4. Calcd for $C_{28}H_{22}CuN_4Na_2O_8S_2$·2.4 $H_2O$: C, 44.3; H, 3.6; N, 7.4. IR ($\tilde{\nu}$ / $cm^{-1}$): 3404s, 3076w, 2974w, 2937w, 1612w, 1591m, 1557s, 1472m, 1368m, 1305w, 1170s, 1084s, 1016m, 765m, 690m, 648m.

***[(L7)Cu]**$Na_2$·7$H_2O$*

Yield: 59 mg, 0.08 mmol, 49% ESI-MS ($CHCl_3$/MeOH) m/z negative mode: 713.8 $[(L7)Cu+H^+]^-$, 735.8 $[(L7)Cu+Na^+]^-$. HRMS-ESI ($CHCl_3$/MeOH): calcd for $[(L7)Cu]^{2-}$, ($C_{32}H_{18}CuN_4O_8S_2$) : 356.4937, found 356.4933. Elemental analysis (% found): C, 43.4; H, 3.2; N, 6.2. Calcd for $C_{32}H_{18}CuN_4Na_2O_8S_2$·7 $H_2O$: C, 43.4; H, 3.6; N, 6.3. IR ($\tilde{\nu}$ / $cm^{-1}$): 3626m, 3358s, 3078w, 1614w, 1575m, 1552s, 1506m, 1420w, 1390s, 176m, 1285w, 1214w, 1182s, 1156m, 1045s, 1156m, 1045s, 1023m, 759m, 688m, 612w.

***[(L8)Cu]***$Na_2 \cdot 6H_2O$

Yield: 12 mg, 16 mmol, 20% ESI-MS (MeOH) m/z negative mode: 735.8 $[(L8)Cu+Na^+]^-$, 713.8 $[(L8)Cu+H^+]^-$. HRMS-ESI(-ve, MeOH): calcd for $[(L8)Cu+Na]^-$, ($C_{32}H_{18}CuN_4O_8S_2Na$): 735.9765, found 735.9763. Elemental analysis (% found): C, 44.2; H, 3.3; N, 6.5. Calcd for $C_{32}H_{18}CuN_4Na_2O_8S_2$ 6 $H_2O$: C, 44.3; H, 3.5; N, 6.4. IR ($\tilde{\nu}$ / $cm^{-1}$): 3427s, 3081m, 1673w, 1626m, 1577s, 1530m, 1494m, 1470m, 1377m, 1181s, 1096s, 1035s, 819m, 674m, 623m.

**Synthesis of complex $[(L4)Zn](Na)_2 \cdot 4H_2O$.**

The procedure for the synthesis of the zinc complex was similar to the synthesis of the copper complexes. To a suspension of $[H_2L4]^{2-}$ (200 mg (0.36 mmol) in 16 mL of MeOH), 14.4 mL (4 eq.) of 0.1 M $NaOH_{aq.}$ were added to the reaction mixture and vigorously stirred during 30 minutes at room temperature. After complete dissolution of the ligand, 131 mg (0.36 mmol) of zinc trifluoromethanesulfonate dissolved in 4 mL of MeOH was added dropwise to the mixture, which was allowed to react overnight (16 h) at room temperature. Afterwards, a white precipitate appeared, which was filtrated and washed with $H_2O$ (2 x 2 mL) and dried over vacuum yielding **[(L4)Zn]**$Na_2 \cdot 4\ H_2O$ as a white solid.

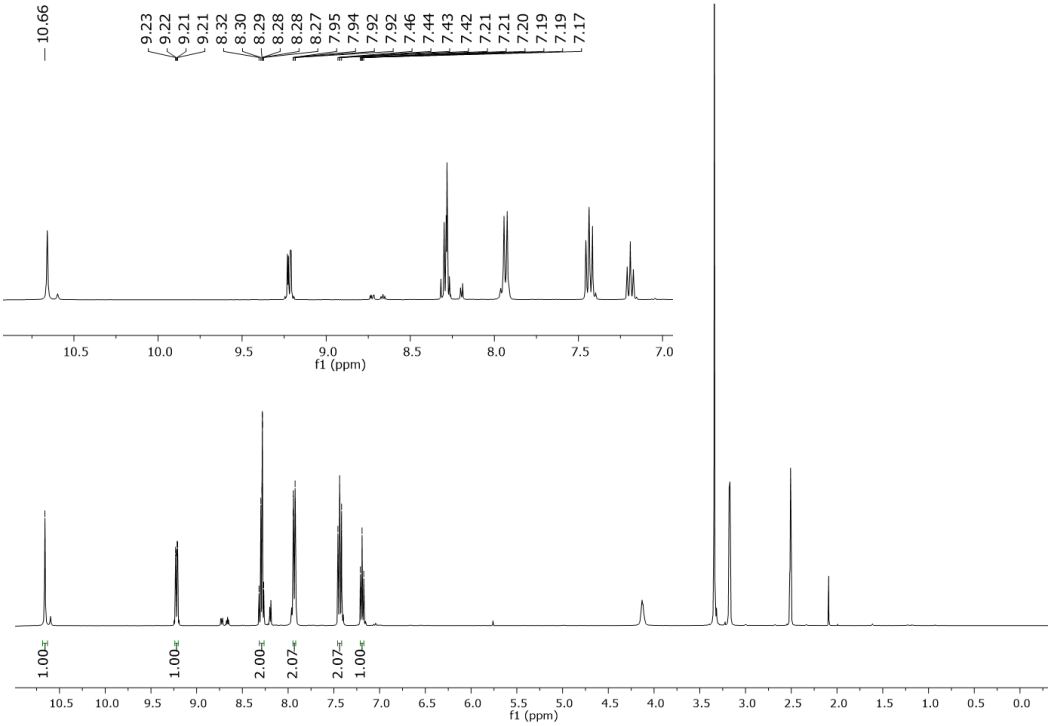
***[(L4)Zn]***$Na_2 \cdot 4\ H_2O$

Yield: 193 mg, 0.29 mmol, 81%. $^1$H-NMR ($D_2O$-$d_2$): δ [ppm] = 8.04 ($H_{1\text{-}2}$, m, 4H), 7.67 ($H_3$, dd, J= 7.5, 1.3 Hz, 2H), 7.20 ($H_4$, d, = 8.5 Hz, 4H), 6.36 ($H_5$, d, J= 8.5 Hz, 4H). Elemental analysis (% found): C, 39.8; H, 3.4; N, 7.6. Calcd for $C_{24}H_{14}CuN_4Na_2O_8S_2Zn \cdot 4\ H_2O$: C, 39.3; H, 3.0; N, 7.6.

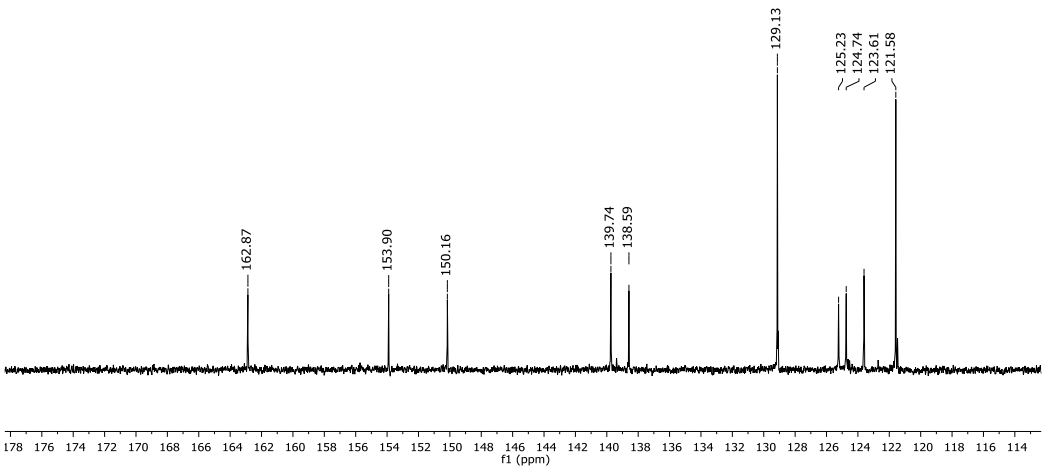
## Spectroscopic Characterization

### NMR Spectroscopy

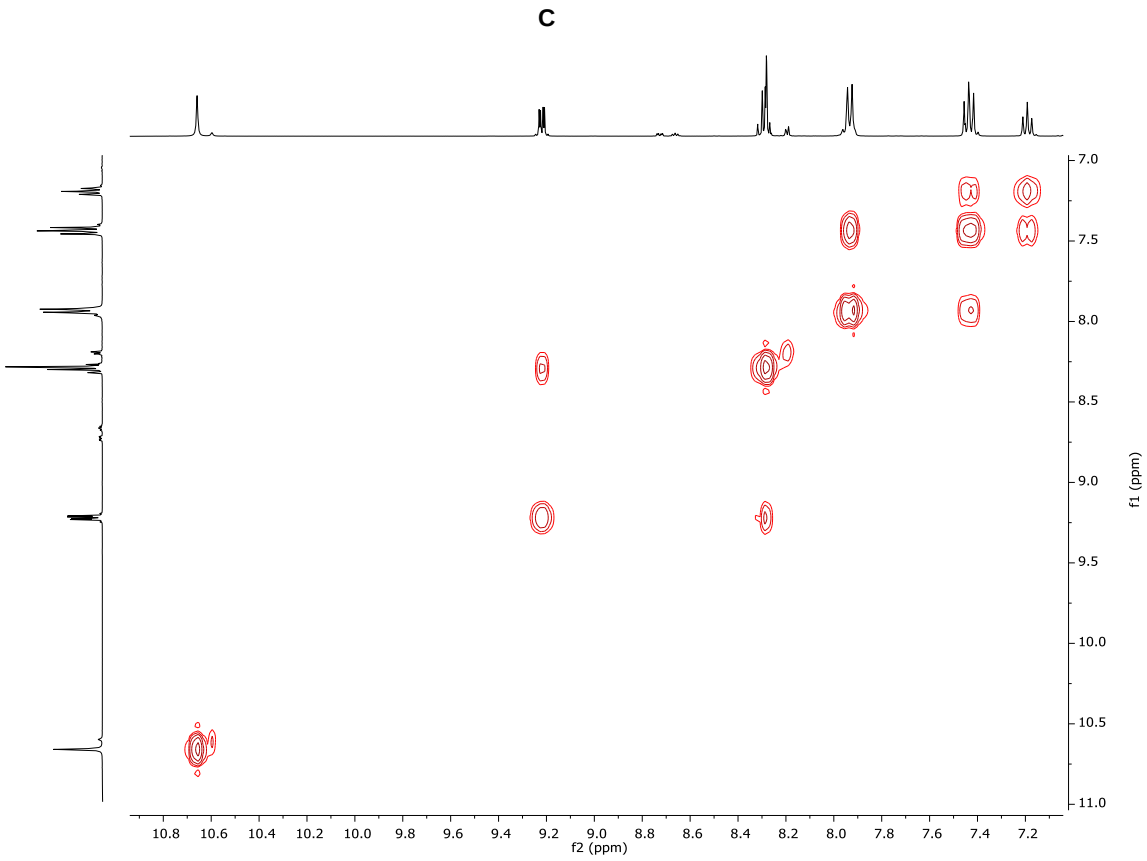
**A**



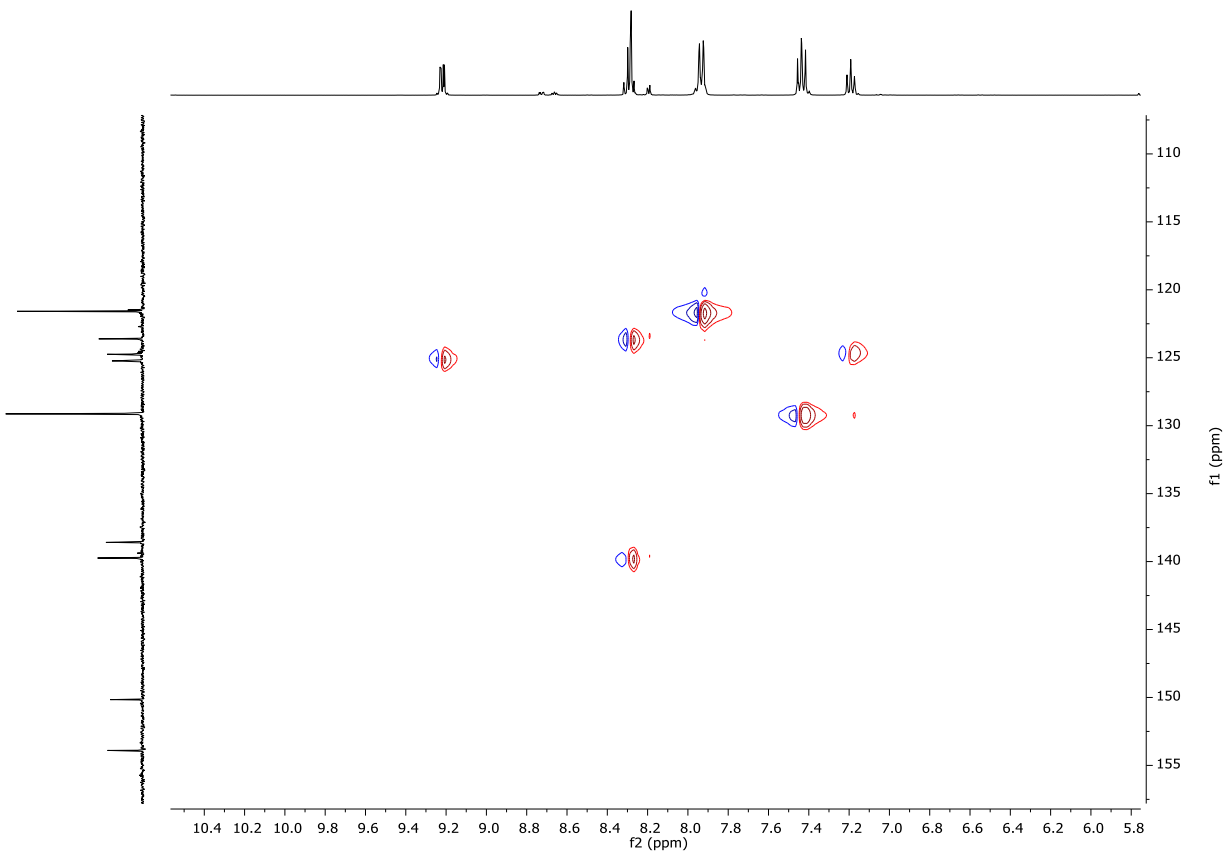

**B**



C


C
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0
f1 (ppm)
10.8 10.6 10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2
f2 (ppm)

D


110
115
120
125
130
135
140
145
150
155
f1 (ppm)
10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8
f2 (ppm)

**E**

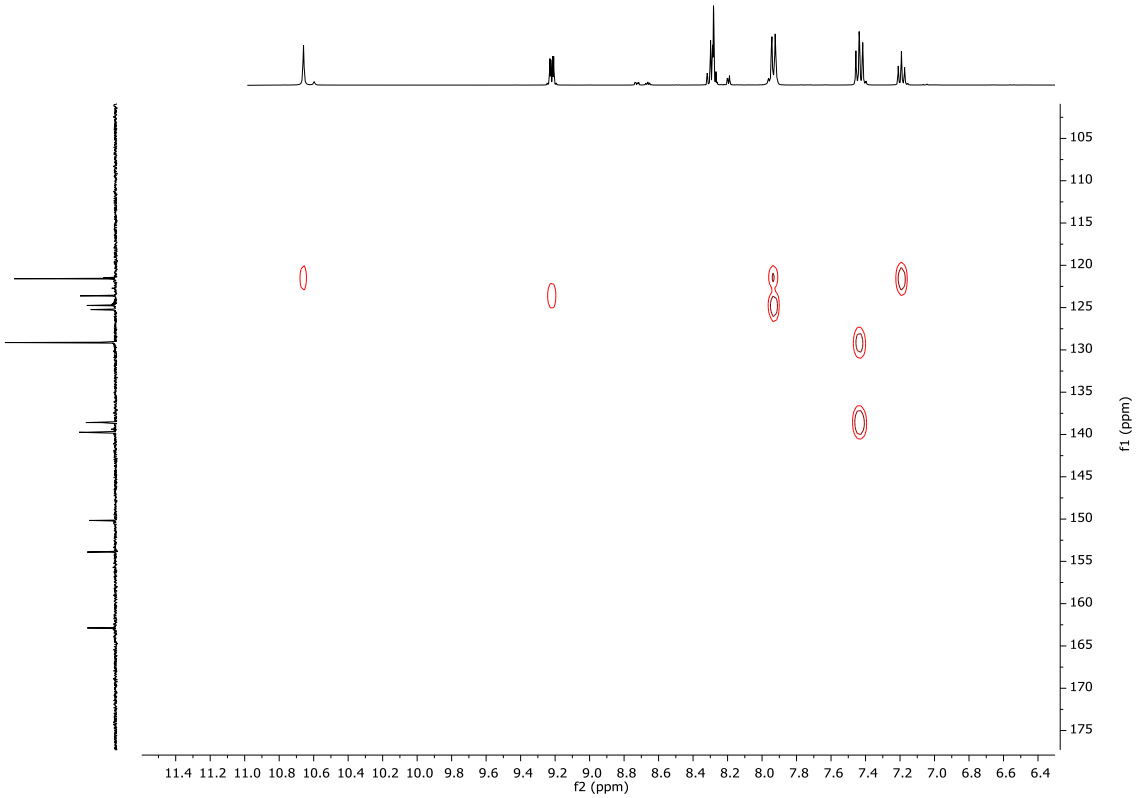
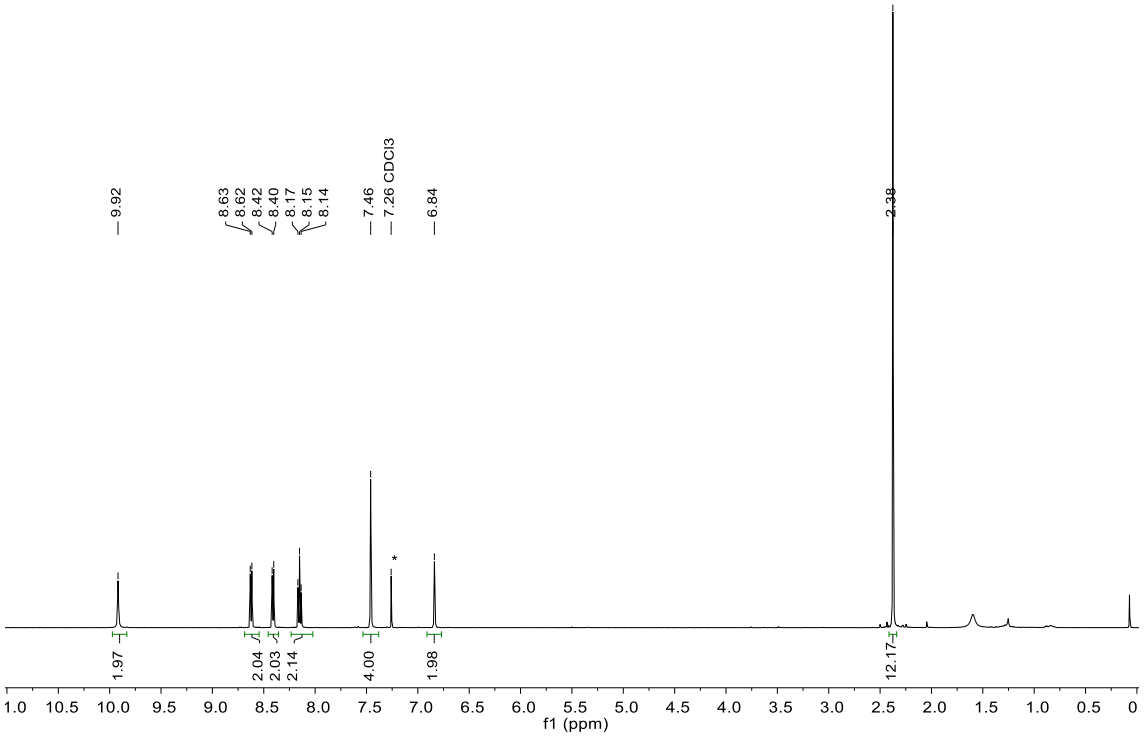
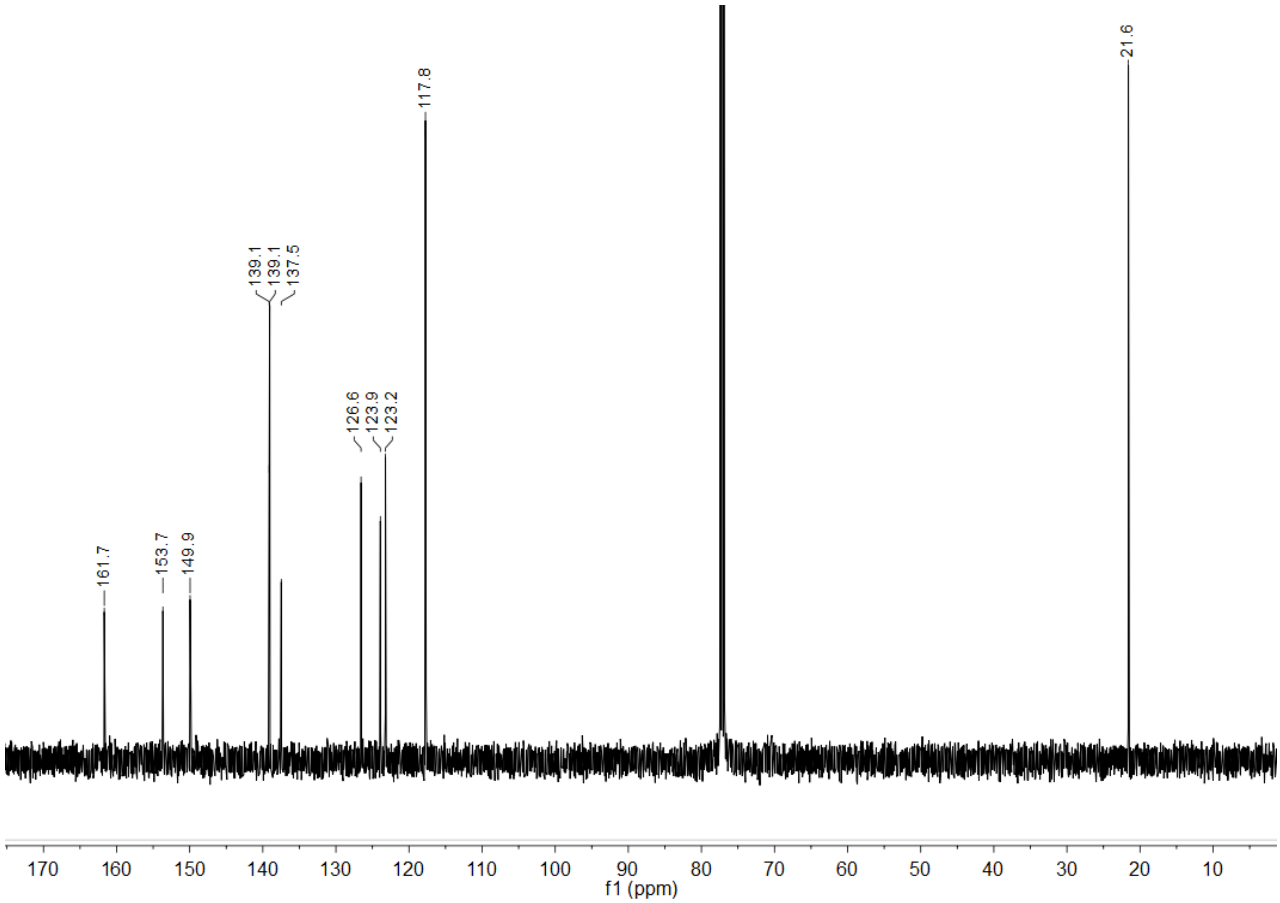



**Figure S2.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2$L1**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

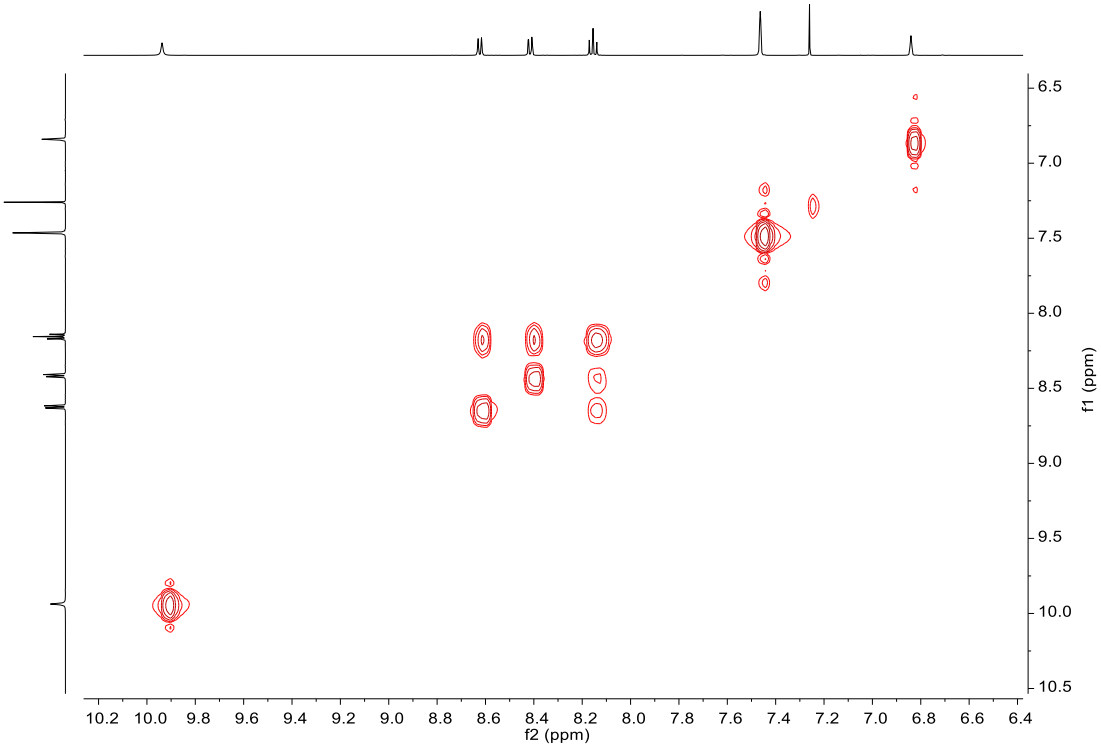
**A**


9.92
8.63
8.62
8.42
8.40
8.17
8.15
8.14
7.46
7.26 CDCl3
6.84
2.38
1.97
2.04
2.03
2.14
4.00
1.98
12.17
f1 (ppm)

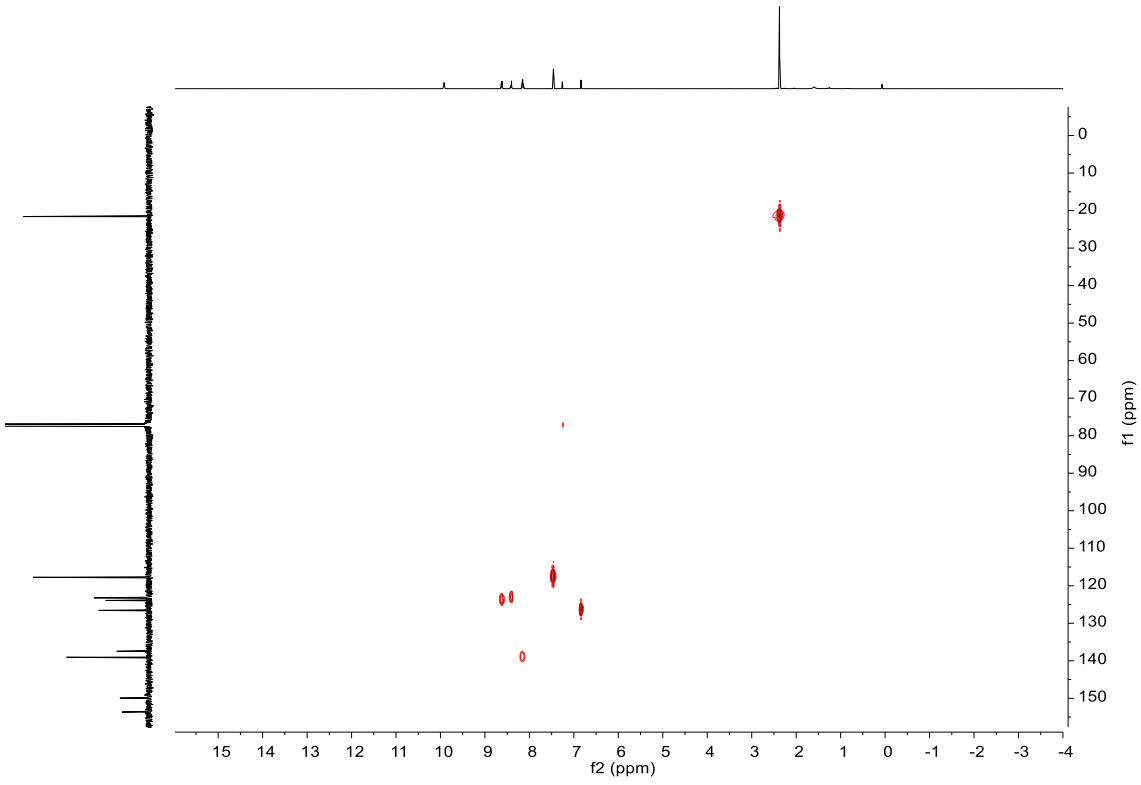
**B**


161.7
153.7
149.9
139.1
139.1
137.5
126.6
123.9
123.2
117.8
21.6
f1 (ppm)

**C**


6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
f1 (ppm)
10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f2 (ppm)

**D**


0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
f1 (ppm)
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f2 (ppm)

**E**

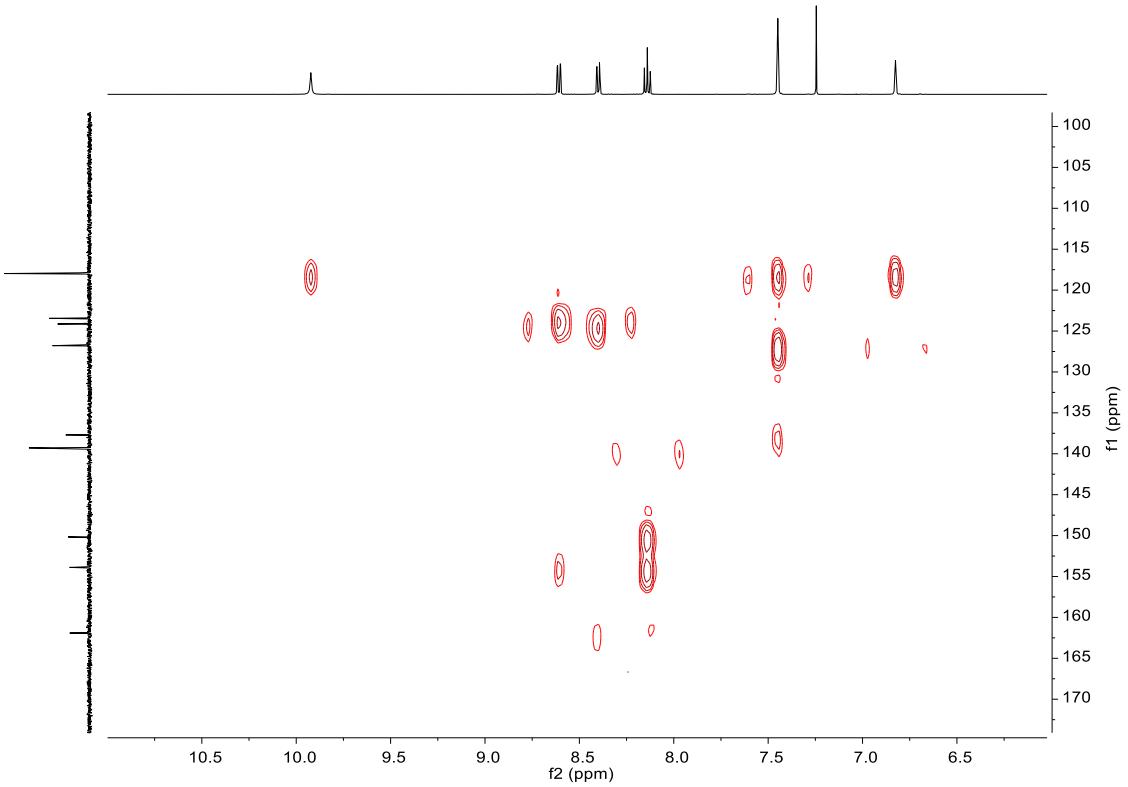
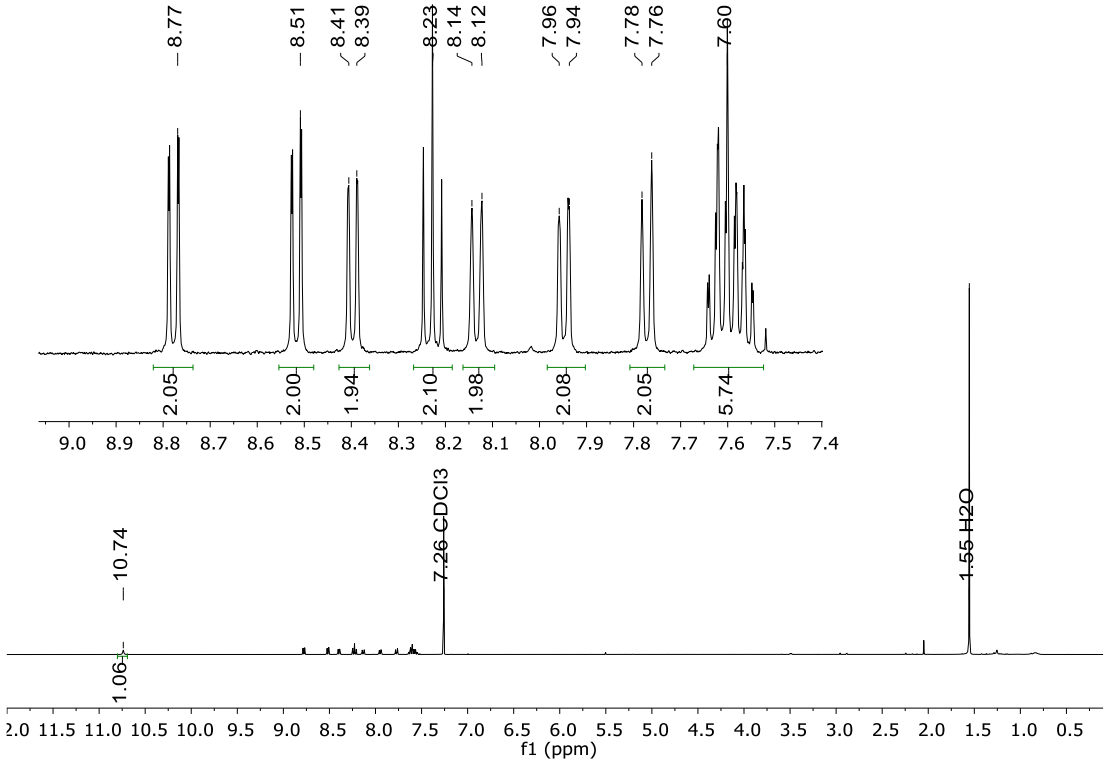



**Figure S3.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2$L2**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

**A**




**B**

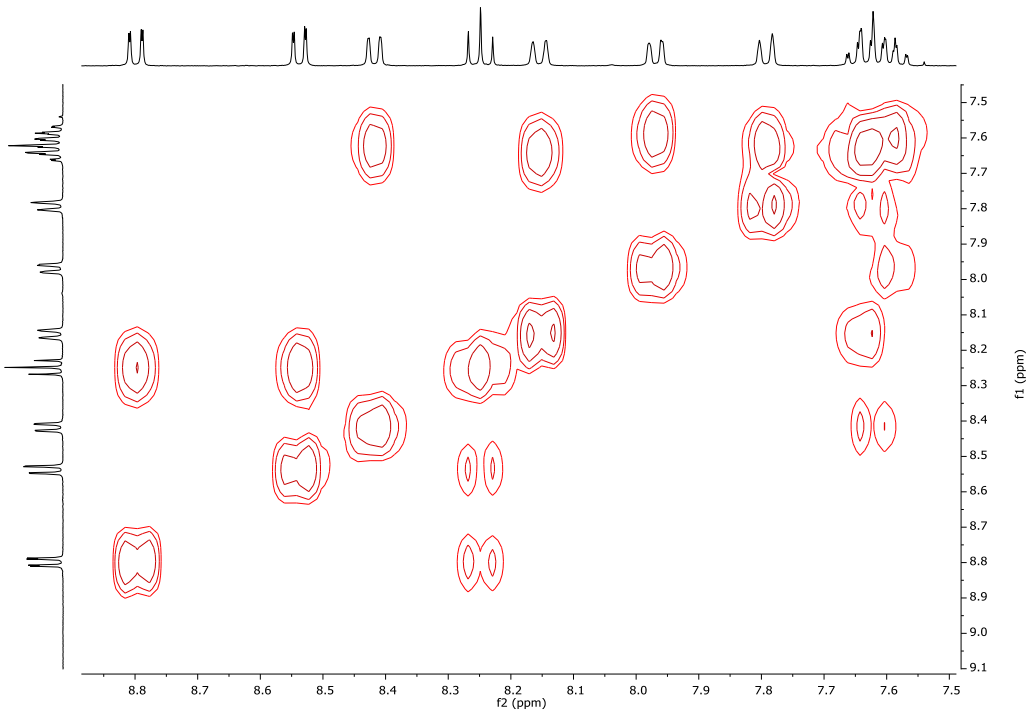
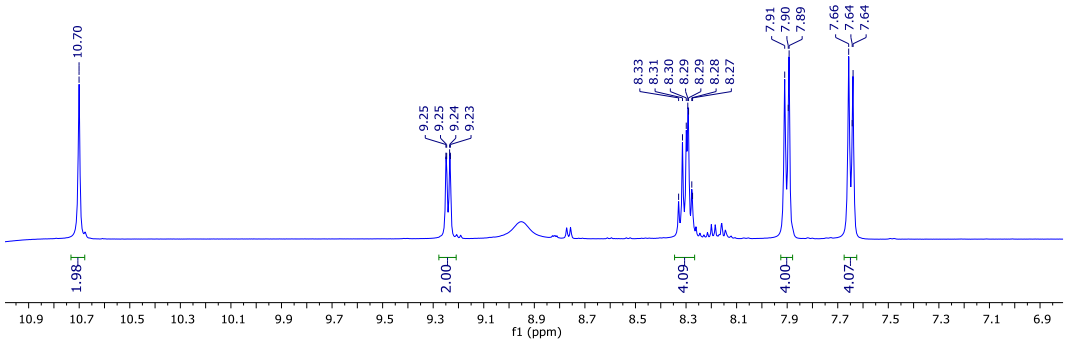
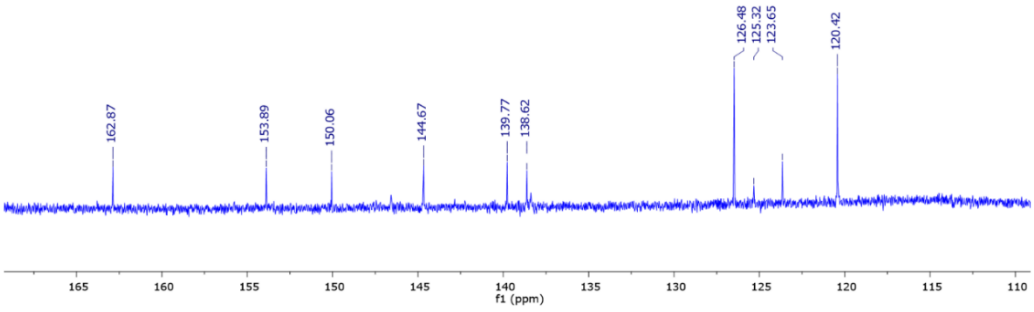



**Figure S4.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2$L3**. (A) $^{1}$H-NMR, (B) COSY. ***Note**:* Due to low solubility of the compound, $^{13}$C-NMR was not measurable.

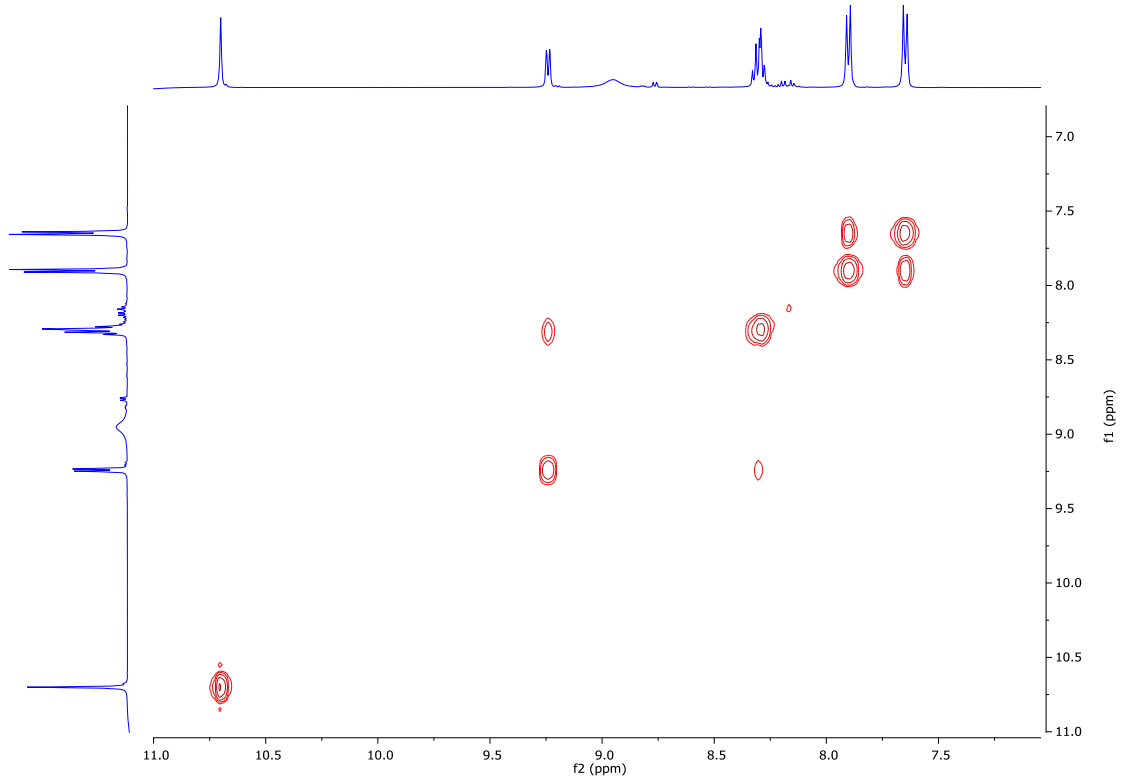
**A**


10.70
9.25
9.25
9.24
9.23
8.33
8.31
8.30
8.29
8.29
8.28
8.27
7.91
7.90
7.89
7.66
7.64
7.64
1.98
2.00
4.09
4.00
4.07
f1 (ppm)

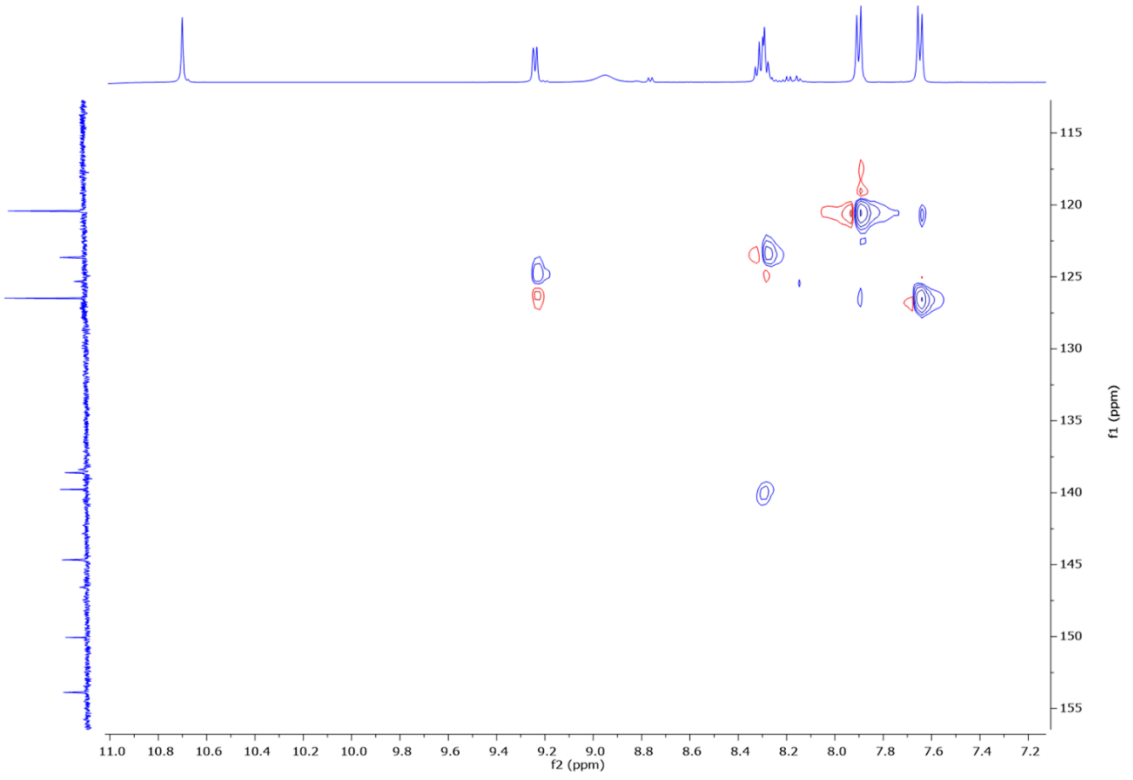
**B**


162.87
153.89
150.06
144.67
139.77
138.62
126.48
125.32
123.65
120.42
f1 (ppm)

**C**


7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0
f1 (ppm)
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
f2 (ppm)

**D**


115
120
125
130
135
140
145
150
155
f1 (ppm)
11.0
10.8
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
f2 (ppm)

**E**

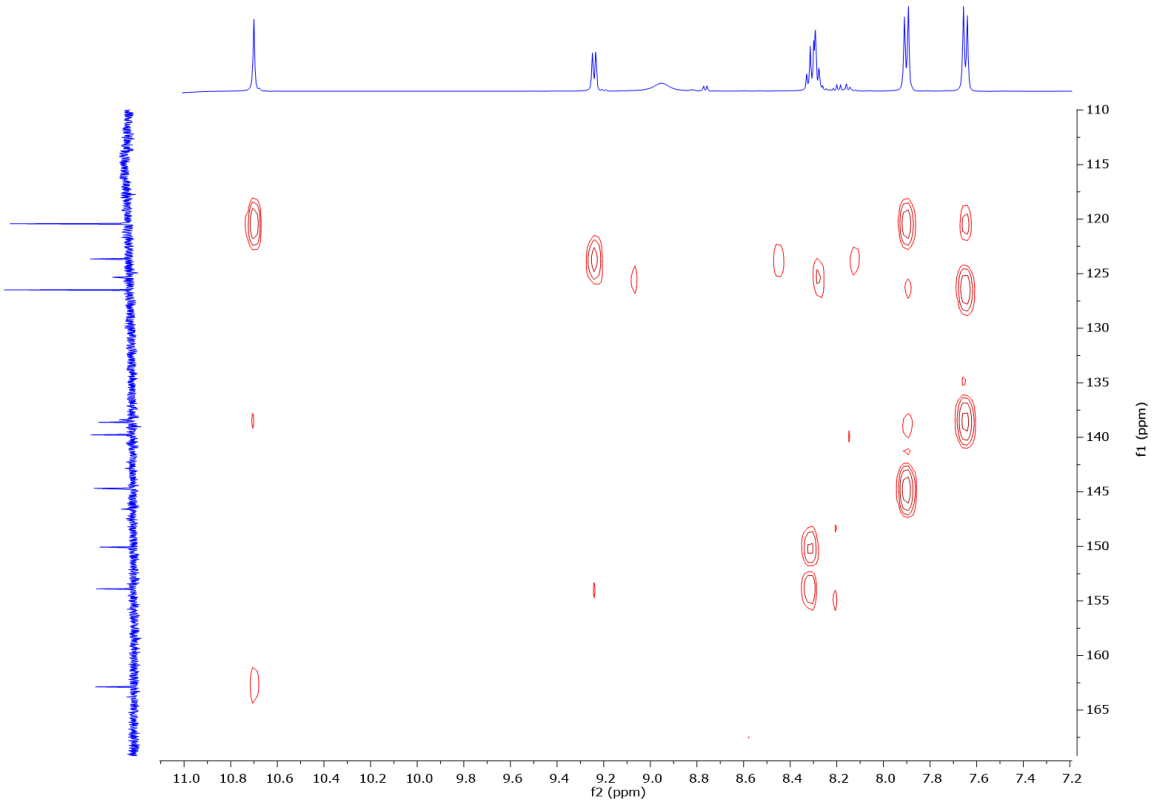
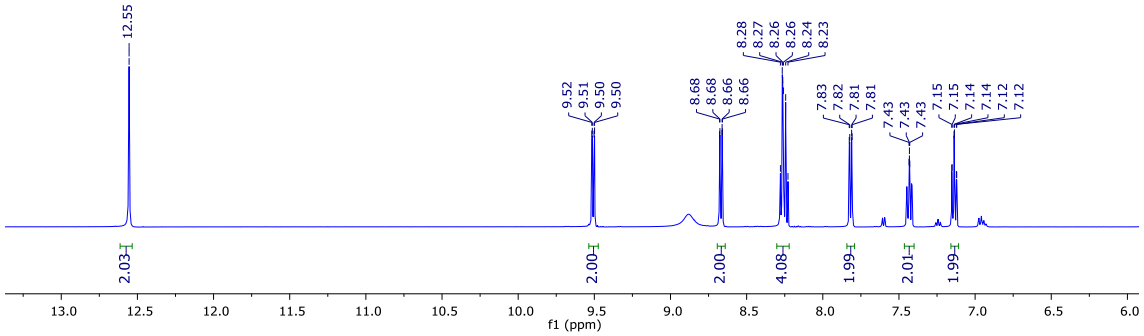
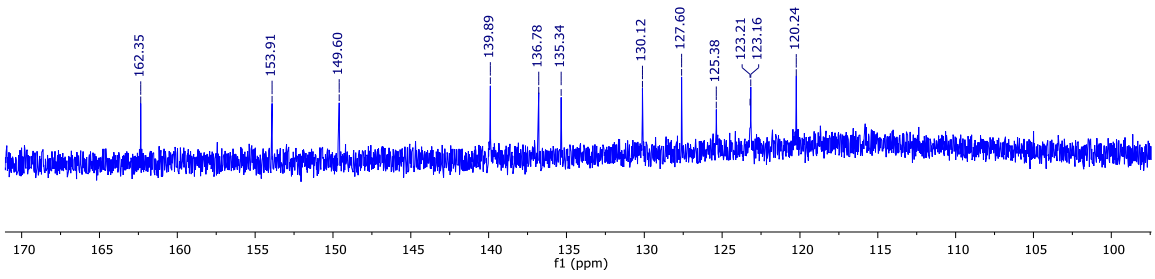



**Figure S5.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2L4^{2-}$**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

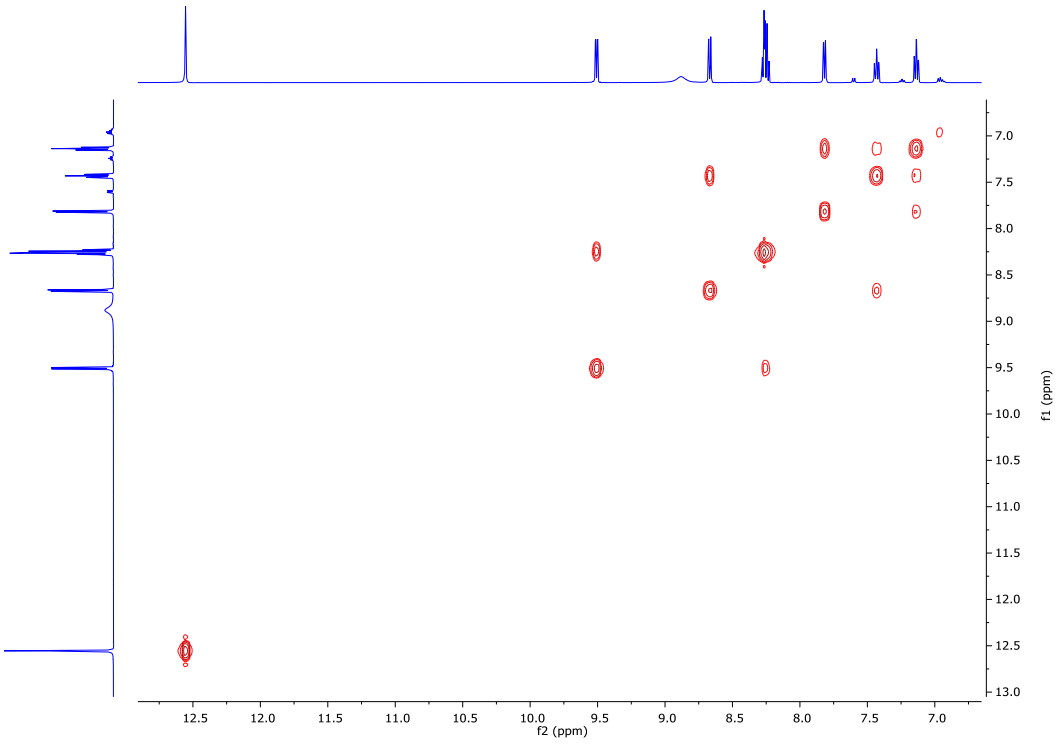
**A**


12.55
9.52
9.51
9.50
9.50
8.68
8.68
8.66
8.66
8.28
8.27
8.26
8.26
8.24
8.23
7.83
7.82
7.81
7.81
7.43
7.43
7.43
7.15
7.15
7.14
7.14
7.12
7.12
2.03
2.00
2.00
4.08
1.99
2.01
1.99
f1 (ppm)

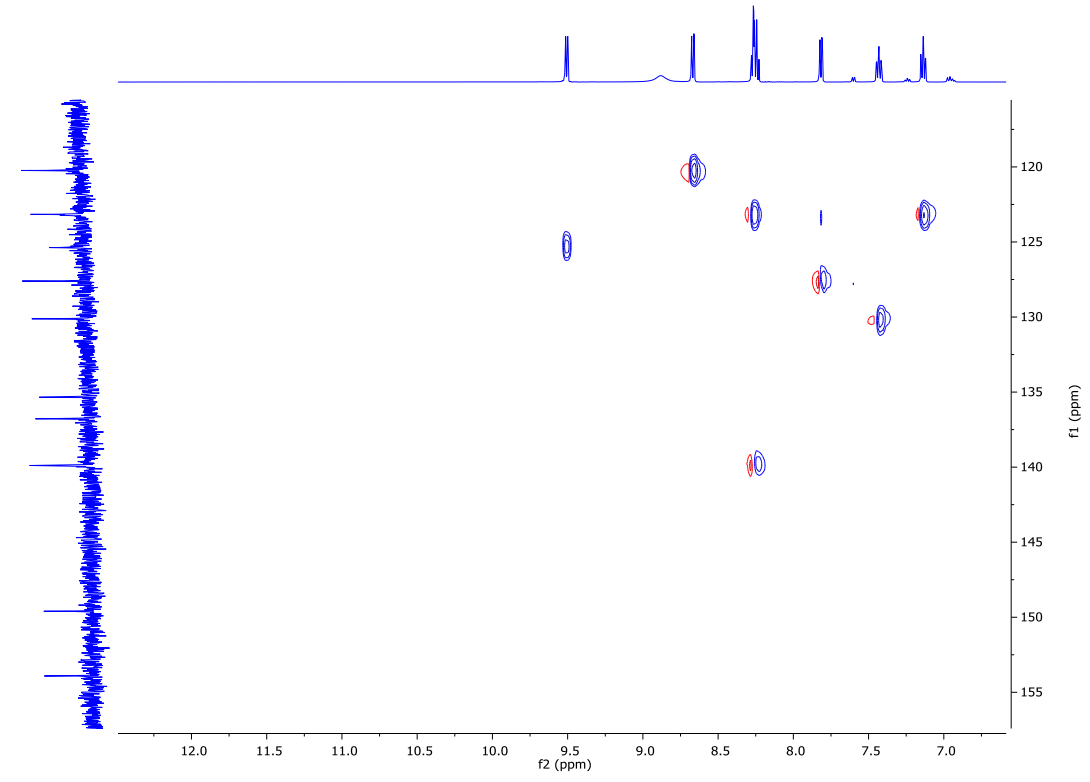
**B**


162.35
153.91
149.60
139.89
136.78
135.34
130.12
127.60
125.38
123.21
123.16
120.24
f1 (ppm)

