Supporting Information

Anion tuning of Zn^{2+} architectures using a tris-base salicylic ligand

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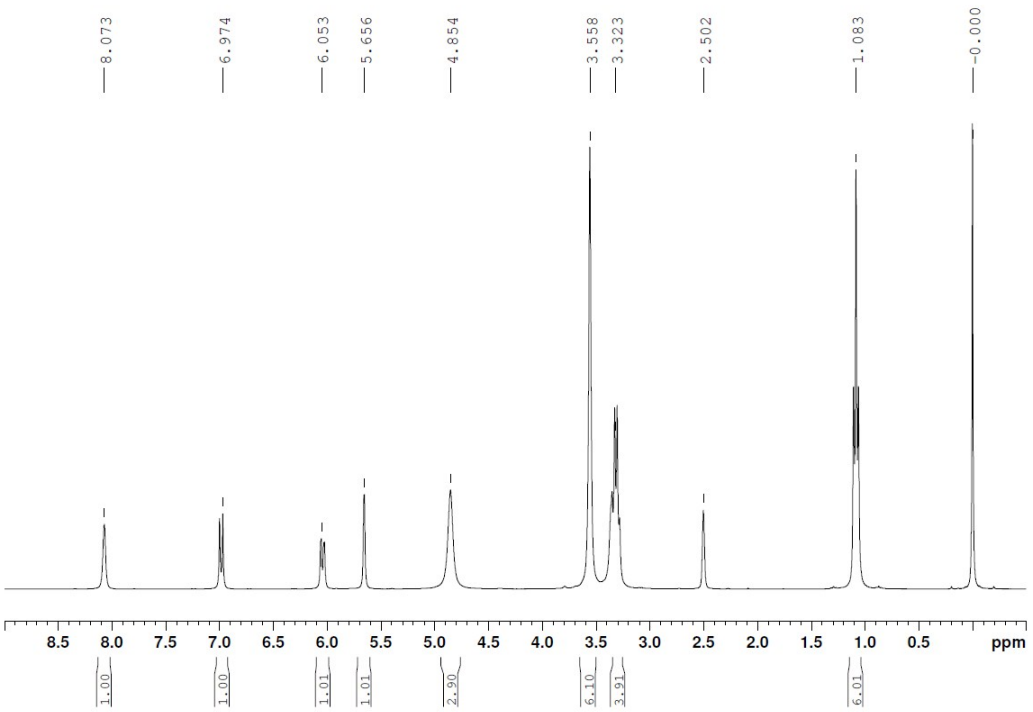

Fig. S1 ^{1}H NMR H_4**L**.