**C**


12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
f2 (ppm)
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0
11.5
12.0
12.5
13.0
f1 (ppm)

**D**


12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
f2 (ppm)
120
125
130
135
140
145
150
155
f1 (ppm)

**E**

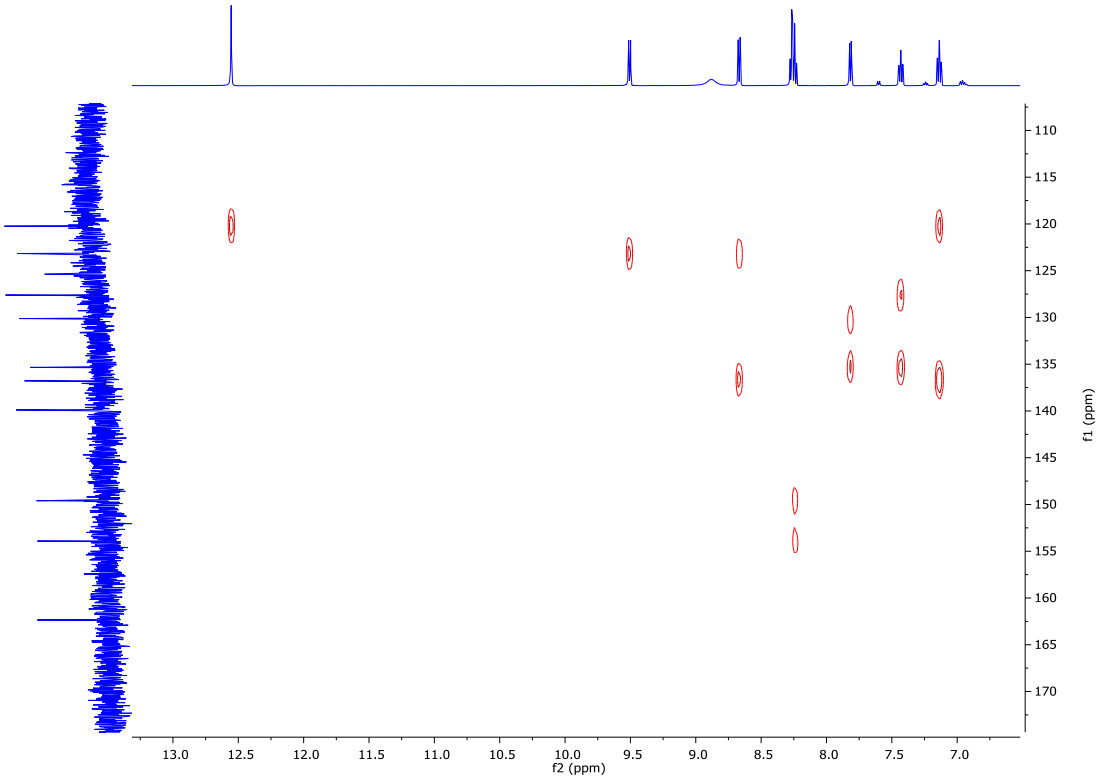
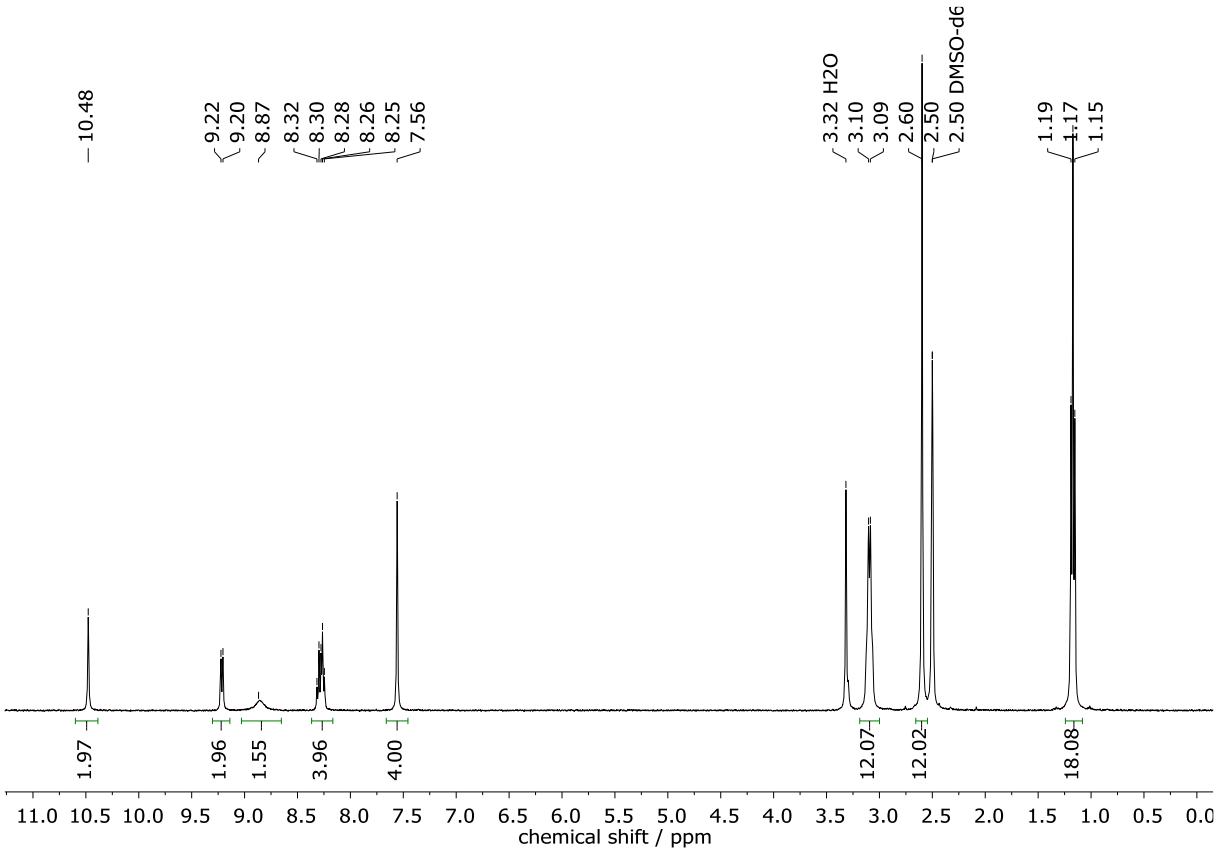
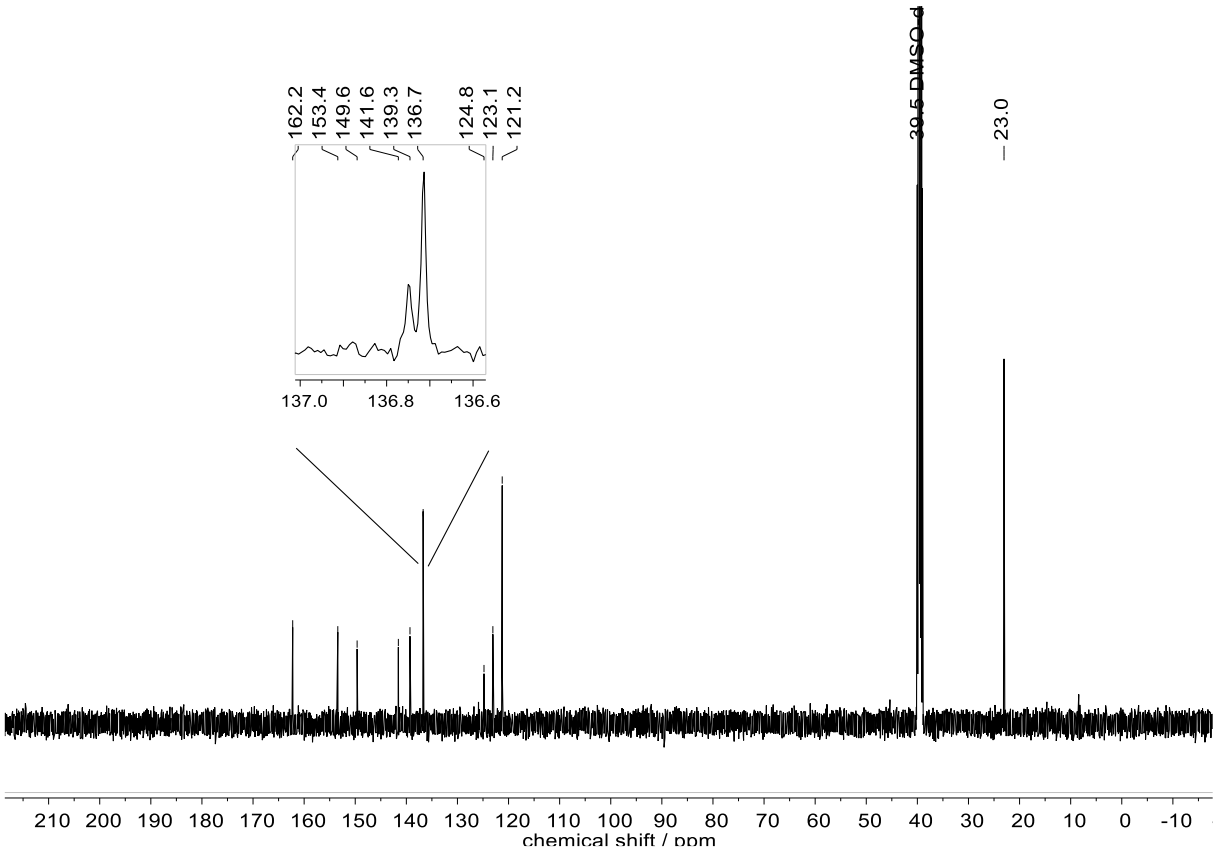



**Figure S6.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2L5^{2-}$**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

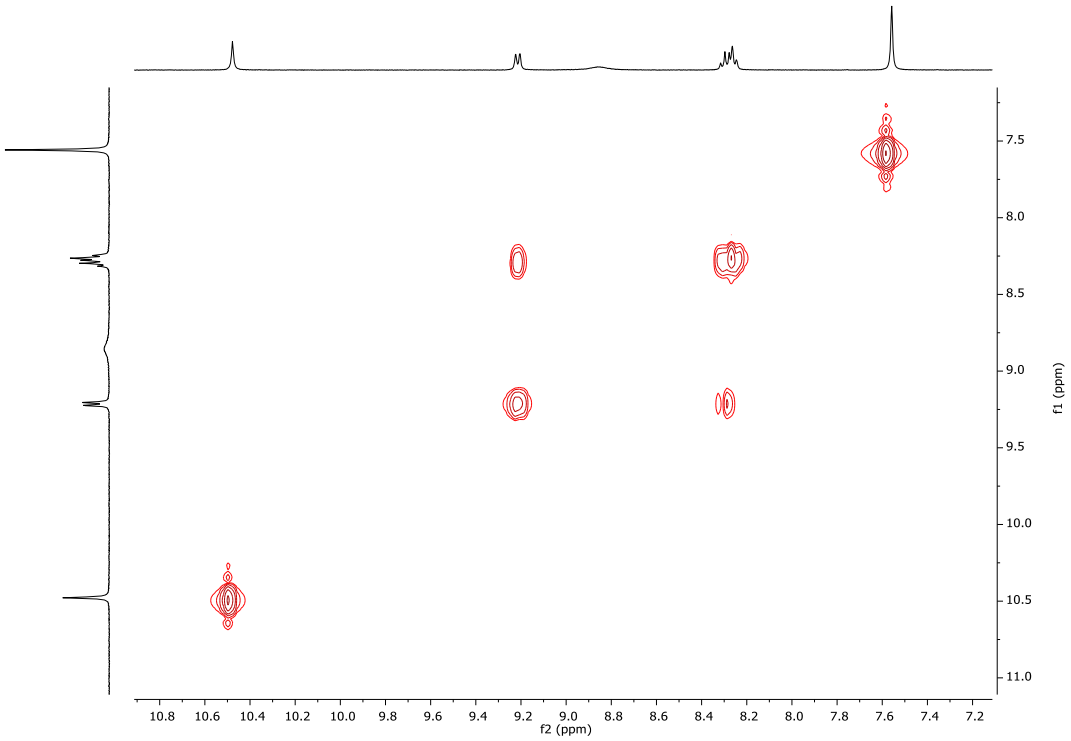
**A**


10.48
9.22
9.20
8.87
8.32
8.30
8.28
8.26
8.25
7.56
3.32 H2O
3.10
3.09
2.60
2.50
2.50 DMSO-d6
1.19
1.17
1.15
1.97
1.96
1.55
3.96
4.00
12.07
12.02
18.08
chemical shift / ppm

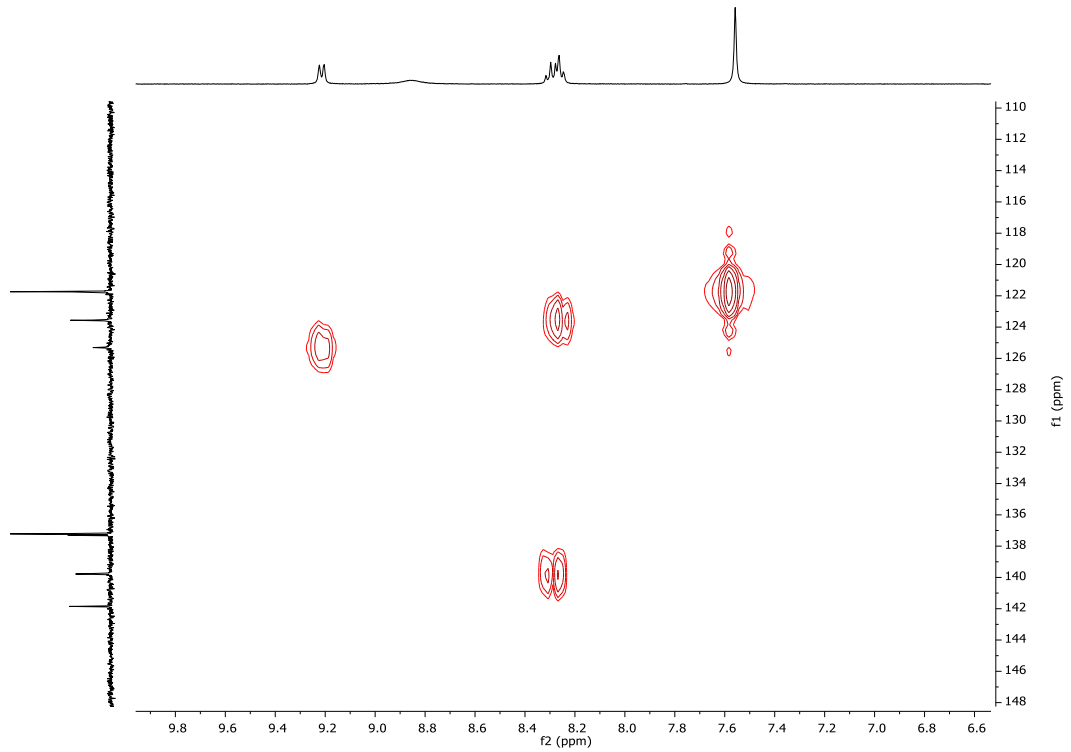
**B**


162.2
153.4
149.6
141.6
139.3
136.7
124.8
123.1
121.2
39.5 DMSO-d6
23.0
137.0
136.8
136.6
chemical shift / ppm

**C**


7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0
f1 (ppm)
10.8 10.6 10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2
f2 (ppm)

**D**


110
112
114
116
118
120
122
124
126
128
130
132
134
136
138
140
142
144
146
148
f1 (ppm)
9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6
f2 (ppm)

**E**

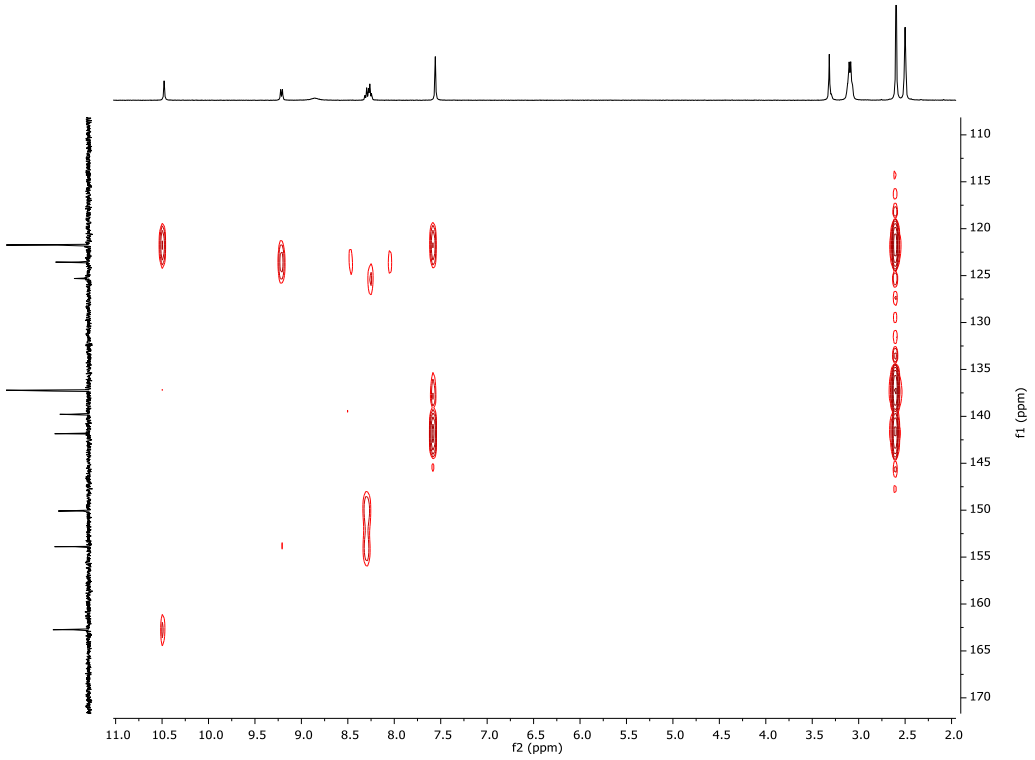
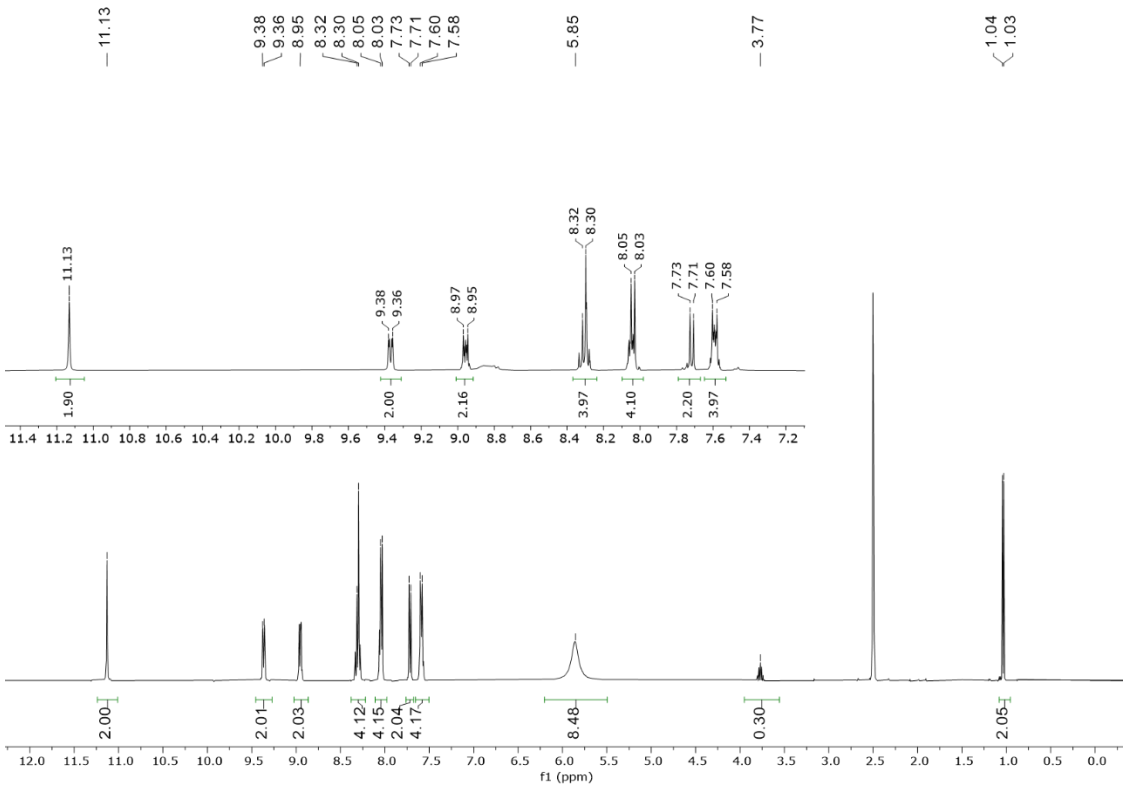
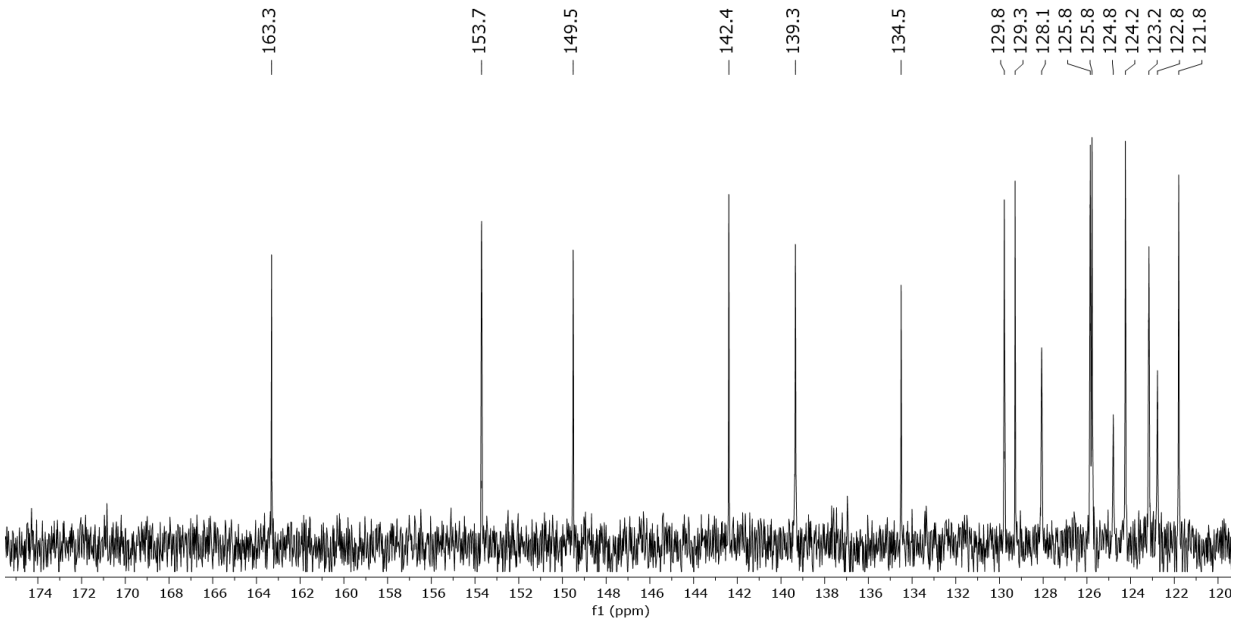



**Figure S7.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2L6^{2-}$**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

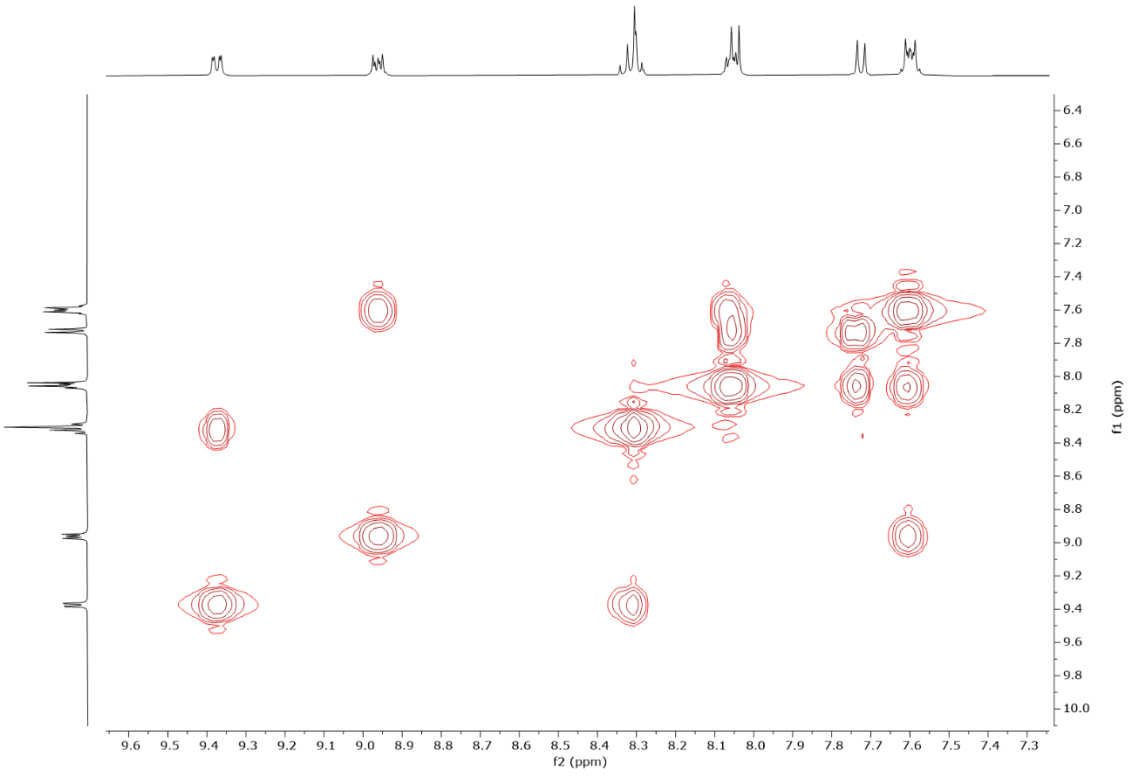
**A**


11.13
9.38
9.36
8.95
8.32
8.30
8.05
8.03
7.73
7.71
7.60
7.58
5.85
3.77
1.04
1.03
f1 (ppm)

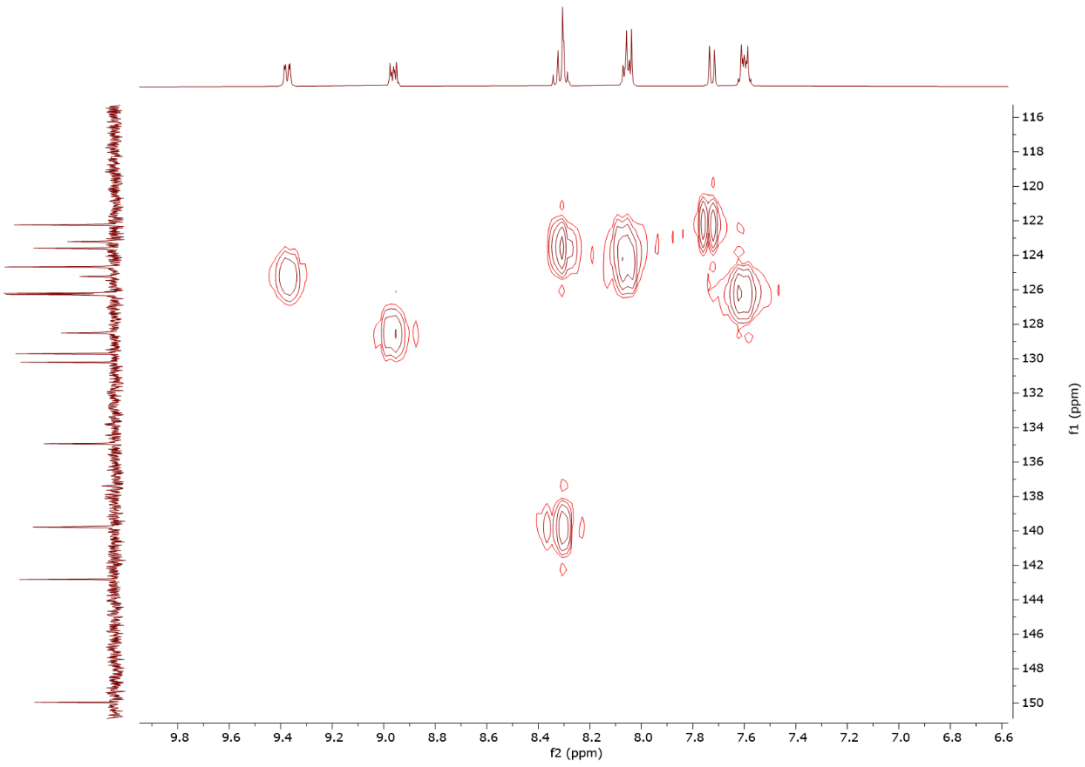
**B**


163.3
153.7
149.5
142.4
139.3
134.5
129.8
129.3
128.1
125.8
125.8
124.8
124.2
123.2
122.8
121.8
f1 (ppm)

**C**




**D**



**E**

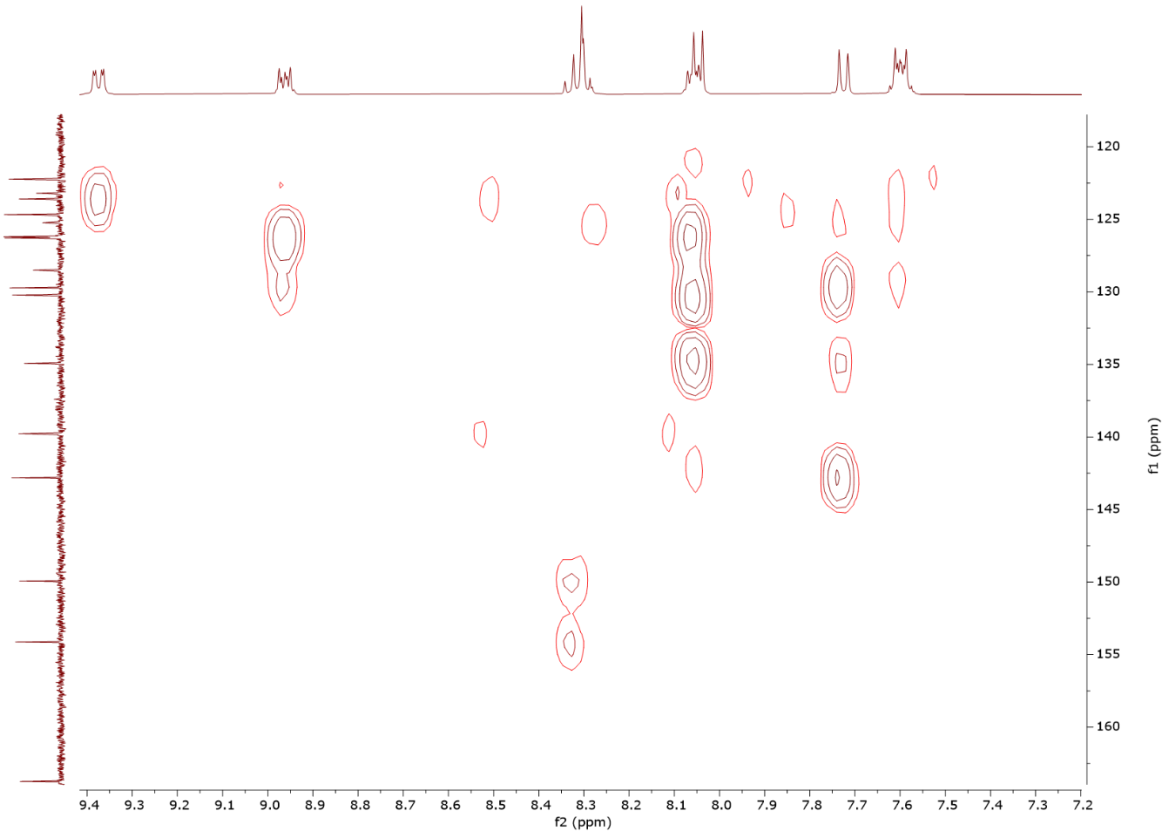
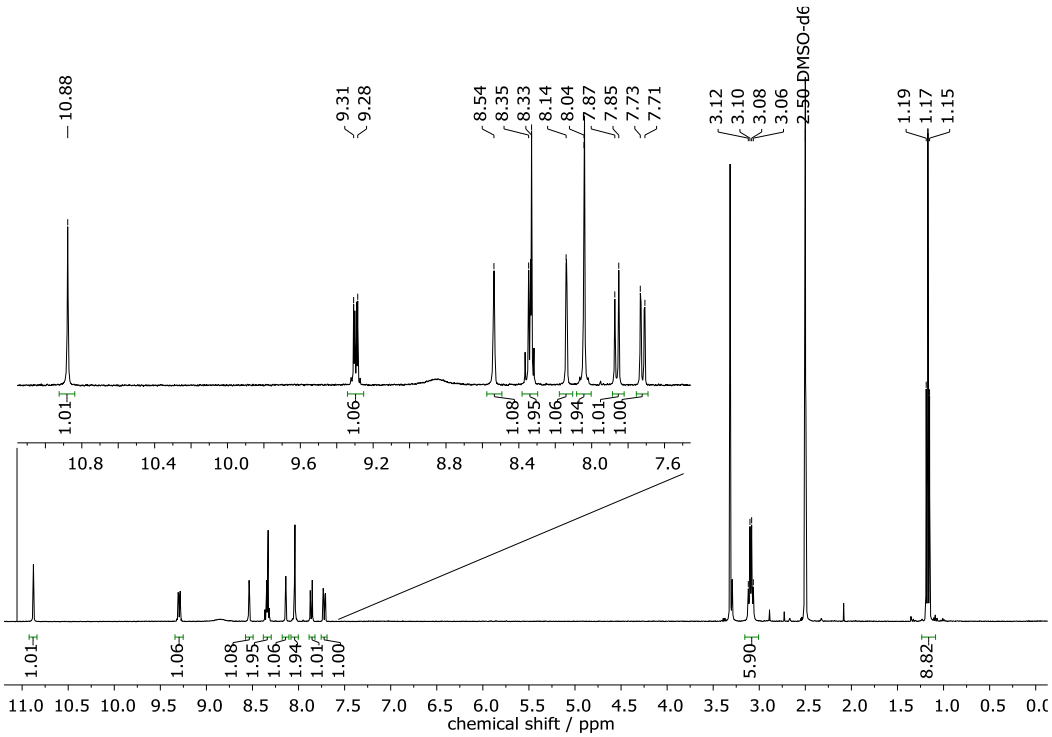
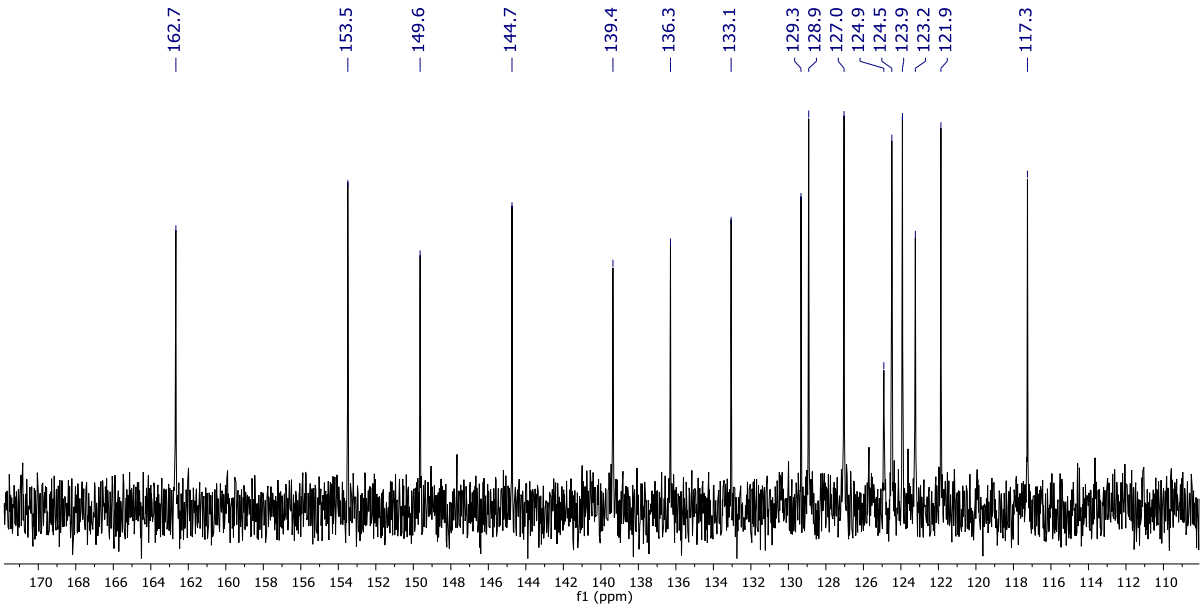



**Figure S8.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2L7^{2-}$**. (A) $^{1}$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

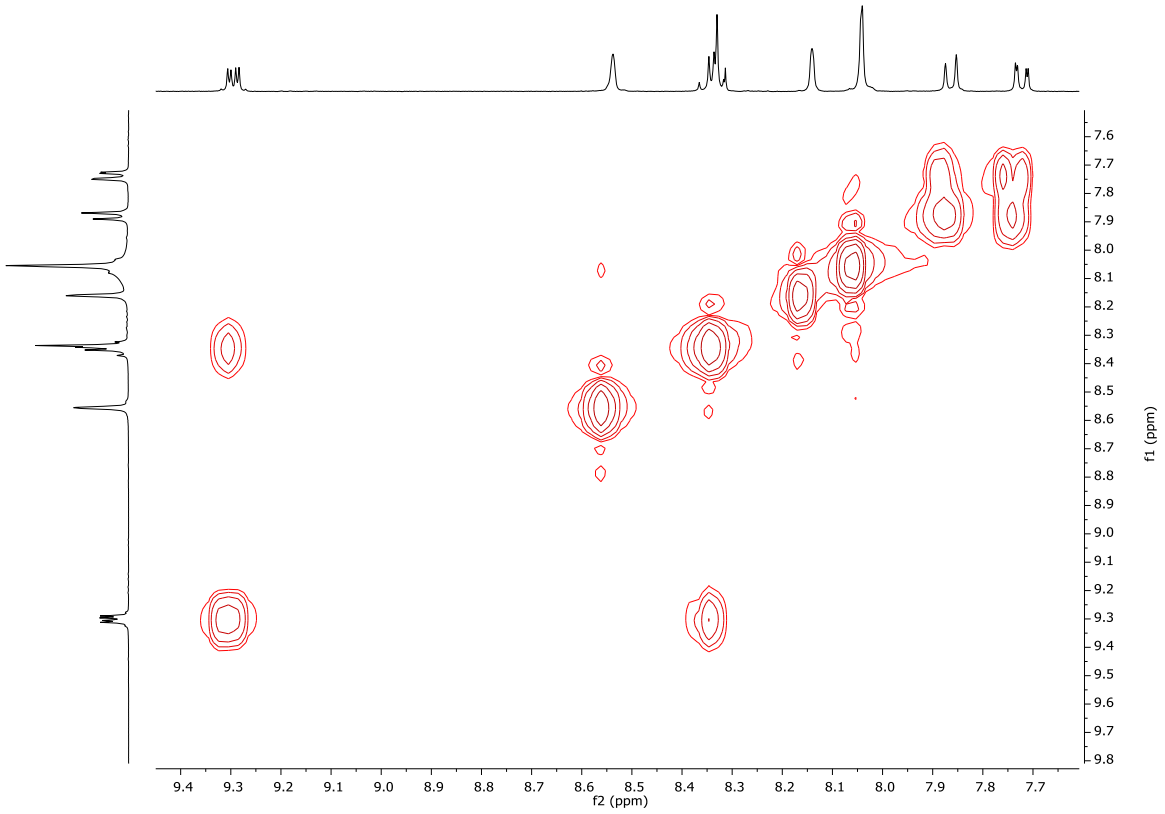
**A**


10.88
9.31
9.28
8.54
8.35
8.33
8.14
8.04
7.87
7.85
7.73
7.71
3.12
3.10
3.08
3.06
2.50 DMSO-d6
1.19
1.17
1.15
1.01
1.06
1.08
1.95
1.06
1.94
1.01
1.00
5.90
8.82
chemical shift / ppm

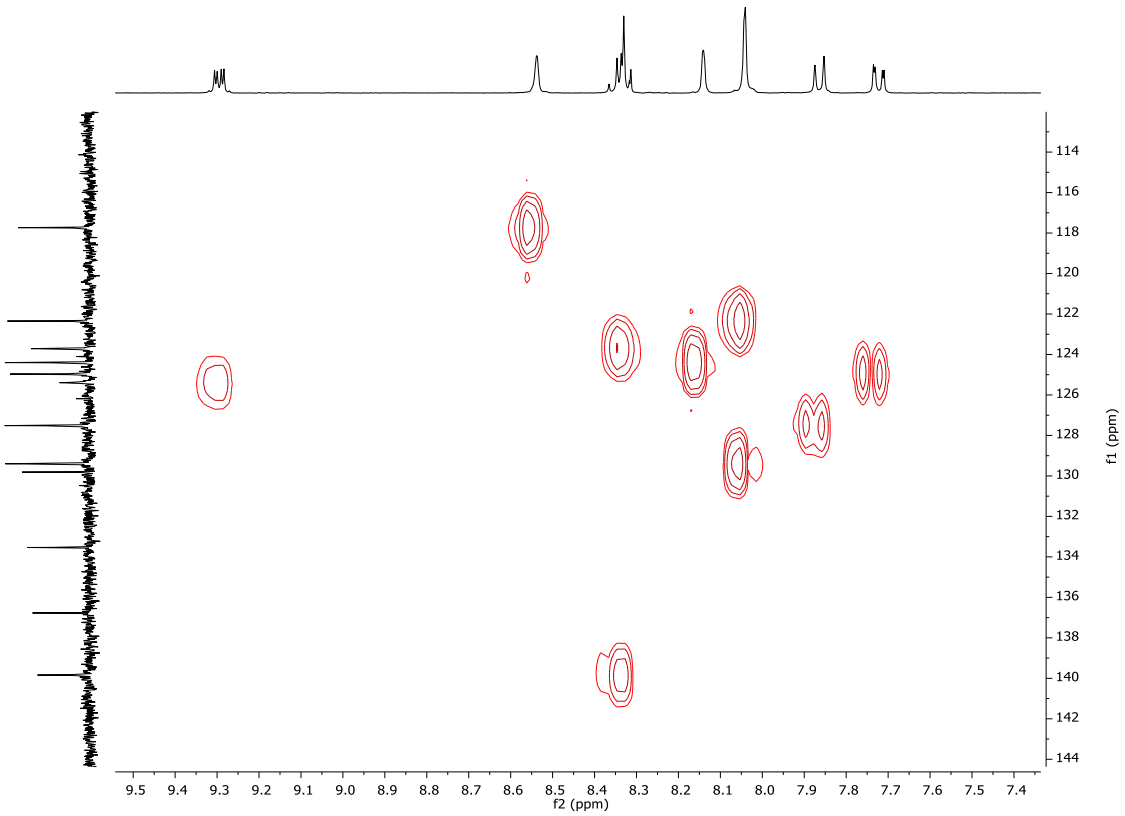
**B**


162.7
153.5
149.6
144.7
139.4
136.3
133.1
129.3
128.9
127.0
124.9
124.5
123.9
123.2
121.9
117.3
f1 (ppm)

**C**




**D**



**E**

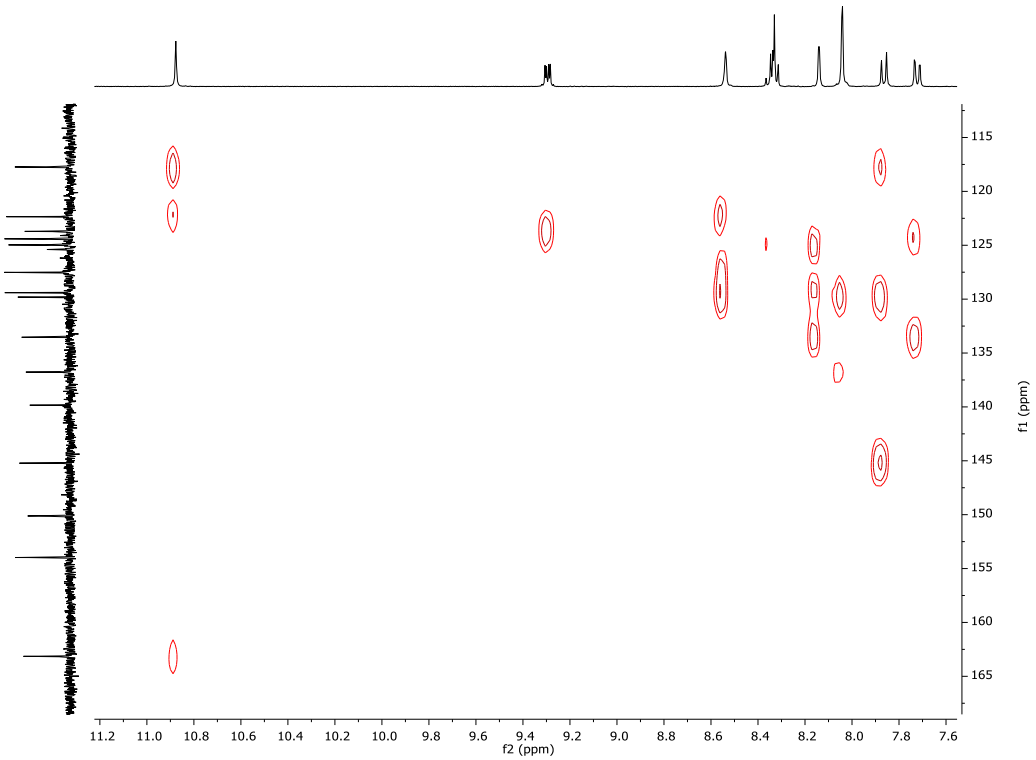



**Figure S9.** NMR spectra (DMSO-$d_6$, 500 MHz, 25 °C) for **$H_2L8^{2-}$**. (A) $^1$H-NMR, (B) $^{13}$C NMR, (C) COSY, (D) HSQC and (E) HMBC.

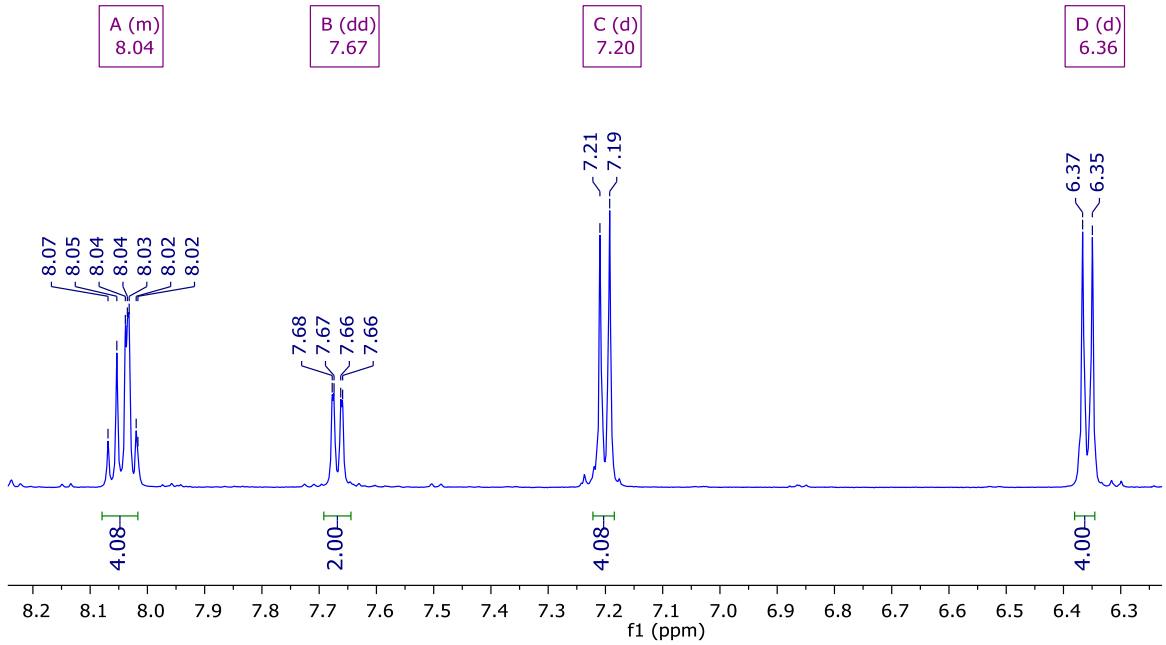



**Figure S10.** $^1$H-NMR spectrum of the complex **$[(L4)Zn]^{2-}$** ($D_2O$-$d_2$, 500 MHz, 25 °C).

**Mass-spectrometry**


**Figure S11.** (+)-ESI-MS for **$H_2$L1**. m/z: 417.0 $[H_2L1+Na^+]^+$

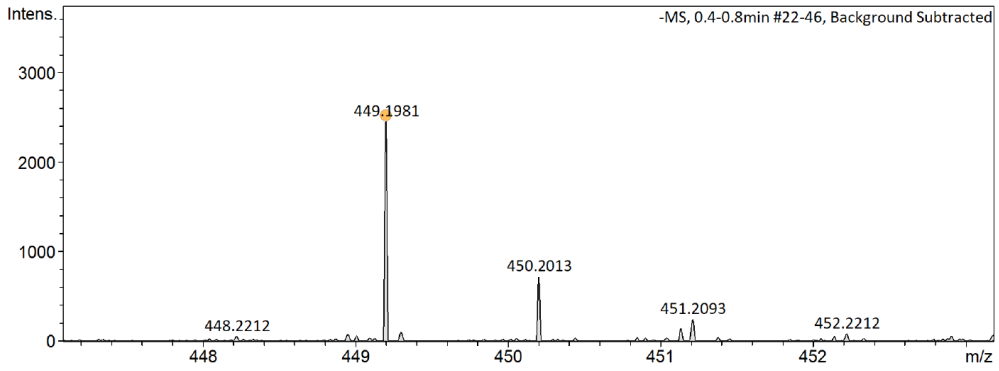



**Figure S12.** (+)-ESI-HRMS for **$H_2$L2**. Calcd for $[H_2L2\text{-}H^+]^+$, ($C_{28}H_{25}N_4O_2$) :449.1983, found: 449.1981.

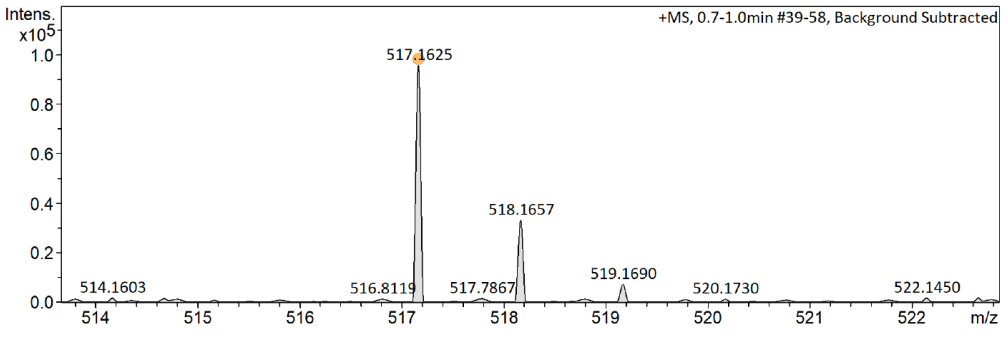



**Figure S13.** (+)-ESI-HRMS for **$H_2$L3**. Calcd for $[H_2L3+Na^+]^+$, ($C_{32}H_{22}N_4O_2Na$): 517.1635, found: 517.1625.

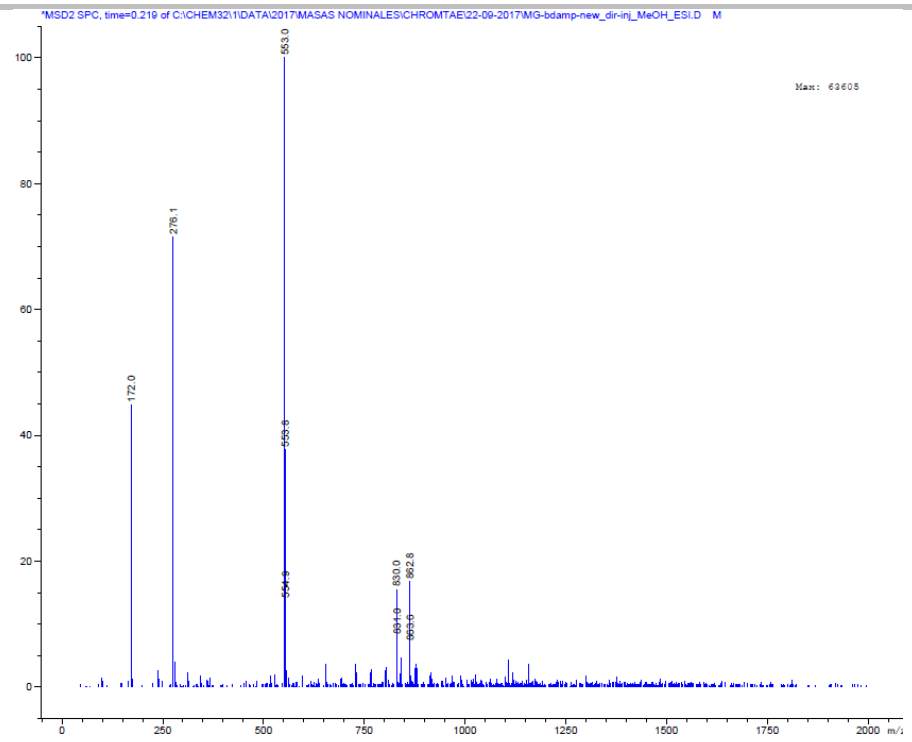



**Figure S14.** (-)-ESI-MS spectrum for **$H_2L4^{2-}$**. m/z: 553.0 $[H_2L4+H^+]^-$, 276.1 $[H_2L4]^{2-}$.

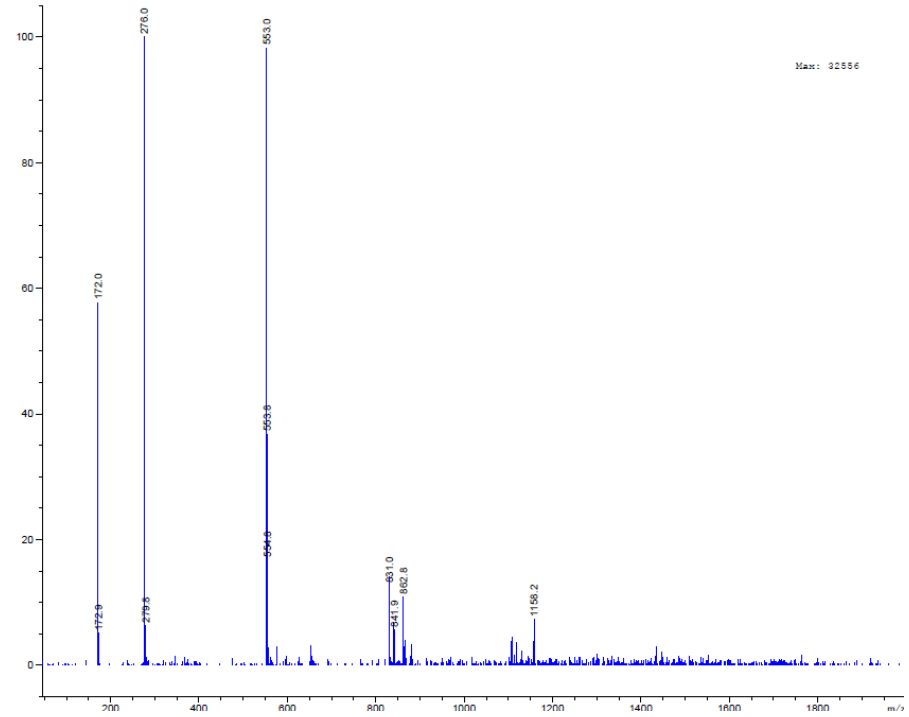



**Figure S15.** (-)-ESI-MS spectrum for the ligand **$H_2L5^{2-}$**. m/z: 553.0 $[H_2L5+H^+]^-$, 276.1 $[H_2L5]^{2-}$

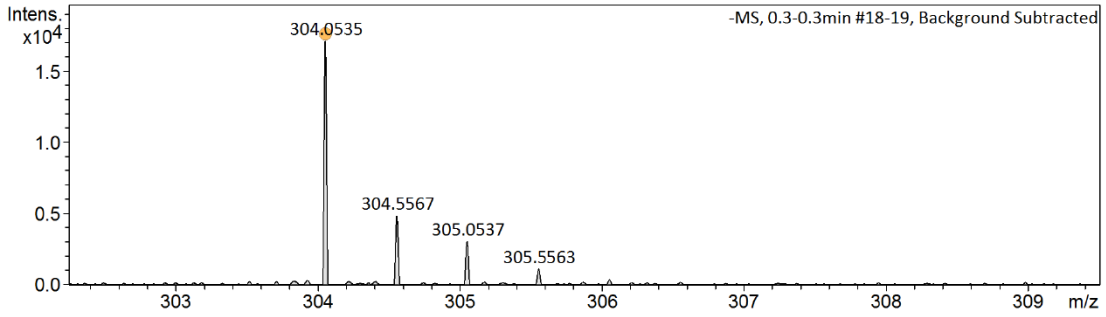



**Figure S16.** (-)-ESI-HRMS for $\mathbf{H_2L6^{2-}}$. Calcd for $[H_2L6]^{2-}$, ($C_{28}H_{24}N_4O_8S_2$) : 304.0523, found 304.0535.

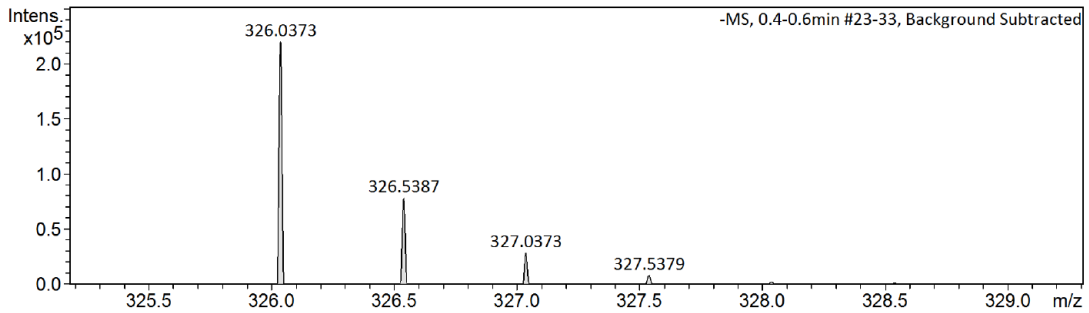



**Figure S17.** (-)-ESI-MS for $\mathbf{H_2L7^{2-}}$. Calcd for $[H_2L7]^{2-}$, ($C_{32}H_{22}N_4O_8S_2$) : 326.0367, found 326.0373.

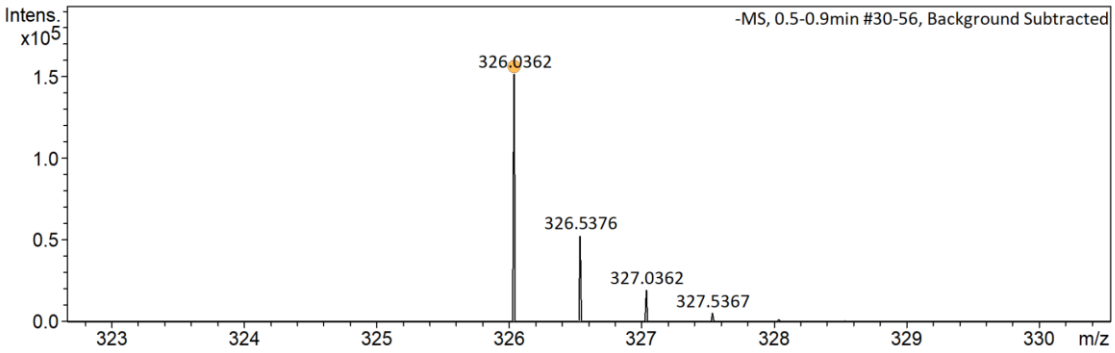



**Figure S18.** (-)-ESI-MS for $\mathbf{H_2L8^{2-}}$. Calcd for $[H_2L8]^{2-}$, ($C_{32}H_{22}N_4O_8S_2$) : 326.0367, found 326.0362.

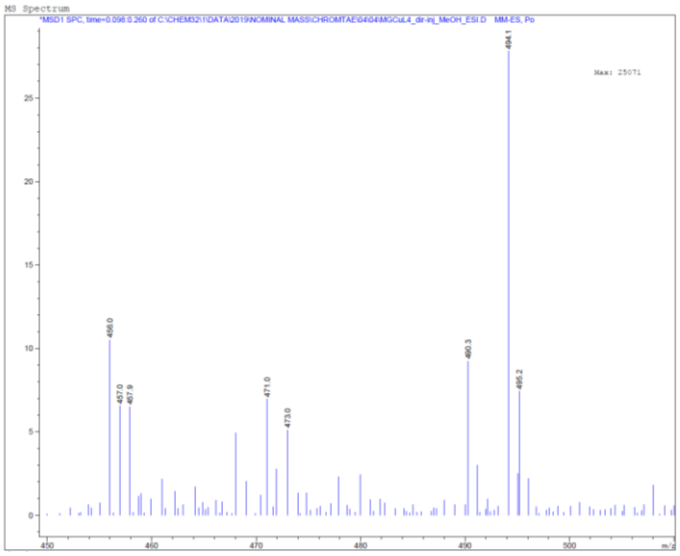


**Figure S19.** (+)-ESI-MS for **[(L1)Cu]**. m/z = 456.0 [(L1)Cu-H$^+$]$^+$; m/z = 494.1[(L1)Cu+K$^+$]$^+$.

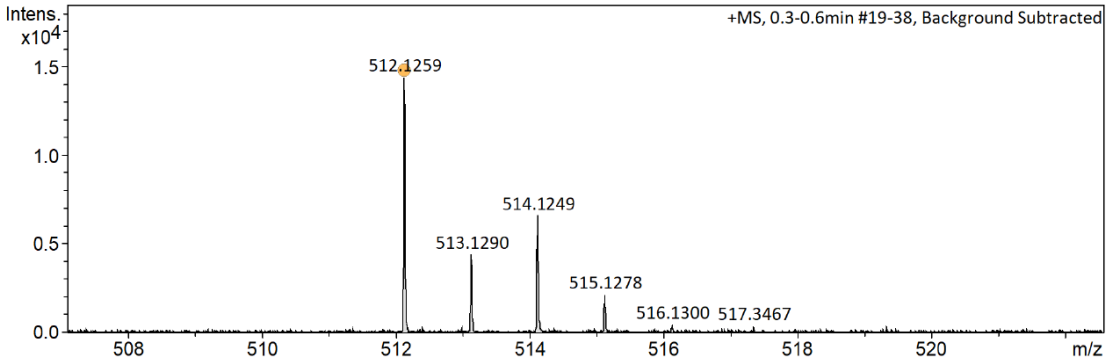



**Figure S20.** (+)-ESI-HRMS for **[(L2)Cu]**. Calcd for [(L2)Cu+H$^+$]$^+$, (C28H25N4O2Cu) : 512.1259, found 512.1268.

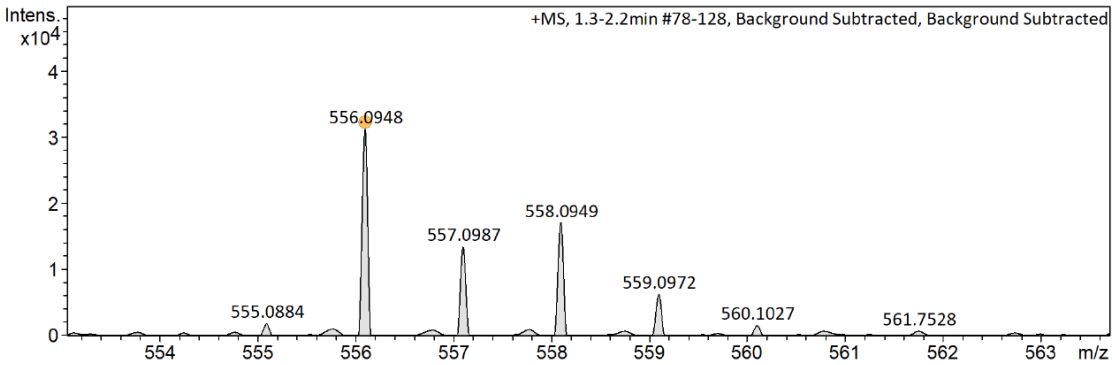



**Figure S21.** (-)-ESI-HRMS for **[(L3)Cu]**. Calcd for [(L3)Cu+H$^+$]$^+$, ($C_{32}H_{21}CuN_4O_2$): 556.0955, found: 556.0948.

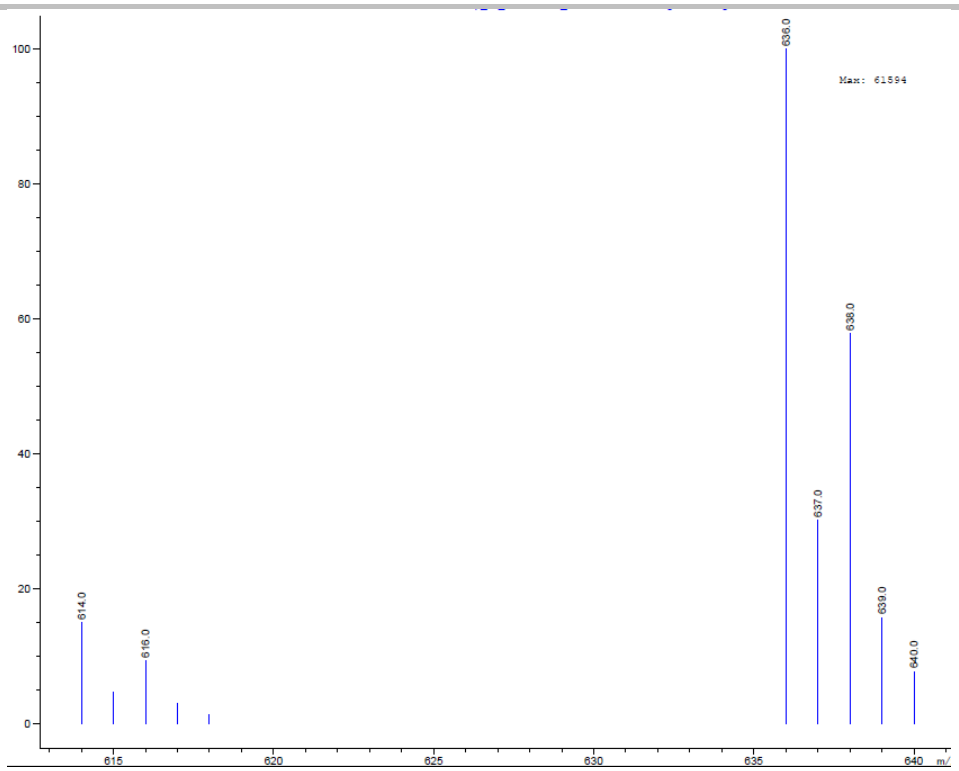



**Figure S22.** (-)-ESI-MS for **[(L4)Cu]$^{2-}$**. m/z: 636.0 [(L4)Cu+Na$^{+}$]$^{-}$, 614.0 [(L4)Cu+H$^{+}$]$^{-}$.

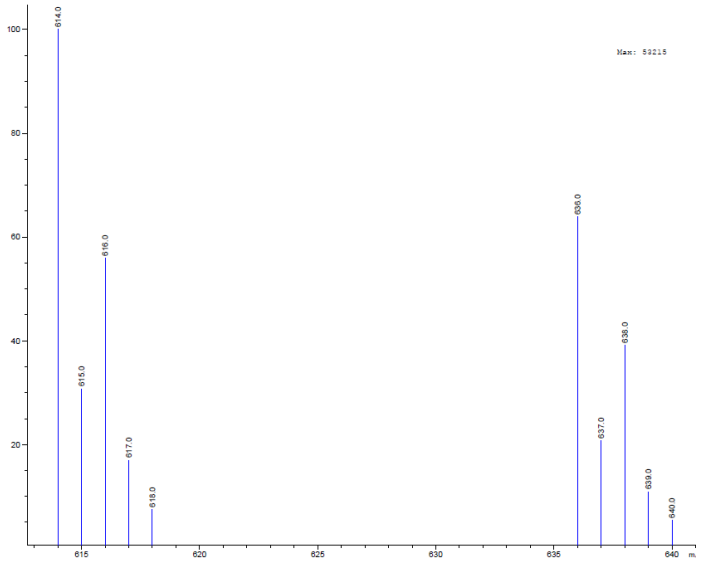



**Figure S23.** (-)-ESI-MS for **[(L5)Cu]$^{2-}$**. m/z: 636.0 [(L5)Cu+Na$^{+}$]$^{-}$, 614.0 [(L5)Cu+H$^{+}$]$^{-}$.

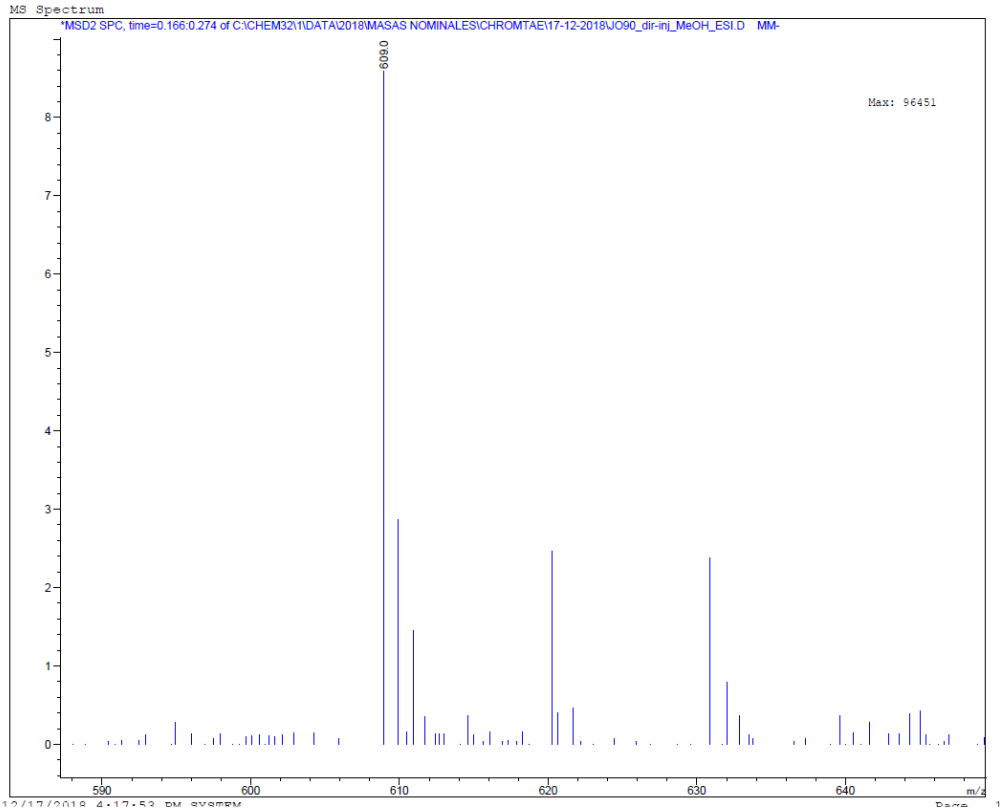



**Figure S24.** (-)-ESI-MS for **[(L6)Cu]$^{2-}$**. m/z = 609.0 [(L6)Cu-Na$^{+}$]$^{-}$.

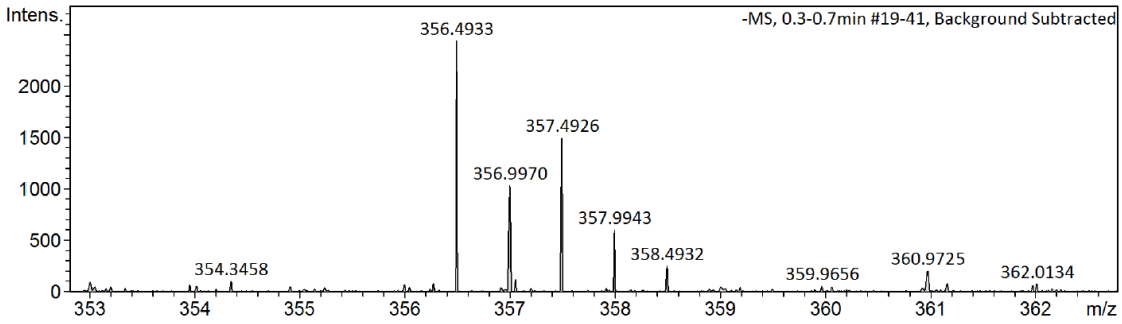



**Figure S25.** (-)-ESI-HRMS for **[(L7)Cu]$^{2-}$**. Calcd for [(L7)Cu]$^{2-}$, ($C_{32}H_{18}CuN_4O_8S_2$) : 356.4937, found 356.4933.

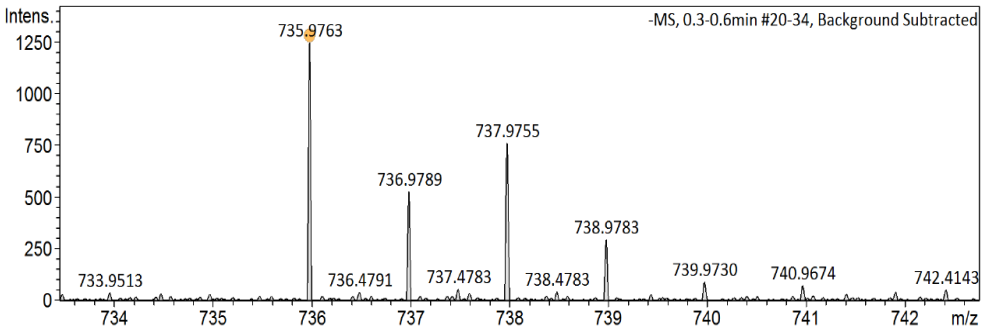



**Figure S26.** (-)-ESI-HRMS for **[(L8)Cu]$^{2-}$**. Calcd for [(L8)Cu+Na$^{+}$]$^{-}$, ($C_{32}H_{18}CuN_4O_8S_2Na$) : 735.9765, found 735.9763.

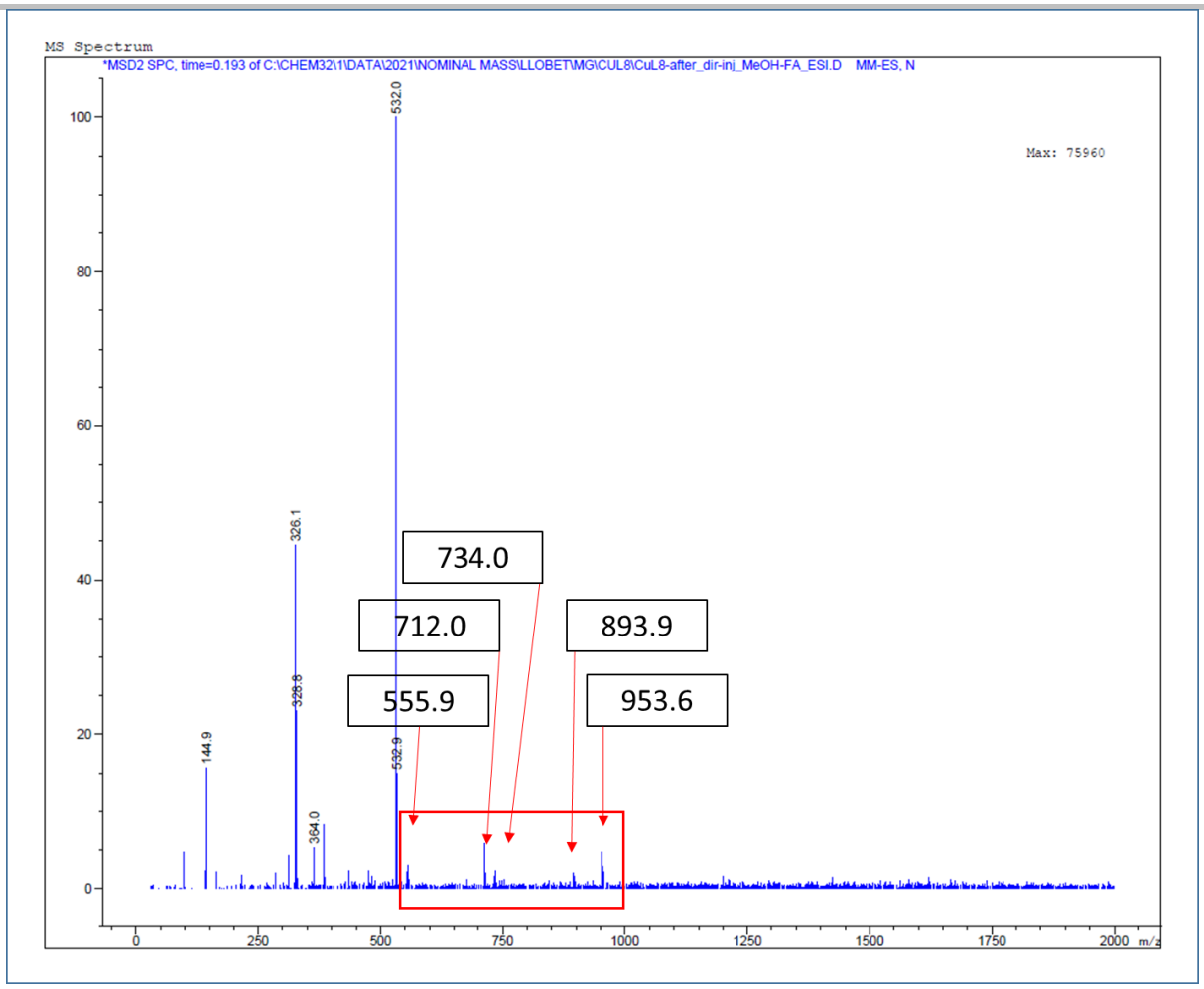



**Figure S27.** (-)-ESI-MS spectrum for **[(L8)Cu]**$^{2-}$ after a CPE experiment at 1.45 V vs. NHE in 0.01 M phosphate buffer pH 11.6 during 12 h. The spectrum shows peaks at m/z= 555.9, 712.0, 734.0, 893.9 and 953.6 can be potentially assigned to molecular Cu degradation products based on the isotopic cracking pattern. The peak at m/z= 712.0 is assigned in Figure S28.

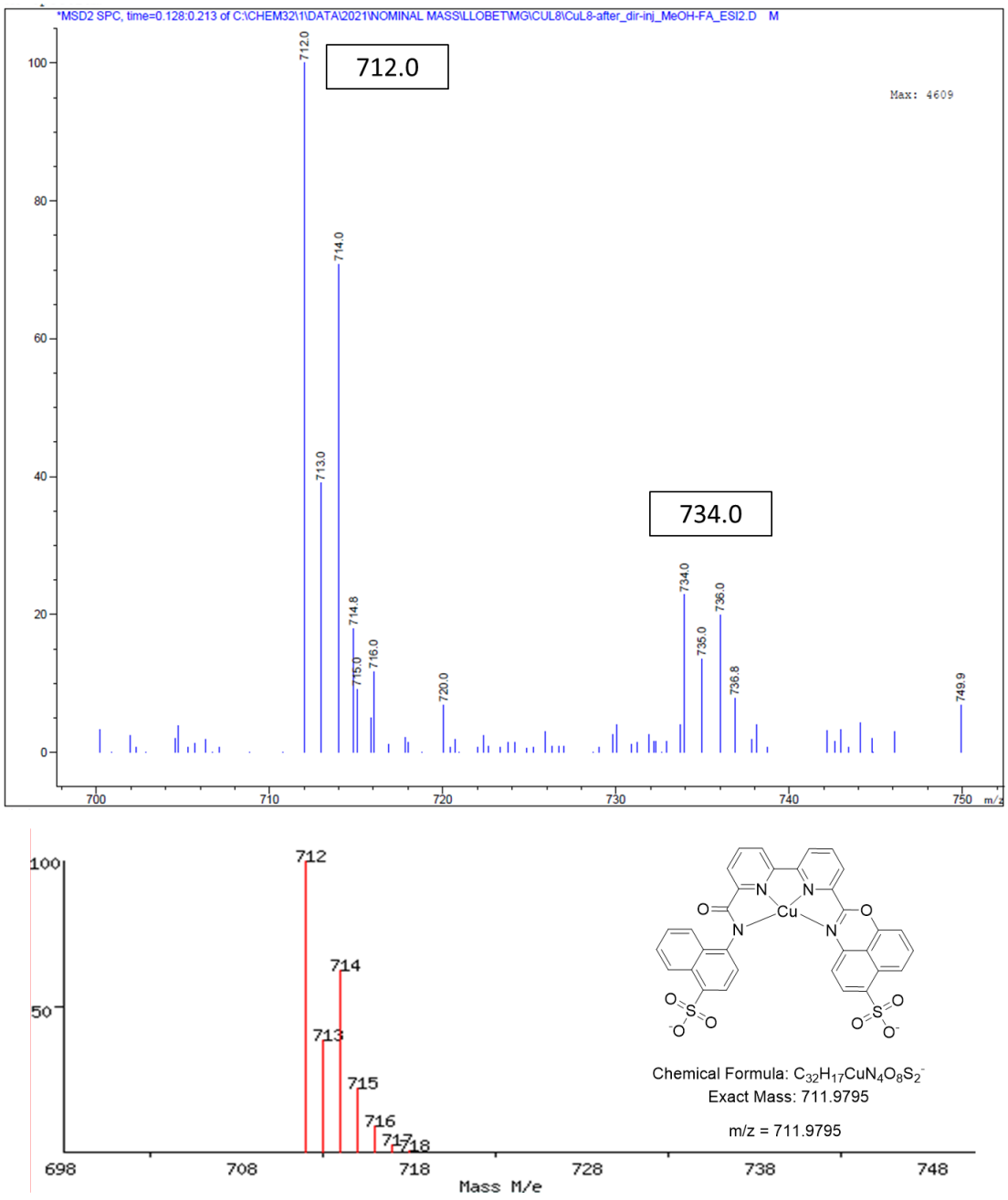



**Figure 28.** Top, zoom in the m/z= 700-750 region of (-)-ESI-MS spectrum from Figure S27. Bottom, simulation and molecular assignment of the m/z =712 peak.

**UV-Vis spectroscopy**

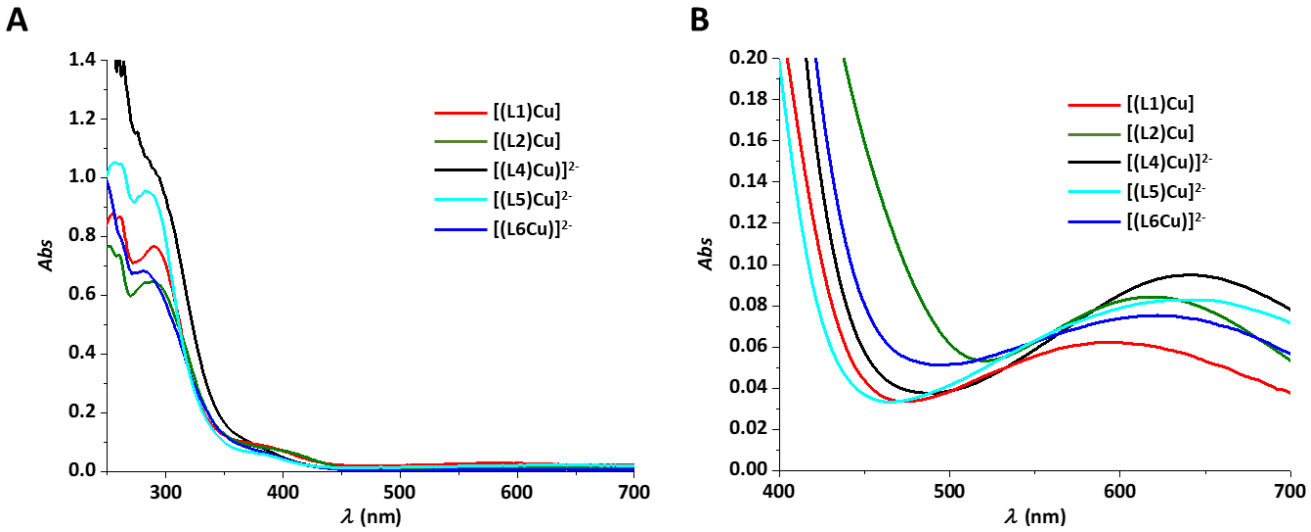



**Figure S29.** (**A**) UV-vis spectra of **[(L1)Cu]** (red line), **[(L2)Cu]** (green line), **[(L4)Cu]$^{2-}$** (black line), **[(L5)Cu]$^{2-}$** (light blue line) and **[(L6)Cu]$^{2-}$** (blue line). (**B**) UV-vis spectra enlargement of the visible region. Conditions: [**Complex**] = ~0.1 mM in 0.1 M phosphate buffer (pH 11.6). ***Note:*** in order to solve low solubility issues with **[(L1)Cu]** and **[(L2)Cu]**, 40% of TFE was added to the mixture used for UV-Vis measurements.

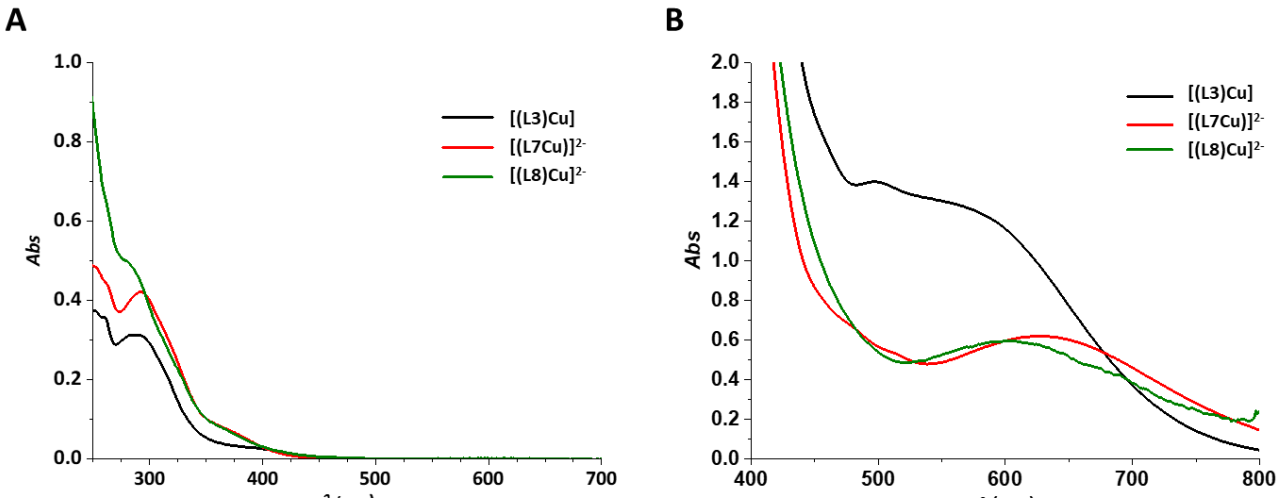



**Figure S30.** (**A**) UV-vis spectra of **[(L3)Cu]** (black line), **[(L7)Cu]$^{2-}$** (red line) and **[(L8)Cu]$^{2-}$** (green line). (**B**) UV-vis spectra enlargement of the visible region. Conditions: **[Complex]** = 0.04 mM (A, *d*= 1 mm) and 1 mM (B, *d*= 10 mm) in 0.1 M phosphate buffer (pH 11.6). ***Note:*** in order to solve low solubility issues with **[(L3)Cu]** 40% of TFE was added to the mixture used for UV-Vis measurements.

# SUPPORTING INFORMATION

## X-Ray Crystallography

### Crystal preparation:

**Table S1.** Summary of the conditions employed for the crystallization of the complexes studied in this work.

| Compound | Methodology |
|---|---|
| **$H_2L5^{2-}$** | Crystals were grown in water by slow diffusion of EtOH. |
| **[(L1)Cu]** | Crystals were grown by slow evaporation in MeOH/Toluene. |
| **[(L2)Cu]** | Crystals were grown in MeOH by slow diffusion of $Et_2O$. |
| **[(L3)Cu]** | Crystals were grown by slow evaporation in MeOH/Toluene. |
| **$[(L4)Cu]^{2-}$** | Crystals were grown in water by slow diffusion of acetone. |
| **$[(L5)Cu]^{2-}$** | Crystals were grown in water by slow diffusion of acetone. |
| **$[(L6)Cu]^{2-}$** | Crystals were grown in MeOH by slow diffusion of layered isopropanol. |
| **$[(L7)Cu]^{2-}$** | Crystals were grown in water by slow diffusion of acetone. |

The crystals were selected using a Zeiss stereomicroscope using polarized light and prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation.

**Data collection:** Crystal structure determinations for samples were carried out using an Apex DUO Kappa 4-axis goniometer equipped with an APPEX 2 4K CCD area detector, a Microfocus Source E025 IuS using $MoK_\alpha$ radiation, a Quazar MX multilayer Optics as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus ($T$ = -173 ˚C). Full-sphere data collection was used with $\omega$ and $\varphi$ scans. *Programs used:* Bruker Device: Data collection APEX-2,[7] data reduction Bruker Saint[8] V/.60A and absorption correction SADABS.[9]

**Structure Solution and Refinement**: Crystal structure solution was achieved using the computer program SHELXT.[10] Visualization was performed with the program SHELXle.[11] Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on $F^2$ using all measured intensities was carried out using the program SHELXL 2015.[12] All non-hydrogen atoms were refined including anisotropic displacement parameters.

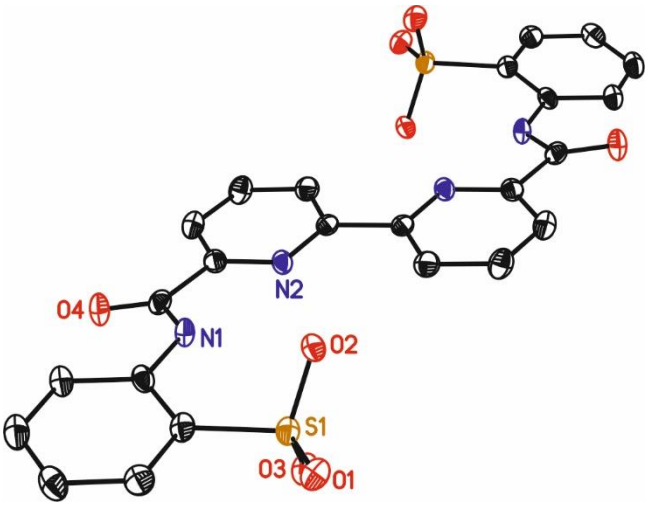



**Figure S31.** ORTEP representation of **$H_2L5^{2-}$** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; S, yellow.

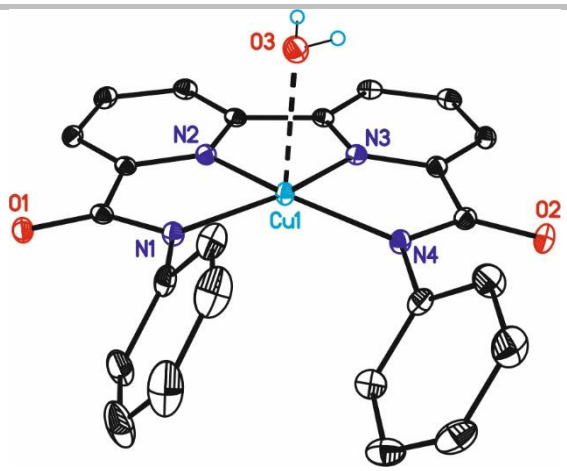



**Figure S32.** ORTEP representation of **[(L1)Cu]** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; Cu, light blue. The ORTEP drawing shows a contact (2.38 Å) with an oxygen from a $H_2O$ molecule in the apical position.

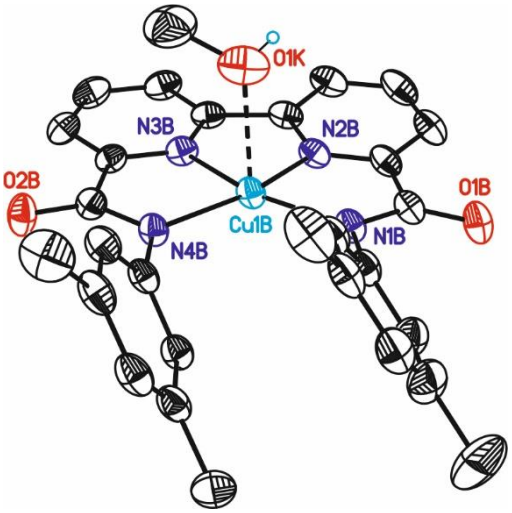



**Figure S33.** ORTEP representation of **[(L2)Cu]** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; Cu, light blue. The ORTEP drawing shows a contact (2.47 Å) with an oxygen from a MeOH molecule in the apical position.

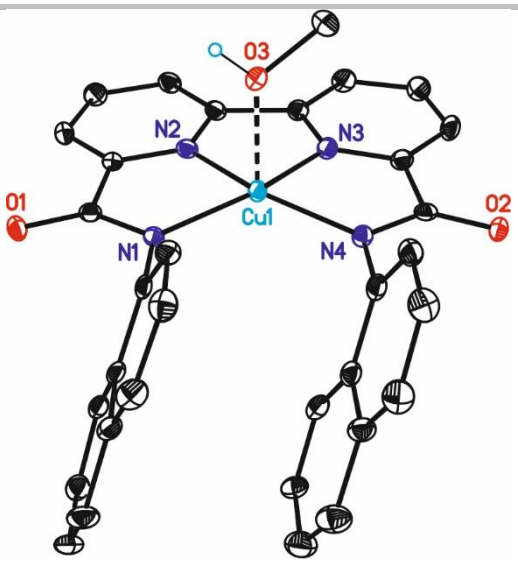



**Figure S34.** ORTEP representation of **[(L3)Cu]** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; Cu, light blue. The ORTEP drawing shows a contact (2.25 Å) with an oxygen from a MeOH molecule in the apical position.

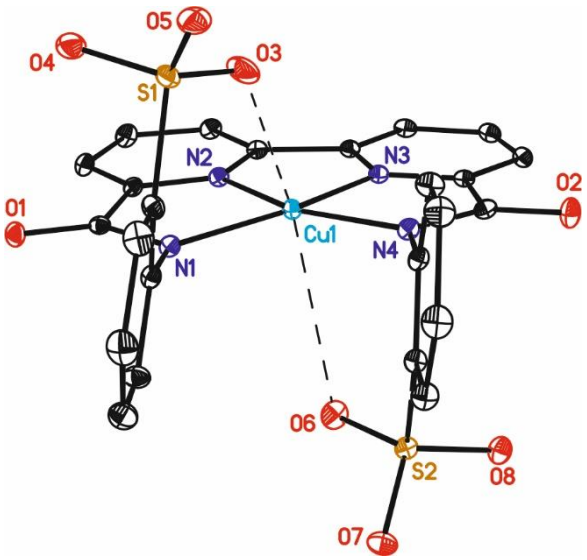



**Figure S35.** ORTEP representation of **[(L5)Cu]**$^{2-}$ at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; Cu, light blue; S, yellow. The ORTEP drawing shows a contact (2.61 Å) between an oxygen from the sulfonate moiety (O3) and the Cu center in the apical position.

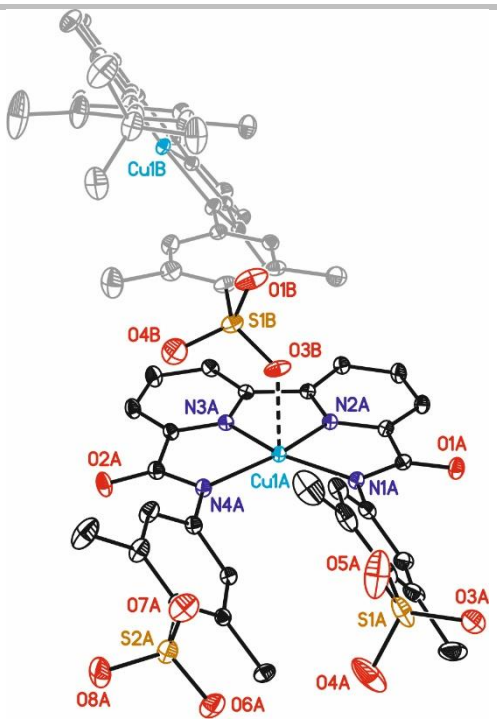



**Figure S36.** ORTEP representation of **[(L6)Cu]$^{2-}$** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, black; N, blue; O, red; Cu, light blue; S, yellow. The ORTEP drawing shows a contact (2.33 Å) with a sulfonate moiety from another **[(L6)Cu]$^{2-}$** unit in the apical position (grey).

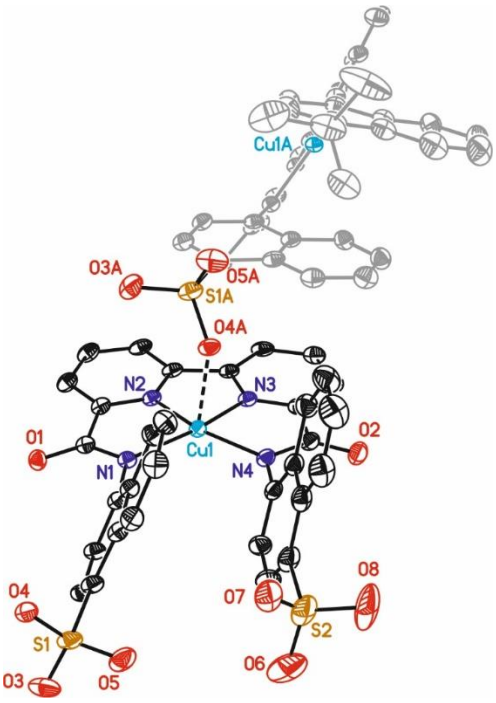



**Figure S37.** ORTEP representation of **[(L7)Cu]$^{2-}$** at 50% probability level. The counter ions, solvent molecules and hydrogen atoms have been omitted for clarity. Color code: C, grey; N, blue; O, red; Cu, light blue; S, yellow. The ORTEP drawing shows a contact (2.38 Å) with a sulfonate moiety from another **[(L7)Cu]$^{2-}$** unit in the apical position (grey).

# SUPPORTING INFORMATION

**Table S2.** Selected interatomic bond distances.

| | Cu-$N_{bpy1}$ | Cu-$N_{bpy2}$ | Cu-$N_{amide1}$ | Cu-$N_{amide2}$ | Cu-$X_{apical}$ | $N_{amide1}$-$C_{ar1}$ | $N_{amide2}$-$C_{ar2}$ |
|---|---|---|---|---|---|---|---|
| [(L1)Cu] | 1.9498(13) | 1.9573(13) | 1.9833(13) | 2.0158(13) | 2.3831(14) | 1.422(2) | 1.433(2) |
| [(L2)Cu] | 1.9522(17) | 1.9546(17) | 1.9855(17) | 1.9913(17) | 2.423(3) | 1.425(3) | 1.423(2) |
| | 1.9475(17) | 1.9517(17) | 1.9759(18) | 1.9828(17) | 2.475(2) | 1.429(2) | 1.421(2) |
| [(L3)Cu] | 1.950(2) | 1.9597(19) | 1.9920(19) | 2.012(5) | 2.2455(18) | 1.434(3) | 1.421(6) |
| $[(L4)Cu]^{2-}$ | 1.9569(14) | 1.9508(14) | 2.0085(14) | 2.0152(14) | 2.3069(14) | 1.415(2) | 1.418(2) |
| $[(L5)Cu]^{2-}$ | 1.9515(14) | 1.9473(13) | 1.9632(14) | 1.9868(14) | 2.6110(13) | 1.418(2) | 1.424(2) |
| $[(L6)Cu]^{2-}$ | 1.9674(17) | 1.9602(17) | 1.9961(17) | 2.0163(17) | 2.324(6) | 1.419(3) | 1.414(3) |
| | 1.9615(17) | 1.9554(18) | 1.9848(18) | 2.0058(18) | 2.339(3) | 1.420(3) | 1.421(3) |
| $[(L7)Cu]^{2-}$ | 1.943(2) | 1.964(2) | 2.012(2) | 1.979(2) | 2.382(2) | 1.431(3) | 1.421(4) |

**Table S3.** Selected interatomic angles.

| | $N_{bpy1}$-Cu-$N_{bpy2}$ | $N_{amide1}$-Cu-$N_{bpy1}$ | $N_{bpy2}$-Cu-$N_{amide2}$ | $N_{amide1}$-Cu-$N_{amide2}$ | $N_{bpy1}$-Cu-$N_{amide2}$ | $N_{bpy2}$-Cu-$N_{amide1}$ |
|---|---|---|---|---|---|---|
| [(L1)Cu] | 78.02(5) | 80.34(5) | 80.94(5) | 118.99(5) | 156.79(6) | 157.46(6) |
| [(L2)Cu] | 77.41(7) | 80.82(7) | 81.09(6) | 119.66(7) | 158.19(7) | 156.42(7) |
| | 77.96(7) | 81.09(7) | 80.83(7) | 119.73(7) | 157.90(7) | 158.95(7) |
| [(L3)Cu] | 77.99(8) | 80.74(8) | 80.77(15) | 118.44(14) | 157.09(19) | 156.92(8) |
| $[(L4)Cu]^{2-}$ | 78.27(6) | 80.12(6) | 80.74(6) | 119.69(6) | 158.81(6) | 155.51(6) |
| $[(L5)Cu]^{2-}$ | 78.49(6) | 80.16(6) | 80.56(6) | 120.78(6) | 159.03(6) | 158.00(6) |
| $[(L6)Cu]^{2-}$ | 77.43(7) | 80.58(7) | 80.53(7) | 120.23(7) | 156.08(7) | 157.57(7) |
| | 77.76(7) | 80.80(7) | 80.58(7) | 119.75(7) | 156.63(8) | 158.13(7) |
| $[(L7)Cu]^{2-}$ | 77.78(10) | 81.30(10) | 80.62(10) | 118.57(10) | 157.37(10) | 157.09(10) |

## Electron Paramagnetic Resonance (EPR)

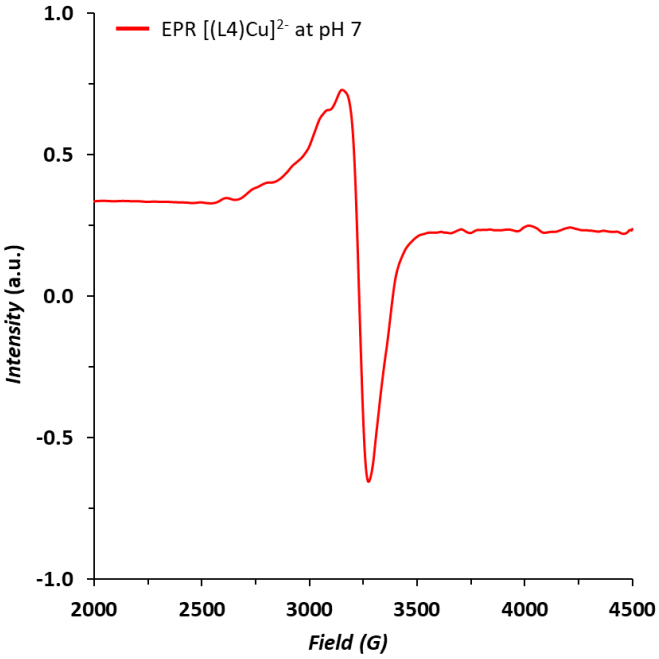



**Figure 38.** EPR spectra measured for **$[(L4)Cu]^{2-}$** in 0.1 M phosphate buffer (pH 7). The spectrum shows the characteristic EPR signal for a $Cu^{II}$ complex with $g_{II}$ = 2.074.

## Electrochemical behavior in organic solvents

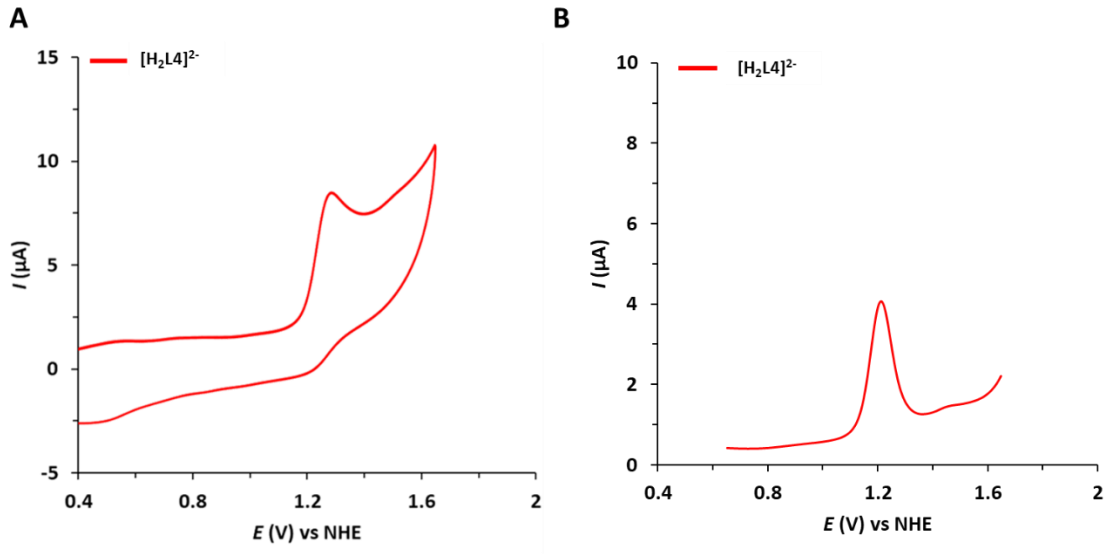



**Figure S39.** (**A**) Cyclic Voltammogram of a 1 mM solution of $H_2L4^{2-}$ in DMF containing 0.1 M $TBAPF_6$ at a scan rate of 100 mV/s (**B**) DPV experiments of a 1 mM solution of $H_2L4^{2-}$ in DMF containing 0.1 M $TBAPF_6$.

## Electrochemical behavior in water

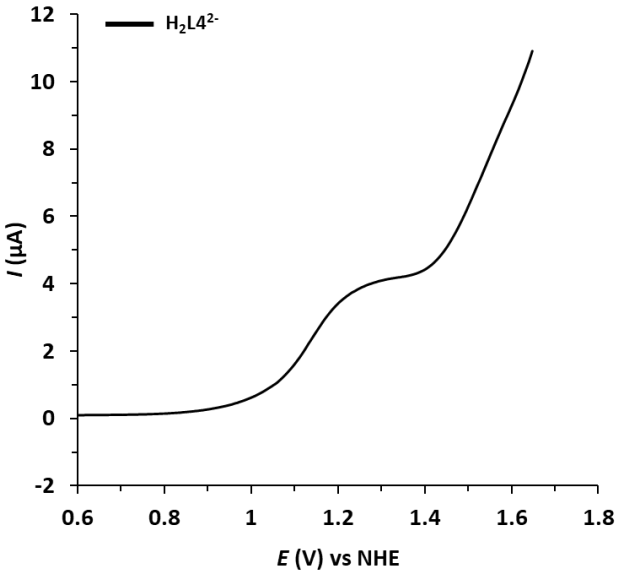



**Figure S40.** DPV experiment of a 1 mM solution of $[H_2L4]^{2-}$ in 0.1 M phosphate buffer pH 11.6. Conditions: scan rate of 100 mV/s, GC as working electrode.

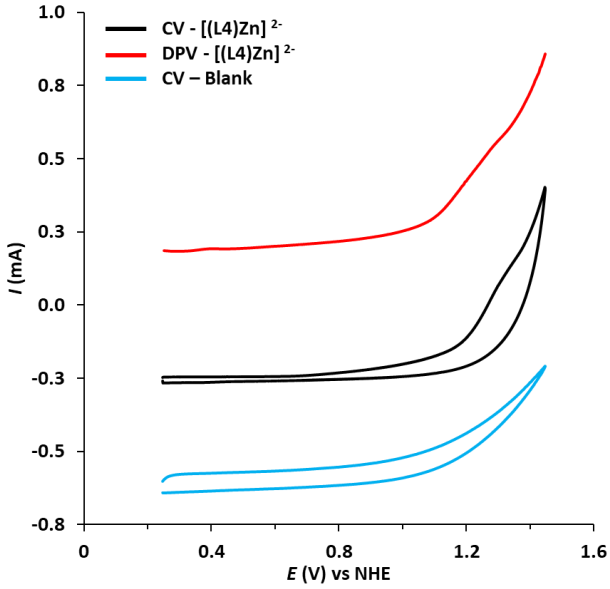



**Figure S41.** CV (black line) and DPV (red line) experiments of 1 mM solution of **$[(L4)Zn]^{2-}$** in a 0.1 M phosphate buffer pH 11.6. Blue line corresponds to a blank with no complex. Conditions: scan rate of 100 mV/s, GC-paper as working electrode.

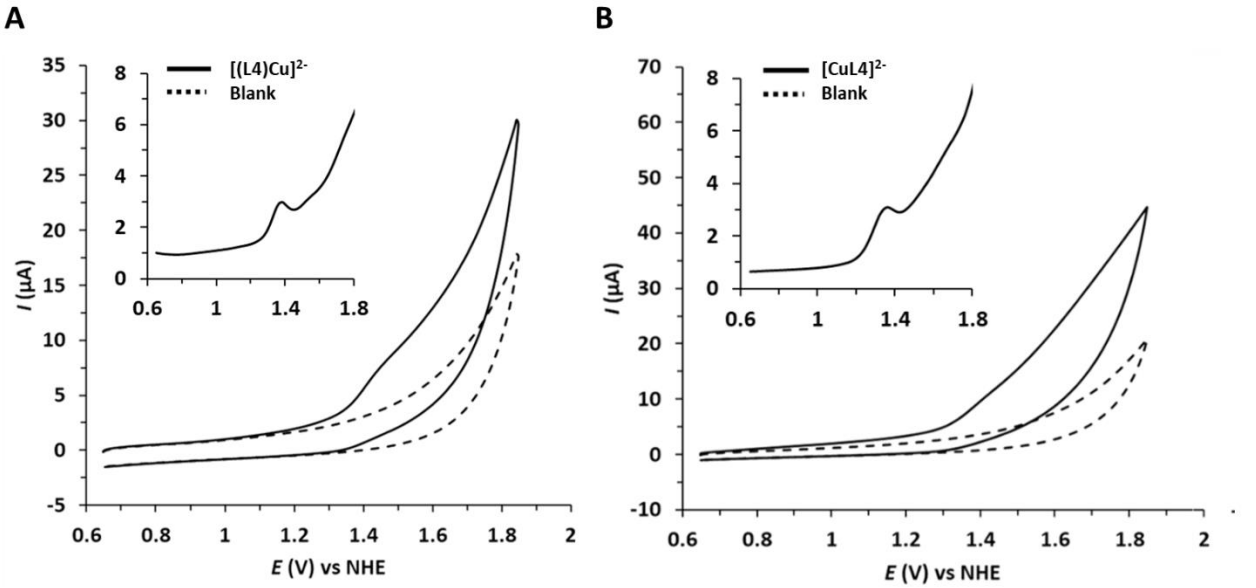



**Figure S42.** Cyclic Voltammograms of a 1 mM solution of **[(L4)Cu]²⁻** at pH 7 (**A**) and 11.6 (**B**) in 0.1 M phosphate buffer solutions. *Inset:* Differential Pulse Voltammograms for **[(L4)Cu]²⁻** at each pH value. Dashed black line corresponds to a blank with no catalyst. Conditions: scan rate of 100 mV/s, GC as working electrode.