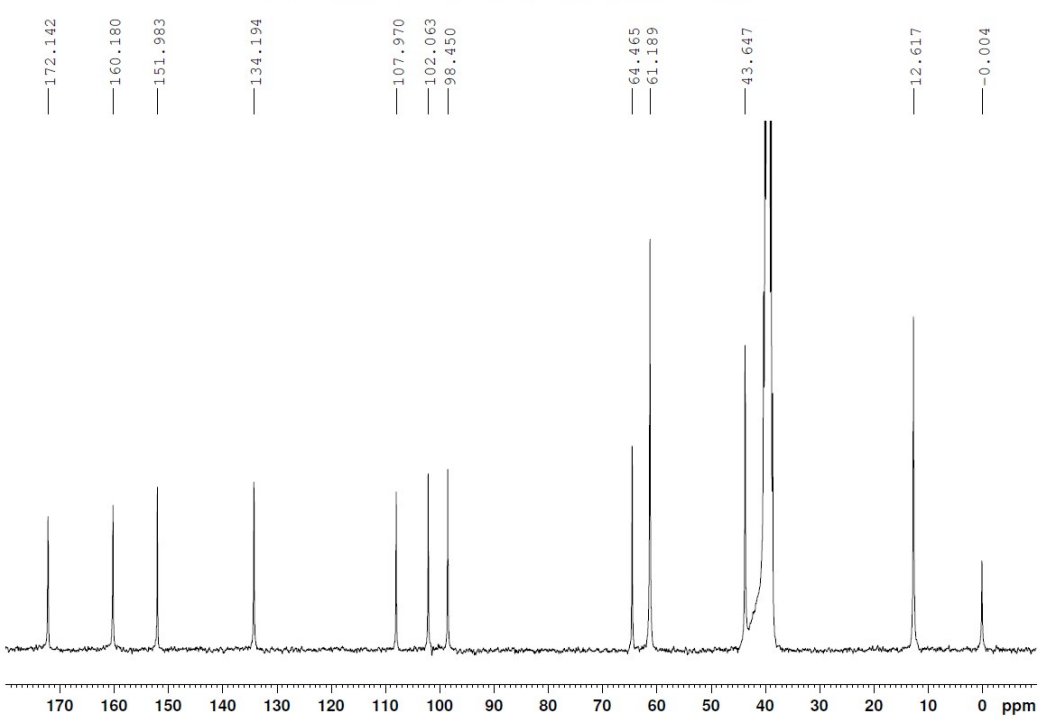

Fig. S2 ^{13}C NMR of H_4**L**.

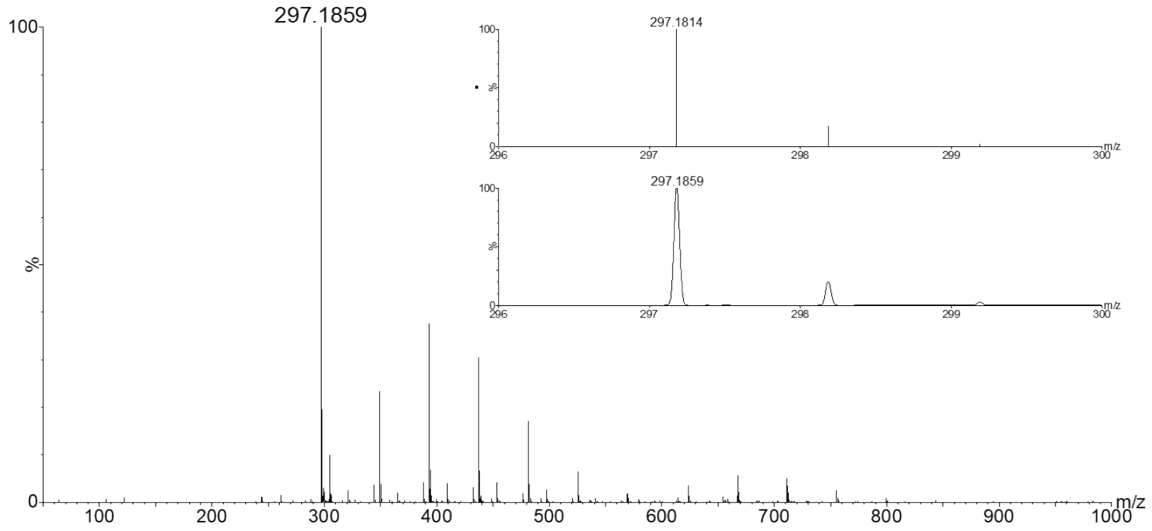

Fig. S3 ESI-HRMS (positive-ion detection, MeOH, *m/z*): calculated for $[H_4\mathbf{L}+H]^+$, 297.1814; found 297.1859. Insert, theoretical isotope model (top) and measured isotope distribution (bottom).