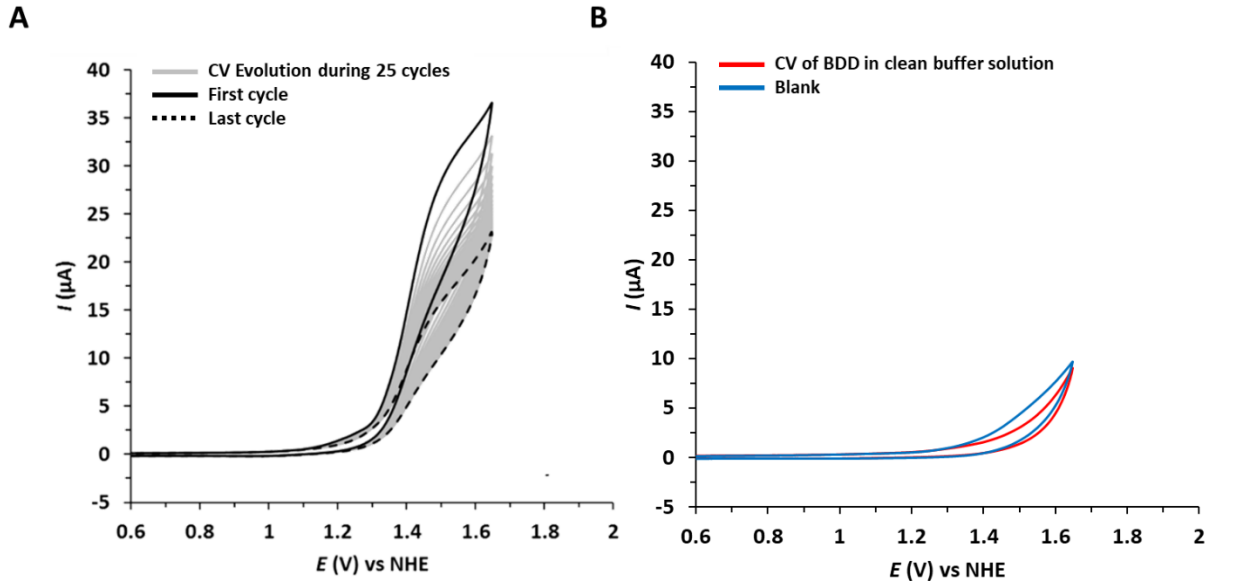



**Figure S43.** (**A**) Evolution of CV profile of a 1 mM solution of **[(L4)Cu]²⁻** in 0.1 M phosphate buffer (pH 11.6) during 25 cycles. (**B**) CV measurement with a BDD electrode that has performed the previous 25 cycles of the complex (red line) or of a blank solution (blue line) immersed in a freshly-prepared 0.1 M phosphate buffer pH 11.6. Conditions: scan rate of 100 mV/s, BDD disk as working electrode.

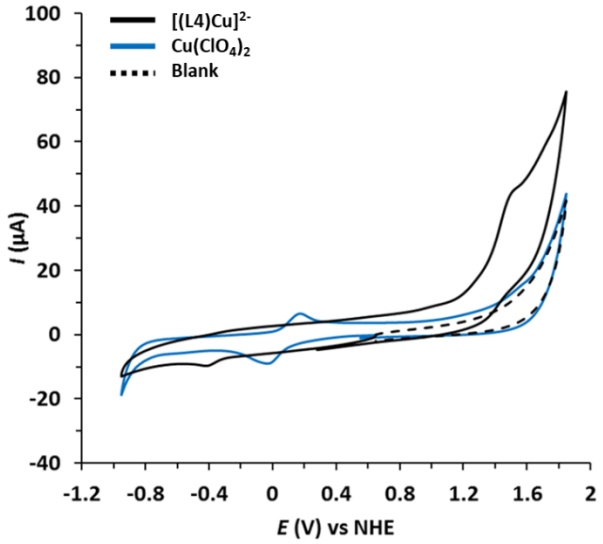



**Figure S44.** Cyclic Voltammograms of a 1 mM solution of **[(L4)Cu]$^{2-}$** in 0.1 M phosphate buffer pH 11.6, showing the electrocatalytic response of the complex (solid black line), of a 1 mM solution of $Cu(ClO_4)_2$ (solid blue line) and the blank (dashed line). Conditions: scan rate of 100 mV/s, BDD disk as working electrode.

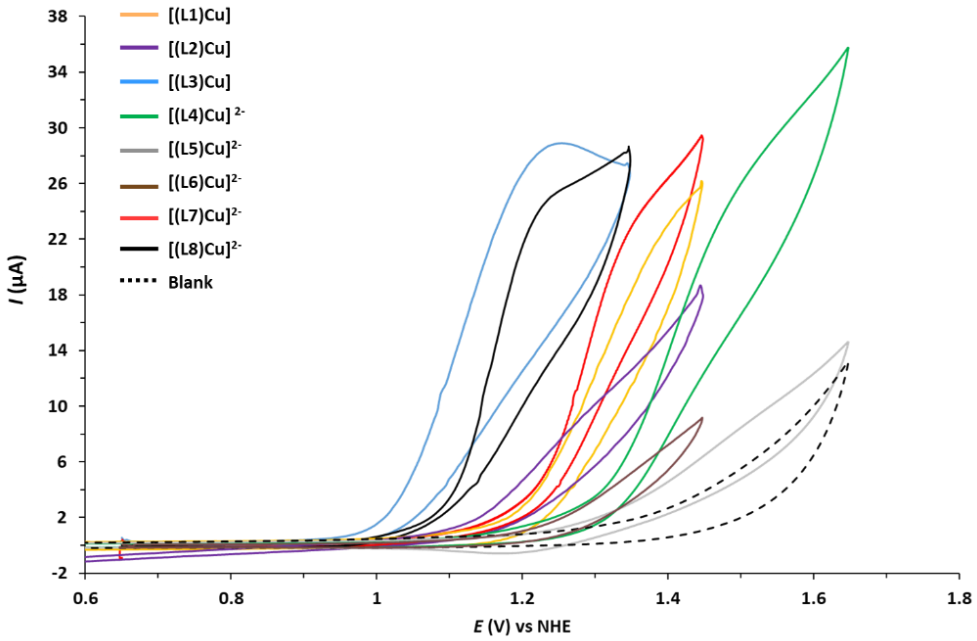



**Figure S45.** Cyclic Voltammograms for the complexes studied in this work in 0.1 M phosphate buffer pH 11.6. *Note:* In case of complexes **[(L1-3)Cu]** the experiments were performed in a mixture of 0.1 M phosphate buffer/TFE (6:4) to fully solubilize the complexes. [**Complex**] = ~1 mM. BDD disk as working electrode.

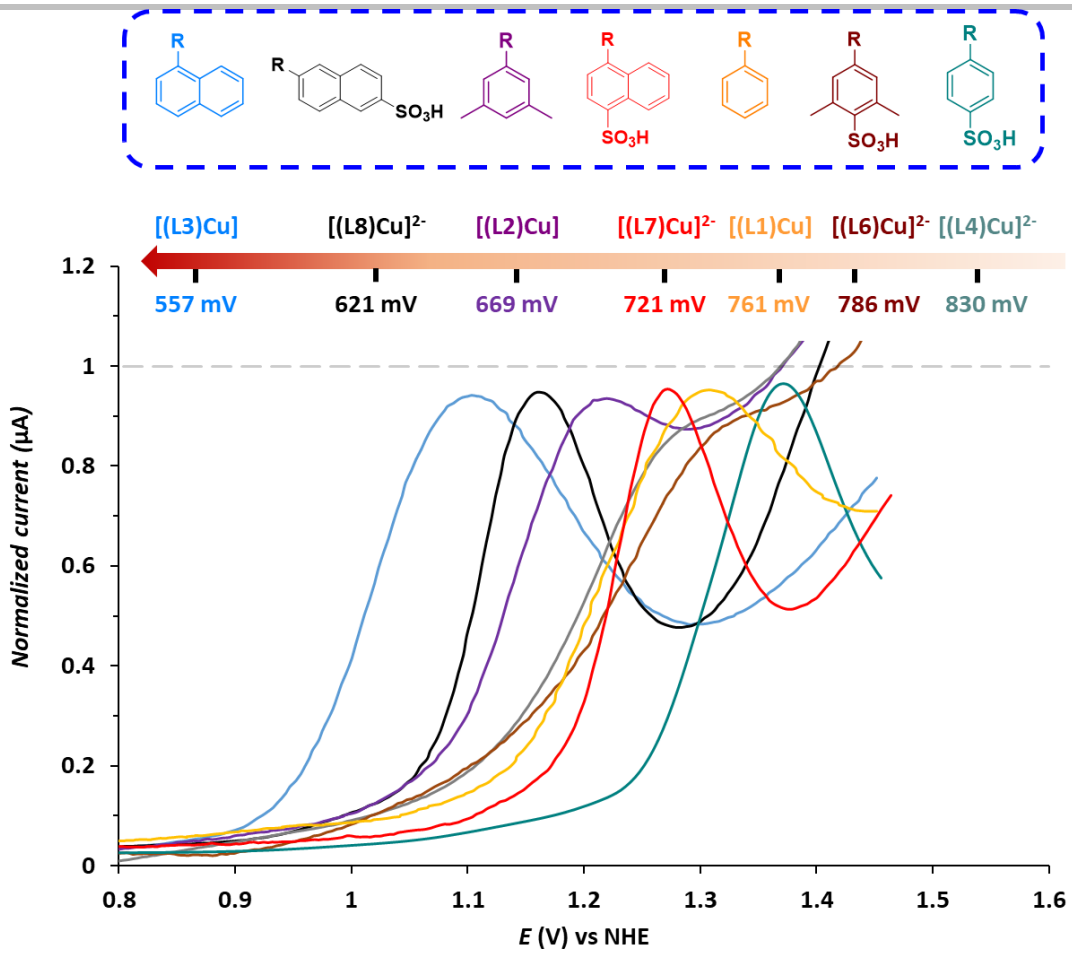
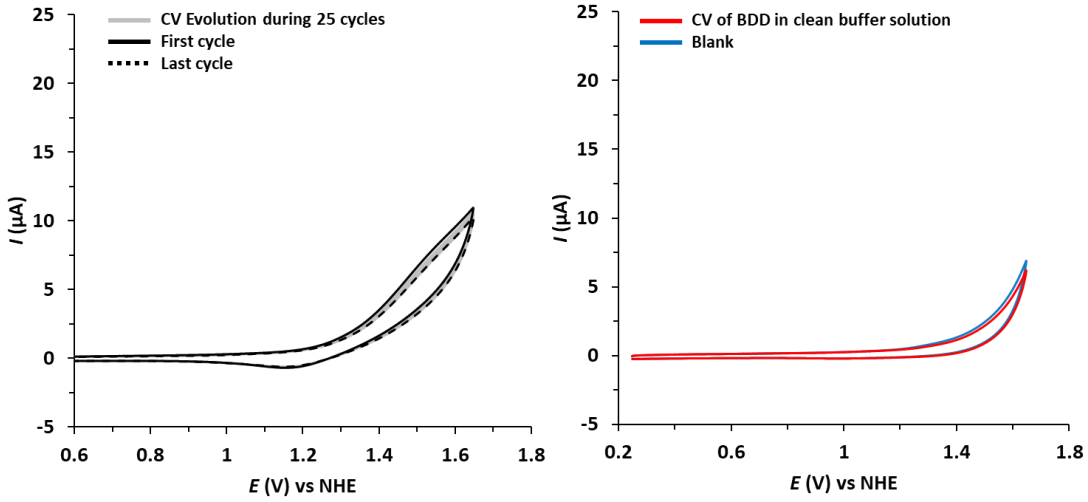
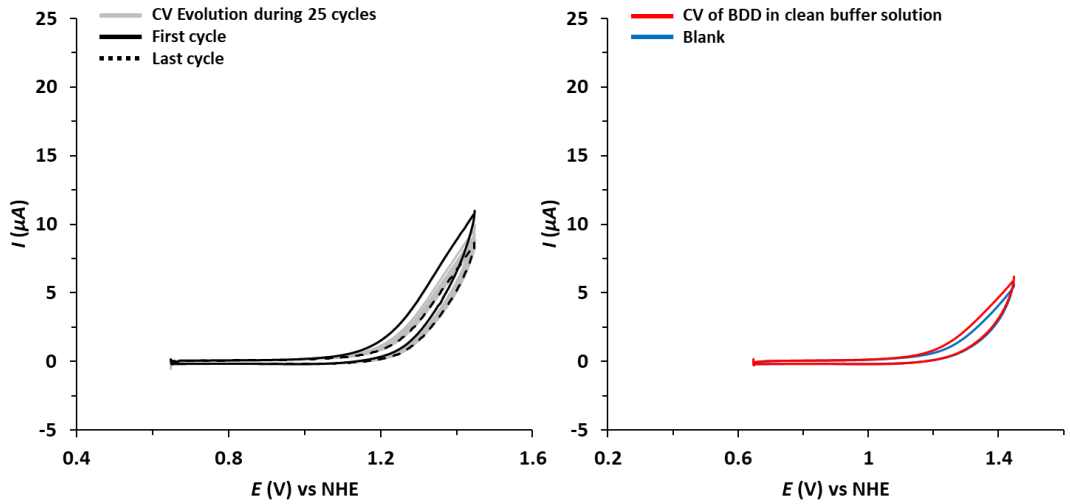



**Figure S46.** DPV experiments for the complexes studied in this work in 0.1 M phosphate buffer pH 11.6. The current (μA) has been normalized between 0 and 1 values for comparison purposes. *Note:* In case of complexes **[(L1-3)Cu]** the experiments were performed in a mixture of 0.1 M phosphate buffer/TFE (6:4) to fully solubilize the complexes. [**Complex**] = ~1 mM. BDD disk as working electrode. *Top inset:* Influence of the substituents in $[(LN)Cu]^{n-}$ complexes on the $\eta$ (mV) of the water oxidation reaction.

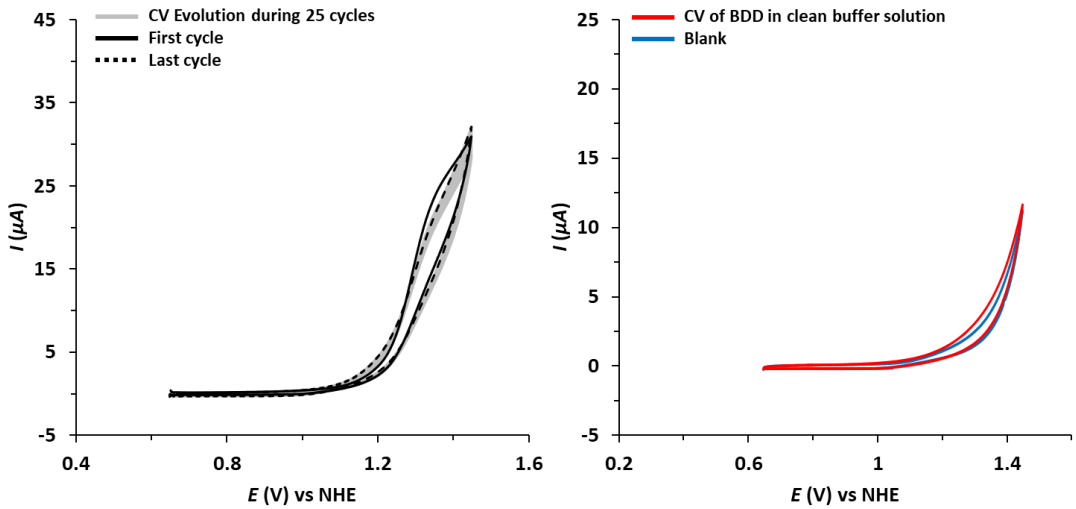
A


CV Evolution during 25 cycles
First cycle
Last cycle
I (µA)
E (V) vs NHE
CV of BDD in clean buffer solution
Blank
I (µA)
E (V) vs NHE

B


CV Evolution during 25 cycles
First cycle
Last cycle
I (µA)
E (V) vs NHE
CV of BDD in clean buffer solution
Blank
I (µA)
E (V) vs NHE

C


CV Evolution during 25 cycles
First cycle
Last cycle
I (µA)
E (V) vs NHE
CV of BDD in clean buffer solution
Blank
I (µA)
E (V) vs NHE

**D**

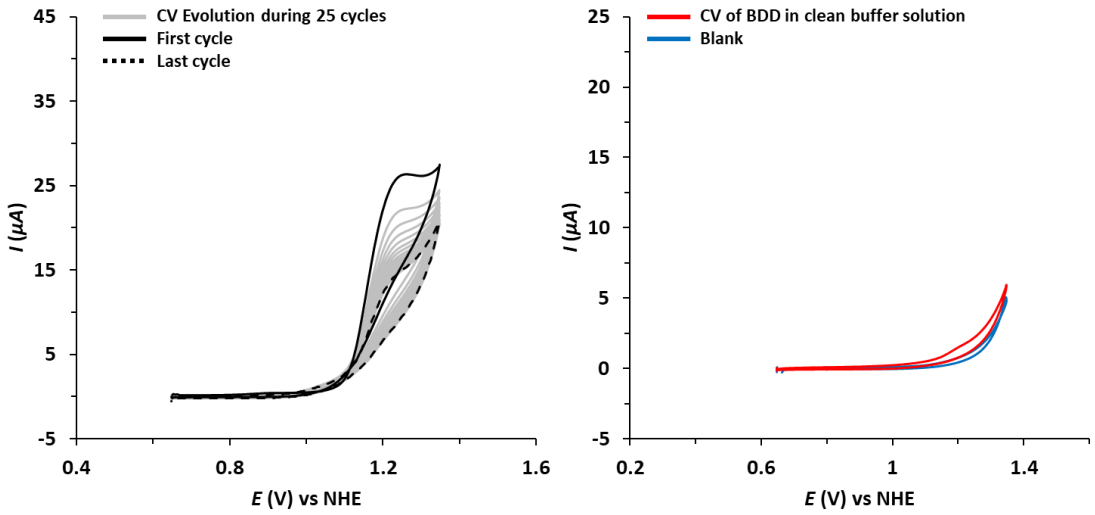



**Figure S47.** Evolution of CV profile for the complexes in 0.1 M phosphate buffer pH 11.6 after 25 cycles (Left) and CV measurement with a BDD electrode that has performed the previous 25 cycles of the complex (red line) or of a blank solution (blue line) immersed in a freshly-prepared catalyst-free 0.1 M phosphate buffer pH 11.6 (Right). Code: (**A**) **[(L5)Cu]**$^{2-}$,(**B**) **[(L6)Cu]**$^{2-}$,(**C**) **[(L7)Cu]**$^{2-}$ and (**D**) **[(L8)Cu]**$^{2-}$. Conditions: scan rate of 100 mV/s, [**Complex**] = 1 mM. BDD as working electrode.

**Determination of the kinetic constant. Foot of the Wave Analysis (FOWA).**

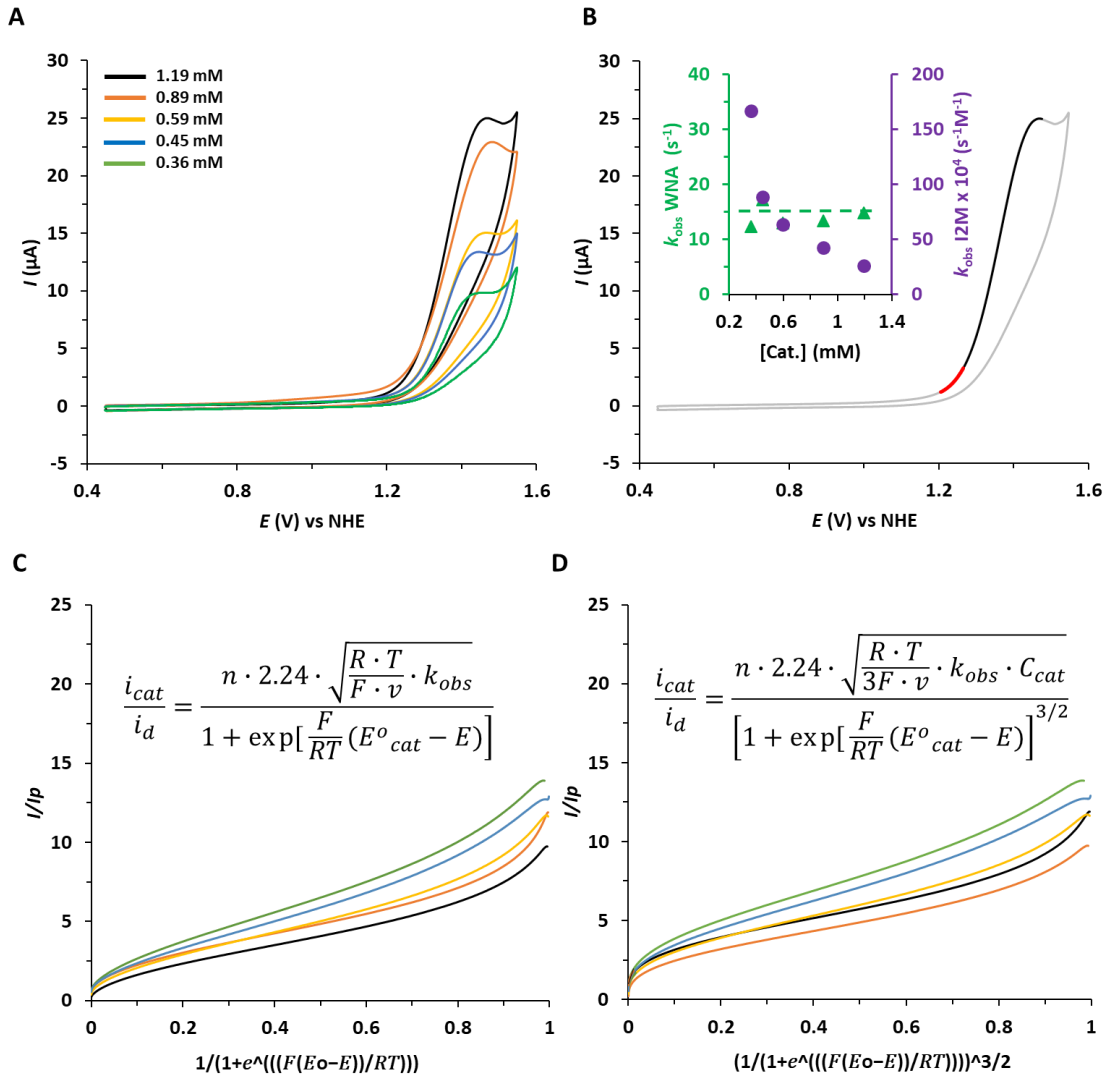
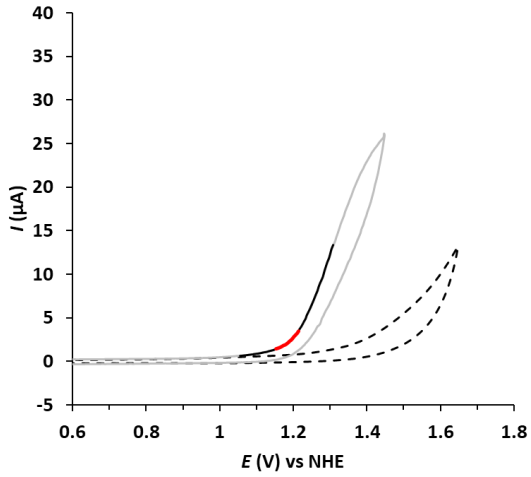
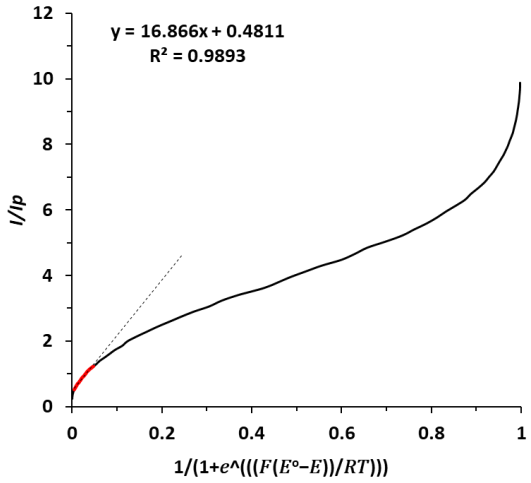


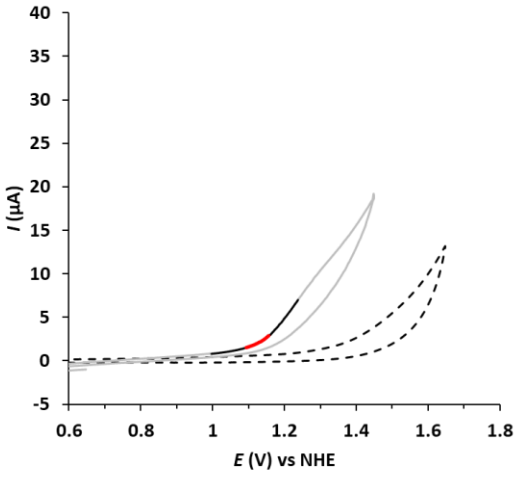

**Figure S48.** (**A**) CVs of [**(L4)Cu**]$^{2-}$ at different concentrations in 0.1 M phosphate buffer pH 11.6 at 100 mV/s scan rate. (**B**) CV of a 1.19 mM solution of [**(L4)Cu**]$^{2-}$ in 0.1 M phosphate buffer pH 11.6 at 100 mV/s scan rate (grey line), experimental data used for FOWA analysis (black line) and region used for the determination of $k_{obs}$ (red line) by plotting $i/i_p^0$ vs. $1/\{1+\exp[(F/RT)(E^0_{PQ}-E)]\}$ for a WNA mechanism and $i/i_p^0$ vs. $(1/\{1+\exp[(F/RT)(E^0_{PQ}-E)]\})^{3/2}$ for an I2M mechanism. *Inset:* Plot of $k_{obs}$ vs. [**(L4)Cu**]$^{2-}$ assuming a WNA mechanism (green trace) or an I2M mechanism (purple trace). The linear trend indicates that the electrochemical oxidation of water to dioxygen is following a WNA mechanism.[3] (**C**) FOWA region obtained by plotting $i/i_p^0$ vs. $1/\{1+\exp[(F/RT)(E^0_{PQ}-E)]\}$ for a WNA mechanism and (**D**) FOWA region obtained by plotting $i/i_p^0$ vs. $(1/\{1+\exp[(F/RT)(E^0_{PQ}-E)]\})^{3/2}$ for an I2M mechanism used for the calculation of $k_{obs}$.

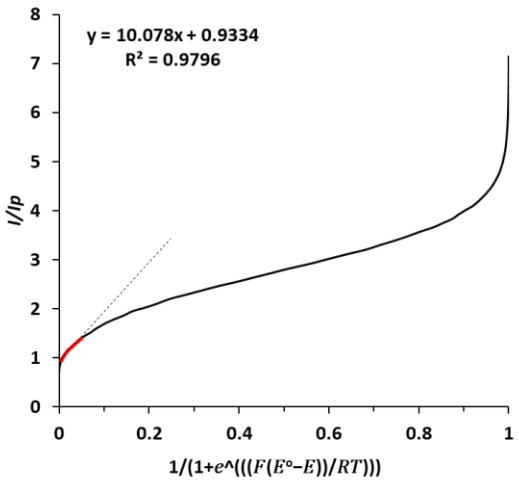
A


I (μA)
E (V) vs NHE

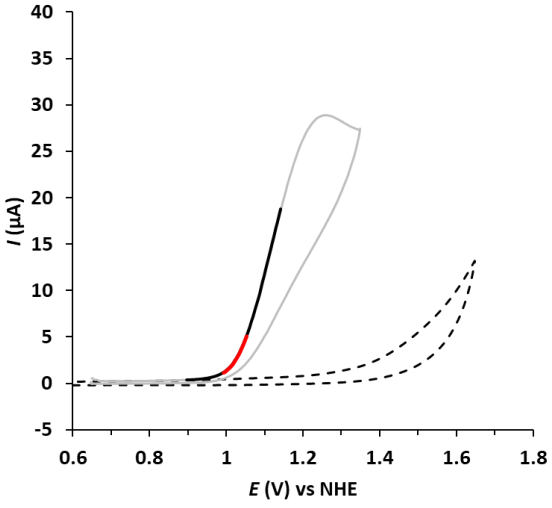

y = 16.866x + 0.4811
R² = 0.9893
I/Ip
1/(1+e^(((F(E°−E))/RT)))

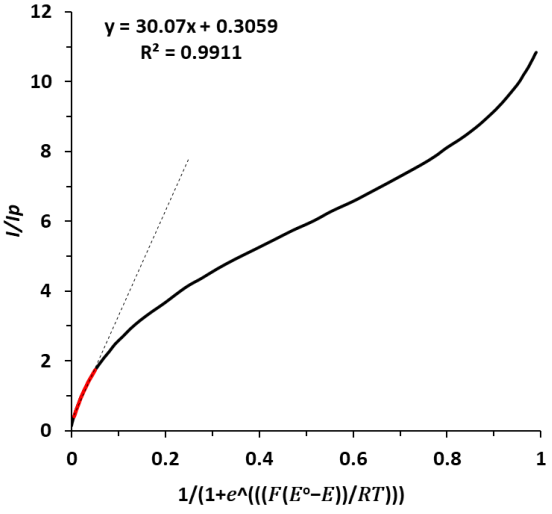
B


I (μA)
E (V) vs NHE

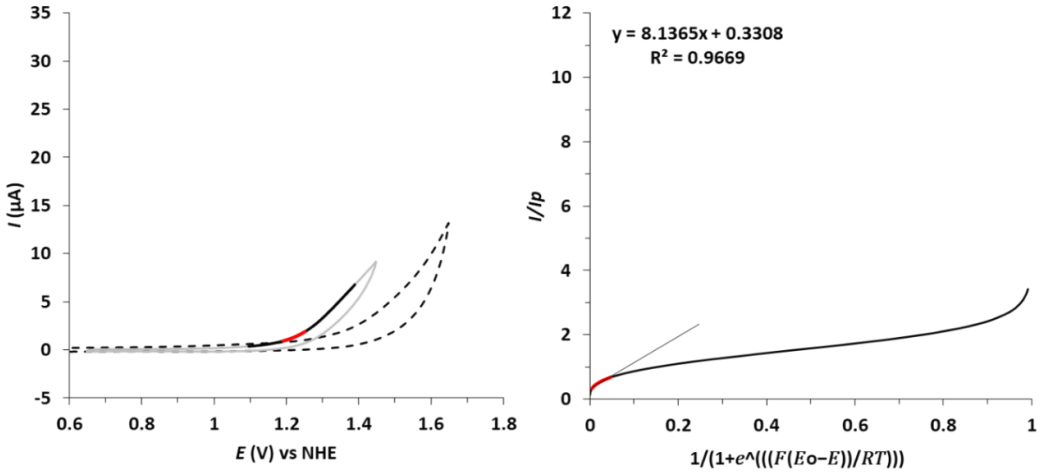

y = 10.078x + 0.9334
R² = 0.9796
I/Ip
1/(1+e^(((F(E°−E))/RT)))

C

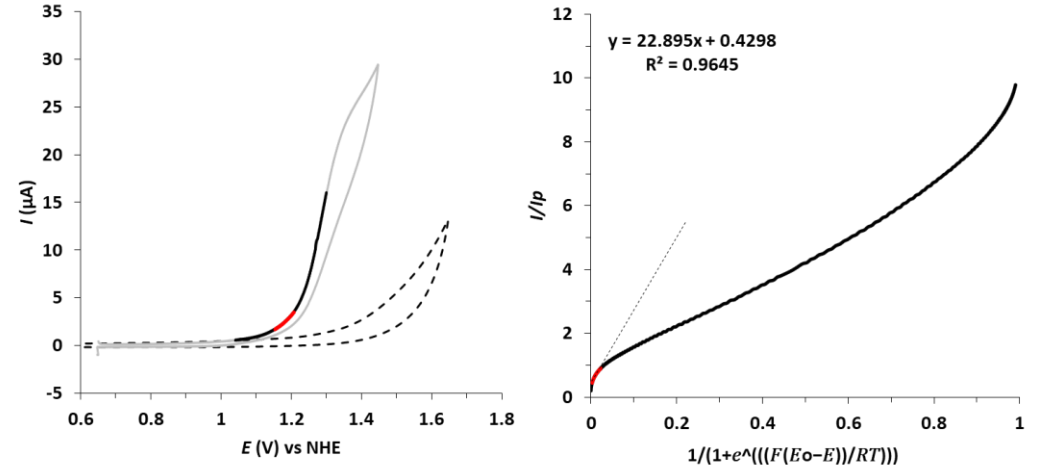

I (μA)
E (V) vs NHE


y = 30.07x + 0.3059
R² = 0.9911
I/Ip
1/(1+e^(((F(E°−E))/RT)))

**D**




**E**




**F**

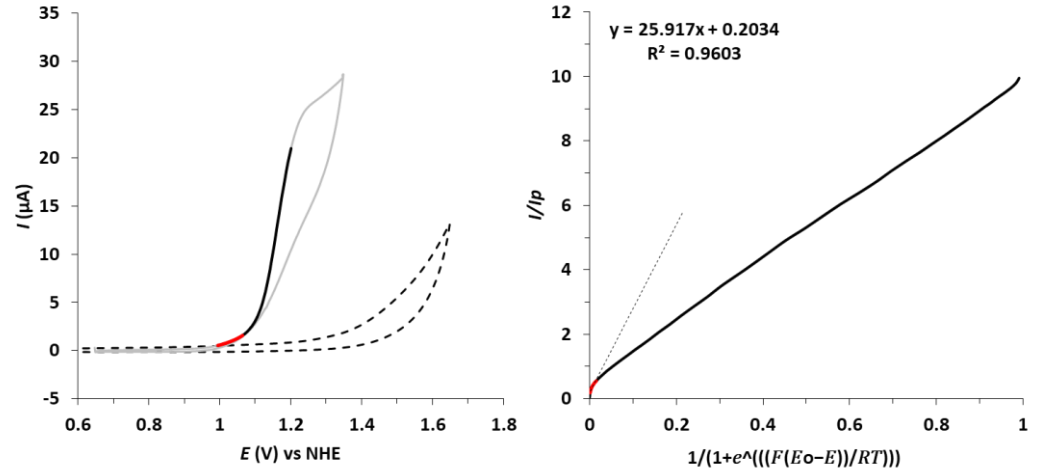



**Figure S49.** (Left) CVs of 1 mM solution of complexes in 0.1 M phosphate buffer pH 11.6 at 100 mV/s scan rate (grey line) and the blank (dashed line). Code: (**A**) **[(L1)Cu]**, (**B**) **[(L2)Cu]**,(**C**) **[(L3)Cu]**, (**D**) **[(L6)Cu]$^{2-}$**, (**E**) **[(L7)Cu]$^{2-}$**, (**F**) **[(L8)Cu]$^{2-}$**. Solid red line corresponds to the experimental data used for FOWA analysis and solid black line shows the region used for the determination of $k_{obs}$. (Right) FOWA obtained by plotting $i/i_p^o$ vs. $1/\{1+\exp[(F/RT)(E^o_{PQ}-E)]\}$. *Note:* In case of complexes **[(L1-3)Cu]** the experiments were performed in a mixture of 0.1 M phosphate buffer/TFE (6:4) to fully solubilize the complexes.

## $O_2$ Evolution experiments.

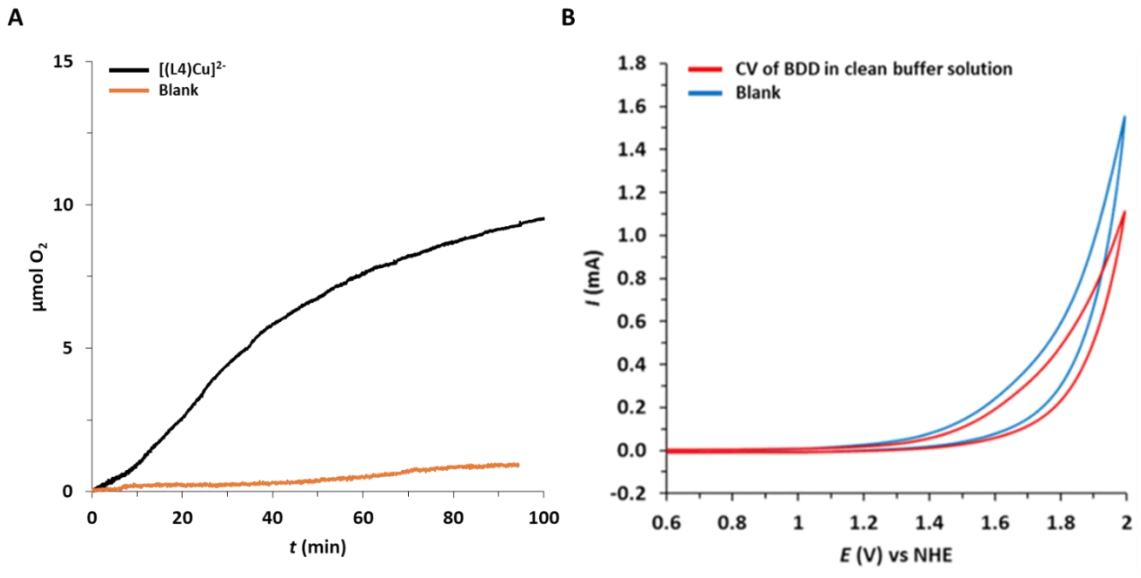



**Figure S50.** (**A**) Oxygen evolution measurements given in µmol $O_2$ vs. time (min) for complex **[(L4)Cu]$^{2-}$** at 1.5 mM concentration ($V_{total}$= 3 mL) using a Clark probe electrode during a CPE at 1.6 V vs. NHE in 0.1 M phosphate buffer pH 11.6. Blank data in the absence of complex is shown in orange. (**B**) Comparison of CVs of a blank solution after a CPE at 1.6 V during 95 mins and of the mechanically polished BDD electrode under a blank solution, showing no catalytic response due to the presence of heterogeneous materials deposited onto the surface of the electrode. Conditions: scan rate of 100 mV/s, BDD disk as working electrode, Pt mesh counter electrode and AgCl as reference electrode. Q = 4.58 C, moles $e^-$= 4.75 x $10^{-5}$ mol, FE= 76 %. TON= (µmol $O_2$)/(µmol cat.)= 1.86. A TON of 58993 was obtained using the methodology developed by Savéant and co-workers based on the electroactive catalyst (i.e. catalyst in contact with the electrode).[4]

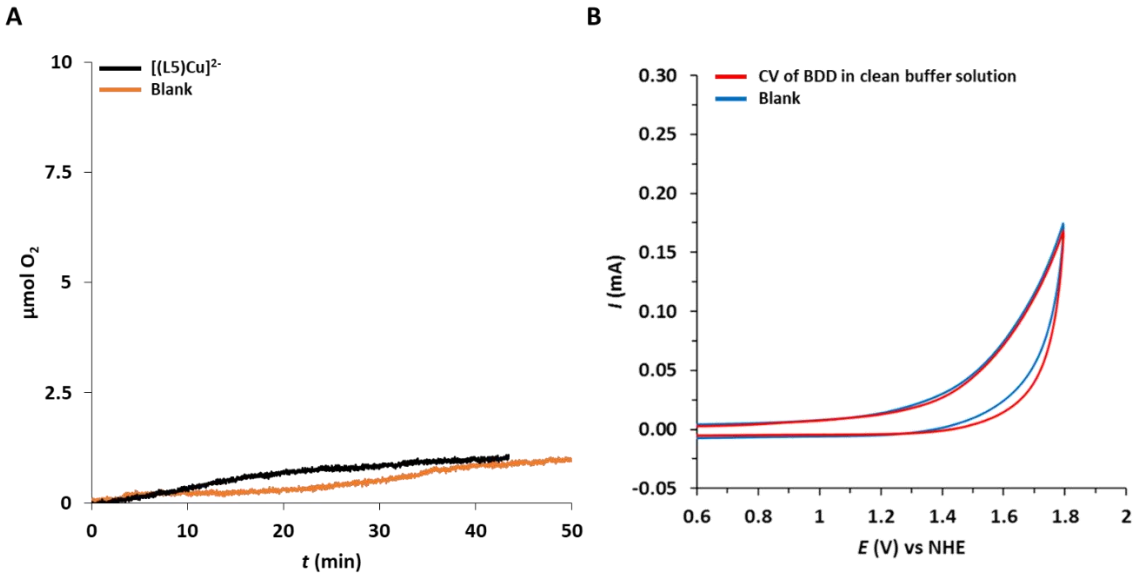



**Figure S51.** (**A**) Oxygen evolution measurements given in µmol $O_2$ vs. time (min) for complex **[(L5)Cu]$^{2-}$** at 1.5 mM concentration ($V_{total}$= 3 mL) using a Clark probe electrode during a CPE at 1.6 V vs. NHE in 0.1 M phosphate buffer pH 11.6. Blank data in the absence of complex is shown in orange. (**B**) Comparison of CVs of a blank solution after a CPE at 1.6 V during 43 min and of the mechanically polished BDD electrode under a blank solution, showing no catalytic response due to the presence of heterogeneous materials deposited onto the surface of the electrode. Conditions: scan rate of 100 mV/s, BDD disk as working electrode, Pt mesh counter electrode and AgCl as reference electrode.

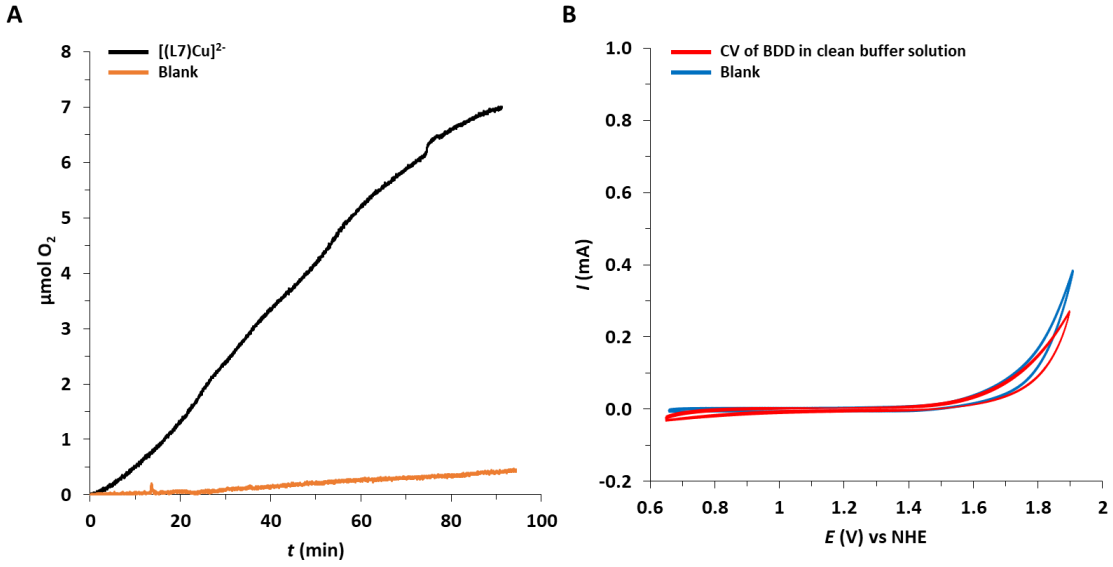



**Figure S52.** (**A**) Oxygen evolution measurements given in µmol $O_2$ vs. time (min) for complex **[(L7)Cu]$^{2-}$** at 1.5 mM concentration ($V_{total}$= 3 mL) using a Clark probe electrode during a CPE at 1.45 V vs. NHE in 0.1 M phosphate buffer pH 11.6 V. Blank data in the absence of complex is shown in orange. (**B**) Comparison of CVs of a blank solution after a CPE at 1.45 V during 94 min and of the mechanically polished BDD electrode under a blank solution. Conditions: scan rate of 100 mV/s, BDD disk as working electrode, Pt mesh counter electrode and AgCl as reference electrode. Q = 4.98 C, moles $e^-$= 5.16 x $10^{-5}$ mol, FE= 52 %. TON= (µmol $O_2$)/(µmol cat.)= 1.35. TON of 130409 was obtained using the methodology developed by Savéant and coworkers based on the electroactive catalyst (i.e. catalyst in contact with the electrode).[4]

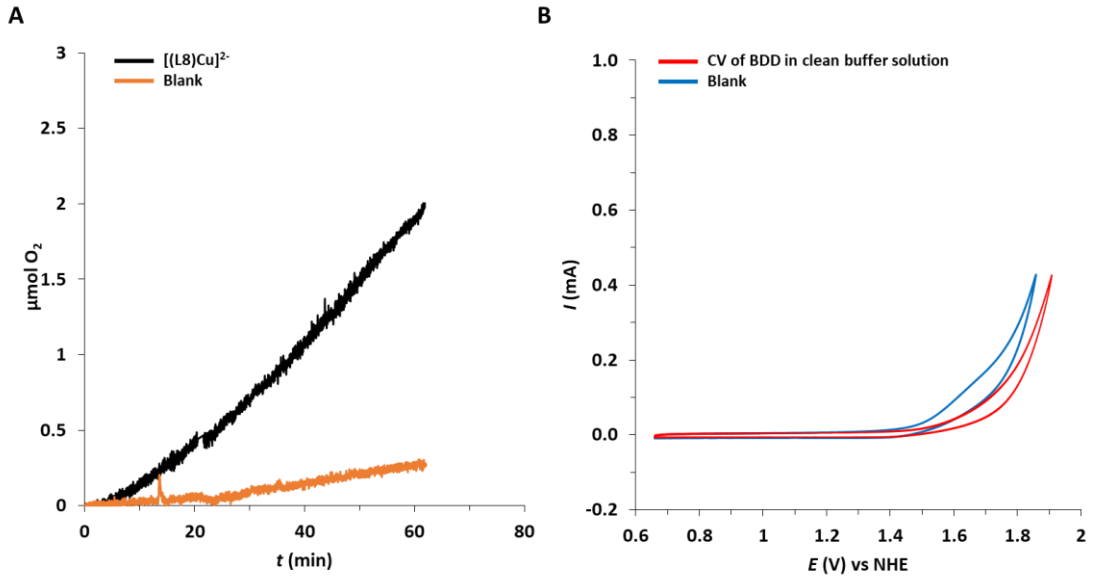
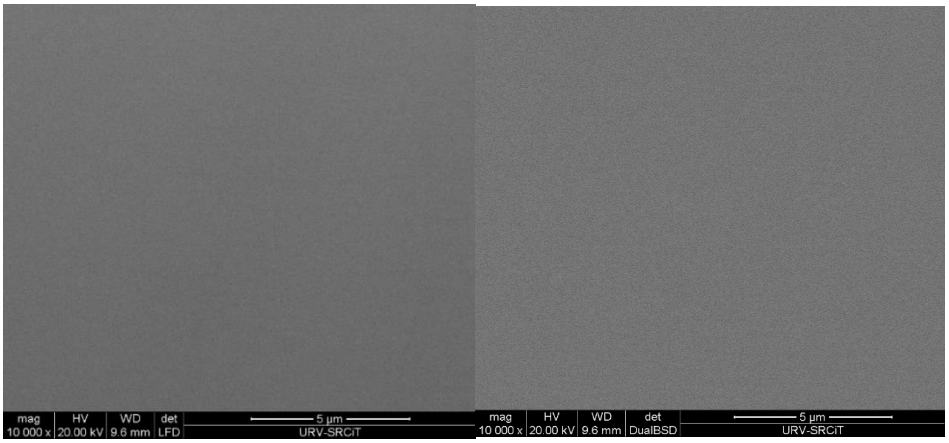



**Figure S53.** (**A**) Oxygen evolution measurements given in µmol $O_2$ vs. time (min) for complex **[(L8)Cu]$^{2-}$** at 1.5 mM concentration ($V_{total}$= 3 mL) using a Clark probe electrode During a CPE at 1.45 V vs. NHE in 0.1 M phosphate buffer pH 11.6. Blank data in the absence of complex is shown in orange. (**B**) Comparison of CVs of a blank solution after a CPE at 1.45 V during 95 min and of the mechanically polished BDD electrode under a blank solution. Conditions: scan rate of 100 mV/s, BDD disk as working electrode, Pt mesh counter electrode and AgCl as reference electrode. Q= 1.84 C, moles $e^-$= 1.9 x $10^{-5}$ mol, FE= 40%. TON= (µmol $O_2$)/(µmol cat.)= 0.4. A TON of 97964 was obtained using the methodology developed by Savéant and coworkers based on the electroactive catalyst (i.e. catalyst in contact with the electrode).[4]

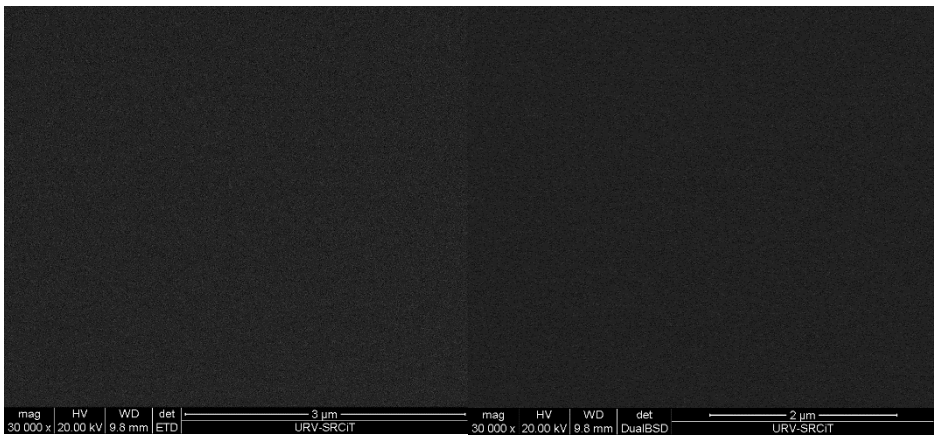
# SUPPORTING INFORMATION

## Scanning Electron Microscopy

**A**




**B**




**C**

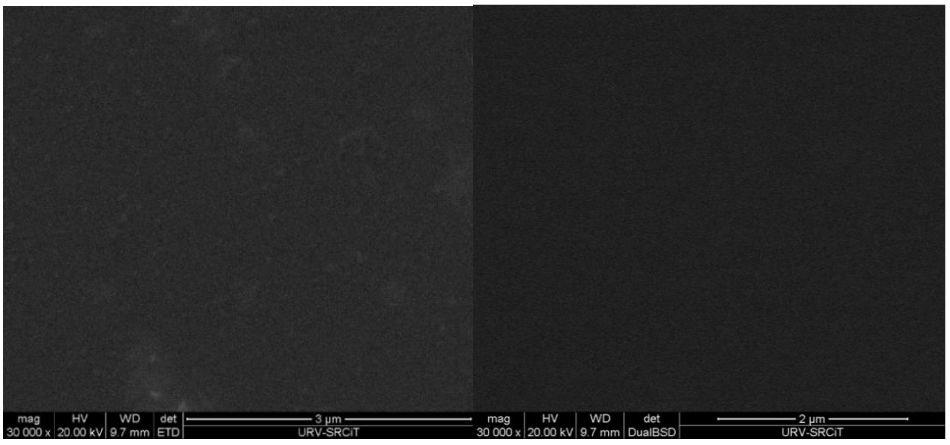



**Figure S54.** SEM micrographs (left) and corresponding back-scattered electron micrographs (right) of a glassy carbon plate after a 30 minute electrolysis of a 1.5 mM solution of the complexes in phosphate buffer pH 11.6 at 1.6 V vs. NHE. Code: (**A**) **[(L4)Cu]$^{2-}$**,(**B**) **[(L7)Cu]$^{2-}$**,(**C**) **[(L8)Cu]$^{2-}$**.There is no appreciable presence of copper oxide nanoparticles or deposited materials on the electrode.

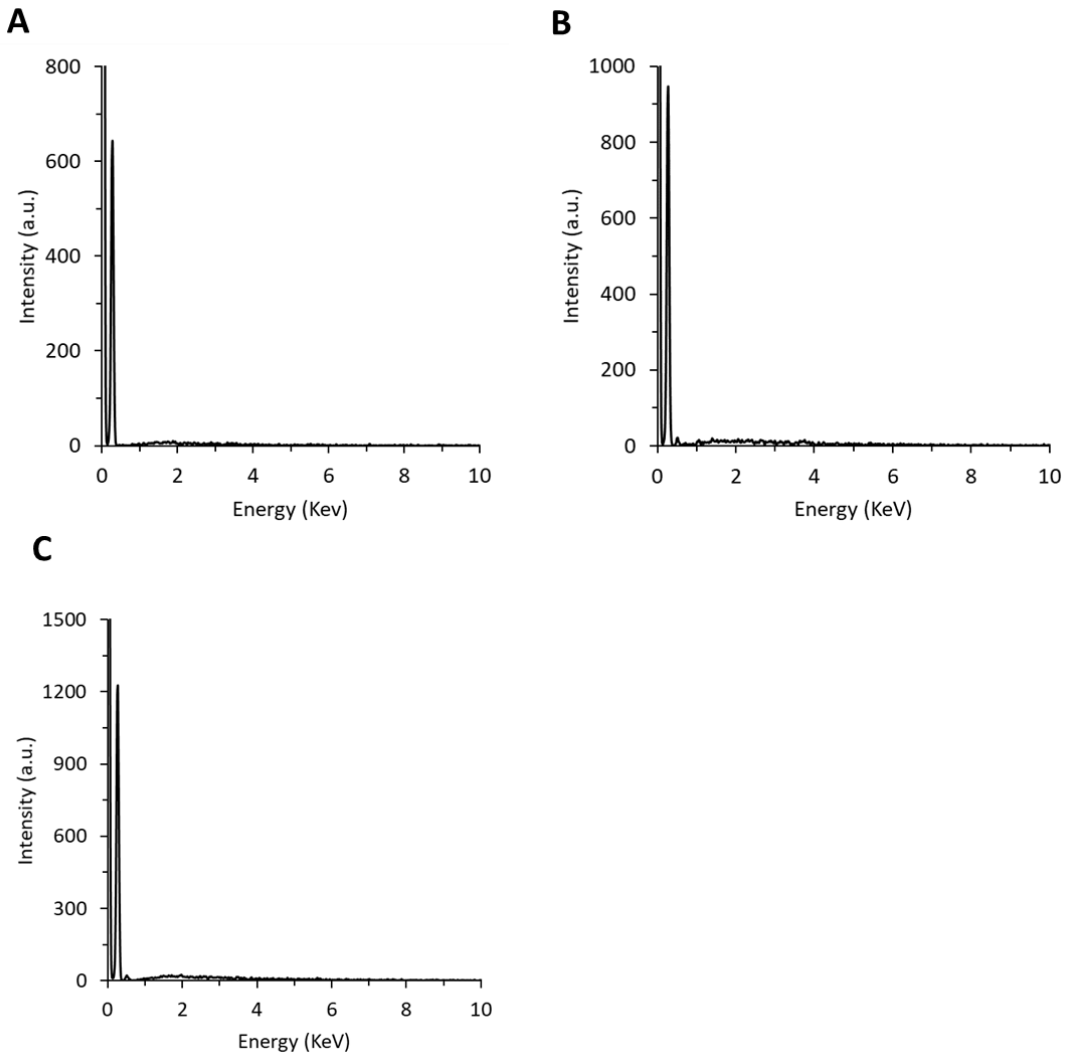



**Figure S55**. EDX spectra of the glassy carbon electrodes after a 30 minute electrolysis in phosphate buffer pH 11.6 at 1.6 V vs. NHE. Code: (**A**) **[(L4)Cu]$^{2-}$**, (**B**) **[(L7)Cu]$^{2-}$**, (**C**) **[(L8)Cu]$^{2-}$**.There is no appreciable presence of copper on the surface of the electrode (Cu expected peaks, Kα= 8.04 KeV and Lα= 0.930 KeV).

# SUPPORTING INFORMATION

## Computational studies

*Computational Details*

All calculations were carried out with the Gaussian09 program package[13] using DFT methodology. We used B3LYP as the functional, including D3 empirical dispersion correction developed by Grimme (B3LYP-D3).[14,1514,15] The basis set was split into 6-31+G(d) for C, N, S, O and H[16,17,18] and LANL2TZ(f) for Cu.[19,20,21,22,23] Implicit solvation was introduced through the SMD model,[24] with water as the solvent. All geometry optimizations were computed in solution without symmetry restrictions. The nature of all computed stationary points as minima or transition states was confirmed through vibrational frequency calculations. Free energy corrections were calculated at 298.15 K and 105 Pa pressure, including zero point energy corrections (ZPE). In addition, a correction term of 1.89 kcal/mol (at 298 K) was added when necessary to account for the standard state concentration of 1 M, except for water, whose concentration was considered to be 55.6 M and its correction term 4.3 kcal/mol. Unless otherwise mentioned, all reported energy values are free energies in solution. In addition, stability of the wave function was checked for the calculations (stable option in G16).

The reaction energy barriers of the Minimum Energy Crossing Points (MECP) were estimated from potential energy relaxed scan from the crossing point of the quartet and doublet potential energy surfaces, along the O-O internal reaction coordinate, when the transition states could be found (or do not exist), applying entropic corrections from the minima to compute an estimated free energy change.

In the transformation from free energies to electrochemical magnitudes the values of 4.28 V for the absolute potential of the standard hydrogen electrode[25] and -11.72 eV for the free energy of the proton in aqueous solution at pH=0 were taken from the literature.[26] The value for the free energy of the proton was translated to the experimental pH value by adding a correction term of -0.059*pH, following the same procedure described elsewhere.[27]

The functional for the DFT calculations was B3LYP-D3 based on the calibration carried out in a previous work on related systems,[6,28] where its performance was compared with that of M06, M06-D3, M06L, M06-2X, ωB97xD and B97D. In order to validate this DFT methodology, the calculated optimized structures were compared to the X-Ray ones. Table S4 summarizes all the main metrics for the coordination environment of the copper metal center. In addition, we have recalculated as single points all the species involved in Figure 3 using a larger basis set (6-311++G(3d,2p) for all the atoms except Cu/LANL2TZ(f) for Cu) and no significant differences were found (see Figure S65).

**Table S4**. Comparison of the main metrics for the X-Ray structure and the DFT optimized structure of complexes **[(L4)Cu]$^{2-}$** and **[(L5)Cu]$^{2-}$**.

| COMPLEX | METRIC | X-RAY (SOLID) | DFT OPTIMIZED (WATER) |
|---|---|---|---|
| **[(L4)Cu]$^{2-}$** | $Cu\text{-}N_{bpy}$ | 1.95 Å, 1.95 Å | 2.00 Å, 2.00 Å |
| | $Cu\text{-}N_{amide}$ | 2.00 Å, 2.00 Å | 2.04 Å, 2.05 Å |
| | $N_{bpy}\text{-}Cu\text{-}N_{bpy}$ | 78.27° | 77.55° |
| | $N_{amide}\text{-}Cu\text{-}N_{amide}$ | 119.69° | 123.15° |
| | | | |
| **[(L5)Cu]$^{2-}$** | $Cu\text{-}N_{bpy}$ | 1.95 Å, 1.95 Å | 1.99 Å, 1.99 Å |
| | $Cu\text{-}N_{amide}$ | 2.00 Å, 2.00 Å | 2.02 Å, 2.03 Å |
| | $N_{bpy}\text{-}Cu\text{-}N_{bpy}$ | 78.49° | 78.02° |
| | $N_{amide}\text{-}Cu\text{-}N_{amide}$ | 120.78° | 123.01° |

**Table S5**. Comparison of the experimental and calculated redox potential for the Cu(III)/Cu(II) couples in complexes **[(L4)Cu]$^{2-}$** and **[(L5)Cu]$^{2-}$**.

| COMPLEX | $E_{1/2}^{o}$ (EXP) | $E_{1/2}^{o}$ (CALC) |
|---|---|---|
| **[(L4)Cu]$^{2-}$** | 1.37 V | 1.27 V |
| **[(L5)Cu]$^{2-}$** | 1.27 V | 1.14 V |

# SUPPORTING INFORMATION

*Speciation for complex $[(L4)Cu]^{2-}$ in water*

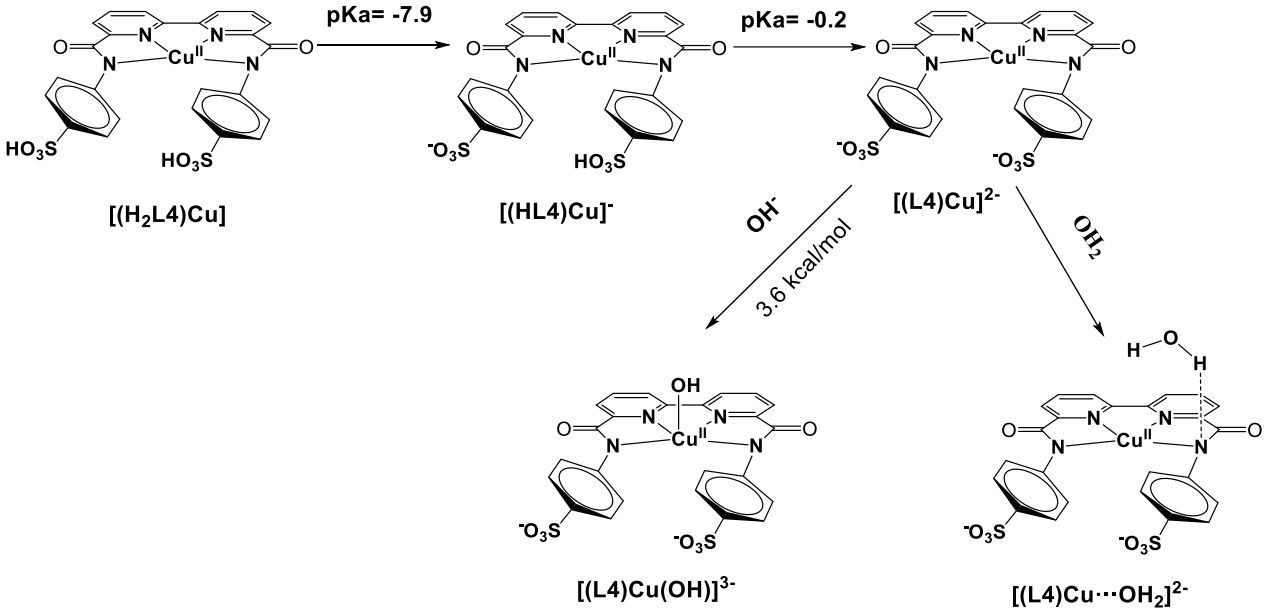



**Figure S56.** Deprotonation processes in complex **$[(L4)Cu]^{2-}$** and apical coordination of hydroxo or water molecules. The corresponding $pK_a$ values or the free energy changes for each process are indicated above the arrows.

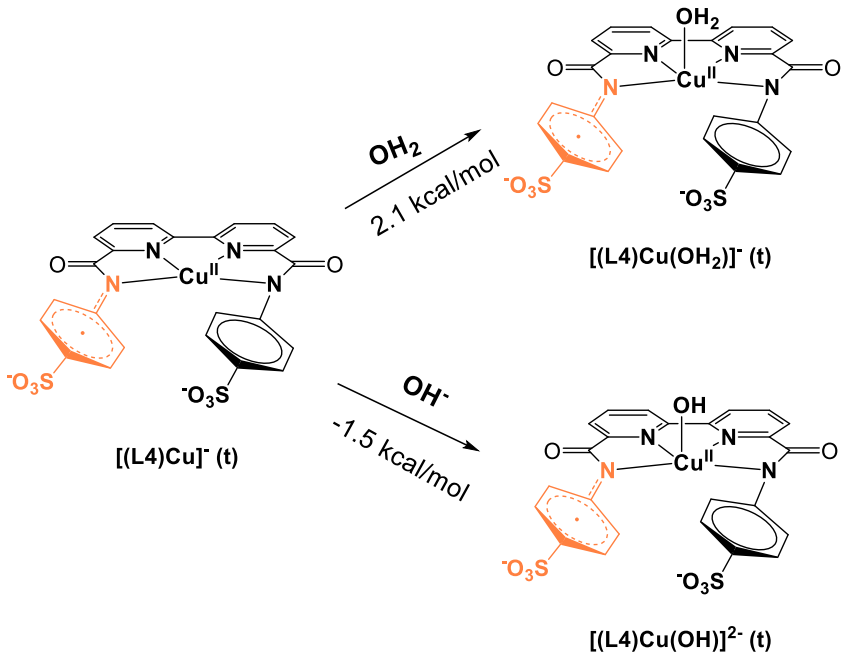



**Figure S57.** Apical coordination of hydroxo or water molecules in the one electron oxidized complex **$[(L4)Cu]^{2-}$**. The corresponding values of the free energy changes for each process are indicated above the arrows.

*Electrochemical activation for complex [(L4)Cu]$^{2-}$*

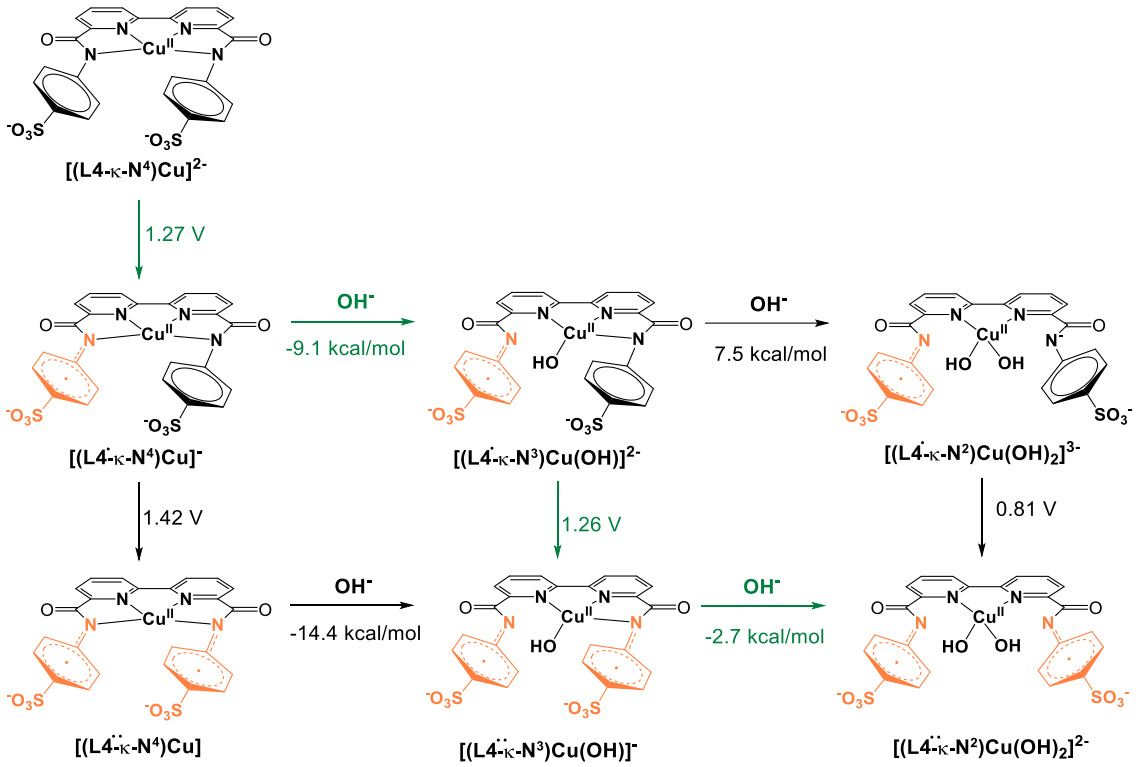



**Figure S58.** Possible pathways for the oxidation of catalyst **[(L4)Cu]$^{2-}$** to generate an active species for the O-O bond formation step.

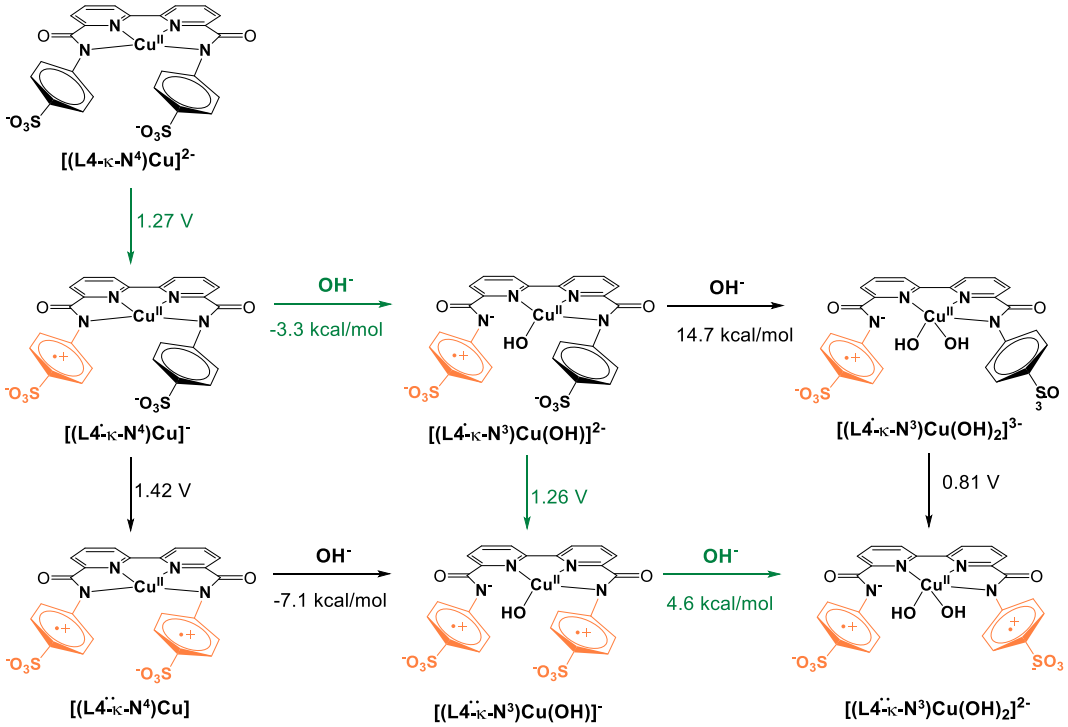



**Figure S59.** Possible pathways for the oxidation of catalyst **[(L4)Cu]$^{2-}$** to generate an active species for the O-O bond formation step using the experimental value for the energy of $OH^-$ solvation at standard state (-102.8 kcal·mol$^{-1}$).[29] This results suggest that the energy of solvation for $OH^-$ might be underestimated by SMD calculations, leading to less favorable coordination of the $OH^-$ to the Cu center. However, the calculated speciation in the different oxidation states is not substantially altered from that proposed using SMD, with the exception of formation of complex $[(L4^{\bullet\bullet}\text{-k-}N^3)Cu(OH)_2]^{2-}$ that is now slightly uphill but still accessible at room temperature towards formation of $O_2$. Therefore, the proposed reaction pathways are still supported by DFT but the calculated barrier for the O-O bond formation step might be overestimated when using the SMD model.

*Potential energy relaxed scan for [(L4)Cu(OH)]$^{-}$ and [(L4)Cu(OH)$_2$]*

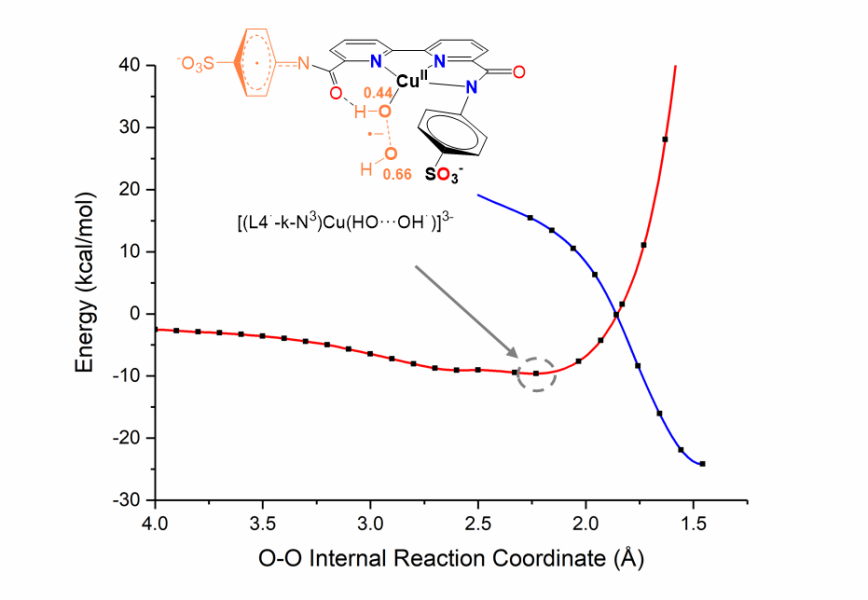



**Figure S60.** Potential energy relaxed scan for catalyst **[(L4)Cu]$^{2-}$** of the O-O reaction coordinate considering a monohydroxylation pathway. Red color represents the quartet state while blue color indicates the doublet state. The inset represents the optimized structure of the 2c-3e$^{-}$ intermediate.

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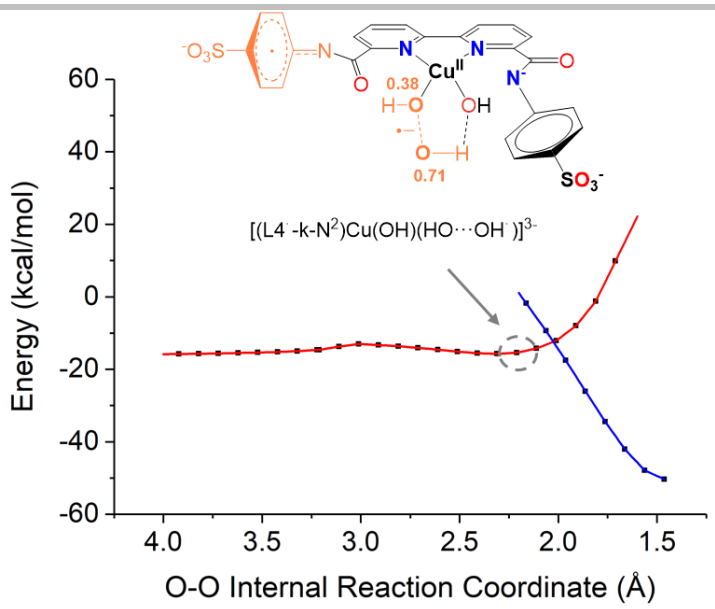


**Figure S61.** Potential energy relaxed scan for catalyst of **[(L4)Cu]$^{2-}$** of the O-O reaction coordinate considering a dihydroxylation pathway. Red color represents the quartet state while blue color indicates the doublet state. The inset represents the optimized structure of the 2c-3e$^{-}$ intermediate.

*Structure and spin density distribution of 2c-3e intermediates*

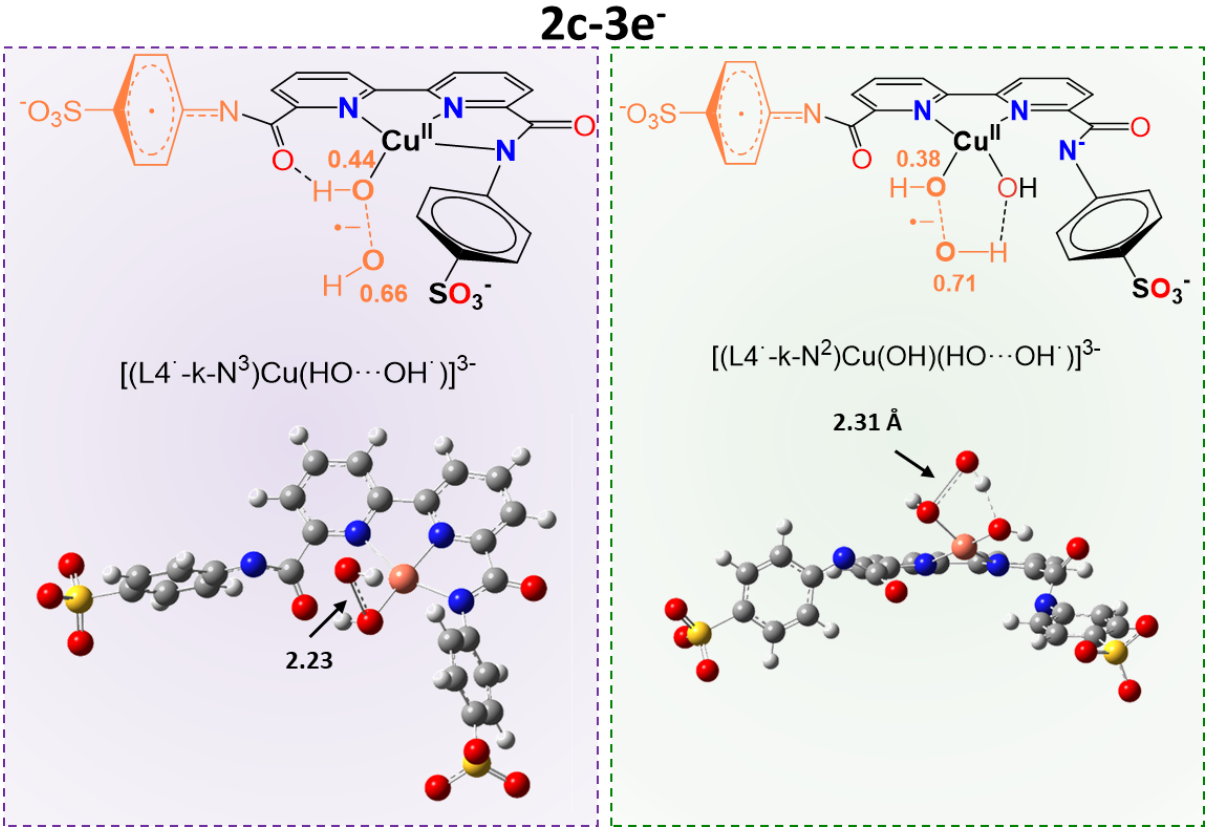


**Figure S62.** Schematic drawing with the spin distribution of each oxygen atom in orange (top) and optimized structure (bottom) of the 2c-3e intermediates for **[(L4˙-*κ*-N$^3$)Cu(OH)]$^{2-}$** (left) and **[(L4˙-*κ*-N$^2$)Cu(OH)$_2$]$^{3-}$** (right) catalysts.

*Intramolecular relaxed scan for [(L4-κ-N²)Cu(OH)₂]²⁻*

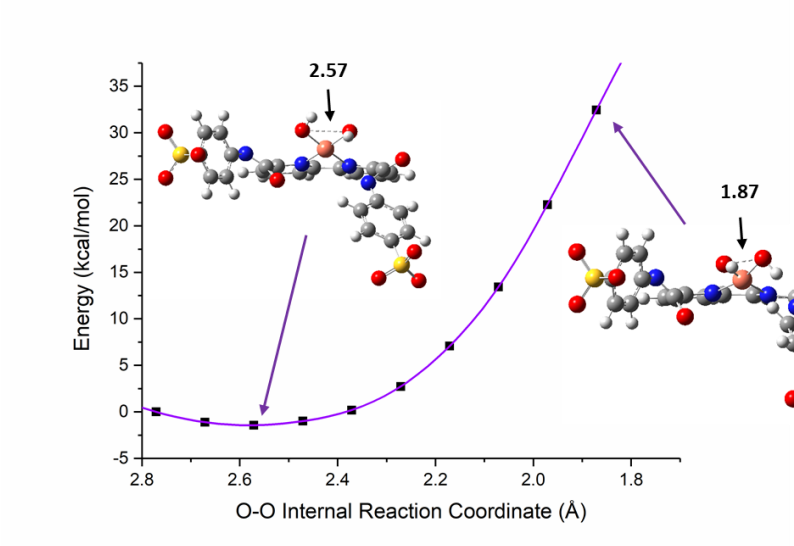


**Figure S63.** Potential energy relaxed scan of the intramolecular HO---OH coupling using catalyst **[(L4·⁻-κ-N²)Cu(OH)₂]²⁻**.

*Structure of complex [(L5)Cu]²⁻ and its oxidized species*

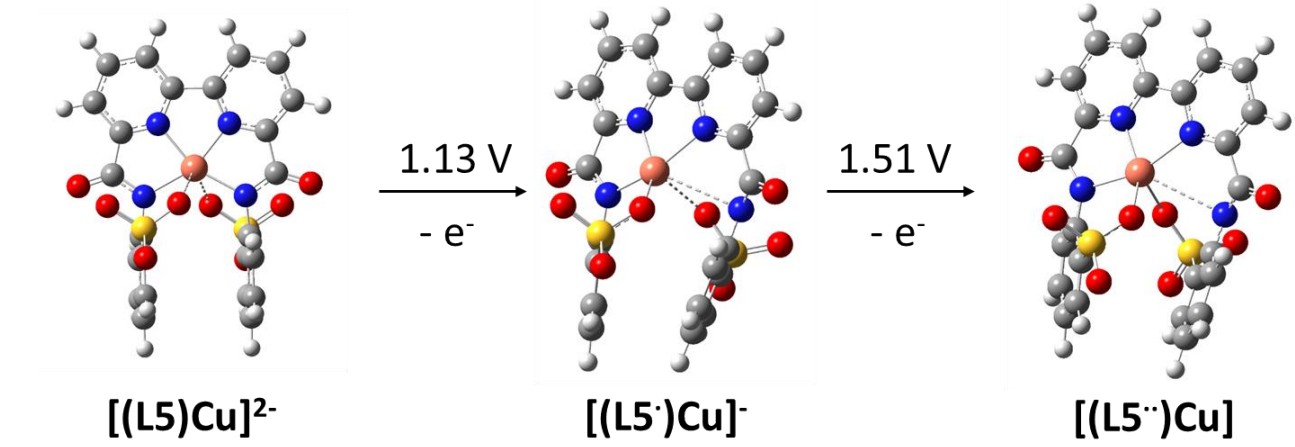


**Figure S64.** Optimized structures of complex **[(L5)Cu]²⁻** and its oxidized species with the calculated redox potential above the arrows. All the structures feature coordination of the copper center to at least one of the sulfonate groups.

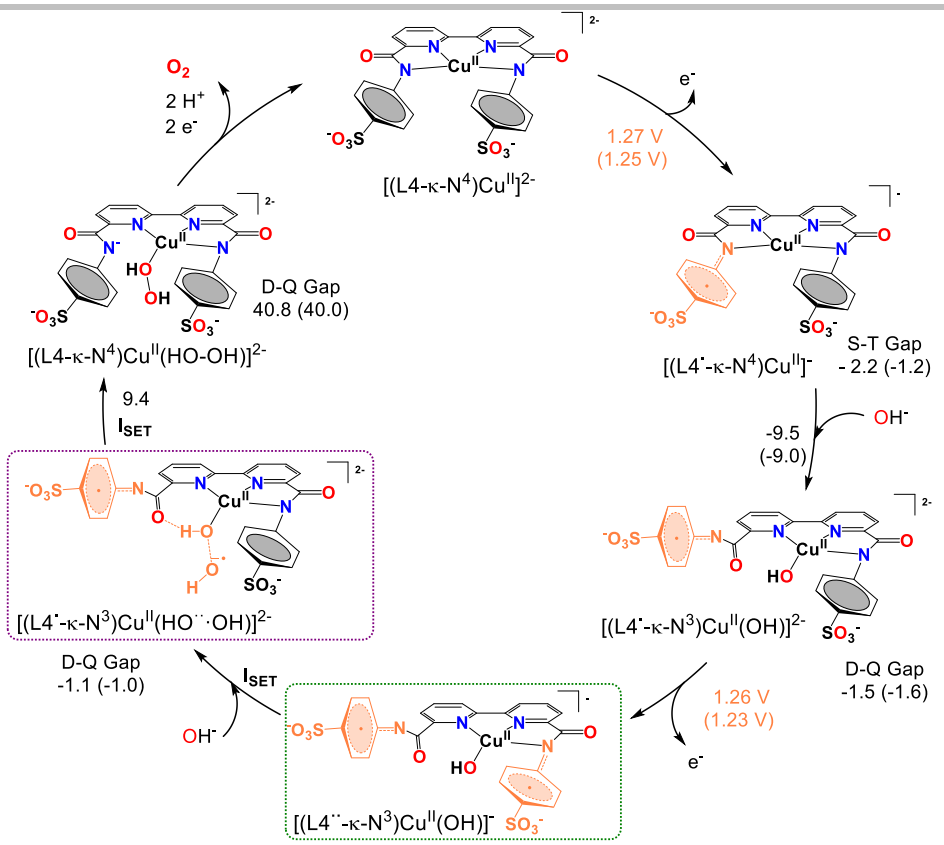


**Figure S65.** Influence of the basis set size in the catalytic cycle depicted in Figure 3 of the main text. Small basis set (6-31+G(d)/LANL2TZ(f)) and large basis set (6-311++G(3d,2p)) shown in brackets, calculated energies are very similar and no influence is observed in oxidation potentials, OH coordination or spin state gap. Energies in kcal/mol.

*Effect of explicit solvation in spin state and reaction profile for the SET-WNA mechanism*

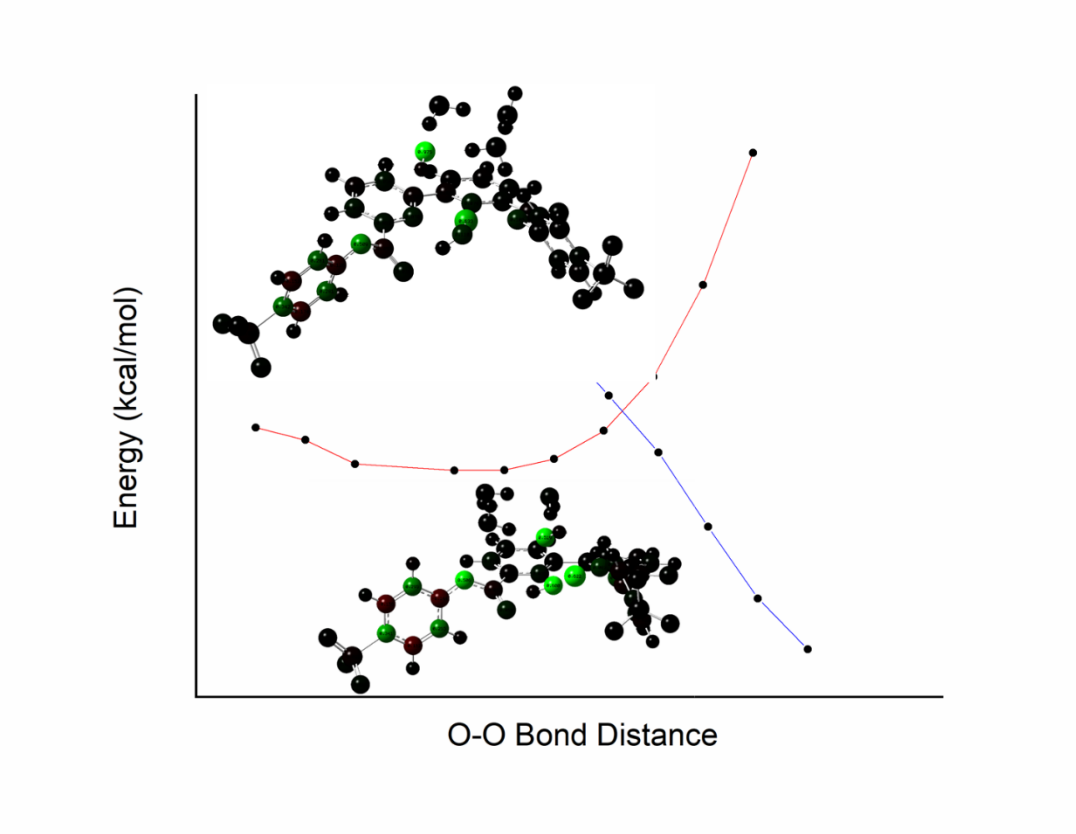


**Figure S66.** Potential energy relaxed scan of the intramolecular $(H_2O)_3HO$---OH SET- WNA using catalyst for **[(L4$^{\cdot}$-*κ*-N$^3$)Cu(OH)]$^{2-}$** in the quartet state.

*Water Nucleophilic Attack potential energy surface*

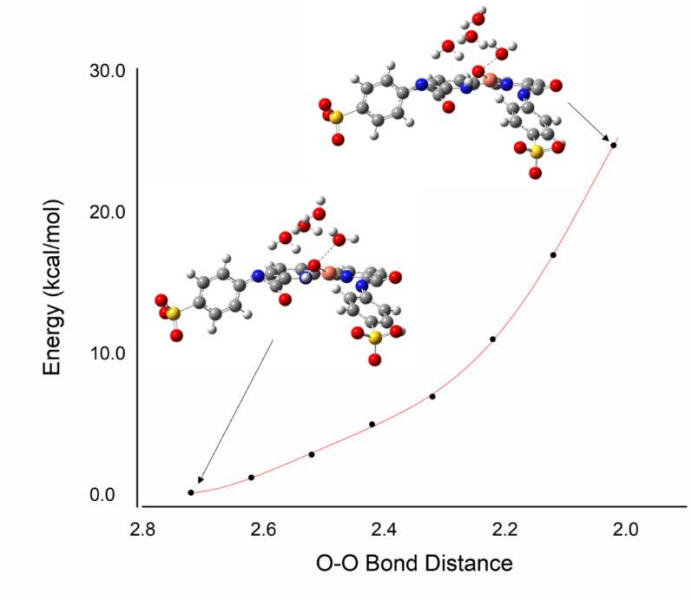


**Figure S67.** Potential energy relaxed scan of the intramolecular $(H_2O)_3H_2O$---OH Water Nucleophilic Attack using catalyst for **[(L4$^{\cdot}$-*κ*-N$^3$)Cu(OH)]$^{2-}$** in the quartet state.

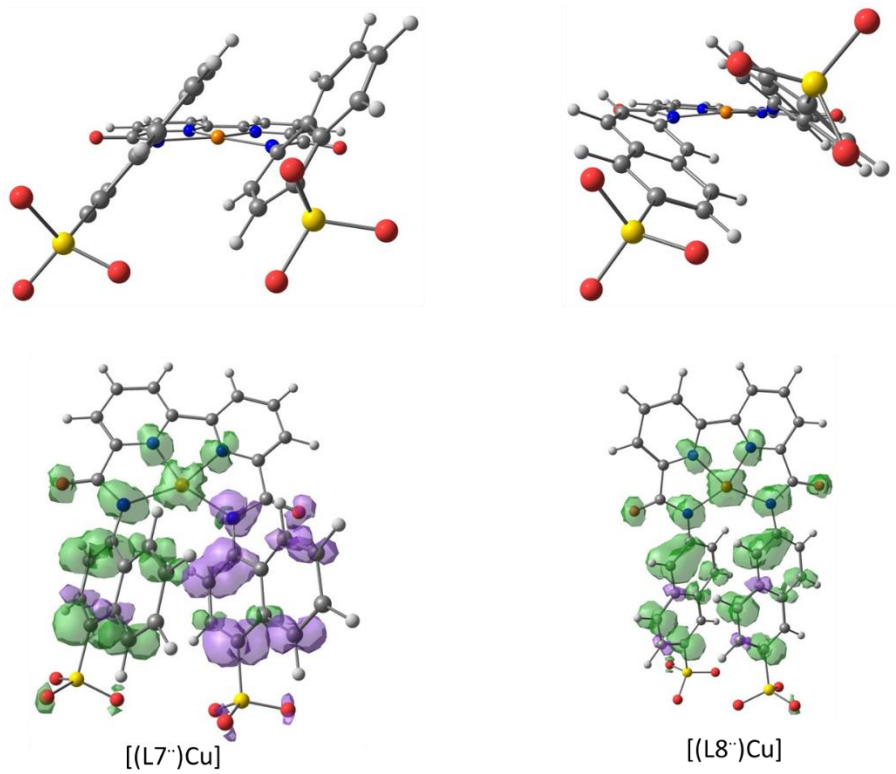


**Figure S68.** DFT optimized structures with representation of the spin distribution for the species **[(L7·)Cu] and [(L8·)Cu]** showing the delocalization of the radicals over the naphtyl-amide moiety.

# SUPPORTING INFORMATION

**Table S6**. Summary of energy data

| Complex (multiplicity) | Ep (H) | ZPVCs (H) | G (H) |
|---|---|---|---|
| $OH^-$ | -75.947690 | -0.00776 | -75.95545 |
| $[(L4)Cu]^{2-}$ (d) | -2736.833258 | 0.290922 | -2736.542336 |
| $[(H_2L4)Cu]$ (d) | -2737.702827 | 0.316735 | -2737.386092 |
| $[(HL4)Cu]^-$ (d) | -2737.275645 | 0.303058 | -2736.972587 |
| $\{[(L4)Cu]\cdots H_2O\}^{2-}$ (d) | -2813.280029 | 0.310897 | -2812.969132 |
| $[(L4)Cu(OH)_{apical}]^{3-}$ (d) | -2812.786660 | 0.297645 | -2812.489015 |
| $[(L4)Cu]^-$ (s) | -2736.628191 | 0.293373 | -2736.334818 |
| $[(L4)Cu]^-$ (t) | -2736.629034 | 0.290744 | -2736.33829 |
| $[(L4)Cu(OH_2)_{apical}]^-$ (s) | -2813.074690 | 0.315265 | -2812.759425 |
| $[(L4)Cu(OH_2)_{apical}]^-$ (t) | -2813.071800 | 0.310034 | -2812.761766 |
| $[(L4)Cu(OH)_{apical}]^{2-}$ (s) | -2812.585820 | 0.301714 | -2812.284106 |
| $[(L4)Cu(OH)_{apical}]^{2-}$ (t) | -2812.592184 | 0.299074 | -2812.29311 |
| $[(L4)Cu(OH)]^{3-}$ (d) | -2812.787172 | 0.296464 | -2812.490708 |
| $[(L4)Cu(OH)]^{2-}$ (s) | -2812.585856 | 0.299376 | -2812.28648 |
| $[(L4)Cu(OH)]^{2-}$ (t) | -2812.602386 | 0.294792 | -2812.307594 |
| $[(L4)Cu(OH_2)]^-$ (s) | -2813.036962 | 0.312095 | -2812.724867 |
| $[(L4)Cu(OH_2)]^-$ (t) | -2813.069746 | 0.309626 | -2812.76012 |
| $[(L4)Cu(OH)]^-$ (d) | -2812.397681 | 0.295942 | -2812.101739 |
| $[(L4)Cu(OH)]^-$ (q) | -2812.400366 | 0.296262 | -2812.104105 |
| $[(L4)Cu(OH_2)]$ (d) | -2812.847401 | 0.310589 | -2812.536812 |
| $[(L4)Cu(OH_2)]$ (q) | -2812.858131 | 0.308672 | -2812.549459 |
| $[(L4)Cu(O)]^{2-}$ (d) | -2811.927027 | 0.285831 | -2811.641196 |
| $[(L4)Cu(O)]^{2-}$ (q) | -2811.926833 | 0.28338 | -2811.643453 |
| $[(L4)Cu(HO\cdots OH)]^{2-}$ (d) | -2888.362321 | 0.304879 | -2888.057442 |
| $[(L4)Cu(HO\cdots OH)]^{2-}$ (q) | -2888.363391 | 0.304178 | -2888.059213 |
| $[(L4)Cu(HO\text{-}OH)]^{2-}$ (d) | -2888.386577 | 0.311244 | -2888.075334 |
| $[(L4)Cu(HO\text{-}OH)]^{2-}$ (q) | -2888.316567 | 0.306258 | -2888.01031 |
| $[(L4)Cu(OH)_2]^{4-}$ (d) | -2888.732095 | 0.304238 | -2888.427857 |
| $[(L4)Cu(OH)_2]^{3-}$ (s) | -2888.530842 | 0.307416 | -2888.223427 |
| $[(L4)Cu(OH)_2]^{3-}$ (t) | -2888.548855 | 0.300718 | -2888.248137 |
| $[(L4)Cu(OH)_2]^{2-}$ (dos) | -2888.350618 | 0.308289 | -2888.042329 |
| $[(L4)Cu(OH)_2]^{2-}$ (q) | -2888.364446 | 0.303684 | -2888.060762 |

| | | | |
|---|---|---|---|
| **[(L4)Cu(OH)(O)]$^{3-}$ (d)** | -2887.887073 | 0.297118 | -2887.589955 |
| **[(L4)Cu(OH)(O)]$^{3-}$ (q)** | -2887.874387 | 0.291281 | -2887.583106 |
| **[(L4)Cu(OH)(HO···OH)]$^{3-}$ (d)** | -2964.313943 | 0.313294 | -2964.000649 |
| **[(L4)Cu(OH)(HO···OH)]$^{3-}$ (q)** | -2964.314770 | 0.313757 | -2964.001013 |
| **[(L4)Cu(OH)(HO-OH)]$^{3-}$ (d)** | -2964.379201 | 0.32112 | -2964.058081 |
| **[(L4)Cu(OH)(HO-OH)]$^{3-}$ (q)** | -2964.298809 | 0.317063 | -2963.981746 |
| **[(L5)Cu]$^{2-}$ (d)** | -2736.83333164 | 0.292585 | -2736.5407 |
| **[(L5)Cu(OH)]$^{3-}$ (d)** | -2812.783247 | 0.296405 | -2812.4868 |
| **[(L5)Cu]$^{-}$ (s)** | -2736.633847 | 0.294614 | -2736.3392 |
| **[(L5)Cu]$^{-}$ (t)** | -2736.632465 | 0.290809 | -2736.3417 |
| **[(L5)Cu(OH)]$^{2-}$ (s)** | -2812.585527 | 0.301584 | -2812.2839 |
| **[(L5)Cu(OH)]$^{2-}$ (t)** | -2812.590105 | 0.299515 | -2812.2906 |
| **[(L5)Cu] (d)** | -2736.422273 | 0.293613 | -2736.1287 |
| **[(L5)Cu] (q)** | -2736.4213 | 0.292433 | -2736.1289 |
| **[(L7)Cu] (dos)** | -3043.74310150 | 0.381056 | -3043.362046 |
| **[(L8)Cu] (q)** | -3043.74912970 | 0.379864 | -3043.369266 |

## Cartesian coordinates (Å) and calculated potential energies (atomic units)

**$OH^-$** E= -75.947690 H

| | | | |
|---|---|---|---|
| O | -1.77132600 | 0.29368800 | 0.00000000 |
| H | -2.09552100 | 1.20918600 | 0.00000000 |

**Complex $[(L4)Cu]^{2-}$ and related species:**

**$[(L4)Cu]^{2-}$ (d)** E= -2736.833258 H

| | | | |
|---|---|---|---|
| Cu | 11.11623100 | 10.97931500 | 17.36338100 |
| S | 8.72740800 | 11.35298500 | 10.43890800 |
| S | 13.48464600 | 12.18400600 | 10.49693100 |
| N | 9.40666100 | 10.49060200 | 16.34875600 |
| N | 9.97455400 | 10.33433600 | 18.86902400 |
| N | 12.29167600 | 11.27054700 | 18.95008500 |
| N | 12.79833600 | 11.66855500 | 16.44441500 |
| O | 7.27965100 | 9.58900900 | 16.71571200 |
| O | 14.92505600 | 12.49733400 | 16.94821200 |
| O | 7.23564200 | 11.38690600 | 10.24231100 |
| O | 9.35512000 | 10.18326200 | 9.73702700 |
| O | 9.37956800 | 12.65925900 | 10.10167100 |
| O | 12.89332600 | 13.49785200 | 10.07698300 |
| O | 12.81858600 | 11.00500600 | 9.85539400 |
| O | 14.97985000 | 12.16089300 | 10.32275500 |
| C | 9.23456100 | 10.66480500 | 14.95970300 |
| C | 9.60350000 | 11.89271500 | 14.38667100 |
| C | 9.47847700 | 12.10918200 | 13.01432900 |
| C | 8.98801000 | 11.08612300 | 12.19949800 |
| C | 8.63958300 | 9.84629200 | 12.74971900 |
| C | 8.76422900 | 9.63648500 | 14.12064100 |
| C | 8.41837900 | 9.96295200 | 17.09526900 |
| C | 8.76038400 | 9.88023800 | 18.56789000 |
| C | 7.92177200 | 9.40434800 | 19.57615500 |
| C | 8.39764900 | 9.43356300 | 20.89245200 |
| C | 9.67547600 | 9.92742600 | 21.18298500 |
| C | 10.46015300 | 10.38153400 | 20.12199300 |
| C | 11.83295300 | 10.94645100 | 20.17107500 |
| C | 12.64136300 | 11.16169800 | 21.28821400 |
| C | 13.91123500 | 11.71658100 | 21.08584800 |
| C | 14.35719800 | 12.03913700 | 19.79827200 |
| C | 13.49652200 | 11.78991900 | 18.72907800 |
| C | 13.79972500 | 12.03462800 | 17.26596100 |
| C | 12.95206000 | 11.81387000 | 15.04820500 |
| C | 13.27182700 | 13.05088300 | 14.46023600 |
| C | 13.39399600 | 13.16500300 | 13.07769000 |
| C | 13.19239100 | 12.04131000 | 12.26733000 |
| C | 12.84761900 | 10.81147700 | 12.83375400 |
| C | 12.72246000 | 10.70448500 | 14.21926500 |
| H | 14.55703800 | 11.89628900 | 21.93986600 |
| H | 15.33883800 | 12.46592000 | 19.62698700 |
| H | 12.29331300 | 10.90545900 | 22.28308200 |
| H | 10.04693600 | 9.95993400 | 22.20153900 |
| H | 7.76861400 | 9.07230500 | 21.70027600 |
| H | 6.93259400 | 9.03035200 | 19.33788200 |
| H | 8.50444100 | 8.67283900 | 14.54497600 |
| H | 10.00112800 | 12.67438300 | 15.02708400 |
| H | 9.76921700 | 13.06136500 | 12.58407400 |
| H | 8.27439200 | 9.04506800 | 12.11377100 |
| H | 12.43831400 | 9.75749500 | 14.66893800 |
| H | 13.42010700 | 13.92097300 | 15.09154800 |
| H | 13.64318300 | 14.12442600 | 12.63446800 |
| H | 12.67022700 | 9.94733700 | 12.20221900 |

**$[(H_2L4)Cu]$ (d)** E= -2737.702827 H

| | | | |
|---|---|---|---|
| Cu | 11.16912300 | 10.98999100 | 17.38722000 |
| S | 9.04134800 | 11.38747200 | 10.47216700 |
| S | 13.18105500 | 12.15055900 | 10.54984000 |
| N | 9.42014900 | 10.61566600 | 16.36417900 |
| N | 9.99772400 | 10.37382100 | 18.87769200 |
| N | 12.35073900 | 11.22157200 | 18.96968400 |
| N | 12.86424000 | 11.63668700 | 16.47288500 |
| O | 7.26590600 | 9.78472100 | 16.71940600 |
| O | 15.03040200 | 12.35536000 | 16.97461400 |
| O | 7.68642400 | 11.11410900 | 9.98214000 |
| O | 9.94220500 | 10.20608300 | 9.84042000 |
| O | 9.65344600 | 12.69125800 | 10.12070400 |
| O | 12.27592000 | 13.43762200 | 10.18968000 |
| O | 12.56592500 | 10.95225100 | 9.93115300 |
| O | 14.53309600 | 12.52401900 | 10.12180900 |
| C | 9.26672300 | 10.78812500 | 14.97958000 |
| C | 9.64521400 | 12.01654100 | 14.40893800 |
| C | 9.58825100 | 12.21464500 | 13.03279400 |
| C | 9.14555200 | 11.16316600 | 12.22439000 |
| C | 8.75737500 | 9.92916900 | 12.76391000 |
| C | 8.81984900 | 9.74736700 | 14.13940700 |
| C | 8.41455500 | 10.11007200 | 17.10618100 |
| C | 8.75590400 | 9.99959100 | 18.57740200 |
| C | 7.88803500 | 9.58043300 | 19.58566700 |
| C | 8.36487800 | 9.57983000 | 20.90204600 |
| C | 9.67087200 | 9.99308600 | 21.19242800 |
| C | 10.48266300 | 10.39723000 | 20.13189700 |
| C | 11.87961200 | 10.89848500 | 20.18603000 |
| C | 12.69653800 | 11.06414300 | 21.30544200 |
| C | 13.98845500 | 11.56809000 | 21.10973200 |
| C | 14.44692800 | 11.89137400 | 19.82648300 |
| C | 13.57646200 | 11.69401400 | 18.75493800 |
| C | 13.88890800 | 11.94663500 | 17.29498500 |
| C | 12.99801600 | 11.77199600 | 15.08203000 |
| C | 13.46420000 | 12.95920800 | 14.48113200 |
| C | 13.51329200 | 13.07560200 | 13.09786000 |
| C | 13.09119900 | 11.99563300 | 12.31031400 |
| C | 12.62504200 | 10.80622800 | 12.87876000 |
| C | 12.58150400 | 10.70554100 | 14.26551700 |
| H | 14.64229700 | 11.70687500 | 21.96518700 |
| H | 15.44584400 | 12.27836700 | 19.66055600 |
| H | 12.33813400 | 10.80826400 | 22.29659700 |
| H | 10.04189400 | 10.00676600 | 22.21159000 |
| H | 7.71333000 | 9.26242900 | 21.71035500 |
| H | 6.87578800 | 9.27405600 | 19.34768000 |
| H | 8.54253800 | 8.79144100 | 14.56908300 |
| H | 10.01013200 | 12.80878200 | 15.05467200 |
| H | 9.90018500 | 13.15838300 | 12.59929200 |
| H | 8.42385300 | 9.11905100 | 12.12258400 |
| H | 12.19689100 | 9.80444700 | 14.73256800 |
| H | 13.76806400 | 13.79319400 | 15.10352500 |
| H | 13.86467100 | 13.99661200 | 12.64270500 |
| H | 12.28462200 | 9.98587500 | 12.25665900 |
| H | 10.91538000 | 10.41899800 | 9.92455200 |
| H | 11.30410300 | 13.20659300 | 10.22691600 |

**$[(HL4)Cu]^-$ (d)** E= -2737.275645 H

| | | | |
|---|---|---|---|
| Cu | 11.15877700 | 10.98593500 | 17.38530900 |
| S | 8.94947500 | 11.53170300 | 10.49633600 |
| S | 13.30102800 | 12.04483500 | 10.49896300 |
| N | 9.42244800 | 10.56864300 | 16.36691800 |
| N | 9.99960200 | 10.35588900 | 18.88169000 |
| N | 12.33640500 | 11.24487200 | 18.96775400 |
| N | 12.84179900 | 11.64138600 | 16.46661200 |
| O | 7.27385600 | 9.72087300 | 16.72918000 |
| O | 14.99020300 | 12.41774700 | 16.95862800 |

| | | | |
|---|---|---|---|
| O | 7.61400200 | 11.11087200 | 10.03683300 |
| O | 9.95276400 | 10.48022800 | 9.81580300 |
| O | 9.39500700 | 12.90293900 | 10.19164600 |
| O | 12.76053500 | 13.37634800 | 10.09134200 |
| O | 12.49786800 | 10.89276000 | 9.92611000 |
| O | 14.75521800 | 11.87835900 | 10.18813000 |
| C | 9.26336000 | 10.77272600 | 14.98651600 |
| C | 9.69813800 | 11.99422100 | 14.44145700 |
| C | 9.61753700 | 12.23876600 | 13.07383000 |
| C | 9.09395000 | 11.24391300 | 12.24330200 |
| C | 8.66323100 | 10.01362000 | 12.75718600 |
| C | 8.75033300 | 9.78157600 | 14.12513500 |
| C | 8.42239900 | 10.05491300 | 17.11032300 |
| C | 8.76896500 | 9.94701600 | 18.58104200 |
| C | 7.91509500 | 9.49931600 | 19.58919400 |
| C | 8.39334100 | 9.50916800 | 20.90507400 |
| C | 9.68705700 | 9.95969300 | 21.19558800 |
| C | 10.48593300 | 10.38907600 | 20.13502100 |
| C | 11.87162400 | 10.92236900 | 20.18658800 |
| C | 12.68480200 | 11.11609100 | 21.30415800 |
| C | 13.96504200 | 11.64750500 | 21.10318500 |
| C | 14.41666000 | 11.96894500 | 19.81695600 |
| C | 13.55102600 | 11.74205400 | 18.74707200 |
| C | 13.85642400 | 11.98365600 | 17.28282400 |
| C | 12.98345100 | 11.75650400 | 15.06808300 |
| C | 13.34678000 | 12.96595800 | 14.44906900 |
| C | 13.41593700 | 13.05413000 | 13.06088600 |
| C | 13.12131000 | 11.93001800 | 12.28058200 |
| C | 12.75213600 | 10.72174500 | 12.87782600 |
| C | 12.67982100 | 10.64302400 | 14.26747000 |
| H | 14.61514100 | 11.80955300 | 21.95744900 |
| H | 15.40660000 | 12.37704800 | 19.64776400 |
| H | 12.33266500 | 10.86140400 | 22.29793100 |
| H | 10.05882900 | 9.98090500 | 22.21436000 |
| H | 7.75248800 | 9.16957700 | 21.71296600 |
| H | 6.91210300 | 9.16343100 | 19.35183800 |
| H | 8.43357800 | 8.82734400 | 14.53016700 |
| H | 10.11909000 | 12.74479900 | 15.10296400 |
| H | 9.96341400 | 13.18059000 | 12.66290300 |
| H | 8.26856800 | 9.24434500 | 12.10043000 |
| H | 12.36812800 | 9.71907300 | 14.74558500 |
| H | 13.55882400 | 13.83781200 | 15.05908800 |
| H | 13.68813600 | 13.99443400 | 12.59119200 |
| H | 12.50670200 | 9.85809200 | 12.26890900 |
| H | 10.93842800 | 10.74246400 | 9.92904100 |

**{[(L4)Cu]···$H_2O$}$^{2-}$ (d)** E= -2813.280029 H

| | | | |
|---|---|---|---|
| Cu | 11.07591900 | 10.98853100 | 17.35803700 |
| S | 8.69338600 | 11.34579700 | 10.42733800 |
| S | 13.46328100 | 12.13197800 | 10.48624400 |
| N | 9.36925500 | 10.51275400 | 16.33934100 |
| N | 9.93155100 | 10.33312200 | 18.85552300 |
| N | 12.24610800 | 11.27843600 | 18.94887900 |
| N | 12.76874900 | 11.66961500 | 16.43941600 |
| O | 7.25132900 | 9.58599300 | 16.68330800 |
| O | 14.91882400 | 12.43237300 | 16.95725500 |
| O | 7.20044000 | 11.37868100 | 10.23793400 |
| O | 9.31897300 | 10.17339100 | 9.72934400 |
| O | 9.34166200 | 12.65185900 | 10.08124600 |
| O | 12.88013400 | 13.44849100 | 10.06092500 |
| O | 12.78129600 | 10.95550300 | 9.85735100 |
| O | 14.95663000 | 12.09694700 | 10.30193400 |
| C | 9.20166700 | 10.68406700 | 14.94876100 |
| C | 9.46594400 | 11.94277000 | 14.38637400 |
| C | 9.34106500 | 12.15150300 | 13.01273600 |
| C | 8.96329300 | 11.08919700 | 12.18803900 |
| C | 8.72166600 | 9.82073200 | 12.72941100 |
| C | 8.84063700 | 9.62007200 | 14.10233700 |
| C | 8.38245400 | 9.97056700 | 17.07533800 |
| C | 8.71712700 | 9.88280400 | 18.54935100 |
| C | 7.87540700 | 9.40370600 | 19.55318100 |
| C | 8.34881500 | 9.42487100 | 20.87066600 |
| C | 9.62794200 | 9.91225800 | 21.16616200 |
| C | 10.41568900 | 10.37031900 | 20.10910800 |
| C | 11.79238700 | 10.92495500 | 20.16346000 |
| C | 12.61300900 | 11.09376300 | 21.27967500 |
| C | 13.89476700 | 11.62200700 | 21.08125500 |
| C | 14.34235500 | 11.95725000 | 19.79755400 |
| C | 13.46791700 | 11.75680100 | 18.72920900 |
| C | 13.78115300 | 12.00324700 | 17.26829900 |
| C | 12.92862200 | 11.80712600 | 15.04300200 |
| C | 13.40431300 | 12.99363900 | 14.45377500 |
| C | 13.53284800 | 13.09172900 | 13.07101500 |
| C | 13.18181500 | 12.00585700 | 12.25945200 |
| C | 12.68075600 | 10.83156500 | 12.82607900 |
| C | 12.55026800 | 10.74044800 | 14.21217100 |
| H | 14.55129700 | 11.76393200 | 21.93417100 |
| H | 15.33733000 | 12.35252000 | 19.62791800 |
| H | 12.26729900 | 10.81692000 | 22.26976300 |
| H | 9.99794200 | 9.93694900 | 22.18548900 |
| H | 7.71685900 | 9.06188800 | 21.67541400 |
| H | 6.88576800 | 9.03351300 | 19.31081200 |
| H | 8.66321900 | 8.63593400 | 14.52334000 |
| H | 9.78211700 | 12.75439000 | 15.03529700 |
| H | 9.54688400 | 13.12858800 | 12.58866300 |
| H | 8.44506100 | 8.99148800 | 12.08503800 |
| H | 12.13991200 | 9.84078400 | 14.66086200 |
| H | 13.66893300 | 13.83684200 | 15.08255200 |
| H | 13.90457900 | 14.01133800 | 12.62875500 |
| H | 12.38563900 | 9.99974600 | 12.19547000 |
| O | 13.01143300 | 8.44482600 | 17.21317000 |
| H | 12.48552600 | 8.61511600 | 18.01326600 |
| H | 13.05586900 | 9.31908200 | 16.78450500 |