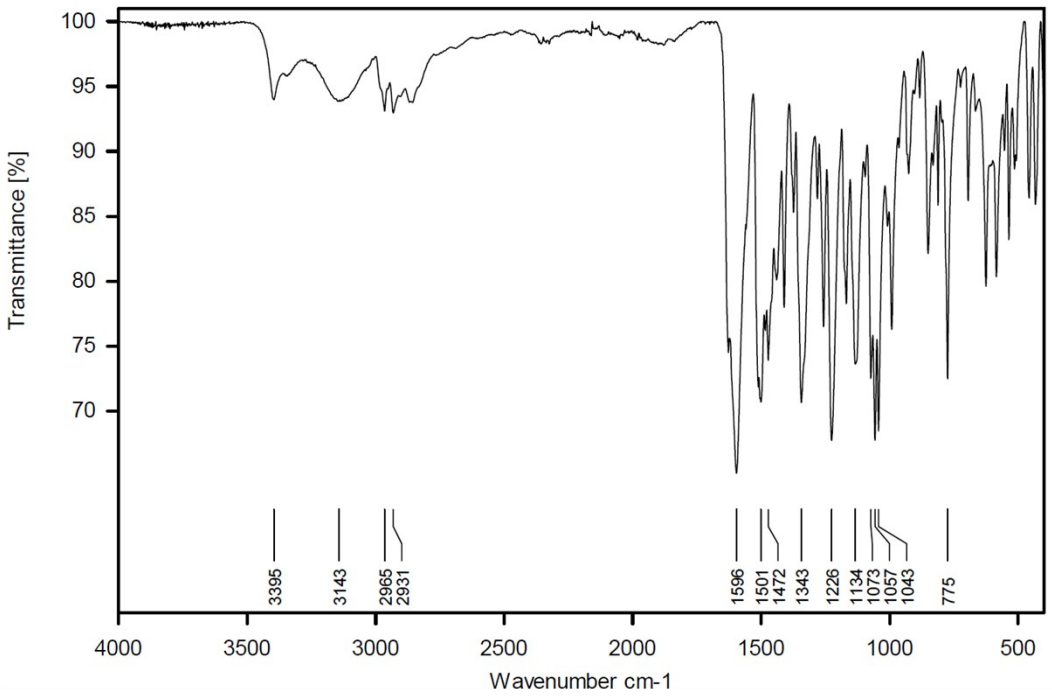

Fig. S4 FT-IR of $H_4\mathbf{L}$.

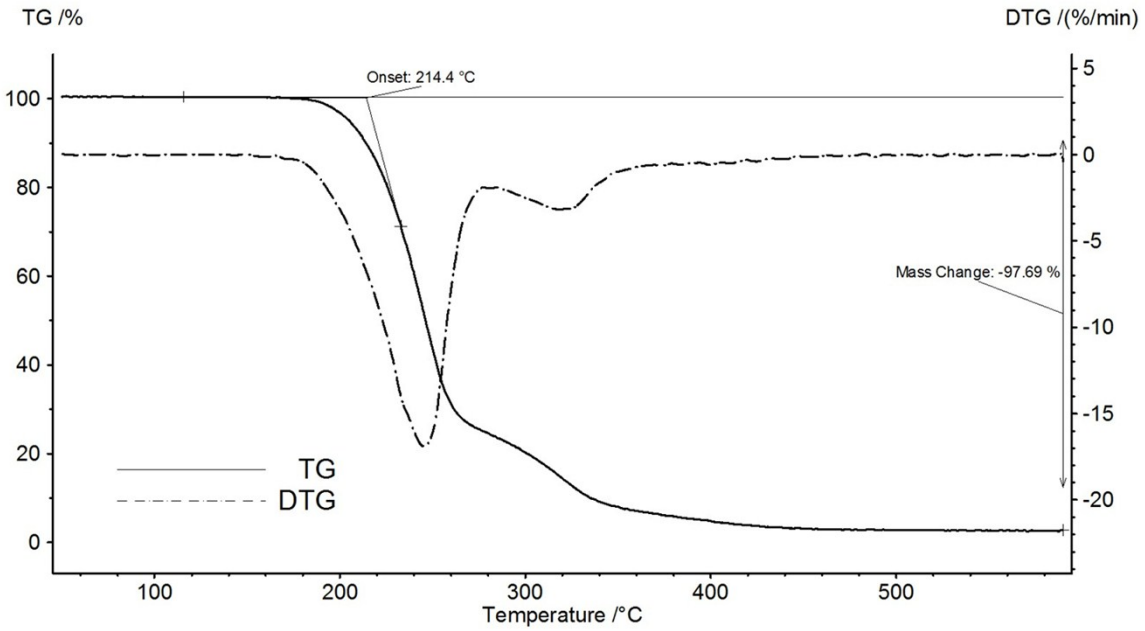

Fig. S5 TGA spectrum of H_4**L** under argon gas measured from 50-590 ˚C at 10 ˚C per/min. Solid line (TG) is the samples thermogravimetric mass loss, while DTG is the first derivative of TG.