**[(L4)Cu(OH)$_{apical}$]$^{3-}$ (d)** E= -2812.786660 H

| | | | |
|---|---|---|---|
| Cu | 11.24523900 | 10.66285000 | 17.32412900 |
| S | 8.68520600 | 11.36095400 | 10.44551600 |
| S | 13.48163800 | 12.22351500 | 10.48058700 |
| N | 9.39721300 | 10.41446400 | 16.33937700 |
| N | 10.00522500 | 10.24926500 | 18.85403300 |
| N | 12.31186000 | 11.22937200 | 18.93607300 |
| N | 12.85706000 | 11.66433900 | 16.43429500 |
| O | 7.24555000 | 9.58386100 | 16.74365100 |
| O | 14.96565400 | 12.51676400 | 16.98590500 |
| O | 12.06202800 | 8.64792000 | 17.03442200 |
| O | 7.29032700 | 10.90254400 | 10.12113400 |
| O | 9.72370400 | 10.52680900 | 9.75009200 |
| O | 8.87680400 | 12.83015500 | 10.21950000 |
| O | 12.46016200 | 13.22606800 | 10.02358600 |
| O | 13.26737200 | 10.86402700 | 9.88621100 |
| O | 14.88604800 | 12.72609800 | 10.28362300 |
| C | 9.20316100 | 10.60721000 | 14.95873000 |
| C | 9.58045600 | 11.83862600 | 14.39635300 |
| C | 9.42999300 | 12.08087300 | 13.03122900 |
| C | 8.90172500 | 11.08187700 | 12.20993500 |
| C | 8.54780300 | 9.83728300 | 12.74630400 |
| C | 8.69742300 | 9.60215900 | 14.11097200 |
| C | 8.40957000 | 9.92021400 | 17.09904400 |
| C | 8.76733200 | 9.84860100 | 18.56824300 |
| C | 7.90032200 | 9.46377800 | 19.59282200 |
| C | 8.36857600 | 9.52800200 | 20.90998400 |
| C | 9.66251000 | 9.98497400 | 21.18605900 |
| C | 10.47402900 | 10.35169000 | 20.11053500 |
| C | 11.84647900 | 10.91601200 | 20.15802100 |
| C | 12.63639300 | 11.15777200 | 21.28375500 |
| C | 13.90086400 | 11.72741100 | 21.09255700 |
| C | 14.35290500 | 12.04738400 | 19.80737500 |
| C | 13.50963700 | 11.77349800 | 18.72868200 |
| C | 13.83630000 | 12.03179000 | 17.27440700 |
| C | 13.02220700 | 11.81727900 | 15.04396500 |

| | | | |
|---|---|---|---|
| C | 13.42168200 | 13.03601300 | 14.46014800 |
| C | 13.54381100 | 13.15169900 | 13.07819600 |
| C | 13.26770300 | 12.04960700 | 12.25845200 |
| C | 12.84296700 | 10.84259200 | 12.81822300 |
| C | 12.71723200 | 10.73325700 | 14.20350100 |
| H | 12.95180800 | 8.85188400 | 16.70302800 |
| H | 14.53444800 | 11.92411000 | 21.95211200 |
| H | 15.32784800 | 12.49192500 | 19.64288100 |
| H | 12.27891800 | 10.90978500 | 22.27738800 |
| H | 10.02338200 | 10.06253400 | 22.20608800 |
| H | 7.71810500 | 9.23648500 | 21.72903300 |
| H | 6.89273100 | 9.13550900 | 19.36432100 |
| H | 8.42562700 | 8.63766800 | 14.52597200 |
| H | 10.00012400 | 12.60575700 | 15.03999500 |
| H | 9.72198000 | 13.03772500 | 12.61210100 |
| H | 8.15021200 | 9.05512900 | 12.10607600 |
| H | 12.37212100 | 9.80556600 | 14.64976200 |
| H | 13.63252100 | 13.89036800 | 15.09459700 |
| H | 13.85844300 | 14.09612200 | 12.64333800 |
| H | 12.60957300 | 9.99574300 | 12.18164200 |

**[(L4)Cu]$^-$ (s)** E= -2736.628191 H

| | | | |
|---|---|---|---|
| Cu | 11.15923000 | 10.95481100 | 17.46817700 |
| S | 8.94358300 | 10.83494500 | 10.42884700 |
| S | 13.22360000 | 12.67087700 | 10.60349300 |
| N | 9.56617400 | 10.74079500 | 16.37695700 |
| N | 9.97453000 | 10.49527400 | 18.87726000 |
| N | 12.36190500 | 11.10855500 | 18.92917100 |
| N | 12.73207700 | 11.43790900 | 16.43450200 |
| O | 7.34615800 | 10.09396400 | 16.59475100 |
| O | 14.94456200 | 12.06293900 | 16.76145000 |
| O | 7.50464800 | 10.41835700 | 10.30711200 |
| O | 9.87637100 | 9.83041400 | 9.82285900 |
| O | 9.18505500 | 12.23279400 | 9.95452700 |
| O | 12.29229100 | 13.79631500 | 10.26794700 |
| O | 12.94880100 | 11.42064200 | 9.83040400 |
| O | 14.66593500 | 13.08898300 | 10.53779300 |
| C | 9.52529200 | 10.76573800 | 14.97353200 |
| C | 9.58496900 | 11.99096200 | 14.29019400 |
| C | 9.45879400 | 12.02118700 | 12.90125200 |
| C | 9.27862400 | 10.82480900 | 12.20337700 |
| C | 9.27055100 | 9.59071600 | 12.87013100 |
| C | 9.40901900 | 9.56159400 | 14.25063900 |
| C | 8.46279200 | 10.33573400 | 17.07597600 |
| C | 8.71174200 | 10.24075800 | 18.55725200 |
| C | 7.79470200 | 9.92888200 | 19.55669400 |
| C | 8.25667000 | 9.90260600 | 20.87859900 |
| C | 9.59541000 | 10.18326500 | 21.18351300 |
| C | 10.46137500 | 10.48841800 | 20.13603800 |
| C | 11.89290400 | 10.83936100 | 20.16544600 |
| C | 12.76994000 | 10.92282600 | 21.24468700 |
| C | 14.10104100 | 11.28102200 | 20.99199700 |
| C | 14.54260000 | 11.55228400 | 19.69083400 |
| C | 13.61580700 | 11.44980400 | 18.65801900 |
| C | 13.84102300 | 11.69482500 | 17.19049400 |
| C | 12.74883000 | 11.72500300 | 15.06053900 |
| C | 12.84820500 | 13.05995000 | 14.62073300 |
| C | 12.95568300 | 13.33780200 | 13.26545400 |
| C | 12.93324600 | 12.28211800 | 12.34193700 |
| C | 12.77326400 | 10.95933800 | 12.76078300 |
| C | 12.67935900 | 10.68079100 | 14.12436000 |
| H | 14.79924200 | 11.34846600 | 21.82012900 |
| H | 15.56806300 | 11.83340400 | 19.47891800 |
| H | 12.42278900 | 10.71057500 | 22.25003300 |
| H | 9.95568500 | 10.17212200 | 22.20624000 |
| H | 7.56766900 | 9.66578600 | 21.68280800 |
| H | 6.76196500 | 9.71668000 | 19.30391600 |
| H | 9.39780400 | 8.61908800 | 14.78941400 |
| H | 9.70930600 | 12.91062500 | 14.85237300 |
| H | 9.49076900 | 12.96484000 | 12.36839700 |
| H | 9.15134100 | 8.66485000 | 12.31613200 |
| H | 12.57222700 | 9.65865000 | 14.47244300 |
| H | 12.86986100 | 13.86021000 | 15.35421400 |
| H | 13.06073800 | 14.36372000 | 12.92669300 |
| H | 12.73120000 | 10.15558000 | 12.03425400 |

**[(L4)Cu]$^-$ (t)** E= -2736.629034 H

| | | | |
|---|---|---|---|
| Cu | 11.14799100 | 11.05888300 | 17.35713600 |
| S | 8.72937700 | 11.30409100 | 10.44428700 |
| S | 13.51195000 | 12.15348500 | 10.49495600 |
| N | 9.33567700 | 10.56632300 | 16.32285700 |
| N | 10.01586900 | 10.30050600 | 18.83701000 |
| N | 12.31040500 | 11.32329000 | 18.94299500 |
| N | 12.82170100 | 11.75836900 | 16.45071600 |
| O | 7.26799500 | 9.56492900 | 16.76532100 |
| O | 14.91543100 | 12.65116600 | 16.96941400 |
| O | 7.24627000 | 11.34622600 | 10.23809600 |
| O | 9.36463500 | 10.09498100 | 9.83276000 |
| O | 9.41485700 | 12.58283100 | 10.09976600 |
| O | 12.89681200 | 13.45090400 | 10.06085100 |
| O | 12.84947500 | 10.95414200 | 9.88847500 |
| O | 15.00399900 | 12.14313000 | 10.29992100 |
| C | 9.17432900 | 10.66800800 | 14.98269800 |
| C | 9.80597400 | 11.78703400 | 14.34495400 |
| C | 9.66475400 | 12.00186600 | 12.98846000 |
| C | 8.93332100 | 11.07795300 | 12.22565900 |
| C | 8.34355800 | 9.93662400 | 12.81792200 |
| C | 8.44307100 | 9.73269300 | 14.17481300 |
| C | 8.38985100 | 9.91788400 | 17.12783500 |
| C | 8.81535300 | 9.79001100 | 18.56050800 |
| C | 8.02450000 | 9.22832100 | 19.56270600 |
| C | 8.52865600 | 9.22844700 | 20.86707200 |
| C | 9.78186100 | 9.78453400 | 21.14254000 |
| C | 10.51918700 | 10.32339900 | 20.08511900 |
| C | 11.86063500 | 10.95352600 | 20.15306300 |
| C | 12.65302500 | 11.18230800 | 21.27908900 |
| C | 13.89649000 | 11.79969600 | 21.09569800 |
| C | 14.33642500 | 12.16212500 | 19.81705400 |
| C | 13.49464800 | 11.89510700 | 18.73798700 |
| C | 13.80399700 | 12.15746300 | 17.28048600 |
| C | 12.99782800 | 11.87366500 | 15.05373600 |
| C | 13.25498800 | 13.11112700 | 14.43807500 |
| C | 13.37830100 | 13.19572400 | 13.05344200 |
| C | 13.24482600 | 12.04102700 | 12.27237000 |
| C | 12.97789100 | 10.80678800 | 12.86876000 |
| C | 12.84688400 | 10.72888600 | 14.25570800 |
| H | 14.52722500 | 11.99420900 | 21.95756100 |
| H | 15.29959100 | 12.63355800 | 19.65830700 |
| H | 12.31294400 | 10.89143600 | 22.26714600 |
| H | 10.17569200 | 9.79841300 | 22.15266100 |
| H | 7.94201100 | 8.80023700 | 21.67349400 |
| H | 7.05113100 | 8.81397000 | 19.32699100 |
| H | 8.01975500 | 8.84533000 | 14.62528500 |
| H | 10.35777600 | 12.48277700 | 14.96659400 |
| H | 10.12260700 | 12.86337300 | 12.51664800 |
| H | 7.81830900 | 9.21451300 | 12.20121800 |
| H | 12.61783600 | 9.77945400 | 14.73123300 |
| H | 13.34449600 | 14.00413600 | 15.04822400 |
| H | 13.56934700 | 14.15629000 | 12.58485700 |
| H | 12.85869200 | 9.91704700 | 12.25947800 |

**[(L4)Cu(OH$_2$)$_{apical}$]$^-$ (s)** E= -2813.074690 H

| | | | |
|---|---|---|---|
| Cu | 11.09202300 | 11.05388900 | 17.47512000 |
| S | 9.05682800 | 10.57263700 | 10.43733600 |
| S | 13.13257200 | 12.87915600 | 10.64706300 |
| N | 9.48364400 | 10.95111300 | 16.39325200 |
| N | 9.88942400 | 10.66799900 | 18.88802400 |
| N | 12.31977300 | 11.09570200 | 18.92159400 |

| | | | |
|---|---|---|---|
| N | 12.69478700 | 11.34856500 | 16.41504800 |
| O | 7.24965500 | 10.35889800 | 16.60719600 |
| O | 14.93804800 | 11.86283200 | 16.72748200 |
| O | 12.28502500 | 8.15390000 | 17.10176200 |
| O | 7.65290400 | 10.05984400 | 10.28116700 |
| O | 10.07810900 | 9.58610800 | 9.95734000 |
| O | 9.23931200 | 11.94306600 | 9.86687500 |
| O | 12.14519300 | 13.97394700 | 10.37427400 |
| O | 12.90684500 | 11.65506400 | 9.81853500 |
| O | 14.55316700 | 13.36596900 | 10.58730000 |
| C | 9.47240600 | 10.87404900 | 14.99091400 |
| C | 9.53663700 | 12.04300400 | 14.21708900 |
| C | 9.44738200 | 11.96402700 | 12.82676300 |
| C | 9.30609100 | 10.71451800 | 12.21950600 |
| C | 9.29449200 | 9.53562900 | 12.97915600 |
| C | 9.38952200 | 9.61540000 | 14.36086900 |
| C | 8.36801500 | 10.57921800 | 17.09314000 |
| C | 8.61415800 | 10.47467100 | 18.57357200 |
| C | 7.69423200 | 10.17004600 | 19.57242700 |
| C | 8.16783300 | 10.08003700 | 20.88733800 |
| C | 9.52221300 | 10.28319600 | 21.18495200 |
| C | 10.39145200 | 10.58187000 | 20.13790400 |
| C | 11.84677200 | 10.82509400 | 20.15601100 |
| C | 12.74486700 | 10.79372600 | 21.22088200 |
| C | 14.09916700 | 11.03887700 | 20.95596700 |
| C | 14.54578500 | 11.30085300 | 19.65439600 |
| C | 13.59761000 | 11.31143100 | 18.63547400 |
| C | 13.82332900 | 11.55044600 | 17.16661500 |
| C | 12.70951100 | 11.70091000 | 15.05420300 |
| C | 12.78654500 | 13.05783500 | 14.68177200 |
| C | 12.88071700 | 13.40551100 | 13.34185700 |
| C | 12.87648800 | 12.39628700 | 12.36790900 |
| C | 12.74690600 | 11.05105900 | 12.72110200 |
| C | 12.65969100 | 10.70298000 | 14.06948500 |
| H | 12.58930700 | 8.97308300 | 16.67092300 |
| H | 14.81211400 | 11.01934300 | 21.77399600 |
| H | 15.59036200 | 11.48718400 | 19.43160300 |
| H | 12.39498200 | 10.57702600 | 22.22440100 |
| H | 9.89435900 | 10.21052600 | 22.20099600 |
| H | 7.47775700 | 9.84410200 | 21.69087500 |
| H | 6.65228100 | 10.00290600 | 19.32357600 |
| H | 9.37834700 | 8.71645100 | 14.96954200 |
| H | 9.63186100 | 13.00493200 | 14.70976400 |
| H | 9.48133800 | 12.86456400 | 12.22405700 |
| H | 9.20810000 | 8.56786100 | 12.49496400 |
| H | 12.57390700 | 9.66335900 | 14.36862600 |
| H | 12.79481600 | 13.82103800 | 15.45408600 |
| H | 12.96047800 | 14.44957000 | 13.05534800 |
| H | 12.71816300 | 10.28489700 | 11.95453700 |
| H | 11.76710900 | 8.47602600 | 17.85946900 |

**[(L4)Cu(OH$_2$)$_{apical}$]$^{-}$ (t)** E= -2813.071800 H

| | | | |
|---|---|---|---|
| Cu | 11.23570200 | 10.94872700 | 17.32289000 |
| S | 9.02812800 | 10.55797100 | 10.46109100 |
| S | 13.43921800 | 12.76470700 | 10.56540000 |
| N | 9.12372200 | 10.87111800 | 16.40181100 |
| N | 9.95367000 | 10.46785200 | 18.87097600 |
| N | 12.38986400 | 11.17492100 | 18.92627400 |
| N | 12.91351000 | 11.63903300 | 16.44336900 |
| O | 6.99450200 | 10.12237800 | 16.96864100 |
| O | 15.06607300 | 12.36855500 | 16.95166300 |
| O | 11.30299900 | 8.88086400 | 16.29575700 |
| O | 7.64242900 | 10.15082200 | 10.06993900 |
| O | 10.04970300 | 9.50155000 | 10.16780300 |
| O | 9.41543900 | 11.91094200 | 9.96376300 |
| O | 12.45073600 | 13.84789400 | 10.24410600 |
| O | 13.16726900 | 11.48674600 | 9.83257200 |
| O | 14.85995700 | 13.23269100 | 10.40259000 |
| C | 9.02403100 | 10.76622500 | 15.06084800 |
| C | 9.76081800 | 11.72245500 | 14.28855800 |
| C | 9.73187500 | 11.69067400 | 12.90955000 |
| C | 9.00346100 | 10.67584800 | 12.26450800 |
| C | 8.29858400 | 9.69587200 | 12.99773900 |
| C | 8.29218900 | 9.73817100 | 14.37476300 |
| C | 8.17561400 | 10.33699100 | 17.26000100 |
| C | 8.66985600 | 10.15784100 | 18.66493700 |
| C | 7.84696800 | 9.73401600 | 19.70836700 |
| C | 8.39982800 | 9.65096000 | 20.98870800 |
| C | 9.73516500 | 10.00241900 | 21.19791200 |
| C | 10.49936700 | 10.41422300 | 20.10225600 |
| C | 11.91608400 | 10.84999400 | 20.13895200 |
| C | 12.74394300 | 10.97225200 | 21.25742200 |
| C | 14.04760500 | 11.44331800 | 21.06646200 |
| C | 14.50609000 | 11.78031500 | 19.78768900 |
| C | 13.62750400 | 11.62364900 | 18.71743200 |
| C | 13.93462900 | 11.92189700 | 17.26814400 |
| C | 13.05482700 | 11.89956000 | 15.05971200 |
| C | 13.10788900 | 13.22223300 | 14.58692300 |
| C | 13.20147000 | 13.47817700 | 13.22189800 |
| C | 13.24097400 | 12.40777700 | 12.31914600 |
| C | 13.18085200 | 11.08974800 | 12.77427500 |
| C | 13.08461700 | 10.83872600 | 14.14499800 |
| H | 12.22442600 | 8.59266700 | 16.41873000 |
| H | 14.70737600 | 11.55062800 | 21.92183900 |
| H | 15.51137700 | 12.15063000 | 19.62242800 |
| H | 12.38540000 | 10.71574900 | 22.24790800 |
| H | 10.17078100 | 9.95822900 | 22.18981200 |
| H | 7.78987400 | 9.32349200 | 21.82459100 |
| H | 6.80939400 | 9.48544600 | 19.51806700 |
| H | 7.77610000 | 8.97441100 | 14.94275400 |
| H | 10.31938700 | 12.48622100 | 14.81681200 |
| H | 10.27337600 | 12.42985900 | 12.33082200 |
| H | 7.76567900 | 8.90742100 | 12.47658300 |
| H | 13.02773800 | 9.81797300 | 14.50936500 |
| H | 13.06734000 | 14.04299300 | 15.29714800 |
| H | 13.23801300 | 14.50264100 | 12.86370500 |
| H | 13.19917700 | 10.26558100 | 12.06915500 |
| H | 10.78181400 | 8.29817900 | 16.87586700 |

**[(L4)Cu(OH)$_{apical}$]$^{2-}$ (s)** E= -2812.585820 H

| | | | |
|---|---|---|---|
| Cu | 11.16187400 | 10.83682400 | 17.43880600 |
| S | 9.06001300 | 10.59122700 | 10.44080000 |
| S | 13.19372200 | 12.80996500 | 10.61050600 |
| N | 9.49175200 | 10.93850800 | 16.39960000 |
| N | 9.95558700 | 10.54587400 | 18.87237800 |
| N | 12.36816400 | 11.03811700 | 18.90438100 |
| N | 12.71953500 | 11.47918100 | 16.42526900 |
| O | 7.27680800 | 10.27529800 | 16.62783900 |
| O | 14.95584000 | 12.01813700 | 16.74403600 |
| O | 11.55016100 | 8.67508200 | 17.17163200 |
| O | 7.64854300 | 10.10000400 | 10.27946900 |
| O | 10.06619500 | 9.59141600 | 9.95543500 |
| O | 9.26387800 | 11.96122600 | 9.87543500 |
| O | 12.22640700 | 13.91043000 | 10.28999200 |
| O | 12.95736600 | 11.56370500 | 9.81750500 |
| O | 14.62235500 | 13.27430100 | 10.54584000 |
| C | 9.46916700 | 10.86541600 | 14.99802300 |
| C | 9.56453600 | 12.03478300 | 14.22784600 |
| C | 9.47503200 | 11.96434100 | 12.83654400 |
| C | 9.30890100 | 10.72136000 | 12.22299600 |
| C | 9.26803800 | 9.54004800 | 12.97838800 |
| C | 9.35609100 | 9.61218200 | 14.36079000 |
| C | 8.40262200 | 10.50474200 | 17.10154300 |
| C | 8.67476000 | 10.36174800 | 18.57121800 |
| C | 7.76295100 | 10.05206100 | 19.57730900 |
| C | 8.24584900 | 9.95220900 | 20.88726100 |
| C | 9.60141200 | 10.16091600 | 21.17396500 |
| C | 10.46275400 | 10.46377700 | 20.12109100 |
| C | 11.90706800 | 10.75414100 | 20.13966500 |
| C | 12.79763200 | 10.78860700 | 21.21140700 |

| | | | |
|---|---|---|---|
| C | 14.13276600 | 11.12705700 | 20.95415200 |
| C | 14.56268600 | 11.43034600 | 19.65650900 |
| C | 13.62353700 | 11.37124000 | 18.62982100 |
| C | 13.84072700 | 11.66114200 | 17.17001200 |
| C | 12.73818800 | 11.78081900 | 15.05326100 |
| C | 12.79853300 | 13.12358600 | 14.63311400 |
| C | 12.90324900 | 13.42641000 | 13.28185700 |
| C | 12.91567000 | 12.38614800 | 12.34217500 |
| C | 12.79431900 | 11.05294300 | 12.74151100 |
| C | 12.70470200 | 10.75026500 | 14.10078300 |
| H | 12.25442600 | 8.66786600 | 16.50263700 |
| H | 14.84079700 | 11.16007500 | 21.77609300 |
| H | 15.58932500 | 11.70537800 | 19.44178100 |
| H | 12.45571000 | 10.56139400 | 22.21538900 |
| H | 9.97976300 | 10.09549100 | 22.18827700 |
| H | 7.56210400 | 9.71359200 | 21.69547500 |
| H | 6.71781200 | 9.89342000 | 19.33607900 |
| H | 9.32272300 | 8.71208900 | 14.96609200 |
| H | 9.68354600 | 12.99247300 | 14.72364500 |
| H | 9.53037100 | 12.86682400 | 12.23832800 |
| H | 9.16200800 | 8.57626400 | 12.48992000 |
| H | 12.62455000 | 9.72025400 | 14.43301900 |
| H | 12.79304000 | 13.91365800 | 15.37799500 |
| H | 12.97751600 | 14.46082900 | 12.96068800 |
| H | 12.77692800 | 10.25972500 | 12.00237500 |

**[(L4)Cu(OH)$_{apical}$]$^{2-}$ (t)** E= -2812.592184 H

| | | | |
|---|---|---|---|
| Cu | 11.13347900 | 10.88375000 | 17.31941200 |
| S | 8.98076100 | 10.75542100 | 10.41091600 |
| S | 13.36891900 | 12.67344600 | 10.53311600 |
| N | 9.30663600 | 10.77257000 | 16.39523500 |
| N | 9.93665500 | 10.44966900 | 18.88982900 |
| N | 12.34051400 | 11.15335600 | 18.92487400 |
| N | 12.79863900 | 11.59539700 | 16.41548500 |
| O | 7.16183900 | 9.95449800 | 16.78054300 |
| O | 14.99971100 | 12.20744900 | 16.86545700 |
| O | 11.57760500 | 8.95698400 | 16.93291000 |
| O | 7.56228600 | 10.36691000 | 10.10275200 |
| O | 9.96111000 | 9.71892300 | 9.94470600 |
| O | 9.31856800 | 12.13638100 | 9.94340700 |
| O | 12.41776800 | 13.78185700 | 10.18440200 |
| O | 13.08314700 | 11.40132400 | 9.79647500 |
| O | 14.80406400 | 13.10674000 | 10.40524800 |
| C | 9.21540300 | 10.75307000 | 14.99916700 |
| C | 9.55820300 | 11.91373900 | 14.28260400 |
| C | 9.49348400 | 11.93053300 | 12.89040600 |
| C | 9.10260900 | 10.77525200 | 12.20874400 |
| C | 8.79400800 | 9.59825800 | 12.90642600 |
| C | 8.85018200 | 9.58619700 | 14.29392000 |
| C | 8.30999300 | 10.25749300 | 17.16407900 |
| C | 8.67099800 | 10.14237000 | 18.62439400 |
| C | 7.80826300 | 9.75986500 | 19.65070900 |
| C | 8.32207000 | 9.71862500 | 20.95251800 |
| C | 9.65627100 | 10.05685600 | 21.20671500 |
| C | 10.46033100 | 10.42880500 | 20.12760500 |
| C | 11.88629600 | 10.83509800 | 20.14745100 |
| C | 12.74881700 | 10.91388100 | 21.24224200 |
| C | 14.06930200 | 11.31969700 | 21.01212100 |
| C | 14.50914500 | 11.63644300 | 19.72084200 |
| C | 13.58937900 | 11.53356600 | 18.67756100 |
| C | 13.86202800 | 11.81629900 | 17.21779300 |
| C | 12.91086600 | 11.84211500 | 15.02729100 |
| C | 13.15782600 | 13.14429700 | 14.55539100 |
| C | 13.26679800 | 13.38816300 | 13.19049800 |
| C | 13.12357200 | 12.32989400 | 12.28388300 |
| C | 12.84328700 | 11.03956700 | 12.73586100 |
| C | 12.73245700 | 10.79952800 | 14.10793000 |
| H | 12.50219700 | 9.00571800 | 16.62504200 |
| H | 14.75989700 | 11.38738100 | 21.84706600 |
| H | 15.52908900 | 11.94896600 | 19.52780700 |
| H | 12.40384600 | 10.66455900 | 22.23987700 |
| H | 10.05840500 | 10.03407600 | 22.21377000 |
| H | 7.67896600 | 9.42520200 | 21.77636200 |
| H | 6.77656200 | 9.50522100 | 19.43629700 |
| H | 8.61783100 | 8.67964100 | 14.84263000 |
| H | 9.87270000 | 12.79845600 | 14.82731200 |
| H | 9.75337500 | 12.82921100 | 12.34223200 |
| H | 8.51011100 | 8.69769000 | 12.36996400 |
| H | 12.50177800 | 9.80262600 | 14.46881600 |
| H | 13.26879100 | 13.95745700 | 15.26619000 |
| H | 13.46599600 | 14.39515300 | 12.83591600 |
| H | 12.70717700 | 10.22927400 | 12.02776100 |

**[(L4)Cu(OH)]$^{3-}$ (d)** E= -2812.787172 H

| | | | |
|---|---|---|---|
| Cu | 11.51383100 | 10.87527900 | 17.08771600 |
| S | 5.86325100 | 7.66600700 | 10.88428500 |
| S | 14.70938800 | 12.55893600 | 10.63674800 |
| N | 8.37939600 | 8.57885800 | 16.27216600 |
| N | 10.00329000 | 10.23408500 | 18.57098700 |
| N | 12.35439600 | 11.36085400 | 18.82366900 |
| N | 13.27754400 | 11.75899600 | 16.42308600 |
| O | 7.64522100 | 10.78264100 | 16.64639500 |
| O | 15.16040900 | 12.86202900 | 17.24961100 |
| O | 10.85701200 | 10.36889600 | 15.38953500 |
| O | 5.02732200 | 8.87321400 | 10.56510600 |
| O | 5.01891400 | 6.43150600 | 11.05880800 |
| O | 6.98103100 | 7.45711400 | 9.90532900 |
| O | 13.49612000 | 13.18470800 | 10.00768000 |
| O | 15.02414300 | 11.20859900 | 10.06576400 |
| O | 15.89336300 | 13.48529700 | 10.61965200 |
| C | 7.77626200 | 8.44413300 | 15.01258700 |
| C | 8.52851700 | 7.87906200 | 13.96309800 |
| C | 7.96686000 | 7.65872000 | 12.70524800 |
| C | 6.62866100 | 7.99197000 | 12.47647800 |
| C | 5.85366300 | 8.53693800 | 13.50906200 |
| C | 6.42242100 | 8.76426900 | 14.75941900 |
| C | 8.21769800 | 9.68846800 | 16.96569600 |
| C | 8.80444000 | 9.66485800 | 18.36059400 |
| C | 8.03630200 | 9.14300000 | 19.41016700 |
| C | 8.51832500 | 9.23500100 | 20.71064800 |
| C | 9.74692600 | 9.85848500 | 20.93635600 |
| C | 10.46480100 | 10.34746700 | 19.84556500 |
| C | 11.77007500 | 11.03423200 | 19.98694400 |
| C | 12.39217200 | 11.36216800 | 21.19831000 |
| C | 13.61609300 | 12.03085600 | 21.16360300 |
| C | 14.20404100 | 12.35682600 | 19.93784500 |
| C | 13.53513600 | 11.99288600 | 18.77280200 |
| C | 14.06182800 | 12.25557700 | 17.38411100 |
| C | 13.64145700 | 11.95492500 | 15.07254900 |
| C | 13.72543600 | 13.24680800 | 14.51906700 |
| C | 14.05369300 | 13.42308300 | 13.17761400 |
| C | 14.30060500 | 12.30393100 | 12.37151500 |
| C | 14.21507000 | 11.01548800 | 12.90253400 |
| C | 13.88510100 | 10.84578600 | 14.24916200 |
| H | 10.10478800 | 9.76929100 | 15.52489000 |
| H | 14.11070600 | 12.29733700 | 22.09268700 |
| H | 15.15493900 | 12.87336000 | 19.87933500 |
| H | 11.93566500 | 11.10929500 | 22.14778500 |
| H | 10.13390300 | 9.95584900 | 21.94368000 |
| H | 7.94638000 | 8.83696300 | 21.54344800 |
| H | 7.07732300 | 8.68369200 | 19.19237800 |
| H | 5.81675900 | 9.18634700 | 15.55464900 |
| H | 9.56884100 | 7.62036000 | 14.14195700 |
| H | 8.56891000 | 7.23427000 | 11.90827400 |
| H | 4.81105500 | 8.78970900 | 13.33786900 |
| H | 13.81257900 | 9.84711300 | 14.66862200 |
| H | 13.52898200 | 14.10977100 | 15.14812400 |
| H | 14.11529000 | 14.42591000 | 12.76470900 |
| H | 14.40544500 | 10.15137800 | 12.27502700 |

# SUPPORTING INFORMATION

**[(L4)Cu(OH)]$^{2-}$ (s)** E= -2812.585856 H

| | | | |
|---|---|---|---|
| Cu | 11.64512900 | 10.77920800 | 17.32850500 |
| S | 6.34180200 | 8.04066800 | 10.65608900 |
| S | 13.87408800 | 12.16024800 | 10.64357500 |
| N | 8.61978400 | 8.79448400 | 16.17495700 |
| N | 10.13527100 | 10.26508600 | 18.60755000 |
| N | 12.45364500 | 11.32258200 | 18.94431000 |
| N | 13.28386700 | 11.49077500 | 16.56678300 |
| O | 7.71801400 | 10.91835900 | 16.64968200 |
| O | 15.15808500 | 12.70268200 | 17.17604100 |
| O | 11.13392700 | 10.19298400 | 15.68909900 |
| O | 5.52986400 | 9.26538700 | 10.34174700 |
| O | 5.48165700 | 6.80841500 | 10.74857300 |
| O | 7.50367800 | 7.85759800 | 9.72507900 |
| O | 12.46871400 | 12.33598400 | 10.14595900 |
| O | 14.52705200 | 10.92025800 | 10.11756900 |
| O | 14.70854700 | 13.39123200 | 10.44695500 |
| C | 8.06375800 | 8.68500600 | 14.88806300 |
| C | 8.88051500 | 8.20672100 | 13.84488700 |
| C | 8.37583500 | 8.02380800 | 12.55686000 |
| C | 7.03268000 | 8.30567600 | 12.29403900 |
| C | 6.19468700 | 8.75986600 | 13.32121500 |
| C | 6.70557600 | 8.95037500 | 14.60214500 |
| C | 8.35762900 | 9.85414600 | 16.91470600 |
| C | 8.90566100 | 9.80351200 | 18.32845800 |
| C | 8.04292800 | 9.37698700 | 19.35000500 |
| C | 8.45610600 | 9.44614600 | 20.67197700 |
| C | 9.71310500 | 9.98415200 | 20.96384800 |
| C | 10.52693400 | 10.39308700 | 19.91686500 |
| C | 11.84005300 | 11.02657000 | 20.10120700 |
| C | 12.47461800 | 11.36387000 | 21.30207500 |
| C | 13.71787400 | 11.99746200 | 21.25168500 |
| C | 14.32413600 | 12.28614900 | 20.02250800 |
| C | 13.64865700 | 11.91418600 | 18.86974900 |
| C | 14.11398100 | 12.09631000 | 17.45901800 |
| C | 13.43761000 | 11.64957400 | 15.18169700 |
| C | 13.14885500 | 12.88679100 | 14.57446900 |
| C | 13.30247300 | 13.03899200 | 13.20224400 |
| C | 13.72940300 | 11.94696200 | 12.43162900 |
| C | 14.00432600 | 10.71046300 | 13.01974300 |
| C | 13.85252100 | 10.56124000 | 14.39815500 |
| H | 10.36110500 | 9.60123300 | 15.81748800 |
| H | 14.21749600 | 12.26723400 | 22.17658300 |
| H | 15.28900700 | 12.77583800 | 19.95378200 |
| H | 12.00915400 | 11.13919100 | 22.25437200 |
| H | 10.04655500 | 10.08611300 | 21.98999300 |
| H | 7.80745300 | 9.10755200 | 21.47366600 |
| H | 7.06003800 | 9.00319400 | 19.08261800 |
| H | 6.05086100 | 9.30050400 | 15.39311600 |
| H | 9.92435400 | 7.98497500 | 14.05090200 |
| H | 9.02553200 | 7.66792300 | 11.76392900 |
| H | 5.14753800 | 8.97063900 | 13.12301000 |
| H | 14.05693900 | 9.60869000 | 14.87571000 |
| H | 12.81402300 | 13.71638600 | 15.18972500 |
| H | 13.08902500 | 13.99532900 | 12.73486400 |
| H | 14.32965800 | 9.87379800 | 12.41147000 |

**[(L4)Cu(OH)]$^{2-}$ (t)** E= -2812.602386 H

| | | | |
|---|---|---|---|
| Cu | 12.07759000 | 11.10599500 | 16.53725000 |
| S | 3.28686500 | 6.63162400 | 13.01567300 |
| S | 16.56449900 | 13.71113300 | 11.30541600 |
| N | 8.65641400 | 8.21291500 | 15.02048300 |
| N | 10.26729500 | 10.06883500 | 17.60469800 |
| N | 12.33469200 | 11.49448200 | 18.47058100 |
| N | 13.78464700 | 12.26847400 | 16.43595500 |
| O | 9.06979500 | 10.46393700 | 15.03416600 |
| O | 15.16329800 | 13.55018700 | 17.81245700 |
| O | 11.96245800 | 10.70473600 | 14.70055900 |
| O | 2.51274200 | 7.88727600 | 12.76588100 |
| O | 2.73219300 | 5.82247300 | 14.15096500 |
| O | 3.51664700 | 5.81974000 | 11.78047800 |
| O | 15.83100700 | 14.88432500 | 10.72375800 |
| O | 16.51366800 | 12.49669000 | 10.42530400 |
| O | 17.96979200 | 14.06532700 | 11.70869500 |
| C | 7.43681200 | 7.91534100 | 14.55703900 |
| C | 7.28079400 | 6.71390900 | 13.79151700 |
| C | 6.03923400 | 6.34470600 | 13.31126400 |
| C | 4.92185400 | 7.15843300 | 13.57561400 |
| C | 5.04212500 | 8.34160400 | 14.33032500 |
| C | 6.27670000 | 8.72188400 | 14.81709100 |
| C | 8.97599600 | 9.39392600 | 15.64409900 |
| C | 9.28329900 | 9.29637300 | 17.11209400 |
| C | 8.47182600 | 8.49223700 | 17.91666000 |
| C | 8.66962500 | 8.51842600 | 19.29648700 |
| C | 9.66645300 | 9.33559200 | 19.81744000 |
| C | 10.45452500 | 10.09616700 | 18.94158700 |
| C | 11.54266000 | 10.98047500 | 19.42692000 |
| C | 11.76742700 | 11.29544200 | 20.77277700 |
| C | 12.82420900 | 12.14495700 | 21.09861100 |
| C | 13.64024400 | 12.65959800 | 20.08936400 |
| C | 13.36251900 | 12.30463100 | 18.77229300 |
| C | 14.18770900 | 12.77960300 | 17.60158400 |
| C | 14.44803200 | 12.62650100 | 15.24354900 |
| C | 14.50728100 | 13.96271400 | 14.80871900 |
| C | 15.13195600 | 14.28975800 | 13.60646700 |
| C | 15.69877200 | 13.27725300 | 12.82350400 |
| C | 15.64636000 | 11.94396700 | 13.24055400 |
| C | 15.01924600 | 11.62342000 | 14.44473500 |
| H | 11.03242900 | 10.48538600 | 14.53038000 |
| H | 13.00947900 | 12.40241200 | 22.13684400 |
| H | 14.47265500 | 13.31822400 | 20.30745100 |
| H | 11.13069200 | 10.89629300 | 21.55299100 |
| H | 9.83668900 | 9.37037200 | 20.88665600 |
| H | 8.05323000 | 7.91442200 | 19.95463600 |
| H | 7.69457700 | 7.87990700 | 17.47302700 |
| H | 6.37615200 | 9.63063100 | 15.40210200 |
| H | 8.15784300 | 6.10424400 | 13.59850000 |
| H | 5.92675100 | 5.43753700 | 12.72745200 |
| H | 4.16803200 | 8.95391400 | 14.52564800 |
| H | 14.96115900 | 10.58961800 | 14.77091800 |
| H | 14.05344600 | 14.74086600 | 15.41485500 |
| H | 15.16726500 | 15.32360100 | 13.27742800 |
| H | 16.08212400 | 11.16010900 | 12.62945300 |

**[(L4)Cu(OH$_2$)]$^{-}$ (s)** E= -2813.036962 H

| | | | |
|---|---|---|---|
| Cu | 11.68746300 | 10.91979500 | 17.15037000 |
| S | 6.30062900 | 7.43151700 | 10.80583500 |
| S | 13.98052400 | 12.93670700 | 10.71737000 |
| N | 8.21209600 | 8.55696400 | 16.39606300 |
| N | 10.12420100 | 10.40168800 | 18.49512400 |
| N | 12.58303200 | 11.16882700 | 18.81289600 |
| N | 13.52096300 | 11.27138800 | 16.43672900 |
| O | 8.45699800 | 10.86809400 | 16.08718100 |
| O | 15.51670200 | 12.16986200 | 17.16259400 |
| O | 10.91690200 | 10.80312400 | 15.35970700 |
| O | 5.50893500 | 8.62152200 | 10.34704600 |
| O | 5.44353400 | 6.20194100 | 10.94487300 |
| O | 7.51778900 | 7.18199400 | 9.96419500 |
| O | 12.96727400 | 14.02456700 | 10.54336400 |
| O | 13.70086600 | 11.72504800 | 9.88907700 |
| O | 15.39032200 | 13.42991700 | 10.58348600 |
| C | 7.77893200 | 8.35597300 | 15.06982800 |
| C | 8.54552100 | 7.55755300 | 14.20304600 |
| C | 8.11313800 | 7.29634400 | 12.90223800 |
| C | 6.89846400 | 7.82586300 | 12.45595100 |
| C | 6.11333800 | 8.60968000 | 13.30989200 |
| C | 6.55456600 | 8.87516200 | 14.60468900 |
| C | 8.47350600 | 9.77411600 | 16.77837700 |
| C | 8.90237600 | 9.91521300 | 18.22086200 |

| | | | |
|---|---|---|---|
| C | 8.01250500 | 9.57034800 | 19.24805100 |
| C | 8.39968100 | 9.73446200 | 20.57216200 |
| C | 9.67999200 | 10.21436000 | 20.85200300 |
| C | 10.52398100 | 10.52692800 | 19.79067500 |
| C | 11.90773300 | 10.98602500 | 19.96212100 |
| C | 12.56702000 | 11.21549800 | 21.17633400 |
| C | 13.89415000 | 11.64166700 | 21.16409100 |
| C | 14.56122200 | 11.82960300 | 19.94909100 |
| C | 13.85753100 | 11.57415700 | 18.78245100 |
| C | 14.38964400 | 11.73988100 | 17.40488300 |
| C | 13.64969300 | 11.66985900 | 15.11488900 |
| C | 13.72843200 | 13.04297500 | 14.76954000 |
| C | 13.82476100 | 13.41375200 | 13.44022900 |
| C | 13.83168700 | 12.41914000 | 12.44499000 |
| C | 13.74640800 | 11.06035600 | 12.76786700 |
| C | 13.64329100 | 10.68388900 | 14.10206200 |
| H | 9.90861300 | 10.88156900 | 15.49309600 |
| H | 14.40844300 | 11.82586700 | 22.10164700 |
| H | 15.58916100 | 12.17037800 | 19.89546900 |
| H | 12.05028400 | 11.05811300 | 22.11554300 |
| H | 10.01412800 | 10.33240300 | 21.87581000 |
| H | 7.72133600 | 9.48413800 | 21.38158400 |
| H | 7.03289600 | 9.18517900 | 18.98919600 |
| H | 5.95082900 | 9.48813300 | 15.26778600 |
| H | 9.49040700 | 7.14952600 | 14.55149100 |
| H | 8.72243200 | 6.68914400 | 12.24020400 |
| H | 5.16844200 | 9.01907100 | 12.96578500 |
| H | 13.56219100 | 9.63893000 | 14.38155100 |
| H | 13.70423200 | 13.79202000 | 15.55458400 |
| H | 13.88186200 | 14.46344500 | 13.17084300 |
| H | 13.74895600 | 10.31066800 | 11.98475400 |
| H | 11.16699800 | 11.59575800 | 14.84447800 |

**[(L4)Cu(OH$_2$)]$^-$ (t)** E= -2813.069746 H

| | | | |
|---|---|---|---|
| Cu | 12.11174300 | 11.06049100 | 16.62462700 |
| S | 3.35418400 | 6.68527000 | 13.04582500 |
| S | 16.37661300 | 13.66179000 | 11.25663700 |
| N | 8.76515100 | 8.20331800 | 14.97429700 |
| N | 10.34905400 | 10.04983900 | 17.59803900 |
| N | 12.35576700 | 11.48661700 | 18.52748400 |
| N | 13.79089900 | 12.22035600 | 16.48932500 |
| O | 9.34431600 | 10.41304800 | 14.95060500 |
| O | 15.16336600 | 13.54043300 | 17.83136500 |
| O | 12.04654500 | 10.46777600 | 14.69645000 |
| O | 2.58746200 | 7.94607800 | 12.80158500 |
| O | 2.81567100 | 5.88906500 | 14.19769600 |
| O | 3.55427200 | 5.86250400 | 11.81264700 |
| O | 15.60709400 | 14.82241600 | 10.69810800 |
| O | 16.30592900 | 12.44122600 | 10.38753300 |
| O | 17.78970700 | 14.03364800 | 11.61020000 |
| C | 7.54202100 | 7.92574700 | 14.51360600 |
| C | 7.35410700 | 6.70420300 | 13.78710700 |
| C | 6.10126900 | 6.34985300 | 13.32721700 |
| C | 5.00480000 | 7.19875600 | 13.57127800 |
| C | 5.15894400 | 8.40655800 | 14.27952500 |
| C | 6.40507400 | 8.77322300 | 14.74626200 |
| C | 9.13896200 | 9.36791500 | 15.58397200 |
| C | 9.36991500 | 9.29336300 | 17.06780100 |
| C | 8.49982100 | 8.52943100 | 17.84966600 |
| C | 8.62370500 | 8.58373800 | 19.23707700 |
| C | 9.61125400 | 9.38843200 | 19.79284700 |
| C | 10.46592600 | 10.10397200 | 18.94476000 |
| C | 11.54816500 | 10.97172400 | 19.46658900 |
| C | 11.76378000 | 11.28107900 | 20.81442600 |
| C | 12.82321700 | 12.12640400 | 21.14739000 |
| C | 13.65116000 | 12.64403600 | 20.14757500 |
| C | 13.38392600 | 12.29180800 | 18.82843100 |
| C | 14.19871400 | 12.75736800 | 17.64786800 |
| C | 14.41969100 | 12.58123700 | 15.27734600 |
| C | 14.45951900 | 13.91757900 | 14.83938300 |
| C | 15.03792600 | 14.24118300 | 13.61428600 |
| C | 15.57267100 | 13.22733500 | 12.80979800 |
| C | 15.53630000 | 11.89513900 | 13.22800900 |
| C | 14.96166900 | 11.57644100 | 14.45975800 |
| H | 11.09415200 | 10.52520600 | 14.46201000 |
| H | 13.00215400 | 12.37961900 | 22.18766100 |
| H | 14.48263000 | 13.30051300 | 20.37608700 |
| H | 11.12096700 | 10.88000800 | 21.58862800 |
| H | 9.72392700 | 9.45149600 | 20.86847600 |
| H | 7.95643100 | 8.01186200 | 19.87371000 |
| H | 7.73144700 | 7.92408800 | 17.38282400 |
| H | 6.53276400 | 9.70068100 | 15.29574700 |
| H | 8.21457200 | 6.06599400 | 13.61308300 |
| H | 5.96257500 | 5.42519100 | 12.77735400 |
| H | 4.30134900 | 9.04713000 | 14.45577900 |
| H | 14.92469100 | 10.54349500 | 14.79347100 |
| H | 14.02750600 | 14.69586500 | 15.46062700 |
| H | 15.06014100 | 15.27439700 | 13.28230400 |
| H | 15.94753400 | 11.11037800 | 12.60154000 |
| H | 12.51386600 | 11.07378000 | 14.09235000 |

**[(L4)Cu(OH)]$^-$ (d)** E= -2812.397681 H

| | | | |
|---|---|---|---|
| Cu | 11.70722400 | 10.75989200 | 16.83312900 |
| S | 5.16694700 | 6.16492900 | 11.82874000 |
| S | 15.11515900 | 13.69338500 | 11.00189600 |
| N | 8.60453500 | 9.20087800 | 15.61383100 |
| N | 9.95414200 | 10.48477800 | 18.11917500 |
| N | 12.45688600 | 11.14672600 | 18.63104700 |
| N | 13.76102000 | 11.40490600 | 16.33239600 |
| O | 7.62730300 | 11.26730300 | 15.91853600 |
| O | 15.66757500 | 12.07214000 | 17.46218700 |
| O | 11.24062000 | 10.34488500 | 15.08157400 |
| O | 4.39953900 | 7.20787000 | 11.07570600 |
| O | 4.29151400 | 5.32092900 | 12.70423600 |
| O | 6.08400100 | 5.36386200 | 10.96291000 |
| O | 14.16486500 | 14.83710200 | 10.82297700 |
| O | 14.92362900 | 12.59955000 | 10.00434500 |
| O | 16.53937600 | 14.13688600 | 11.13411800 |
| C | 7.79171200 | 8.55136700 | 14.76657100 |
| C | 8.39638000 | 7.66835400 | 13.81560000 |
| C | 7.61540000 | 6.95518300 | 12.92444300 |
| C | 6.21794500 | 7.09019900 | 12.97121700 |
| C | 5.59331700 | 7.93902900 | 13.91062500 |
| C | 6.36002900 | 8.66144500 | 14.79892900 |
| C | 8.23513800 | 10.28478200 | 16.35531100 |
| C | 8.66963200 | 10.26218600 | 17.79932100 |
| C | 7.66971800 | 10.06747100 | 18.75636500 |
| C | 8.02224400 | 10.09919600 | 20.10150100 |
| C | 9.34567900 | 10.36701200 | 20.44570000 |
| C | 10.28558600 | 10.57161100 | 19.43343000 |
| C | 11.69218900 | 10.93429100 | 19.71580400 |
| C | 12.23595100 | 11.08321500 | 20.99900500 |
| C | 13.56877000 | 11.46572800 | 21.13245800 |
| C | 14.34290900 | 11.69232500 | 19.99274400 |
| C | 13.74305100 | 11.51371100 | 18.75042200 |
| C | 14.48110200 | 11.72964300 | 17.47068900 |
| C | 14.06814600 | 11.95948700 | 15.13451400 |
| C | 14.59461900 | 13.28815600 | 15.00708400 |
| C | 14.89621300 | 13.79309700 | 13.76246600 |
| C | 14.69561000 | 12.99294500 | 12.61499100 |
| C | 14.17065900 | 11.69500200 | 12.71084100 |
| C | 13.84013200 | 11.18577600 | 13.95383900 |
| H | 14.00081600 | 11.58666600 | 22.12058300 |
| H | 15.38039000 | 11.99879100 | 20.05509000 |
| H | 11.63374900 | 10.90199000 | 21.88071000 |
| H | 9.63385700 | 10.42455600 | 21.48806400 |
| H | 7.27692200 | 9.93623900 | 20.87331500 |
| H | 6.64675200 | 9.89472100 | 18.43867500 |
| H | 5.88832900 | 9.30731300 | 15.53114700 |
| H | 9.47851100 | 7.58428900 | 13.80158700 |

| | | | |
|---|---|---|---|
| H | 8.07403700 | 6.29581200 | 12.19621400 |
| H | 4.51134800 | 8.02153500 | 13.93843200 |
| H | 13.43853800 | 10.18713300 | 14.06065000 |
| H | 14.72772300 | 13.89925100 | 15.89209000 |
| H | 15.28275100 | 14.80239800 | 13.66495500 |
| H | 14.02948200 | 11.09724200 | 11.81751600 |

**[(L4)Cu(OH)]$^-$ (q)** E= -2812.400366 H

| | | | |
|---|---|---|---|
| Cu | 12.34102300 | 10.45297100 | 16.68810100 |
| S | 3.65335300 | 6.64766700 | 12.67674600 |
| S | 15.32798600 | 14.58617300 | 11.30451800 |
| N | 8.86485700 | 8.02824500 | 15.18158300 |
| N | 10.42766300 | 10.00392800 | 17.65378900 |
| N | 12.58846700 | 11.22281300 | 18.51198000 |
| N | 14.07576600 | 11.80143600 | 16.41842900 |
| O | 9.59041100 | 10.18587000 | 14.89851200 |
| O | 15.82019500 | 12.46227700 | 17.81495600 |
| O | 12.54833400 | 9.36195000 | 15.17610500 |
| O | 3.60665600 | 7.46003700 | 11.41705100 |
| O | 2.61210600 | 7.06354100 | 13.67024600 |
| O | 3.67585700 | 5.17407100 | 12.42695100 |
| O | 14.52129900 | 15.84655800 | 11.38124300 |
| O | 14.89586300 | 13.67287800 | 10.20493100 |
| O | 16.80358000 | 14.83594400 | 11.32673400 |
| C | 7.68719300 | 7.76330400 | 14.60643900 |
| C | 7.48539300 | 6.45658100 | 14.05460100 |
| C | 6.27457100 | 6.11556600 | 13.48009400 |
| C | 5.23574100 | 7.06085000 | 13.44249100 |
| C | 5.40462300 | 8.35605000 | 13.97590300 |
| C | 6.60698100 | 8.70979000 | 14.55082600 |
| C | 9.25643800 | 9.26046800 | 15.64105500 |
| C | 9.35009500 | 9.38771800 | 17.13948800 |
| C | 8.28500600 | 8.95040700 | 17.93081700 |
| C | 8.32898100 | 9.19561100 | 19.30231100 |
| C | 9.43164500 | 9.85511000 | 19.83687500 |
| C | 10.47225700 | 10.24119300 | 18.98485000 |
| C | 11.68479000 | 10.94542300 | 19.46548100 |
| C | 11.92567900 | 11.32060300 | 20.79406600 |
| C | 13.11788000 | 11.97129500 | 21.10884600 |
| C | 14.05035100 | 12.24033900 | 20.10440900 |
| C | 13.74120000 | 11.84444000 | 18.80637400 |
| C | 14.65771100 | 12.09521600 | 17.65187100 |
| C | 14.41292600 | 12.45764500 | 15.28858200 |
| C | 15.14225600 | 13.69796100 | 15.26376800 |
| C | 15.40912000 | 14.31270600 | 14.06125600 |
| C | 14.97474300 | 13.72333100 | 12.85286000 |
| C | 14.24704200 | 12.52175500 | 12.84943300 |
| C | 13.95480900 | 11.90141200 | 14.04838900 |
| H | 13.31822200 | 12.26667800 | 22.13365000 |
| H | 14.98756700 | 12.74368900 | 20.31154700 |
| H | 11.20250000 | 11.10852300 | 21.57190600 |
| H | 9.48133500 | 10.06103000 | 20.89913400 |
| H | 7.51292300 | 8.88112000 | 19.94483100 |
| H | 7.43702300 | 8.44831000 | 17.47857600 |
| H | 6.74165000 | 9.70095500 | 14.97262100 |
| H | 8.30121600 | 5.74199000 | 14.09925100 |
| H | 6.12337300 | 5.12493200 | 13.06585400 |
| H | 4.58871500 | 9.07127500 | 13.94277700 |
| H | 13.38643900 | 10.97664500 | 14.08673000 |
| H | 15.45480000 | 14.16391100 | 16.18891100 |
| H | 15.94779800 | 15.25469200 | 14.04555700 |
| H | 13.91405500 | 12.08964600 | 11.91245400 |

**[(L4)Cu(OH$_2$)] (d)** E= -2812.847401 H

| | | | |
|---|---|---|---|
| Cu | 12.11523300 | 11.04334900 | 16.60515200 |
| S | 3.34888400 | 6.69648000 | 13.15744900 |
| S | 16.35626200 | 13.66491900 | 11.25941700 |
| N | 8.75273500 | 8.26897100 | 14.87817800 |
| N | 10.33112900 | 10.03876600 | 17.57152300 |
| N | 12.33495000 | 11.46571400 | 18.51587600 |
| N | 13.79799800 | 12.19829700 | 16.49778500 |
| O | 9.37497500 | 10.44303400 | 14.92478000 |
| O | 15.13509600 | 13.54020400 | 17.85162400 |
| O | 12.10326100 | 10.43824200 | 14.67404000 |
| O | 2.73332000 | 7.92084000 | 12.57859200 |
| O | 2.79257800 | 6.30321200 | 14.48645500 |
| O | 3.50877400 | 5.57239700 | 12.20225200 |
| O | 15.45794300 | 14.68961500 | 10.63072000 |
| O | 16.45247400 | 12.40230900 | 10.45653100 |
| O | 17.70542800 | 14.22867300 | 11.60799500 |
| C | 7.55298500 | 7.99732900 | 14.47650400 |
| C | 7.37432000 | 6.75331900 | 13.72446500 |
| C | 6.12366900 | 6.37263800 | 13.32409000 |
| C | 5.02549000 | 7.21361200 | 13.62806400 |
| C | 5.15525300 | 8.44423900 | 14.33513800 |
| C | 6.38807900 | 8.84306600 | 14.75596000 |
| C | 9.13831500 | 9.42280100 | 15.56041100 |
| C | 9.34749000 | 9.29138400 | 17.03408500 |
| C | 8.48640600 | 8.50266000 | 17.79934600 |
| C | 8.62482200 | 8.52437200 | 19.18818700 |
| C | 9.60577500 | 9.32704100 | 19.75347600 |
| C | 10.44975800 | 10.07245700 | 18.91500500 |
| C | 11.51949800 | 10.94864400 | 19.44749700 |
| C | 11.71117700 | 11.26598800 | 20.79653800 |
| C | 12.76002800 | 12.12039700 | 21.14127500 |
| C | 13.59906300 | 12.63732400 | 20.15116500 |
| C | 13.35318800 | 12.27813200 | 18.82912700 |
| C | 14.18216400 | 12.74584100 | 17.65931400 |
| C | 14.43438900 | 12.56562300 | 15.29179300 |
| C | 14.43525900 | 13.89798700 | 14.83938800 |
| C | 15.01041700 | 14.22471100 | 13.61425000 |
| C | 15.58092400 | 13.21828000 | 12.82393500 |
| C | 15.58898700 | 11.89188800 | 13.25912500 |
| C | 15.01777800 | 11.56968600 | 14.49249800 |
| H | 11.20759400 | 10.59117100 | 14.31338500 |
| H | 12.92112100 | 12.38097800 | 22.18258000 |
| H | 14.42291400 | 13.30035300 | 20.38817200 |
| H | 11.05768800 | 10.86611400 | 21.56250200 |
| H | 9.72607200 | 9.36630900 | 20.82931800 |
| H | 7.96930900 | 7.92954600 | 19.81547900 |
| H | 7.71414800 | 7.90253000 | 17.33272100 |
| H | 6.52579600 | 9.77292200 | 15.29864000 |
| H | 8.25430900 | 6.15293000 | 13.51741900 |
| H | 5.96381900 | 5.45208100 | 12.77488600 |
| H | 4.27766500 | 9.05068200 | 14.53002900 |
| H | 15.01798500 | 10.54071600 | 14.84124800 |
| H | 13.97434800 | 14.66879700 | 15.44919300 |
| H | 15.00036800 | 15.25423800 | 13.26985100 |
| H | 16.03080800 | 11.11436500 | 12.64496800 |
| H | 12.71679400 | 10.94193100 | 14.10665300 |

**[(L4)Cu(OH$_2$)] (q)** E= -2812.858131 H

| | | | |
|---|---|---|---|
| Cu | 12.04526300 | 11.11923600 | 16.58068500 |
| S | 3.38303900 | 6.60588700 | 12.83153300 |
| S | 16.55370700 | 13.55517100 | 11.26740500 |
| N | 8.65813200 | 8.08936900 | 15.13269600 |
| N | 10.33454600 | 10.03665400 | 17.63356900 |
| N | 12.35277400 | 11.55304000 | 18.47932200 |
| N | 13.81174300 | 12.33117400 | 16.41763200 |
| O | 9.07143700 | 10.33482700 | 15.05704000 |
| O | 15.16491800 | 13.60484900 | 17.83034100 |
| O | 11.66232000 | 10.83679000 | 14.63179000 |
| O | 2.63022800 | 7.87507900 | 12.58869200 |
| O | 2.77092900 | 5.76151800 | 13.90950400 |
| O | 3.67000500 | 5.83573400 | 11.58196700 |
| O | 16.09160400 | 14.91774100 | 10.86267000 |
| O | 16.15227000 | 12.47832600 | 10.31531200 |
| O | 18.00471400 | 13.51332600 | 11.63720400 |
| C | 7.46262100 | 7.81202500 | 14.60144900 |

| | | | |
|---|---|---|---|
| C | 7.32706800 | 6.61084300 | 13.83137500 |
| C | 6.10794400 | 6.26610100 | 13.28227900 |
| C | 4.99260700 | 7.10051000 | 13.48802900 |
| C | 5.09228900 | 8.28032600 | 14.25135100 |
| C | 6.30497500 | 8.63859600 | 14.80408100 |
| C | 9.00956000 | 9.27604800 | 15.70338900 |
| C | 9.37260100 | 9.22088900 | 17.15950700 |
| C | 8.59969600 | 8.40345500 | 17.98851400 |
| C | 8.80712400 | 8.45378600 | 19.36501700 |
| C | 9.77454800 | 9.31702900 | 19.86397600 |
| C | 10.52595400 | 10.09163900 | 18.97034900 |
| C | 11.57456900 | 11.02545800 | 19.43886700 |
| C | 11.77683900 | 11.37952700 | 20.78022200 |
| C | 12.79080000 | 12.27830700 | 21.10257900 |
| C | 13.59465600 | 12.80616500 | 20.09142300 |
| C | 13.34141500 | 12.41264800 | 18.78161200 |
| C | 14.18624900 | 12.88448200 | 17.64335300 |
| C | 14.43861300 | 12.67034400 | 15.26499400 |
| C | 15.03556800 | 13.95390600 | 15.01901900 |
| C | 15.63883100 | 14.20891600 | 13.80702300 |
| C | 15.69377900 | 13.20232000 | 12.81868000 |
| C | 15.12645900 | 11.93348400 | 13.03783100 |
| C | 14.48842300 | 11.67636500 | 14.23242300 |
| H | 10.68022800 | 10.73342000 | 14.61051500 |
| H | 12.95419000 | 12.56238800 | 22.13698000 |
| H | 14.40025000 | 13.49952800 | 20.30189100 |
| H | 11.15056100 | 10.96978500 | 21.56268500 |
| H | 9.95203300 | 9.37533300 | 20.93064300 |
| H | 8.21944500 | 7.83637100 | 20.03645500 |
| H | 7.83891300 | 7.76026000 | 17.56077200 |
| H | 6.38978100 | 9.54430800 | 15.39579800 |
| H | 8.20218900 | 5.98530100 | 13.68695100 |
| H | 6.01059600 | 5.36193800 | 12.69109400 |
| H | 4.21946100 | 8.90683400 | 14.40109900 |
| H | 14.06033900 | 10.70130600 | 14.43370800 |
| H | 14.95646900 | 14.73628600 | 15.76136000 |
| H | 16.05604500 | 15.19059700 | 13.60824700 |
| H | 15.18859400 | 11.16742100 | 12.27311100 |
| H | 11.84709700 | 11.64713200 | 14.12003600 |

**[(L4)Cu(O)]$^{2-}$ (d)** E= -2812.858131 H

| | | | |
|---|---|---|---|
| Cu | 12.03666300 | 11.05819700 | 16.72376300 |
| S | 3.70216800 | 6.65976900 | 12.61428000 |
| S | 16.04303600 | 13.57290800 | 11.14742800 |
| N | 8.82933700 | 8.38291900 | 15.08660900 |
| N | 10.30186000 | 10.16530000 | 17.74929800 |
| N | 12.37530200 | 11.48868400 | 18.62493900 |
| N | 13.73488600 | 12.22092000 | 16.53057500 |
| O | 9.08459700 | 10.66409200 | 15.16732500 |
| O | 15.23553400 | 13.43504600 | 17.84677800 |
| O | 11.83684600 | 10.50881300 | 14.95997400 |
| O | 3.27591100 | 7.80022300 | 11.74043700 |
| O | 2.77894000 | 6.44521200 | 13.77568200 |
| O | 3.98929100 | 5.40754800 | 11.85005200 |
| O | 14.97904200 | 14.37451000 | 10.45057500 |
| O | 16.33106600 | 12.27425600 | 10.45561000 |
| O | 17.28210200 | 14.38476200 | 11.39939600 |
| C | 7.66175000 | 8.03884900 | 14.52909900 |
| C | 7.61718300 | 6.84162400 | 13.74415900 |
| C | 6.43328500 | 6.42524200 | 13.16172600 |
| C | 5.26612300 | 7.18363000 | 13.34929700 |
| C | 5.27623400 | 8.36356200 | 14.12296500 |
| C | 6.44941000 | 8.79003400 | 14.70806300 |
| C | 9.04399300 | 9.57295900 | 15.73899900 |
| C | 9.28987300 | 9.45829300 | 17.22069000 |
| C | 8.40321100 | 8.71236000 | 18.00060600 |
| C | 8.55321500 | 8.73706900 | 19.38664300 |
| C | 9.58357000 | 9.48932700 | 19.94307000 |
| C | 10.45106500 | 10.18621000 | 19.09472800 |
| C | 11.58835600 | 10.99615600 | 19.59299700 |
| C | 11.87180500 | 11.27376400 | 20.93470700 |
| C | 12.97801700 | 12.07259800 | 21.23105100 |
| C | 13.78041100 | 12.57445500 | 20.20254000 |
| C | 13.44369900 | 12.25059600 | 18.89051700 |
| C | 14.22373600 | 12.70531300 | 17.68079500 |
| C | 14.31654500 | 12.55917300 | 15.29367400 |
| C | 14.60762300 | 13.89142800 | 14.93771400 |
| C | 15.13537100 | 14.18845300 | 13.68408900 |
| C | 15.38022500 | 13.15645600 | 12.76838200 |
| C | 15.08816800 | 11.83202300 | 13.10107200 |
| C | 14.55854100 | 11.53903500 | 14.35911700 |
| H | 13.21247800 | 12.30261700 | 22.26578900 |
| H | 14.64490800 | 13.19592500 | 20.40497500 |
| H | 11.24856800 | 10.88507000 | 21.73104200 |
| H | 9.71772400 | 9.52318100 | 21.01775400 |
| H | 7.87446300 | 8.17978900 | 20.02437000 |
| H | 7.60429200 | 8.14856200 | 17.53136400 |
| H | 6.46196700 | 9.69273000 | 15.31031900 |
| H | 8.53217100 | 6.27244200 | 13.61385000 |
| H | 6.40320000 | 5.52117200 | 12.56395200 |
| H | 4.36305100 | 8.93356600 | 14.26344500 |
| H | 14.32761300 | 10.51246900 | 14.62819000 |
| H | 14.40667000 | 14.69076800 | 15.64285500 |
| H | 15.35174300 | 15.22044000 | 13.42315600 |
| H | 15.27283100 | 11.03466800 | 12.38921700 |

**[(L4)Cu(O)]$^{2-}$ (q)** E= -2811.926833 H

| | | | |
|---|---|---|---|
| Cu | 12.03879000 | 11.04318600 | 16.71851700 |
| S | 3.67326200 | 6.65563500 | 12.67367500 |
| S | 15.70291700 | 13.93736800 | 11.10578100 |
| N | 8.79708300 | 8.49023500 | 15.07179100 |
| N | 10.32109300 | 10.14937400 | 17.75992500 |
| N | 12.47267200 | 11.35540000 | 18.62221200 |
| N | 13.74646300 | 12.18326500 | 16.51202500 |
| O | 8.98509400 | 10.77501100 | 15.24197600 |
| O | 15.37101200 | 13.23397200 | 17.82109300 |
| O | 11.74327500 | 10.59842600 | 14.93881900 |
| O | 3.18376100 | 7.80587700 | 11.84697700 |
| O | 2.78896200 | 6.37363300 | 13.85073200 |
| O | 3.98402800 | 5.43763000 | 11.86488600 |
| O | 14.57812000 | 14.76286100 | 10.54471600 |
| O | 15.96114400 | 12.69761000 | 10.30308400 |
| O | 16.94309200 | 14.75556500 | 11.32857400 |
| C | 7.62899900 | 8.12248000 | 14.53080000 |
| C | 7.60848900 | 6.95170500 | 13.70603900 |
| C | 6.42600500 | 6.50947300 | 13.14003100 |
| C | 5.23622100 | 7.21415000 | 13.38501800 |
| C | 5.22267500 | 8.36683900 | 14.19861600 |
| C | 6.39398600 | 8.81827100 | 14.76831400 |
| C | 8.99072700 | 9.65945500 | 15.76612000 |
| C | 9.27687200 | 9.48764900 | 17.23535100 |
| C | 8.39954700 | 8.72592400 | 18.01068200 |
| C | 8.59747700 | 8.68222900 | 19.39010200 |
| C | 9.66611800 | 9.38178400 | 19.94373800 |
| C | 10.52018700 | 10.09881700 | 19.09921300 |
| C | 11.69998200 | 10.84846900 | 19.59394200 |
| C | 12.03708300 | 11.05755700 | 20.93575700 |
| C | 13.18298100 | 11.80050700 | 21.22709400 |
| C | 13.96948000 | 12.31835000 | 20.19388200 |
| C | 13.57514800 | 12.06887600 | 18.88169500 |
| C | 14.31804500 | 12.56324500 | 17.66419800 |
| C | 14.26417600 | 12.60540300 | 15.27245400 |
| C | 14.57848200 | 13.95468300 | 15.01257000 |
| C | 15.02447100 | 14.34669100 | 13.75352400 |
| C | 15.16295200 | 13.39447300 | 12.73501800 |
| C | 14.85126100 | 12.05434400 | 12.97355600 |
| C | 14.40510800 | 11.66575500 | 14.23799800 |
| H | 13.46005700 | 11.97628200 | 22.26192200 |
| H | 14.86268500 | 12.89878500 | 20.39355400 |

| | | | |
|---|---|---|---|
| H | 11.42448000 | 10.66067000 | 21.73640300 |
| H | 9.84201300 | 9.35651400 | 21.01264300 |
| H | 7.92855900 | 8.10995800 | 20.02494200 |
| H | 7.57432600 | 8.19941100 | 17.54369500 |
| H | 6.38875300 | 9.69906500 | 15.40230600 |
| H | 8.54029200 | 6.42234400 | 13.53345800 |
| H | 6.41418000 | 5.62490000 | 12.51309200 |
| H | 4.29254300 | 8.89541400 | 14.38312100 |
| H | 14.16152600 | 10.62559500 | 14.43329300 |
| H | 14.45745300 | 14.69420400 | 15.79667500 |
| H | 15.25745600 | 15.39110300 | 13.56727500 |
| H | 14.95690100 | 11.31810300 | 12.18388300 |

**[(L4)Cu(HO···OH)]$^{2-}$ (d)** E= -2888.362321 H

| | | | |
|---|---|---|---|
| Cu | 12.14961800 | 11.07702500 | 16.64937800 |
| S | 3.40297900 | 6.74463500 | 12.89334400 |
| S | 16.23704700 | 13.86433700 | 11.26794000 |
| N | 8.72938200 | 8.14991600 | 15.12976700 |
| N | 10.38626400 | 9.97605300 | 17.71053700 |
| N | 12.48173800 | 11.35685800 | 18.57992400 |
| N | 13.85191800 | 12.21560100 | 16.53089200 |
| O | 9.15980600 | 10.39674700 | 15.14573400 |
| O | 15.28757300 | 13.43472400 | 17.90279400 |
| O | 11.93084700 | 10.84400100 | 14.76188000 |
| O | 2.96972200 | 7.93806700 | 12.09805900 |
| O | 2.54328800 | 6.51129500 | 14.09914200 |
| O | 3.59623900 | 5.51803500 | 12.06109500 |
| O | 15.17374700 | 13.50988100 | 10.26471300 |
| O | 17.48578900 | 13.05357700 | 11.07505000 |
| O | 16.50147400 | 15.33934100 | 11.32338500 |
| C | 7.52046000 | 7.87981500 | 14.62496500 |
| C | 7.37002300 | 6.69207000 | 13.83874200 |
| C | 6.13838100 | 6.35052000 | 13.30950900 |
| C | 5.02835100 | 7.17632700 | 13.55243200 |
| C | 5.14328200 | 8.34848600 | 14.32985000 |
| C | 6.36492300 | 8.70155300 | 14.86202700 |
| C | 9.06884800 | 9.32262700 | 15.75221500 |
| C | 9.39562800 | 9.21303800 | 17.21489200 |
| C | 8.59161800 | 8.39584800 | 18.01393800 |
| C | 8.80528100 | 8.39243500 | 19.39119900 |
| C | 9.81758700 | 9.18824100 | 19.91477200 |
| C | 10.59920600 | 9.96154900 | 19.04472600 |
| C | 11.71308200 | 10.80911500 | 19.53578200 |
| C | 11.98875500 | 11.05803800 | 20.88599500 |
| C | 13.06425400 | 11.88305800 | 21.21342000 |
| C | 13.84943600 | 12.44029100 | 20.20172900 |
| C | 13.52476200 | 12.14736600 | 18.88074700 |
| C | 14.30480600 | 12.67308700 | 17.70111300 |
| C | 14.45635300 | 12.63163100 | 15.32484700 |
| C | 14.44896500 | 13.98001400 | 14.93128200 |
| C | 15.00791400 | 14.36528200 | 13.71239800 |
| C | 15.57960200 | 13.39903400 | 12.87908700 |
| C | 15.59184400 | 12.05132800 | 13.25612900 |
| C | 15.03142600 | 11.67308100 | 14.47476300 |
| H | 10.99778900 | 10.59371700 | 14.63222500 |
| H | 13.28780300 | 12.08942000 | 22.25549100 |
| H | 14.69342700 | 13.08329300 | 20.42195700 |
| H | 11.37676200 | 10.62706300 | 21.66884900 |
| H | 10.00547400 | 9.19589400 | 20.98147100 |
| H | 8.19263400 | 7.77958700 | 20.04460400 |
| H | 7.80717900 | 7.79535100 | 17.56667300 |
| H | 6.45992300 | 9.59898100 | 15.46485900 |
| H | 8.24297600 | 6.07051900 | 13.66617200 |
| H | 6.02764300 | 5.45398000 | 12.70997800 |
| H | 4.27333800 | 8.97172600 | 14.51198100 |
| H | 15.03549900 | 10.63005400 | 14.77645500 |
| H | 13.99850000 | 14.72338100 | 15.58208600 |
| H | 14.99811300 | 15.40889900 | 13.41565800 |
| H | 16.03629000 | 11.30189800 | 12.60841600 |
| O | 12.47125500 | 8.66518500 | 14.89034300 |
| H | 13.34763100 | 9.06329500 | 15.04723200 |

**[(L4)Cu(HO···OH)]$^{2-}$ (q)** E= -2888.363391 H

| | | | |
|---|---|---|---|
| Cu | 12.15960800 | 11.06851400 | 16.63283600 |
| S | 3.41191400 | 6.69312500 | 12.91624900 |
| S | 16.20786000 | 13.91731800 | 11.25708400 |
| N | 8.73797900 | 8.14067500 | 15.12619400 |
| N | 10.37887500 | 9.98199500 | 17.70239000 |
| N | 12.48733800 | 11.34863300 | 18.56736300 |
| N | 13.86039600 | 12.20768400 | 16.51681700 |
| O | 9.17241600 | 10.38631900 | 15.12787600 |
| O | 15.30402100 | 13.41352200 | 17.89148300 |
| O | 11.94084300 | 10.83873500 | 14.74744500 |
| O | 2.96600200 | 7.88115600 | 12.11983400 |
| O | 2.55936700 | 6.45670600 | 14.12654500 |
| O | 3.61027900 | 5.46568800 | 12.08644800 |
| O | 15.02971500 | 13.89495700 | 10.32196000 |
| O | 17.25426900 | 12.91120500 | 10.87833300 |
| O | 16.76358300 | 15.30030300 | 11.43457400 |
| C | 7.52912600 | 7.86104100 | 14.62656700 |
| C | 7.38169000 | 6.66613500 | 13.85069800 |
| C | 6.15004000 | 6.31507200 | 13.32776400 |
| C | 5.03715800 | 7.13825800 | 13.56658200 |
| C | 5.14918700 | 8.31742800 | 14.33372500 |
| C | 6.37080400 | 8.68000900 | 14.85960400 |
| C | 9.07251900 | 9.31789400 | 15.74304000 |
| C | 9.38662900 | 9.22014800 | 17.20906400 |
| C | 8.57525400 | 8.41282800 | 18.01072800 |
| C | 8.78493200 | 8.41801900 | 19.38867600 |
| C | 9.80174100 | 9.20987600 | 19.90957900 |
| C | 10.59009400 | 9.97327200 | 19.03652100 |
| C | 11.71040500 | 10.81456600 | 19.52444700 |
| C | 11.98252600 | 11.07121300 | 20.87404900 |
| C | 13.06318900 | 11.88977600 | 21.20028800 |
| C | 13.85558400 | 12.43488800 | 20.18773300 |
| C | 13.53324200 | 12.13589000 | 18.86748800 |
| C | 14.31655800 | 12.65803100 | 17.68836900 |
| C | 14.46319200 | 12.63069700 | 15.31232500 |
| C | 14.45383100 | 13.98317800 | 14.92906700 |
| C | 15.00786500 | 14.37722700 | 13.71242500 |
| C | 15.57662300 | 13.41684500 | 12.86800200 |
| C | 15.59104000 | 12.06756300 | 13.23391400 |
| C | 15.03628900 | 11.68002900 | 14.45392500 |
| H | 11.00743100 | 10.58243600 | 14.62702600 |
| H | 13.28414300 | 12.10179600 | 22.24178300 |
| H | 14.70240900 | 13.07465400 | 20.40650700 |
| H | 11.36321000 | 10.65155900 | 21.65734700 |
| H | 9.98807300 | 9.22163900 | 20.97650700 |
| H | 8.16677700 | 7.81338400 | 20.04455400 |
| H | 7.78933400 | 7.81293800 | 17.56527200 |
| H | 6.46376100 | 9.58294700 | 15.45454200 |
| H | 8.25670500 | 6.04661800 | 13.68129800 |
| H | 6.04141100 | 5.41303500 | 12.73614400 |
| H | 4.27719700 | 8.93868200 | 14.51281200 |
| H | 15.04414300 | 10.63494700 | 14.74840400 |
| H | 14.00541800 | 14.72098800 | 15.58756600 |
| H | 14.99645200 | 15.42396700 | 13.42532800 |
| H | 16.03326700 | 11.32518400 | 12.57729400 |
| O | 12.47888100 | 8.70594200 | 15.11597300 |
| H | 13.38186200 | 9.06903300 | 15.05827100 |

**[(L4)Cu(HO-OH)]$^{2-}$ (d)**E= -2888.386577 H

| | | | |
|---|---|---|---|
| Cu | 11.69255900 | 11.00398900 | 17.20650100 |
| S | 5.84031600 | 7.67243800 | 10.95600800 |
| S | 14.39134600 | 12.96226200 | 10.74119300 |
| N | 8.31722600 | 8.28683200 | 16.40086000 |
| N | 10.30356700 | 10.03964900 | 18.57670300 |
| N | 12.64383600 | 11.15979200 | 18.92284200 |
| N | 13.40497900 | 11.87382700 | 16.56806400 |

| | | | |
|---|---|---|---|
| O | 8.50126200 | 10.62261300 | 16.34022500 |
| O | 15.40987900 | 12.74232400 | 17.36987000 |
| O | 10.78552100 | 11.09568900 | 15.38770800 |
| O | 5.47993900 | 9.04885100 | 10.47334100 |
| O | 4.61994900 | 6.82161100 | 11.18274400 |
| O | 6.85355300 | 6.99651400 | 10.08037400 |
| O | 13.05323900 | 12.72198000 | 10.09954600 |
| O | 15.42942100 | 11.98371000 | 10.27870900 |
| O | 14.83635300 | 14.38966100 | 10.61700200 |
| C | 7.75702400 | 8.20918100 | 15.11370800 |
| C | 8.34348000 | 7.35577200 | 14.16239100 |
| C | 7.78266800 | 7.20022100 | 12.89329100 |
| C | 6.61442900 | 7.89206300 | 12.56402600 |
| C | 6.00333100 | 8.73325000 | 13.50353100 |
| C | 6.57230000 | 8.89205200 | 14.76391700 |
| C | 8.60189400 | 9.45743700 | 16.90194600 |
| C | 9.12556500 | 9.44125000 | 18.31764700 |
| C | 8.36041000 | 8.84908700 | 19.33043000 |
| C | 8.82144500 | 8.88744300 | 20.64150300 |
| C | 10.04573800 | 9.49797800 | 20.91085000 |
| C | 10.76601200 | 10.05858000 | 19.85670100 |
| C | 12.08389000 | 10.70609700 | 20.05163200 |
| C | 12.75938700 | 10.86438700 | 21.26837700 |
| C | 14.00587100 | 11.49221400 | 21.26398800 |
| C | 14.56560300 | 11.94954900 | 20.06550900 |
| C | 13.83842300 | 11.76388000 | 18.89507100 |
| C | 14.29261800 | 12.18373900 | 17.51854700 |
| C | 13.69422300 | 12.15820400 | 15.21332900 |
| C | 13.50410200 | 13.44543200 | 14.68936400 |
| C | 13.73938100 | 13.69776700 | 13.33761100 |
| C | 14.16324900 | 12.65765000 | 12.50344400 |
| C | 14.35370000 | 11.36906600 | 13.01093200 |
| C | 14.12354100 | 11.12423100 | 14.36582400 |
| H | 9.79849000 | 10.91904400 | 15.63791300 |
| H | 14.54331800 | 11.62303900 | 22.19809200 |
| H | 15.53346600 | 12.43644900 | 20.03592000 |
| H | 12.32883600 | 10.51003600 | 22.19719800 |
| H | 10.42997600 | 9.53424200 | 21.92320100 |
| H | 8.23983200 | 8.44781300 | 21.44594900 |
| H | 7.41527600 | 8.38207100 | 19.07819300 |
| H | 6.09931300 | 9.54485500 | 15.49096700 |
| H | 9.25097000 | 6.81740900 | 14.42205800 |
| H | 8.25389600 | 6.54594200 | 12.16717000 |
| H | 5.09188300 | 9.26824400 | 13.25236700 |
| H | 14.27513500 | 10.12910300 | 14.77463900 |
| H | 13.16919000 | 14.24341200 | 15.34560200 |
| H | 13.59435300 | 14.69666700 | 12.93854100 |
| H | 14.68572800 | 10.56483100 | 12.36235600 |
| O | 11.11298700 | 9.90560500 | 14.61316200 |
| H | 11.88823300 | 10.23583700 | 14.11471300 |

**[(L4)Cu(HO-OH)]$^{2-}$ (q)** E= -2888.316567 H

| | | | |
|---|---|---|---|
| Cu | 12.21782100 | 10.88513900 | 16.59602300 |
| S | 3.08955700 | 7.66878100 | 13.87610500 |
| S | 16.35475900 | 13.93422100 | 11.46497200 |
| N | 8.99030500 | 7.55038200 | 14.69820100 |
| N | 10.70481700 | 9.54658300 | 17.34120800 |
| N | 12.23570400 | 11.34475000 | 18.49012900 |
| N | 13.64694300 | 12.32007800 | 16.58024600 |
| O | 10.02685900 | 9.56164900 | 14.48319300 |
| O | 14.60963800 | 13.92655100 | 17.96523000 |
| O | 12.25722700 | 10.62121100 | 14.59302700 |
| O | 2.76308700 | 9.01508600 | 13.30287300 |
| O | 2.52828800 | 7.48155000 | 15.25563900 |
| O | 2.75748800 | 6.53912800 | 12.95278800 |
| O | 15.43190900 | 13.41847300 | 10.39562600 |
| O | 17.69533800 | 13.26425000 | 11.43510800 |
| O | 16.44789500 | 15.43242500 | 11.45820700 |
| C | 7.66032700 | 7.63600800 | 14.50546500 |
| C | 7.01575600 | 6.57059300 | 13.80173400 |
| C | 5.64533300 | 6.57935200 | 13.59867500 |
| C | 4.88137200 | 7.65119500 | 14.08596500 |
| C | 5.48525700 | 8.71931800 | 14.77832200 |
| C | 6.85087800 | 8.71923500 | 14.98565900 |
| C | 9.67543700 | 8.62736300 | 15.30219600 |
| C | 9.93645000 | 8.57511500 | 16.70448200 |
| C | 9.30645600 | 7.54869100 | 17.47410100 |
| C | 9.35296100 | 7.56731200 | 18.84663500 |
| C | 10.03087400 | 8.62877700 | 19.48925000 |
| C | 10.68960800 | 9.56924300 | 18.71419400 |
| C | 11.46751200 | 10.65776300 | 19.34531600 |
| C | 11.46862200 | 11.01860000 | 20.70221500 |
| C | 12.27226200 | 12.08072100 | 21.11364300 |
| C | 13.07367400 | 12.76844300 | 20.19019800 |
| C | 13.02918000 | 12.35987200 | 18.86481800 |
| C | 13.83970400 | 12.95555900 | 17.74142600 |
| C | 14.32846000 | 12.74670900 | 15.41784000 |
| C | 13.93331600 | 13.90931000 | 14.73633100 |
| C | 14.56475600 | 14.28165900 | 13.55081200 |
| C | 15.59760600 | 13.48775900 | 13.03802900 |
| C | 16.00356700 | 12.32941800 | 13.70561100 |
| C | 15.37246600 | 11.96615900 | 14.89742700 |
| H | 11.34383300 | 10.12537500 | 14.47743000 |
| H | 12.27695300 | 12.37524300 | 22.15860000 |
| H | 13.71095100 | 13.59295800 | 20.48860000 |
| H | 10.85052100 | 10.49427900 | 21.42100400 |
| H | 10.05864900 | 8.68383500 | 20.57060900 |
| H | 8.86510300 | 6.79254900 | 19.42992300 |
| H | 8.76594000 | 6.76227300 | 16.95982300 |
| H | 7.31975200 | 9.53809900 | 15.52201600 |
| H | 7.62306100 | 5.75016000 | 13.43154700 |
| H | 5.16368500 | 5.76677800 | 13.06601700 |
| H | 4.88073800 | 9.54192700 | 15.14806100 |
| H | 15.68875800 | 11.07428800 | 15.43164000 |
| H | 13.12433300 | 14.51196700 | 15.13888800 |
| H | 14.25270700 | 15.18225400 | 13.03089000 |
| H | 16.80871900 | 11.72031200 | 13.30814100 |
| O | 13.22464700 | 9.58706500 | 14.25196800 |
| H | 13.99429500 | 10.14907500 | 14.02922400 |

**[(L4)Cu(OH)$_2$]$^{4-}$ (d)** E= -2888.732095 H

| | | | |
|---|---|---|---|
| Cu | 11.10198700 | 10.48303400 | 16.69061100 |
| S | 5.41432900 | 6.51523000 | 11.21341700 |
| S | 16.12547900 | 16.35132500 | 11.76030200 |
| N | 7.95998600 | 8.03970100 | 16.44272900 |
| N | 9.88080800 | 10.06375700 | 18.32922500 |
| N | 12.19141400 | 11.43247300 | 18.36488800 |
| N | 13.77479500 | 13.83128300 | 16.68663700 |
| O | 7.85266900 | 10.37656600 | 16.20891500 |
| O | 14.35276300 | 11.59490900 | 16.25813600 |
| O | 11.04124500 | 8.71346000 | 15.84385100 |
| O | 4.64212900 | 7.69998100 | 10.70744500 |
| O | 4.50962600 | 5.36422300 | 11.56665600 |
| O | 6.51762500 | 6.09944900 | 10.28389700 |
| O | 16.85491600 | 17.56108800 | 12.28240000 |
| O | 14.98533500 | 16.72538900 | 10.85831200 |
| O | 17.06394400 | 15.36063300 | 11.13180100 |
| C | 7.37456400 | 7.76914900 | 15.19843700 |
| C | 8.00436700 | 6.84585600 | 14.33900400 |
| C | 7.42971000 | 6.48296500 | 13.12147000 |
| C | 6.20304000 | 7.03761200 | 12.74049100 |
| C | 5.55129300 | 7.94749100 | 13.58240300 |
| C | 6.13448100 | 8.31250400 | 14.79381800 |
| C | 8.10307200 | 9.29200500 | 16.83313000 |
| C | 8.68571500 | 9.45147300 | 18.22130700 |
| C | 7.96849400 | 9.04313100 | 19.34838800 |
| C | 8.50136700 | 9.29417300 | 20.61034400 |
| C | 9.72543400 | 9.95149800 | 20.71692200 |
| C | 10.39901800 | 10.32968900 | 19.55038700 |
| C | 11.68681800 | 11.07128300 | 19.57016900 |

| | | | |
|---|---|---|---|
| C | 12.33067100 | 11.40906200 | 20.76503700 |
| C | 13.50405100 | 12.15932600 | 20.71426100 |
| C | 13.99816700 | 12.55851100 | 19.47687200 |
| C | 13.31794000 | 12.16751000 | 18.31819100 |
| C | 13.87590200 | 12.54915200 | 16.96557700 |
| C | 14.32741700 | 14.33036200 | 15.50020300 |
| C | 15.66097200 | 14.07952700 | 15.10382100 |
| C | 16.19588900 | 14.67751100 | 13.96529900 |
| C | 15.40385700 | 15.53102800 | 13.18625600 |
| C | 14.08209600 | 15.79601100 | 13.55872800 |
| C | 13.55560500 | 15.20210600 | 14.70551800 |
| H | 10.19367400 | 8.28078200 | 16.04913900 |
| H | 14.01820900 | 12.43253700 | 21.63103500 |
| H | 14.89920500 | 13.15678900 | 19.39325600 |
| H | 11.93076700 | 11.09924100 | 21.72234800 |
| H | 10.13642100 | 10.16865400 | 21.69473300 |
| H | 7.96607600 | 8.99214700 | 21.50570700 |
| H | 7.00995900 | 8.55070700 | 19.22674000 |
| H | 5.62666400 | 9.01848800 | 15.44333900 |
| H | 8.95830800 | 6.41780200 | 14.63575800 |
| H | 7.93706200 | 5.77705300 | 12.47121100 |
| H | 4.59673700 | 8.37568300 | 13.29110800 |
| H | 12.52942200 | 15.40867200 | 14.99790500 |
| H | 16.27997500 | 13.42132800 | 15.70515800 |
| H | 17.22440800 | 14.47469800 | 13.68132400 |
| H | 13.46530500 | 16.45708800 | 12.95801200 |
| O | 11.61846800 | 11.44424800 | 15.10942200 |
| H | 12.57241500 | 11.61476000 | 15.19735500 |

**$[(L4)Cu(OH)_2]^{3-}$ (s)** E= -2888.530842 H

| | | | |
|---|---|---|---|
| Cu | 11.57908900 | 9.99367000 | 17.21417400 |
| S | 5.96521900 | 7.36260900 | 10.85370000 |
| S | 15.10351500 | 15.72986600 | 11.36662400 |
| N | 8.25794500 | 8.47617500 | 16.30058300 |
| N | 10.08491100 | 9.97939500 | 18.50709400 |
| N | 12.40297900 | 11.17695900 | 18.60667800 |
| N | 13.34411900 | 13.37500700 | 16.61355700 |
| O | 7.78444100 | 10.77439600 | 16.50887300 |
| O | 15.04301000 | 11.75458600 | 16.79509400 |
| O | 11.05736800 | 8.48125800 | 16.31449300 |
| O | 5.63052300 | 8.68930400 | 10.23062000 |
| O | 4.73333300 | 6.53496400 | 11.10077000 |
| O | 7.01531200 | 6.61277500 | 10.08906500 |
| O | 15.67609400 | 17.08236900 | 11.68928700 |
| O | 13.88695200 | 15.81093000 | 10.49201900 |
| O | 16.14778600 | 14.79819800 | 10.81463300 |
| C | 7.71181500 | 8.29913800 | 15.01997300 |
| C | 8.41416500 | 7.48040100 | 14.11385200 |
| C | 7.90235100 | 7.19893800 | 12.84730500 |
| C | 6.66545000 | 7.72755200 | 12.46875100 |
| C | 5.94132000 | 8.53239500 | 13.35852800 |
| C | 6.46006300 | 8.81801500 | 14.61915100 |
| C | 8.21706800 | 9.64995000 | 16.90160900 |
| C | 8.79622400 | 9.64747600 | 18.30609200 |
| C | 7.94306800 | 9.41583500 | 19.39015600 |
| C | 8.43815400 | 9.52708400 | 20.68408600 |
| C | 9.75317900 | 9.95282400 | 20.87913400 |
| C | 10.55330300 | 10.20200800 | 19.76806200 |
| C | 11.86794500 | 10.85954200 | 19.82455000 |
| C | 12.47890000 | 11.26674400 | 21.00656000 |
| C | 13.62862900 | 12.05519500 | 20.93831500 |
| C | 14.11183300 | 12.44247300 | 19.69528200 |
| C | 13.47214300 | 11.98856800 | 18.53611900 |
| C | 14.01528800 | 12.41362300 | 17.19043200 |
| C | 13.79451100 | 13.88168100 | 15.38278200 |
| C | 15.09888700 | 14.39209000 | 15.20378200 |
| C | 15.48355900 | 14.95906400 | 13.99225400 |
| C | 14.56985300 | 15.02267100 | 12.93101300 |
| C | 13.27384000 | 14.52544200 | 13.08747300 |
| C | 12.89049200 | 13.96671000 | 14.30856400 |
| H | 10.07295300 | 8.38519100 | 16.36719000 |
| H | 14.11913800 | 12.38371100 | 21.84925300 |
| H | 14.97385400 | 13.09390400 | 19.59748300 |
| H | 12.05868500 | 10.99317000 | 21.96664700 |
| H | 10.13214900 | 10.11488200 | 21.88050400 |
| H | 7.80043100 | 9.32273900 | 21.53840800 |
| H | 6.90845600 | 9.15195200 | 19.19772600 |
| H | 5.89185400 | 9.43587200 | 15.30603100 |
| H | 9.37219600 | 7.06469300 | 14.41402100 |
| H | 8.46245000 | 6.57259200 | 12.16088700 |
| H | 4.97512100 | 8.93821500 | 13.07145300 |
| H | 11.88027300 | 13.58728700 | 14.43668200 |
| H | 15.80401600 | 14.35028500 | 16.02839500 |
| H | 16.49028700 | 15.35100000 | 13.87675700 |
| H | 12.56610400 | 14.57704900 | 12.26671100 |
| O | 12.93755500 | 10.00935400 | 15.98348000 |
| H | 13.73510200 | 10.44153600 | 16.35289400 |

**$[(L4)Cu(OH)_2]^{3-}$ (t)** E= -2888.548855 H

| | | | |
|---|---|---|---|
| Cu | 11.87343300 | 9.68925500 | 16.93038300 |
| S | 5.42032500 | 6.91077600 | 11.14670100 |
| S | 14.69641500 | 16.91351200 | 12.37387900 |
| N | 7.92744600 | 8.49893600 | 16.37716400 |
| N | 10.19929500 | 10.21727000 | 18.19612700 |
| N | 12.70166700 | 11.06862700 | 18.28152400 |
| N | 13.76266600 | 12.18744900 | 15.86614700 |
| O | 8.52961500 | 10.70093300 | 15.81696300 |
| O | 15.80584400 | 11.54531600 | 16.71887500 |
| O | 11.05948200 | 8.39313000 | 15.76211400 |
| O | 5.26023000 | 8.14960300 | 10.31126900 |
| O | 4.08932600 | 6.32235400 | 11.53337600 |
| O | 6.32626000 | 5.89584700 | 10.51254900 |
| O | 14.21582300 | 18.07686400 | 13.18902200 |
| O | 13.89393000 | 16.69489700 | 11.13178600 |
| O | 16.17333900 | 16.95255200 | 12.12713100 |
| C | 7.37578900 | 8.20124200 | 15.12268300 |
| C | 7.75292500 | 7.00135800 | 14.48694300 |
| C | 7.18499200 | 6.61518600 | 13.27286700 |
| C | 6.21722500 | 7.42613400 | 12.67204600 |
| C | 5.81559300 | 8.61770900 | 13.29032600 |
| C | 6.39332300 | 9.00279100 | 14.49769800 |
| C | 8.40462200 | 9.70823600 | 16.60751900 |
| C | 8.89650700 | 9.93506000 | 18.02095000 |
| C | 7.99149100 | 9.95472700 | 19.08829800 |
| C | 8.45294800 | 10.29096600 | 20.35717400 |
| C | 9.79614700 | 10.62740000 | 20.52783800 |
| C | 10.64593100 | 10.59000100 | 19.41973200 |
| C | 12.06083700 | 11.04192100 | 19.46985500 |
| C | 12.69018600 | 11.48143700 | 20.64317900 |
| C | 13.99345600 | 11.96396600 | 20.57446800 |
| C | 14.63174600 | 12.03387200 | 19.33607700 |
| C | 13.94425600 | 11.58152100 | 18.20959500 |
| C | 14.59730800 | 11.76532000 | 16.86796200 |
| C | 14.02675700 | 13.25222600 | 15.09459800 |
| C | 15.03210000 | 14.23185500 | 15.40355400 |
| C | 15.22127400 | 15.31673600 | 14.57393700 |
| C | 14.42688500 | 15.46435500 | 13.41757600 |
| C | 13.42867200 | 14.53034700 | 13.09556300 |
| C | 13.22299500 | 13.44167600 | 13.92441200 |
| H | 10.10595900 | 8.31625600 | 15.93239600 |
| H | 14.49922300 | 12.30119400 | 21.47374300 |
| H | 15.63040900 | 12.44265900 | 19.23114300 |
| H | 12.17574200 | 11.45004900 | 21.59536800 |
| H | 10.15860400 | 10.92575100 | 21.50381400 |
| H | 7.77423100 | 10.31251500 | 21.20458000 |
| H | 6.94742900 | 9.72115100 | 18.90996500 |
| H | 6.07878700 | 9.92634000 | 14.97321300 |
| H | 8.50565500 | 6.37282800 | 14.95548700 |
| H | 7.49782600 | 5.69173600 | 12.79614400 |
| H | 5.05986100 | 9.24731500 | 12.82937100 |

| | | | |
|---|---|---|---|
| H | 12.45674500 | 12.70750000 | 13.69707200 |
| H | 15.63550300 | 14.11743800 | 16.29711800 |
| H | 15.98101800 | 16.05449100 | 14.81210200 |
| H | 12.82673400 | 14.66310500 | 12.20347900 |
| O | 13.62049600 | 8.93365600 | 16.45287000 |
| H | 14.28198000 | 9.15396300 | 17.12788000 |

**$[(L4)Cu(OH)_2]^{2-}$ (dos)** E= -2888.350618 H

| | | | |
|---|---|---|---|
| Cu | 11.61907400 | 9.73420700 | 17.20824900 |
| S | 5.74976600 | 7.07951000 | 11.05778500 |
| S | 15.01869500 | 16.56538500 | 12.02514300 |
| N | 8.36072300 | 8.65928500 | 16.23878400 |
| N | 10.08443400 | 10.10199400 | 18.42596800 |
| N | 12.52301200 | 11.02839800 | 18.40496100 |
| N | 13.45558300 | 12.39256300 | 15.97078100 |
| O | 7.43991100 | 10.79643200 | 16.54532800 |
| O | 15.47713800 | 11.46766100 | 16.62508300 |
| O | 11.00114200 | 8.21156900 | 16.43265200 |
| O | 5.66404900 | 8.32604900 | 10.21817400 |
| O | 4.39017100 | 6.54814600 | 11.41275200 |
| O | 6.63741800 | 6.03944100 | 10.43960600 |
| O | 15.27448600 | 17.80586600 | 12.82512000 |
| O | 13.87854600 | 16.70264400 | 11.06902600 |
| O | 16.26176500 | 16.01956900 | 11.39016500 |
| C | 7.72840800 | 8.37064300 | 15.01953200 |
| C | 8.47516900 | 7.71227900 | 14.02218100 |
| C | 7.88381400 | 7.31381700 | 12.82386800 |
| C | 6.52354200 | 7.55422800 | 12.60941100 |
| C | 5.75997100 | 8.20118800 | 13.58922100 |
| C | 6.35639800 | 8.60630500 | 14.78092200 |
| C | 8.13205900 | 9.78900800 | 16.88036300 |
| C | 8.76285300 | 9.91204600 | 18.25816500 |
| C | 7.89091600 | 9.96189500 | 19.35528800 |
| C | 8.39511200 | 10.20353300 | 20.62525200 |
| C | 9.75322300 | 10.49592700 | 20.77282000 |
| C | 10.57137800 | 10.46997600 | 19.64982300 |
| C | 11.96080700 | 10.96158700 | 19.63775300 |
| C | 12.64698700 | 11.42289400 | 20.76406400 |
| C | 13.91810200 | 11.96706300 | 20.60313900 |
| C | 14.46405400 | 12.06971800 | 19.32412400 |
| C | 13.73275400 | 11.59049800 | 18.23677800 |
| C | 14.31069800 | 11.80197000 | 16.86039700 |
| C | 13.85278100 | 13.34533500 | 15.11044200 |
| C | 15.06849100 | 14.09962700 | 15.24824000 |
| C | 15.39228500 | 15.06632800 | 14.32048300 |
| C | 14.52754400 | 15.31622900 | 13.23388500 |
| C | 13.32208300 | 14.61143300 | 13.08433300 |
| C | 12.97926500 | 13.64829300 | 14.01659200 |
| H | 10.00277500 | 8.32332800 | 16.37378800 |
| H | 14.47046900 | 12.32556100 | 21.46575100 |
| H | 15.43270800 | 12.52622000 | 19.15365100 |
| H | 12.19617000 | 11.36002900 | 21.74690500 |
| H | 10.15366500 | 10.77083100 | 21.74093200 |
| H | 7.73815000 | 10.21117000 | 21.48925200 |
| H | 6.83018000 | 9.80986400 | 19.18656400 |
| H | 5.75597400 | 9.09146500 | 15.54282700 |
| H | 9.52791600 | 7.50882500 | 14.19702100 |
| H | 8.47573200 | 6.80714400 | 12.06844200 |
| H | 4.70053500 | 8.37963900 | 13.42991700 |
| H | 12.05240300 | 13.09138500 | 13.92411500 |
| H | 15.72379400 | 13.91297900 | 16.09085300 |
| H | 16.30943800 | 15.63650200 | 14.42991500 |
| H | 12.66726100 | 14.82444600 | 12.24676600 |
| O | 13.15938700 | 9.42075600 | 16.30484000 |
| H | 12.93409600 | 8.66063000 | 15.73741300 |

**$[(L4)Cu(OH)_2]^{2-}$ (q)** E= -2888.364446 H

| | | | |
|---|---|---|---|
| Cu | 12.65833500 | 9.44445500 | 16.88617900 |
| S | 3.67170200 | 7.34682700 | 12.53725600 |
| S | 14.94986600 | 17.39960700 | 12.57841700 |
| N | 8.88564500 | 7.53531800 | 15.38741400 |
| N | 10.69449300 | 9.73529500 | 17.56343500 |
| N | 12.78443900 | 11.23404400 | 18.14092300 |
| N | 14.09333700 | 12.61869900 | 16.01467600 |
| O | 10.32257000 | 9.22305500 | 14.80954700 |
| O | 15.99041300 | 12.31884900 | 17.29098700 |
| O | 12.43957200 | 7.52273000 | 16.60733400 |
| O | 3.75802400 | 8.34066700 | 11.42086400 |
| O | 2.67963400 | 7.74459000 | 13.58981700 |
| O | 3.49248300 | 5.93927800 | 12.06447100 |
| O | 14.19501700 | 18.49260000 | 13.27363400 |
| O | 14.39475700 | 17.06450300 | 11.23159700 |
| O | 16.42914400 | 17.63631100 | 12.56725500 |
| C | 7.72862700 | 7.53530300 | 14.71695700 |
| C | 7.13134100 | 6.27120600 | 14.40322800 |
| C | 5.92178500 | 6.21149600 | 13.73587400 |
| C | 5.27797000 | 7.40334500 | 13.36126600 |
| C | 5.83914200 | 8.66274200 | 13.65793900 |
| C | 7.04486200 | 8.73685300 | 14.32356500 |
| C | 9.62166400 | 8.66551600 | 15.65641400 |
| C | 9.58286900 | 9.15066000 | 17.08239700 |
| C | 8.39885600 | 9.09025600 | 17.81742700 |
| C | 8.36847200 | 9.68339500 | 19.08065000 |
| C | 9.50596300 | 10.32522800 | 19.55973200 |
| C | 10.66450000 | 10.33353600 | 18.77097200 |
| C | 11.90276000 | 11.06318800 | 19.14918100 |
| C | 12.13077500 | 11.59740300 | 20.42288800 |
| C | 13.29065700 | 12.33780900 | 20.64357100 |
| C | 14.17089300 | 12.56146600 | 19.58536700 |
| C | 13.87203000 | 11.99557000 | 18.34379000 |
| C | 14.75740800 | 12.32973900 | 17.17608200 |
| C | 14.33810500 | 13.70457400 | 15.26709600 |
| C | 15.07247700 | 14.84800000 | 15.73466300 |
| C | 15.24949600 | 15.94121500 | 14.91317700 |
| C | 14.70969000 | 15.93592400 | 13.60955600 |
| C | 13.97969100 | 14.83739600 | 13.12778200 |
| C | 13.78670000 | 13.73822600 | 13.94567500 |
| H | 11.57265100 | 7.23467700 | 16.93686400 |
| H | 13.49491300 | 12.75267100 | 21.62557400 |
| H | 15.06051700 | 13.17038000 | 19.70246400 |
| H | 11.42814500 | 11.43513000 | 21.23147800 |
| H | 9.48443100 | 10.82307700 | 20.52150100 |
| H | 7.46057800 | 9.66263900 | 19.67486400 |
| H | 7.51854500 | 8.61217600 | 17.40345500 |
| H | 7.48332700 | 9.70226800 | 14.55627800 |
| H | 7.64886800 | 5.36494000 | 14.70174300 |
| H | 5.47319900 | 5.25351100 | 13.49726400 |
| H | 5.32615600 | 9.57231000 | 13.36184000 |
| H | 13.22349400 | 12.87858300 | 13.59674800 |
| H | 15.47593400 | 14.85110700 | 16.74123600 |
| H | 15.80179800 | 16.80419700 | 15.27186600 |
| H | 13.57124600 | 14.85398400 | 12.12355800 |
| O | 14.48845000 | 9.36132900 | 16.28898400 |
| H | 15.07684100 | 9.74145800 | 16.96083500 |

**$[(L4)Cu(OH)(O)]^{3-}$ (d)** E= -2887.952624 H

| | | | |
|---|---|---|---|
| Cu | 11.47604200 | 10.02067900 | 16.42655100 |
| S | 5.08513200 | 5.60568400 | 11.85292000 |
| S | 15.84554200 | 17.50531100 | 14.44828800 |
| N | 8.03985700 | 8.36158200 | 16.31117600 |
| N | 9.99277700 | 10.45162200 | 17.78839900 |
| N | 12.46460500 | 11.13865900 | 17.59390500 |
| N | 13.47716900 | 12.04448700 | 14.90510300 |
| O | 7.59994800 | 10.59374200 | 15.70551600 |
| O | 15.23079900 | 10.55414500 | 15.49892300 |
| O | 10.76749200 | 8.81393600 | 15.24477900 |

| | | | |
|---|---|---|---|
| O | 4.35144300 | 6.66410800 | 11.07908400 |
| O | 4.13877300 | 4.65601600 | 12.53757700 |
| O | 6.11113000 | 4.88790700 | 11.02623600 |
| O | 15.70217500 | 18.04053100 | 15.84429700 |
| O | 15.01438000 | 18.25020700 | 13.45098600 |
| O | 17.28033800 | 17.37055100 | 14.03211800 |
| C | 7.34554500 | 7.78507700 | 15.23414900 |
| C | 7.96210400 | 6.74825400 | 14.50692100 |
| C | 7.29271600 | 6.09479800 | 13.47168500 |
| C | 5.98331500 | 6.46395200 | 13.15161400 |
| C | 5.34119700 | 7.47784700 | 13.87498900 |
| C | 6.01682600 | 8.13242000 | 14.90137800 |
| C | 8.04530200 | 9.67226900 | 16.45925900 |
| C | 8.68089200 | 10.16725000 | 17.74299800 |
| C | 7.84271700 | 10.41941700 | 18.83848500 |
| C | 8.37317200 | 10.98081300 | 19.99200500 |
| C | 9.72885300 | 11.31715600 | 20.02242400 |
| C | 10.51154200 | 11.05142200 | 18.90574500 |
| C | 11.92840400 | 11.42699900 | 18.79558600 |
| C | 12.72992300 | 12.03620300 | 19.76040700 |
| C | 14.06483200 | 12.30665300 | 19.44165200 |
| C | 14.57661100 | 11.99844500 | 18.17783600 |
| C | 13.72576900 | 11.40509700 | 17.24899900 |
| C | 14.00783300 | 10.97205500 | 15.78960900 |
| C | 14.12228700 | 13.22449900 | 14.79030100 |
| C | 15.39970500 | 13.56831300 | 15.35020700 |
| C | 15.91118600 | 14.84600600 | 15.21720700 |
| C | 15.18762000 | 15.82847000 | 14.51540100 |
| C | 13.95781400 | 15.52056700 | 13.91645900 |
| C | 13.44310700 | 14.23932000 | 14.03907800 |
| H | 9.91183000 | 8.53085800 | 15.62893800 |
| H | 14.70913900 | 12.76070800 | 20.18830700 |
| H | 15.61238900 | 12.19544000 | 17.92940800 |
| H | 12.33302200 | 12.28104000 | 20.73847700 |
| H | 10.16437900 | 11.78740700 | 20.89633300 |
| H | 7.74291900 | 11.17323400 | 20.85462500 |
| H | 6.78890000 | 10.17235700 | 18.76042600 |
| H | 5.51547400 | 8.91654500 | 15.45964100 |
| H | 8.97948500 | 6.45945400 | 14.75687700 |
| H | 7.78991600 | 5.30715400 | 12.91485200 |
| H | 4.32050300 | 7.76188700 | 13.63523000 |
| H | 12.48975100 | 13.98947100 | 13.58351300 |
| H | 15.98411100 | 12.81255900 | 15.85592100 |
| H | 16.87682000 | 15.08671500 | 15.65203400 |
| H | 13.41515400 | 16.27931600 | 13.36296800 |
| O | 13.12677800 | 9.82638400 | 15.59985400 |

**[(L4)Cu(OH)(O)]$^{3-}$ (q)** E= -2887.874387 H

| | | | |
|---|---|---|---|
| Cu | 11.79698800 | 9.83972100 | 16.88437800 |
| S | 5.34385800 | 6.73498600 | 11.23307000 |
| S | 15.00328900 | 16.90889500 | 12.39926400 |
| N | 8.04324400 | 8.39767000 | 16.34455800 |
| N | 10.14305000 | 10.23119700 | 18.18239300 |
| N | 12.64868600 | 11.11014300 | 18.29459300 |
| N | 13.77054100 | 12.26981700 | 15.91340900 |
| O | 8.24371200 | 10.69506000 | 15.88538200 |
| O | 15.77265900 | 11.49807300 | 16.76249600 |
| O | 11.05881300 | 8.74681200 | 15.47201500 |
| O | 5.16166900 | 7.97008000 | 10.39481400 |
| O | 4.02296100 | 6.15492400 | 11.66157600 |
| O | 6.22979300 | 5.71700300 | 10.57733800 |
| O | 14.79158700 | 18.10688300 | 13.27545700 |
| O | 14.04917300 | 16.84387900 | 11.25040300 |
| O | 16.43470500 | 16.74183600 | 11.98790900 |
| C | 7.43819000 | 8.07995600 | 15.11944400 |
| C | 7.95609200 | 7.01675900 | 14.35500700 |
| C | 7.33985400 | 6.60971900 | 13.17043200 |
| C | 6.18256400 | 7.25927100 | 12.73287300 |
| C | 5.64139100 | 8.31383800 | 13.48211100 |
| C | 6.26477800 | 8.72012500 | 14.65819300 |
| C | 8.33406000 | 9.65469600 | 16.61795200 |
| C | 8.85082000 | 9.89797700 | 18.01941900 |
| C | 7.95315300 | 9.87817900 | 19.09359600 |
| C | 8.40897400 | 10.22537000 | 20.36028300 |
| C | 9.74163400 | 10.60492200 | 20.52316800 |
| C | 10.58596900 | 10.60276700 | 19.41123800 |
| C | 11.99652600 | 11.06704900 | 19.47561500 |
| C | 12.61980300 | 11.48747800 | 20.65933100 |
| C | 13.93055800 | 11.95195500 | 20.60901100 |
| C | 14.58597900 | 12.02125700 | 19.37968000 |
| C | 13.90259400 | 11.59820000 | 18.23957200 |
| C | 14.57660400 | 11.78124500 | 16.90746000 |
| C | 14.10660000 | 13.30919500 | 15.13503700 |
| C | 15.18783100 | 14.21018100 | 15.42546800 |
| C | 15.44208800 | 15.27857900 | 14.59199900 |
| C | 14.63901500 | 15.48656400 | 13.45063100 |
| C | 13.57051300 | 14.62850900 | 13.14506100 |
| C | 13.30028800 | 13.55685500 | 13.97772000 |
| H | 10.16805000 | 8.45204800 | 15.73000100 |
| H | 14.43111300 | 12.27220100 | 21.51736100 |
| H | 15.59502100 | 12.40819700 | 19.29256900 |
| H | 12.09778200 | 11.45217400 | 21.60708300 |
| H | 10.10070700 | 10.90377000 | 21.49999800 |
| H | 7.73639000 | 10.21742300 | 21.21276200 |
| H | 6.91820400 | 9.60262500 | 18.92055200 |
| H | 5.84090200 | 9.53325000 | 15.23942100 |
| H | 8.85420100 | 6.50957200 | 14.69746100 |
| H | 7.75913000 | 5.79240400 | 12.59290600 |
| H | 4.73829900 | 8.81863900 | 13.14980300 |
| H | 12.47767100 | 12.88162100 | 13.76518000 |
| H | 15.79560500 | 14.05170800 | 16.30915700 |
| H | 16.25661700 | 15.95976100 | 14.81760700 |
| H | 12.96273500 | 14.80785500 | 12.26523600 |
| O | 13.52612600 | 9.12716700 | 16.44221400 |

**[(L4)Cu(OH)(HO···OH)]$^{3-}$ (d)** E=-2964.313943 H

| | | | |
|---|---|---|---|
| Cu | 12.36614300 | 10.13490200 | 16.72694500 |
| S | 3.51221600 | 6.99501800 | 12.81703300 |
| S | 15.97506700 | 16.41137700 | 12.04423800 |
| N | 8.93562200 | 7.87869400 | 15.08736800 |
| N | 10.52353800 | 9.82461800 | 17.63767600 |
| N | 12.48474500 | 11.39406300 | 18.45037300 |
| N | 13.54894200 | 13.56811300 | 16.75299500 |
| O | 9.83056200 | 9.97916000 | 14.89491500 |
| O | 15.50781700 | 12.60874900 | 17.63375600 |
| O | 12.29826700 | 8.33934000 | 15.84566200 |
| O | 3.16011500 | 8.23653700 | 12.05756700 |
| O | 2.65301700 | 6.79405500 | 14.03028400 |
| O | 3.59850800 | 5.77692700 | 11.95312300 |
| O | 15.50029700 | 17.83425900 | 12.17882700 |
| O | 15.44381800 | 15.74940100 | 10.80694100 |
| O | 17.47016000 | 16.31030400 | 12.16104900 |
| C | 7.71714100 | 7.73342500 | 14.55676100 |
| C | 7.38766700 | 6.47058700 | 13.96423000 |
| C | 6.13277500 | 6.25182400 | 13.42660500 |
| C | 5.17491100 | 7.27991300 | 13.46169500 |
| C | 5.46821900 | 8.53293700 | 14.03798300 |
| C | 6.71618600 | 8.76455800 | 14.57781000 |
| C | 9.42679800 | 9.05469600 | 15.60353800 |
| C | 9.50096400 | 9.12907700 | 17.10649400 |
| C | 8.48323300 | 8.59178100 | 17.89318800 |
| C | 8.52906200 | 8.80244500 | 19.27328400 |
| C | 9.56812100 | 9.54926200 | 19.81619100 |
| C | 10.56119300 | 10.05694100 | 18.96540800 |
| C | 11.67110600 | 10.92659900 | 19.42959500 |
| C | 11.83982900 | 11.30694100 | 20.76134000 |
| C | 12.87024100 | 12.19367700 | 21.08204300 |
| C | 13.67397300 | 12.70004900 | 20.06654900 |
| C | 13.43778500 | 12.29214600 | 18.74811600 |

| | | | |
|---|---|---|---|
| C | 14.25454900 | 12.87729700 | 17.61964800 |
| C | 14.18753400 | 14.18694200 | 15.67026900 |
| C | 15.27412400 | 15.07814300 | 15.82122200 |
| C | 15.81916100 | 15.73650400 | 14.72181200 |
| C | 15.29372400 | 15.51158400 | 13.44209300 |
| C | 14.21655100 | 14.63767300 | 13.26862100 |
| C | 13.67066800 | 13.98594300 | 14.37507100 |
| H | 11.91163700 | 7.70500300 | 16.47388200 |
| H | 13.02499400 | 12.49749700 | 22.11292600 |
| H | 14.46529000 | 13.41330100 | 20.27203900 |
| H | 11.18758200 | 10.93016800 | 21.53960500 |
| H | 9.60236000 | 9.73578800 | 20.88231400 |
| H | 7.75267500 | 8.39856000 | 19.91525600 |
| H | 7.66819700 | 8.03961200 | 17.43954700 |
| H | 6.94826700 | 9.72686500 | 15.02310100 |
| H | 8.14397400 | 5.69206100 | 13.94821300 |
| H | 5.88840500 | 5.29620000 | 12.97587600 |
| H | 4.71611500 | 9.31530300 | 14.05535700 |
| H | 12.83251100 | 13.30705700 | 14.24252900 |
| H | 15.68058100 | 15.25687800 | 16.81198700 |
| H | 16.65256600 | 16.41941800 | 14.86099800 |
| H | 13.80747800 | 14.46381400 | 12.27863200 |
| O | 14.07538000 | 10.37269300 | 15.86420200 |
| H | 14.63009300 | 11.02419800 | 16.32355300 |
| O | 14.43891100 | 7.71379000 | 16.48896300 |
| H | 14.45336100 | 8.68726800 | 16.27333100 |

**[(L4)Cu(OH)(HO···OH)]$^{3-}$ (q)** E=-2964.314770 H

| | | | |
|---|---|---|---|
| Cu | 12.36723500 | 10.13364800 | 16.72295700 |
| S | 3.51419700 | 6.99340800 | 12.81501500 |
| S | 15.97165200 | 16.41581800 | 12.04391500 |
| N | 8.93643600 | 7.87715900 | 15.08812200 |
| N | 10.52498000 | 9.82415500 | 17.63679700 |
| N | 12.48458500 | 11.39688200 | 18.44849700 |
| N | 13.55010200 | 13.56763600 | 16.75199300 |
| O | 9.83250400 | 9.97677000 | 14.89321100 |
| O | 15.51024400 | 12.61127600 | 17.63308700 |
| O | 12.29047000 | 8.33881600 | 15.84014900 |
| O | 3.16228400 | 8.23490400 | 12.05542800 |
| O | 2.65457700 | 6.79236200 | 14.02795500 |
| O | 3.60090400 | 5.77532500 | 11.95113500 |
| O | 15.49609700 | 17.83831300 | 12.17980800 |
| O | 15.44006300 | 15.75435500 | 10.80648600 |
| O | 17.46690600 | 16.31563300 | 12.15969300 |
| C | 7.71824100 | 7.73181200 | 14.55685000 |
| C | 7.38889600 | 6.46880400 | 13.96462200 |
| C | 6.13432300 | 6.25010700 | 13.42623300 |
| C | 5.17662300 | 7.27839300 | 13.46032700 |
| C | 5.46981700 | 8.53158000 | 14.03629700 |
| C | 6.71747600 | 8.76315000 | 14.57686700 |
| C | 9.42789100 | 9.05354400 | 15.60302500 |
| C | 9.50102700 | 9.13046700 | 17.10595300 |
| C | 8.48099000 | 8.59734100 | 17.89245500 |
| C | 8.52558700 | 8.81112400 | 19.27214300 |
| C | 9.56585200 | 9.55656300 | 19.81459100 |
| C | 10.56157700 | 10.05939900 | 18.96397200 |
| C | 11.67349900 | 10.92660300 | 19.42829200 |
| C | 11.84691800 | 11.30082500 | 20.76122500 |
| C | 12.87993800 | 12.18434500 | 21.08249000 |
| C | 13.68189300 | 12.69310500 | 20.06674700 |
| C | 13.44078200 | 12.29116300 | 18.74733100 |
| C | 14.25654700 | 12.87786000 | 17.61893400 |
| C | 14.18788100 | 14.18748400 | 15.66945400 |
| C | 15.27288700 | 15.08063800 | 15.82057100 |
| C | 15.81676500 | 15.74019400 | 14.72130900 |
| C | 15.29177700 | 15.51460100 | 13.44151400 |
| C | 14.21623600 | 14.63872800 | 13.26784100 |
| C | 13.67152100 | 13.98576800 | 14.37414400 |
| H | 11.91285700 | 7.70478000 | 16.47443000 |
| H | 13.03852700 | 12.48334200 | 22.11420500 |
| H | 14.47560300 | 13.40349900 | 20.27291000 |
| H | 11.19700700 | 10.92124700 | 21.54009200 |
| H | 9.59889400 | 9.74606300 | 20.88022800 |
| H | 7.74722700 | 8.41087700 | 19.91400700 |
| H | 7.66517900 | 8.04614500 | 17.43901600 |
| H | 6.94942200 | 9.72552800 | 15.02208400 |
| H | 8.14505400 | 5.69011700 | 13.94938100 |
| H | 5.89006900 | 5.29436600 | 12.97568800 |
| H | 4.71784300 | 9.31408500 | 14.05292000 |
| H | 12.83456000 | 13.30543800 | 14.24142300 |
| H | 15.67894600 | 15.26000100 | 16.81138700 |
| H | 16.64889400 | 16.42462900 | 14.86069700 |
| H | 13.80748200 | 14.46436300 | 12.27780900 |
| O | 14.07358100 | 10.37103200 | 15.85725800 |
| H | 14.62485800 | 11.02796400 | 16.31286600 |
| O | 14.40452800 | 7.71022700 | 16.52791700 |
| H | 14.44601500 | 8.67817700 | 16.29887800 |

**[(L4)Cu(OH)(HO-OH)]$^{3-}$ (d)** E= -2964.369951 H

| | | | |
|---|---|---|---|
| Cu | 10.76396200 | 10.64121400 | 17.08006400 |
| S | 5.39426900 | 7.27558700 | 11.07044400 |
| S | 15.75148900 | 15.88261600 | 11.78384300 |
| N | 7.70413200 | 7.90402500 | 16.58225900 |
| N | 10.04856200 | 9.63098700 | 18.61403400 |
| N | 12.12592400 | 11.20942200 | 18.69375400 |
| N | 13.42924600 | 13.52651100 | 16.80658800 |
| O | 9.34685100 | 9.50833000 | 16.12261500 |
| O | 14.52738600 | 11.45129500 | 16.75636600 |
| O | 13.29968800 | 9.39253100 | 15.49707500 |
| O | 5.86627400 | 8.42250700 | 10.22521000 |
| O | 3.90736600 | 7.31534800 | 11.30161400 |
| O | 5.84657500 | 5.94216300 | 10.55029100 |
| O | 15.73971500 | 17.36619300 | 12.03889000 |
| O | 14.84118400 | 15.50225300 | 10.65110600 |
| O | 17.14395900 | 15.34769600 | 11.61640700 |
| C | 7.24496400 | 7.80861000 | 15.26220000 |
| C | 6.93422400 | 6.52718800 | 14.76265700 |
| C | 6.40643100 | 6.35961000 | 13.48390900 |
| C | 6.16393400 | 7.48031600 | 12.68236900 |
| C | 6.44490200 | 8.76408900 | 13.16413800 |
| C | 6.98756900 | 8.92601900 | 14.43741100 |
| C | 8.64872700 | 8.74280800 | 16.91084000 |
| C | 9.01382900 | 8.81396600 | 18.36817900 |
| C | 8.38683500 | 8.13742200 | 19.41563000 |
| C | 8.86428900 | 8.33976300 | 20.71190200 |
| C | 9.94575600 | 9.19460800 | 20.94310300 |
| C | 10.53104700 | 9.83998500 | 19.85051800 |
| C | 11.69473800 | 10.75643400 | 19.90146600 |
| C | 12.32889800 | 11.12003900 | 21.08859500 |
| C | 13.43740200 | 11.96712200 | 21.02776600 |
| C | 13.89237700 | 12.40331800 | 19.78791700 |
| C | 13.21272000 | 11.99411000 | 18.63367600 |
| C | 13.77293500 | 12.35040600 | 17.27554600 |
| C | 14.00423300 | 13.99340800 | 15.61171300 |
| C | 15.39626400 | 13.99942300 | 15.38316300 |
| C | 15.92940300 | 14.55517300 | 14.22103900 |
| C | 15.07710000 | 15.10554900 | 13.25766700 |
| C | 13.69295300 | 15.11495600 | 13.46594600 |
| C | 13.16674700 | 14.56943800 | 14.63511000 |
| H | 13.77376500 | 10.10969800 | 16.00211900 |
| H | 13.94260800 | 12.27111600 | 21.93961000 |
| H | 14.76315300 | 13.04456800 | 19.69726000 |
| H | 11.97124500 | 10.75203900 | 22.04306500 |
| H | 10.31726600 | 9.34792200 | 21.94932100 |
| H | 8.39475400 | 7.83024300 | 21.54778600 |
| H | 7.55015700 | 7.47903900 | 19.21690300 |
| H | 7.20272100 | 9.92340100 | 14.80443700 |
| H | 7.11554300 | 5.65896500 | 15.39037700 |
| H | 6.18613500 | 5.36279900 | 13.11477700 |
| H | 6.24931000 | 9.63529800 | 12.54648500 |

| | | | |
|---|---|---|---|
| H | 12.09277900 | 14.58293500 | 14.80141600 |
| H | 16.06086200 | 13.57312000 | 16.12766100 |
| H | 17.00323600 | 14.55403100 | 14.06314200 |
| H | 13.02733100 | 15.54368400 | 12.72254200 |
| O | 11.12756700 | 11.71881300 | 15.54937800 |
| H | 11.71679500 | 12.44211400 | 15.82740500 |
| O | 12.79708600 | 10.13080200 | 14.33947400 |
| H | 12.11095100 | 10.75393900 | 14.77792000 |

**[(L4)Cu(OH)(HO-OH)]$^{3-}$ (q)** E= -2964.298809 H

| | | | |
|---|---|---|---|
| Cu | 11.51086800 | 10.16462100 | 16.45172900 |
| S | 3.52490500 | 7.81695300 | 12.98580300 |
| S | 16.48200800 | 16.24210100 | 12.22930900 |
| N | 8.99906300 | 7.04150200 | 15.20580100 |
| N | 10.33340600 | 9.30848400 | 17.73494900 |
| N | 11.96995100 | 11.25471500 | 18.29659400 |
| N | 13.28587800 | 13.56240200 | 16.56560700 |
| O | 10.53869300 | 8.77794700 | 15.17829500 |
| O | 14.92874600 | 12.08204100 | 17.35955500 |
| O | 14.78480400 | 9.42675600 | 16.83209700 |
| O | 3.59520300 | 9.04189800 | 12.12352400 |
| O | 2.65348800 | 8.01240000 | 14.19149600 |
| O | 3.19482100 | 6.57625900 | 12.21794100 |
| O | 16.81829300 | 17.60631500 | 12.76634300 |
| O | 15.60329800 | 16.30244500 | 11.01432700 |
| O | 17.71560900 | 15.41056300 | 12.00852800 |
| C | 7.77249700 | 7.26929000 | 14.70674100 |
| C | 7.11349100 | 6.18998900 | 14.03361100 |
| C | 5.84274900 | 6.34988800 | 13.50823500 |
| C | 5.19296800 | 7.58817800 | 13.63486500 |
| C | 5.81322700 | 8.67286300 | 14.28814400 |
| C | 7.07990800 | 8.52411200 | 14.81554300 |
| C | 9.67940200 | 8.07815700 | 15.86130900 |
| C | 9.51819300 | 8.30753200 | 17.25055500 |
| C | 8.61372100 | 7.65783800 | 18.13251300 |
| C | 8.57312600 | 8.05168100 | 19.45430400 |
| C | 9.41364700 | 9.09696900 | 19.92262400 |
| C | 10.28037100 | 9.70591200 | 19.02172900 |
| C | 11.21393700 | 10.81154700 | 19.34068200 |
| C | 11.33065200 | 11.37016700 | 20.61420100 |
| C | 12.25250700 | 12.39567100 | 20.82358400 |
| C | 13.04024700 | 12.82613100 | 19.76034300 |
| C | 12.87034900 | 12.23021800 | 18.50543600 |
| C | 13.77999400 | 12.65541400 | 17.37545900 |
| C | 14.08629300 | 14.12823900 | 15.55955100 |
| C | 15.39542800 | 14.60962700 | 15.78952400 |
| C | 16.10979200 | 15.24796300 | 14.78008100 |
| C | 15.53392400 | 15.41458600 | 13.51281300 |
| C | 14.24085100 | 14.94891200 | 13.26308500 |
| C | 13.52454900 | 14.31982700 | 14.28248800 |
| H | 14.85198900 | 10.38194900 | 17.11433800 |
| H | 12.35639800 | 12.84535000 | 21.80658500 |
| H | 13.77874700 | 13.61172200 | 19.88476800 |
| H | 10.71622400 | 11.01336300 | 21.43230900 |
| H | 9.36875900 | 9.40602700 | 20.95952700 |
| H | 7.88958200 | 7.56760100 | 20.14558400 |
| H | 7.96668900 | 6.87135400 | 17.75780800 |
| H | 7.56094000 | 9.35659600 | 15.31933300 |
| H | 7.63295100 | 5.24075500 | 13.94500600 |
| H | 5.35057900 | 5.52756000 | 13.00087600 |
| H | 5.29791000 | 9.62458500 | 14.37511700 |
| H | 12.51423100 | 13.96728200 | 14.09214100 |
| H | 15.84317200 | 14.48976300 | 16.77045800 |
| H | 17.11213700 | 15.61567900 | 14.98196700 |
| H | 13.79172700 | 15.08099700 | 12.28441900 |
| O | 12.56758000 | 10.85719600 | 15.02136000 |
| H | 12.82039300 | 11.76463900 | 15.26093300 |
| O | 14.78507400 | 9.54963100 | 15.37424200 |
| H | 13.90218600 | 10.04679800 | 15.20800900 |

**Complex [(L5)Cu]$^{2-}$ and related species:**

**[(L5)Cu]$^{2-}$ (d)** E= -2736.83333164 H

| | | | |
|---|---|---|---|
| Cu | 9.00221100 | 14.67040800 | 0.97793100 |
| C | 9.62349300 | 11.46738400 | 2.74352500 |
| C | 9.86844100 | 10.09983600 | 2.58627800 |
| H | 10.81957600 | 9.68606400 | 2.90219500 |
| C | 8.89403300 | 9.27287700 | 2.02284600 |
| H | 9.09567500 | 8.21357600 | 1.89190700 |
| C | 7.66833700 | 9.81640000 | 1.62731000 |
| H | 6.90450400 | 9.18063100 | 1.18764400 |
| C | 7.42760900 | 11.18279200 | 1.77494200 |
| H | 6.49064900 | 11.61867000 | 1.44346600 |
| C | 8.40067400 | 12.03092300 | 2.32351600 |
| C | 7.46764100 | 13.99227600 | 3.32339400 |
| C | 7.43171500 | 15.50610300 | 3.21901400 |
| C | 6.77756200 | 16.38067000 | 4.08607600 |
| H | 6.20967400 | 16.00063000 | 4.92776600 |
| C | 6.88332500 | 17.75435000 | 3.83301600 |
| H | 6.38682200 | 18.46128900 | 4.49073200 |
| C | 7.62236900 | 18.23160500 | 2.74288700 |
| H | 7.70753100 | 19.29452900 | 2.54421600 |
| C | 8.24815800 | 17.29726100 | 1.91573600 |
| C | 9.07757300 | 17.54488200 | 0.70552100 |
| C | 9.42559300 | 18.76834100 | 0.13105400 |
| H | 9.08802500 | 19.70276000 | 0.56646600 |
| C | 10.21873100 | 18.75181100 | -1.02323400 |
| H | 10.50113500 | 19.69099700 | -1.48914900 |
| C | 10.64830400 | 17.54269000 | -1.58509800 |
| H | 11.25956900 | 17.51820000 | -2.48013500 |
| C | 10.26130800 | 16.35872100 | -0.95775800 |
| C | 10.59746900 | 14.94948700 | -1.41010300 |
| C | 10.24606800 | 12.64255900 | -0.91698800 |
| C | 11.43367800 | 11.99362300 | -0.54855400 |
| H | 12.22204200 | 12.58256300 | -0.09047700 |
| C | 11.58947000 | 10.62037800 | -0.73931900 |
| H | 12.51451800 | 10.13717000 | -0.43625100 |
| C | 10.55312900 | 9.86823900 | -1.30063100 |
| H | 10.66191900 | 8.79618300 | -1.43763800 |
| C | 9.36811600 | 10.50000400 | -1.68478300 |
| H | 8.56029900 | 9.92656500 | -2.12539800 |
| C | 9.21521300 | 11.87771200 | -1.50057700 |
| N | 8.19439600 | 13.42590500 | 2.35536400 |
| N | 8.12588700 | 15.98743600 | 2.18984700 |
| N | 9.50963900 | 16.40438000 | 0.14035800 |
| N | 10.06474800 | 14.00960800 | -0.62320600 |
| O | 6.86492400 | 13.41950300 | 4.26938600 |
| O | 11.29807300 | 14.77976800 | -2.44331000 |
| O | 11.30887600 | 13.54394400 | 2.54961500 |
| O | 10.23731600 | 13.08986000 | 4.75501600 |
| O | 12.01050800 | 11.56778000 | 3.88676300 |
| O | 7.03485600 | 13.30700700 | -0.87721400 |
| O | 6.85104400 | 11.57594900 | -2.65423200 |
| O | 8.10486700 | 13.68593900 | -3.09728900 |
| S | 10.88567700 | 12.49808600 | 3.53733000 |
| S | 7.68943200 | 12.67447800 | -2.06867400 |

**[(L5)Cu(OH)]$^{3-}$ (d)** E= -2812.783247 H

| | | | |
|---|---|---|---|
| Cu | 7.77402000 | 12.64565100 | 1.83947300 |
| C | 9.02465500 | 9.12933000 | 1.75208800 |
| C | 9.63861200 | 8.14622200 | 0.96977900 |
| H | 10.61959900 | 7.77701100 | 1.24722900 |
| C | 8.99120700 | 7.64630800 | -0.16236700 |
| H | 9.47796400 | 6.89130500 | -0.77304400 |
| C | 7.72174100 | 8.12374900 | -0.50251300 |
| H | 7.20973800 | 7.74047600 | -1.38112600 |
| C | 7.11355400 | 9.11057500 | 0.27381900 |
| H | 6.14104000 | 9.50818800 | 0.00150000 |
| C | 7.75716400 | 9.63761900 | 1.40333200 |

| | | | |
|---|---|---|---|
| C | 6.18964000 | 10.51390200 | 2.97634000 |
| C | 5.72573200 | 11.79344700 | 3.64613000 |
| C | 4.72502800 | 11.90408200 | 4.61085000 |
| H | 4.18925700 | 11.02550600 | 4.95203300 |
| C | 4.44119800 | 13.17909200 | 5.11663300 |
| H | 3.66752500 | 13.29897100 | 5.86895100 |
| C | 5.13988300 | 14.30512100 | 4.66307900 |
| H | 4.92199100 | 15.29463600 | 5.05029200 |
| C | 6.12775300 | 14.11866600 | 3.69500700 |
| C | 6.99704300 | 15.14283000 | 3.05615600 |
| C | 7.02653200 | 16.51874300 | 3.28685400 |
| H | 6.35745600 | 16.97605600 | 4.00789700 |
| C | 7.94203900 | 17.28870600 | 2.55840100 |
| H | 7.98446600 | 18.36126600 | 2.72151100 |
| C | 8.79810700 | 16.69503400 | 1.62265700 |
| H | 9.50745700 | 17.28117600 | 1.04946000 |
| C | 8.70861400 | 15.31532400 | 1.44149600 |
| C | 9.52215500 | 14.48153900 | 0.47011000 |
| C | 9.80968700 | 12.27275900 | -0.38371500 |
| C | 11.06487500 | 11.72744200 | -0.07806700 |
| H | 11.57277600 | 12.07133600 | 0.81717400 |
| C | 11.63402200 | 10.74351200 | -0.88727100 |
| H | 12.60224500 | 10.32550600 | -0.62481100 |
| C | 10.95253400 | 10.28455100 | -2.01856200 |
| H | 11.38236400 | 9.50618000 | -2.64255300 |
| C | 9.70820300 | 10.82834000 | -2.34630300 |
| H | 9.17536900 | 10.48456200 | -3.22591900 |
| C | 9.14214000 | 11.82004600 | -1.53966400 |
| N | 7.18689400 | 10.71543100 | 2.11062700 |
| N | 6.37644700 | 12.88028200 | 3.23529600 |
| N | 7.83584800 | 14.60697300 | 2.15395500 |
| N | 9.19487200 | 13.18609800 | 0.49705800 |
| O | 5.64089000 | 9.42052600 | 3.27850600 |
| O | 10.38238800 | 15.04228300 | -0.25946500 |
| O | 10.09459700 | 11.17076700 | 3.13028600 |
| O | 8.91998800 | 9.36939100 | 4.39201200 |
| O | 11.13345700 | 8.91975200 | 3.33636300 |
| O | 7.79307300 | 14.02088000 | -2.16761400 |
| O | 6.56957900 | 12.23415800 | -0.93058100 |
| O | 7.18358400 | 11.89601600 | -3.31843100 |
| S | 9.85145300 | 9.69758800 | 3.26046400 |
| S | 7.55305800 | 12.54787500 | -2.01744800 |
| O | 5.40619400 | 15.57574600 | -0.37183300 |
| H | 6.12255500 | 14.97649100 | -0.64182300 |

**[(L5)Cu]$^-$ (s)** E= -2736.633847 H

| | | | |
|---|---|---|---|
| Cu | 8.98671100 | 14.72427000 | 0.96857300 |
| C | 9.83026300 | 11.61300700 | 2.84805300 |
| C | 10.16373000 | 10.26094300 | 2.85985000 |
| H | 11.05823400 | 9.93139300 | 3.37603100 |
| C | 9.35495900 | 9.33588400 | 2.18829100 |
| H | 9.62716700 | 8.28459300 | 2.19406800 |
| C | 8.21780400 | 9.76428200 | 1.49744600 |
| H | 7.60289800 | 9.04927100 | 0.95931000 |
| C | 7.87723700 | 11.11530200 | 1.48830100 |
| H | 7.00167500 | 11.47113400 | 0.95555900 |
| C | 8.66201600 | 12.04948500 | 2.17973000 |
| C | 7.52880400 | 13.90387700 | 3.20192300 |
| C | 7.44398500 | 15.40780000 | 3.16316800 |
| C | 6.76840200 | 16.25113200 | 4.03978700 |
| H | 6.19449900 | 15.83853600 | 4.86191900 |
| C | 6.86412000 | 17.63124400 | 3.82061300 |
| H | 6.35091400 | 18.31635000 | 4.48769800 |
| C | 7.61171300 | 18.14582200 | 2.75246600 |
| H | 7.68675000 | 19.21330600 | 2.57611400 |
| C | 8.25954200 | 17.24769700 | 1.90740000 |
| C | 9.08898100 | 17.50140800 | 0.71355800 |
| C | 9.47504300 | 18.70574300 | 0.12920800 |
| H | 9.15476100 | 19.64914300 | 0.55768400 |
| C | 10.28261600 | 18.65993300 | -1.01549800 |
| H | 10.59250300 | 19.58880900 | -1.48340000 |
| C | 10.69480500 | 17.43880700 | -1.56448200 |
| H | 11.31937000 | 17.38752400 | -2.44933700 |
| C | 10.27192500 | 16.27189200 | -0.93551800 |
| C | 10.55298300 | 14.84688600 | -1.33815500 |
| C | 9.98511500 | 12.57551300 | -0.80010400 |
| C | 11.01901200 | 11.77134100 | -0.29795300 |
| H | 11.77238600 | 12.23364000 | 0.33091600 |
| C | 11.07026800 | 10.41386000 | -0.60681800 |
| H | 11.87527700 | 9.80118200 | -0.21243900 |
| C | 10.07952600 | 9.84383600 | -1.41133000 |
| H | 10.11175000 | 8.78490300 | -1.65013200 |
| C | 9.02633500 | 10.62810000 | -1.89718400 |
| H | 8.24666700 | 10.18021600 | -2.50274000 |
| C | 8.96831000 | 11.98442600 | -1.58576200 |
| N | 8.29080400 | 13.40152500 | 2.19116600 |
| N | 8.14551100 | 15.92687000 | 2.16273000 |
| N | 9.50620400 | 16.35083600 | 0.14586400 |
| N | 9.96456100 | 13.94590100 | -0.50496400 |
| O | 6.96055400 | 13.24237100 | 4.08294500 |
| O | 11.24264100 | 14.57777800 | -2.33289700 |
| O | 11.38299500 | 13.75552400 | 2.61011200 |
| O | 10.09165900 | 13.48226100 | 4.72544600 |
| O | 12.03989500 | 11.99853700 | 4.24917400 |
| O | 6.90429500 | 13.53834600 | -0.96617100 |
| O | 6.69509100 | 12.02736700 | -2.93573700 |
| O | 8.15672200 | 14.04389400 | -3.06302100 |
| S | 10.91848500 | 12.80772500 | 3.67412400 |
| S | 7.57392400 | 12.97937700 | -2.18448200 |

**[(L5)Cu]$^-$ (t)** E= -2736.632465 H

| | | | |
|---|---|---|---|
| Cu | 9.27508500 | 14.55644500 | 1.43686500 |
| C | 9.58154900 | 11.34198300 | 2.44569900 |
| C | 9.73419000 | 9.97047800 | 2.23650700 |
| H | 10.72834100 | 9.53848000 | 2.20812900 |
| C | 8.60633100 | 9.16930600 | 2.04904400 |
| H | 8.72294200 | 8.10362200 | 1.87637300 |
| C | 7.33493100 | 9.75304200 | 2.06677800 |
| H | 6.45269700 | 9.14019700 | 1.90305600 |
| C | 7.18437100 | 11.12392300 | 2.27514400 |
| H | 6.19867000 | 11.57584300 | 2.26104500 |
| C | 8.30573800 | 11.94844700 | 2.47551100 |
| C | 7.26586700 | 13.94272400 | 3.35986500 |
| C | 7.25974500 | 15.44484900 | 3.18186300 |
| C | 6.48135600 | 16.34265300 | 3.90693400 |
| H | 5.80069800 | 15.98585100 | 4.67141100 |
| C | 6.61584100 | 17.70583100 | 3.61787700 |
| H | 6.02691700 | 18.43446600 | 4.16629200 |
| C | 7.50235100 | 18.14355300 | 2.62924300 |
| H | 7.60177100 | 19.20024600 | 2.40988300 |
| C | 8.24713300 | 17.18519600 | 1.93316100 |
| C | 9.21489400 | 17.42574300 | 0.83230000 |
| C | 9.56464000 | 18.70041600 | 0.37785200 |
| H | 9.14751800 | 19.58532300 | 0.84395700 |
| C | 10.45911200 | 18.81515200 | -0.68434400 |
| H | 10.75315500 | 19.79476600 | -1.04763100 |
| C | 10.94842000 | 17.66042300 | -1.29420100 |
| H | 11.61543000 | 17.70838900 | -2.14704500 |
| C | 10.54014500 | 16.41896800 | -0.80330200 |
| C | 10.96109500 | 15.16155100 | -1.52801900 |
| C | 10.30277900 | 12.85072600 | -1.33638400 |
| C | 11.61043400 | 12.32613900 | -1.05305100 |
| H | 12.43749600 | 13.01964600 | -0.96236300 |
| C | 11.81070800 | 10.96946600 | -0.88734700 |
| H | 12.80569400 | 10.59180000 | -0.67422800 |
| C | 10.72441700 | 10.08388700 | -0.96028600 |
| H | 10.87537900 | 9.02031000 | -0.80471600 |
| C | 9.42389100 | 10.56569800 | -1.21582700 |
| H | 8.59247400 | 9.87172600 | -1.24976100 |
| C | 9.20506300 | 11.91369100 | -1.40955200 |

| | | | |
|---|---|---|---|
| N | 8.19873300 | 13.34156100 | 2.59740300 |
| N | 8.09009900 | 15.89012200 | 2.23414000 |
| N | 9.72258300 | 16.30799100 | 0.25860700 |
| N | 10.04336800 | 14.15197200 | -1.47007600 |
| O | 6.47202500 | 13.40469300 | 4.16540500 |
| O | 11.97116400 | 15.16169100 | -2.24642600 |
| O | 10.94872200 | 13.44959900 | 1.61082900 |
| O | 10.98893100 | 12.93047900 | 4.05637300 |
| O | 12.23819100 | 11.50491100 | 2.42691300 |
| O | 7.14580900 | 13.43156200 | -0.65465200 |
| O | 6.67077800 | 11.25116000 | -1.75155100 |
| O | 7.57930500 | 13.14058600 | -3.09998800 |
| S | 11.04642500 | 12.35664400 | 2.68083800 |
| S | 7.51699800 | 12.48687900 | -1.75344300 |

**[(L5)Cu(OH)]$^{2-}$ (s)** E= -2812.585527 H

| | | | |
|---|---|---|---|
| Cu | 7.72095700 | 12.66880100 | 1.81369500 |
| C | 9.19239200 | 9.23414000 | 2.03221300 |
| C | 9.91102700 | 8.18789200 | 1.45858600 |
| H | 10.77919400 | 7.78734300 | 1.96947500 |
| C | 9.51917500 | 7.66973600 | 0.21840100 |
| H | 10.08928500 | 6.85943300 | -0.22638600 |
| C | 8.41463300 | 8.20351600 | -0.45199300 |
| H | 8.12338100 | 7.81331100 | -1.42254900 |
| C | 7.69024200 | 9.24698500 | 0.12102100 |
| H | 6.83151900 | 9.67757000 | -0.38324900 |
| C | 8.05572100 | 9.75858300 | 1.37443100 |
| C | 6.27402500 | 10.49441700 | 2.80341100 |
| C | 5.74108700 | 11.71974900 | 3.49877800 |
| C | 4.73243300 | 11.79093500 | 4.45431100 |
| H | 4.20648600 | 10.89359900 | 4.76077900 |
| C | 4.43685500 | 13.04771700 | 4.99774200 |
| H | 3.65709400 | 13.13739000 | 5.74730400 |
| C | 5.13183100 | 14.19496700 | 4.59104600 |
| H | 4.90778100 | 15.16998000 | 5.00967600 |
| C | 6.12841100 | 14.05640400 | 3.62805600 |
| C | 7.01331700 | 15.07125000 | 3.02614500 |
| C | 7.11040400 | 16.43716500 | 3.27996400 |
| H | 6.45975000 | 16.90523800 | 4.01057400 |
| C | 8.06478200 | 17.17883100 | 2.57102300 |
| H | 8.15496900 | 18.24400200 | 2.75804100 |
| C | 8.89989500 | 16.56884600 | 1.62696400 |
| H | 9.64132300 | 17.12825100 | 1.06755400 |
| C | 8.74991600 | 15.20174700 | 1.41777100 |
| C | 9.50158200 | 14.32538600 | 0.45046200 |
| C | 9.53508600 | 12.09443100 | -0.44340000 |
| C | 10.66936800 | 11.31124800 | -0.18498700 |
| H | 11.17623400 | 11.43484400 | 0.76616700 |
| C | 11.12935300 | 10.40178100 | -1.13548900 |
| H | 12.00801100 | 9.79959300 | -0.92513000 |
| C | 10.45103900 | 10.25711600 | -2.34913300 |
| H | 10.80230200 | 9.54551000 | -3.09055100 |
| C | 9.30187800 | 11.01316000 | -2.61006000 |
| H | 8.76350600 | 10.88699900 | -3.54259800 |
| C | 8.83632800 | 11.91924100 | -1.66056200 |
| N | 7.30240400 | 10.78506900 | 1.96161900 |
| N | 6.37909200 | 12.82561800 | 3.13421900 |
| N | 7.84025400 | 14.52628100 | 2.10982000 |
| N | 9.09667300 | 13.02724400 | 0.50789100 |
| O | 5.80658900 | 9.36689000 | 3.02232400 |
| O | 10.37754400 | 14.78233900 | -0.29830200 |
| O | 10.07443900 | 11.36391500 | 3.35041800 |
| O | 8.58855600 | 9.77417200 | 4.56959300 |
| O | 10.93220900 | 9.12359500 | 4.02100400 |
| O | 7.70509900 | 14.30714000 | -1.94943700 |
| O | 6.35789200 | 12.48806900 | -0.90248900 |
| O | 6.85696600 | 12.42207000 | -3.34348600 |
| S | 9.73532500 | 9.92917200 | 3.61852400 |
| S | 7.32024400 | 12.85990500 | -1.98853500 |
| O | 5.42819200 | 15.93070600 | -0.14810100 |
| H | 6.11621300 | 15.32573400 | -0.47286300 |

**[(L5)Cu(OH)]$^{2-}$ (t)** E= -2812.590105 H

| | | | |
|---|---|---|---|
| Cu | 7.74883800 | 12.62275500 | 1.87990400 |
| C | 9.03417300 | 9.12499700 | 1.74112800 |
| C | 9.63866000 | 8.15329000 | 0.93749600 |
| H | 10.63018200 | 7.79312800 | 1.18803700 |
| C | 8.96841000 | 7.65278600 | -0.18100100 |
| H | 9.44798900 | 6.90683600 | -0.80824900 |
| C | 7.68587900 | 8.11846700 | -0.48660200 |
| H | 7.15649800 | 7.73493800 | -1.35476000 |
| C | 7.08665200 | 9.09363800 | 0.31106200 |
| H | 6.10330500 | 9.48182700 | 0.06530300 |
| C | 7.75259600 | 9.62068700 | 1.42773400 |
| C | 6.19586300 | 10.47591500 | 3.02457200 |
| C | 5.72209300 | 11.75038000 | 3.69765100 |
| C | 4.72468200 | 11.85060200 | 4.66728100 |
| H | 4.20326100 | 10.96580500 | 5.01454200 |
| C | 4.42396100 | 13.12340300 | 5.16845300 |
| H | 3.65267600 | 13.23499300 | 5.92446700 |
| C | 5.10236200 | 14.25821400 | 4.70533300 |
| H | 4.86978000 | 15.24634300 | 5.08764600 |
| C | 6.08718600 | 14.08205000 | 3.73232300 |
| C | 6.92977900 | 15.11697200 | 3.07500300 |
| C | 6.91536000 | 16.49994700 | 3.27488300 |
| H | 6.23796600 | 16.94983700 | 3.99273000 |
| C | 7.79488800 | 17.28366600 | 2.52000900 |
| H | 7.80144800 | 18.36059000 | 2.65678200 |
| C | 8.66185800 | 16.69758800 | 1.58754200 |
| H | 9.34411500 | 17.29346600 | 0.99224700 |
| C | 8.62268300 | 15.30945900 | 1.44340100 |
| C | 9.45820900 | 14.48275700 | 0.48332400 |
| C | 9.76532900 | 12.27752400 | -0.36951500 |
| C | 11.03334700 | 11.75070700 | -0.08686000 |
| H | 11.55277300 | 12.10172100 | 0.79878900 |
| C | 11.60098600 | 10.77471400 | -0.90674000 |
| H | 12.57957000 | 10.37063600 | -0.66173700 |
| C | 10.90635700 | 10.30517700 | -2.02564200 |
| H | 11.33629600 | 9.53294300 | -2.65696400 |
| C | 9.64910700 | 10.83094300 | -2.33209500 |
| H | 9.10604600 | 10.48010200 | -3.20251800 |
| C | 9.08518900 | 11.81402400 | -1.51373800 |
| N | 7.18794500 | 10.68825500 | 2.15484800 |
| N | 6.35382600 | 12.84499800 | 3.27856400 |
| N | 7.77947200 | 14.58856700 | 2.18016200 |
| N | 9.14829100 | 13.18318800 | 0.51713100 |
| O | 5.65739100 | 9.37771600 | 3.32570600 |
| O | 10.30734900 | 15.05361400 | -0.24971300 |
| O | 10.11678700 | 11.16882600 | 3.10639400 |
| O | 8.99160200 | 9.34679100 | 4.38291200 |
| O | 11.18426500 | 8.92821400 | 3.27083300 |
| O | 7.71867900 | 14.00269600 | -2.13629400 |
| O | 6.51362600 | 12.22993300 | -0.86491300 |
| O | 7.09803900 | 11.87150100 | -3.26030900 |
| S | 9.89272500 | 9.69222300 | 3.23222700 |
| S | 7.48208800 | 12.52069600 | -1.96709000 |
| O | 6.64021300 | 15.95782300 | -0.52481100 |
| H | 7.04161200 | 15.19615600 | -1.03716300 |

**[(L5)Cu] (d)** E= -2736.422273 H

| | | | |
|---|---|---|---|
| Cu | 9.13762900 | 14.51843300 | 1.37391500 |
| C | 9.26918600 | 11.28250900 | 2.36518100 |
| C | 9.24401800 | 9.93493700 | 2.09560200 |
| H | 10.16694500 | 9.39807300 | 1.90736400 |
| C | 8.00791100 | 9.24874500 | 2.06508900 |
| H | 7.99721700 | 8.18876100 | 1.83206400 |
| C | 6.80498700 | 9.92711800 | 2.32233700 |
| H | 5.86229700 | 9.39187000 | 2.27662800 |
| C | 6.81445900 | 11.27998500 | 2.60024600 |
| H | 5.88684900 | 11.81935100 | 2.74407200 |
| C | 8.05131500 | 12.00790500 | 2.62721100 |
| C | 7.14785400 | 14.05580700 | 3.50645800 |

| | | | |
|---|---|---|---|
| C | 7.15094400 | 15.51356200 | 3.17994800 |
| C | 6.35563000 | 16.44562700 | 3.83690800 |
| H | 5.66841400 | 16.12599200 | 4.61166400 |
| C | 6.48225600 | 17.78697800 | 3.46539900 |
| H | 5.87860000 | 18.54611100 | 3.95210100 |
| C | 7.39130200 | 18.15651900 | 2.47457100 |
| H | 7.49405700 | 19.19827800 | 2.19663500 |
| C | 8.16037300 | 17.16380200 | 1.85077600 |
| C | 9.16603800 | 17.38989900 | 0.78641000 |
| C | 9.52828800 | 18.67400000 | 0.36812500 |
| H | 9.09219500 | 19.55028300 | 0.83162100 |
| C | 10.46550100 | 18.81371000 | -0.64995300 |
| H | 10.76999300 | 19.80016700 | -0.98452400 |
| C | 10.98320100 | 17.66975600 | -1.25032100 |
| H | 11.68472100 | 17.73202200 | -2.07339100 |
| C | 10.56803000 | 16.41485400 | -0.79735600 |
| C | 11.05872200 | 15.20105800 | -1.55382000 |
| C | 10.64564600 | 12.84138500 | -1.39648500 |
| C | 12.01910600 | 12.42397400 | -1.34470200 |
| H | 12.79622900 | 13.17827000 | -1.36007900 |
| C | 12.34508000 | 11.08263000 | -1.28914000 |
| H | 13.38767400 | 10.78100400 | -1.26364100 |
| C | 11.33359300 | 10.10840200 | -1.24100900 |
| H | 11.59280000 | 9.05599900 | -1.17999100 |
| C | 9.97588700 | 10.48657700 | -1.23567900 |
| H | 9.20449500 | 9.73002100 | -1.14971100 |
| C | 9.63053100 | 11.81990500 | -1.31438500 |
| N | 8.12013000 | 13.34084200 | 2.81081600 |
| N | 8.00241400 | 15.88277700 | 2.21159900 |
| N | 9.70312700 | 16.27577000 | 0.22872200 |
| N | 10.24419200 | 14.11102900 | -1.46537900 |
| O | 6.42464400 | 13.58037800 | 4.38031400 |
| O | 12.03260900 | 15.30168300 | -2.31323700 |
| O | 10.75911000 | 13.27299300 | 1.49092500 |
| O | 10.95922000 | 12.62110500 | 3.89805300 |
| O | 11.90449800 | 11.16589500 | 2.09645300 |
| O | 7.75180700 | 13.22250200 | -0.06525600 |
| O | 7.13247300 | 11.01703700 | -1.01723600 |
| O | 7.55909100 | 12.94097400 | -2.54229700 |
| S | 10.85649700 | 12.13355200 | 2.49656800 |
| S | 7.88261100 | 12.28998100 | -1.23508700 |

**[(L5)Cu] (q)** E= -2736.633847 H

| | | | |
|---|---|---|---|
| Cu | 9.13908200 | 14.51404500 | 1.37495800 |
| C | 9.23637800 | 11.27575200 | 2.33849100 |
| C | 9.20648700 | 9.92857200 | 2.06512800 |
| H | 10.12487200 | 9.39718900 | 1.84221200 |
| C | 7.97609600 | 9.23335200 | 2.08891800 |
| H | 7.96030300 | 8.17540300 | 1.84742400 |
| C | 6.78666900 | 9.89955000 | 2.42593200 |
| H | 5.84669800 | 9.35743300 | 2.43253300 |
| C | 6.80019200 | 11.25044100 | 2.71645900 |
| H | 5.87619700 | 11.77946000 | 2.91039300 |
| C | 8.02632200 | 11.99497000 | 2.65162200 |
| C | 7.13675200 | 14.06380200 | 3.50256000 |
| C | 7.14147100 | 15.52036000 | 3.16573400 |
| C | 6.34360300 | 16.45331600 | 3.81912800 |
| H | 5.65552900 | 16.13511900 | 4.59366400 |
| C | 6.47033900 | 17.79416900 | 3.44599500 |
| H | 5.86285300 | 18.55330500 | 3.92789500 |
| C | 7.38427100 | 18.16275200 | 2.45950600 |
| H | 7.48430400 | 19.20343200 | 2.17705200 |
| C | 8.15898000 | 17.16939700 | 1.84313800 |
| C | 9.17058000 | 17.39605500 | 0.78374100 |
| C | 9.54514500 | 18.68112400 | 0.37852100 |
| H | 9.11464600 | 19.55717100 | 0.84793700 |
| C | 10.48957700 | 18.82205600 | -0.63272600 |
| H | 10.80522300 | 19.80882800 | -0.95586400 |
| C | 11.00115200 | 17.67921000 | -1.24031200 |
| H | 11.70939400 | 17.74287900 | -2.05749300 |
| C | 10.57313600 | 16.42390000 | -0.80032400 |
| C | 11.06166100 | 15.21252900 | -1.56184000 |
| C | 10.66038100 | 12.85140100 | -1.40858200 |
| C | 12.03645600 | 12.44255300 | -1.35651400 |
| H | 12.80881000 | 13.20181900 | -1.36593600 |
| C | 12.37140000 | 11.10305300 | -1.30797300 |
| H | 13.41596500 | 10.80830200 | -1.28202100 |
| C | 11.36636700 | 10.12195300 | -1.26710700 |
| H | 11.63237600 | 9.07094100 | -1.21159800 |
| C | 10.00633700 | 10.49128200 | -1.26157700 |
| H | 9.23980100 | 9.72922300 | -1.18092400 |
| C | 9.65209800 | 11.82280500 | -1.33300500 |
| N | 8.07723000 | 13.33629600 | 2.77103900 |
| N | 7.99888300 | 15.88874700 | 2.20220100 |
| N | 9.70135300 | 16.28271800 | 0.21950700 |
| N | 10.25142000 | 14.11920700 | -1.47284100 |
| O | 6.43192700 | 13.60035100 | 4.39613100 |
| O | 12.03162400 | 15.31670600 | -2.32607500 |
| O | 10.75164100 | 13.26917600 | 1.48395600 |
| O | 10.93197600 | 12.58411300 | 3.88036800 |
| O | 11.87044700 | 11.14126300 | 2.06408600 |
| O | 7.76179300 | 13.21358300 | -0.08841600 |
| O | 7.15990400 | 11.00141000 | -1.03586600 |
| O | 7.57490100 | 12.92496000 | -2.56563400 |
| S | 10.83062500 | 12.11325500 | 2.47296100 |
| S | 7.90076800 | 12.28010900 | -1.25546300 |

**[(L7)Cu] (dos)** E= -3043.74310150 H

| | | | |
|---|---|---|---|
| Cu | 11.15256800 | 11.17616200 | 17.33940200 |
| N | 9.33021100 | 10.80249600 | 16.29087900 |
| N | 9.96955300 | 10.49936500 | 18.80116500 |
| N | 12.41283900 | 11.13208900 | 18.89538700 |
| N | 12.96852100 | 11.88198500 | 16.44857200 |
| O | 7.17774300 | 10.01714900 | 16.71113400 |
| O | 15.17612300 | 12.30597700 | 17.05938400 |
| C | 8.30273100 | 10.35945300 | 17.09542000 |
| C | 8.70028700 | 10.19340600 | 18.53229600 |
| C | 7.84469100 | 9.74027700 | 19.53444800 |
| C | 8.36064700 | 9.61445900 | 20.82762300 |
| C | 9.69787600 | 9.92798000 | 21.08891500 |
| C | 10.49517600 | 10.37737100 | 20.03414000 |
| C | 11.92838900 | 10.74201100 | 20.08815900 |
| C | 12.76764200 | 10.71101400 | 21.20363000 |
| C | 14.10409200 | 11.08949100 | 21.04313300 |
| C | 14.58020100 | 11.49124400 | 19.79166100 |
| C | 13.68233200 | 11.49943500 | 18.72539600 |
| C | 14.03438300 | 11.91058400 | 17.32755300 |
| H | 14.77359800 | 11.07143600 | 21.89718800 |
| H | 15.61089100 | 11.79067200 | 19.64118900 |
| H | 12.39024600 | 10.40036400 | 22.17139000 |
| H | 10.10934500 | 9.82143400 | 22.08629300 |
| H | 7.72317700 | 9.26623000 | 21.63399800 |
| H | 6.81333600 | 9.49944900 | 19.30389000 |
| C | 9.13344400 | 11.12361200 | 14.98576600 |
| C | 8.05891000 | 11.96700100 | 14.50085200 |
| C | 10.06909000 | 10.59916200 | 14.05294100 |
| C | 7.28438100 | 12.74170700 | 15.38174900 |
| C | 7.85238800 | 12.09494800 | 13.08639100 |
| C | 9.85758900 | 10.71309900 | 12.69014800 |
| H | 10.91991200 | 10.04569200 | 14.43646200 |
| C | 6.28980100 | 13.58981000 | 14.90241800 |
| H | 7.48363100 | 12.70864400 | 16.44669500 |
| C | 6.81967000 | 12.94951600 | 12.62831300 |
| C | 8.74693500 | 11.41167100 | 12.20117600 |
| H | 10.54768100 | 10.24772400 | 11.99659600 |
| C | 6.04939000 | 13.68108600 | 13.52450300 |
| H | 5.70763800 | 14.18475400 | 15.59944900 |
| H | 6.63827900 | 13.05873500 | 11.56710900 |
| H | 5.27181800 | 14.33917500 | 13.14887300 |
| S | 8.49210200 | 11.43048600 | 10.39562800 |
| O | 7.09657400 | 10.92307800 | 10.21208200 |
| O | 8.65919100 | 12.85740000 | 9.98275500 |

| | | | |
|---|---|---|---|
| O | 9.52975400 | 10.52275700 | 9.83004500 |
| C | 13.20701600 | 12.01986300 | 15.11512100 |
| C | 12.29383000 | 12.77527200 | 14.28843500 |
| C | 14.31707600 | 11.37346200 | 14.49744300 |
| C | 11.22854900 | 13.49806000 | 14.86015600 |
| C | 12.49285000 | 12.82551400 | 12.86774700 |
| C | 14.49313000 | 11.41326600 | 13.12466000 |
| H | 14.98957800 | 10.78035200 | 15.10437300 |
| C | 10.35411700 | 14.23719400 | 14.06539600 |
| H | 11.08382600 | 13.47270300 | 15.93496300 |
| C | 11.57542400 | 13.56756100 | 12.08508800 |
| C | 13.60566000 | 12.12179100 | 12.30861100 |
| H | 15.31923200 | 10.87369600 | 12.67659800 |
| C | 10.52378100 | 14.26119800 | 12.67712900 |
| H | 9.52888500 | 14.77046200 | 14.52595500 |
| H | 11.68531500 | 13.60268600 | 11.00944600 |
| H | 9.82764800 | 14.81045400 | 12.05187000 |
| S | 13.90915600 | 12.10066300 | 10.51357700 |
| O | 12.68366300 | 11.47651000 | 9.92913200 |
| O | 14.08177100 | 13.53551900 | 10.12755300 |
| O | 15.14236300 | 11.28426000 | 10.31490500 |

**[(L8)Cu] (q)** E= -3043.74912970 H

| | | | |
|---|---|---|---|
| Cu | 11.23093400 | 11.01393500 | 17.27515800 |
| N | 9.62035300 | 10.23780000 | 16.15356800 |
| N | 10.18197200 | 10.07302200 | 18.67932700 |
| N | 12.17730300 | 11.59533700 | 18.92011000 |
| N | 12.86086000 | 12.03484500 | 16.45370100 |
| O | 7.88423000 | 8.68795500 | 16.39077500 |
| O | 14.57573200 | 13.47381100 | 17.14868000 |
| C | 8.83256300 | 9.33585200 | 16.84662100 |
| C | 9.16216300 | 9.29404100 | 18.31618900 |
| C | 8.45356400 | 8.56463300 | 19.27004000 |
| C | 8.84012000 | 8.69124300 | 20.60874800 |
| C | 9.90193000 | 9.52844600 | 20.96827700 |
| C | 10.57321100 | 10.21946100 | 19.95767800 |
| C | 11.72624000 | 11.14345400 | 20.10283400 |
| C | 12.35245300 | 11.55566700 | 21.28133500 |
| C | 13.43436500 | 12.43822900 | 21.18407800 |
| C | 13.88423700 | 12.88281700 | 19.93592100 |
| C | 13.21756100 | 12.42047900 | 18.80199200 |
| C | 13.61460100 | 12.73496800 | 17.38235300 |
| H | 13.93340500 | 12.77429500 | 22.08743700 |
| H | 14.72870900 | 13.55570500 | 19.84074300 |
| H | 12.00597600 | 11.19985400 | 22.24534800 |
| H | 10.20155700 | 9.63672200 | 22.00502500 |
| H | 8.30884500 | 8.14067900 | 21.37853900 |
| H | 7.62611000 | 7.93042900 | 18.97341200 |
| C | 9.44827900 | 10.50080900 | 14.83097900 |
| C | 9.03124300 | 9.52848800 | 13.87045400 |
| C | 9.78515800 | 11.81982100 | 14.38159500 |
| C | 8.94453000 | 9.86216100 | 12.50929600 |
| H | 8.84772800 | 8.50863700 | 14.18451500 |
| C | 9.64876700 | 12.16646500 | 13.06711200 |
| H | 10.11967600 | 12.53904400 | 15.12183700 |
| C | 8.58557500 | 8.88739800 | 11.53498700 |
| C | 9.23247400 | 11.20386200 | 12.08580500 |
| H | 9.86822100 | 13.17900900 | 12.74081700 |
| C | 8.48150000 | 9.23281700 | 10.19778200 |
| H | 8.38807300 | 7.86878600 | 11.85594800 |
| C | 9.12361000 | 11.53451400 | 10.73119300 |
| C | 8.73863700 | 10.55869000 | 9.80624500 |
| H | 8.20517700 | 8.49008600 | 9.45760400 |
| H | 9.34247600 | 12.54599700 | 10.40379100 |
| C | 13.10362300 | 12.06844800 | 15.11443100 |
| C | 12.66227400 | 10.91897500 | 14.38553300 |
| C | 13.72420600 | 13.13745800 | 14.38948200 |
| C | 12.80277100 | 10.81897800 | 12.99578200 |
| H | 12.22552400 | 10.09633100 | 14.94225500 |
| C | 13.83817100 | 13.05921300 | 13.02511100 |
| H | 14.05539000 | 14.02149900 | 14.91579800 |
| C | 12.32529900 | 9.68540000 | 12.28324500 |
| C | 13.38762000 | 11.91392200 | 12.28141500 |
| H | 14.26762200 | 13.89070800 | 12.47263300 |
| C | 12.42296900 | 9.63426400 | 10.90177400 |
| H | 11.86627800 | 8.86983700 | 12.83349900 |
| C | 13.48602800 | 11.84179300 | 10.88722200 |
| C | 13.00969900 | 10.71024000 | 10.21552900 |
| H | 12.04289100 | 8.77917700 | 10.35429800 |
| H | 13.92560800 | 12.66589900 | 10.33364400 |
| S | 8.46062600 | 11.04375300 | 8.08407300 |
| S | 13.24408400 | 10.60134300 | 8.42470500 |
| O | 7.01951500 | 11.46068800 | 8.04682100 |
| O | 8.73411700 | 9.82571900 | 7.26279700 |
| O | 9.40057100 | 12.17432600 | 7.81732900 |
| O | 12.22656800 | 9.62352200 | 7.93570700 |
| O | 13.04417600 | 11.98873800 | 7.90243200 |
| O | 14.65400500 | 10.11492000 | 8.25794200 |

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