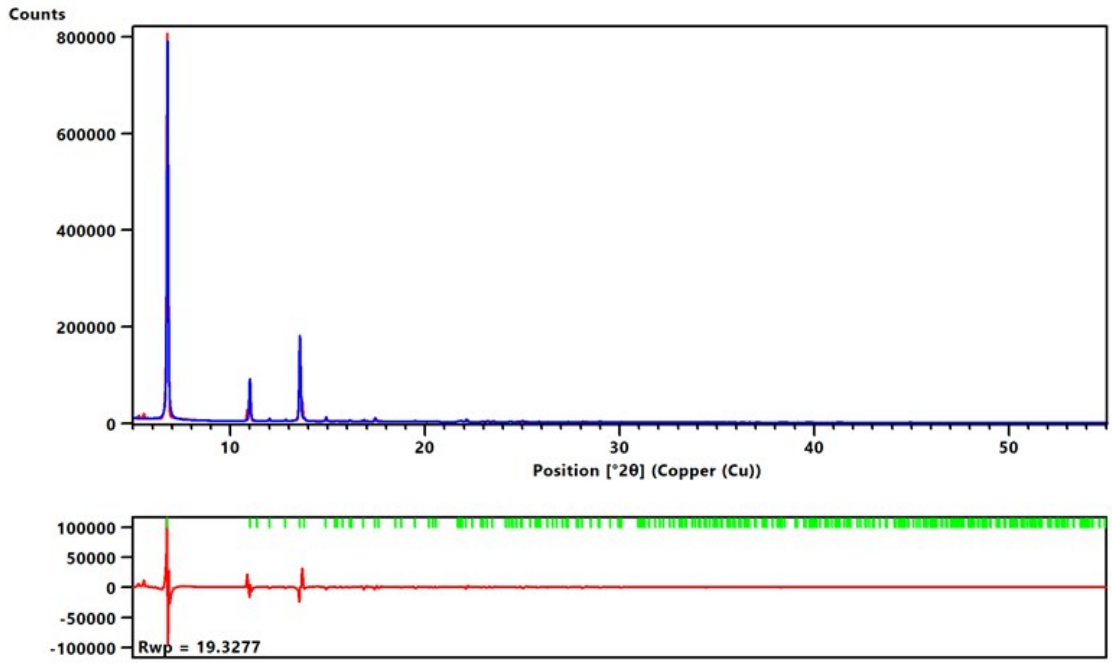

Fig. S6 LeBail fit of complex **1**. The top portion in the figure displays overlap of PXRD experimental pattern of the complex (in red) and the calculated pattern from the crystal structure (in blue). The plot below is the difference between the two patterns.

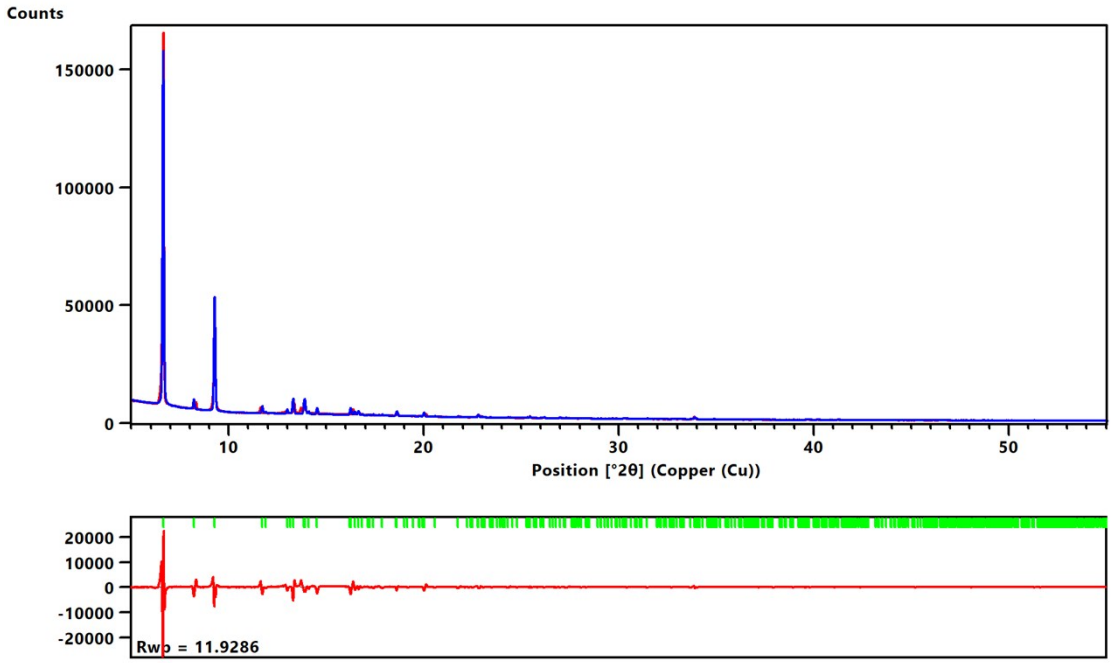

Fig. S7 LeBail fit of complex **2**. The top portion in the figure displays overlap of PXRD experimental pattern of the complex (in red) and the calculated pattern from the crystal structure (in blue). The plot below is the difference between the two patterns.

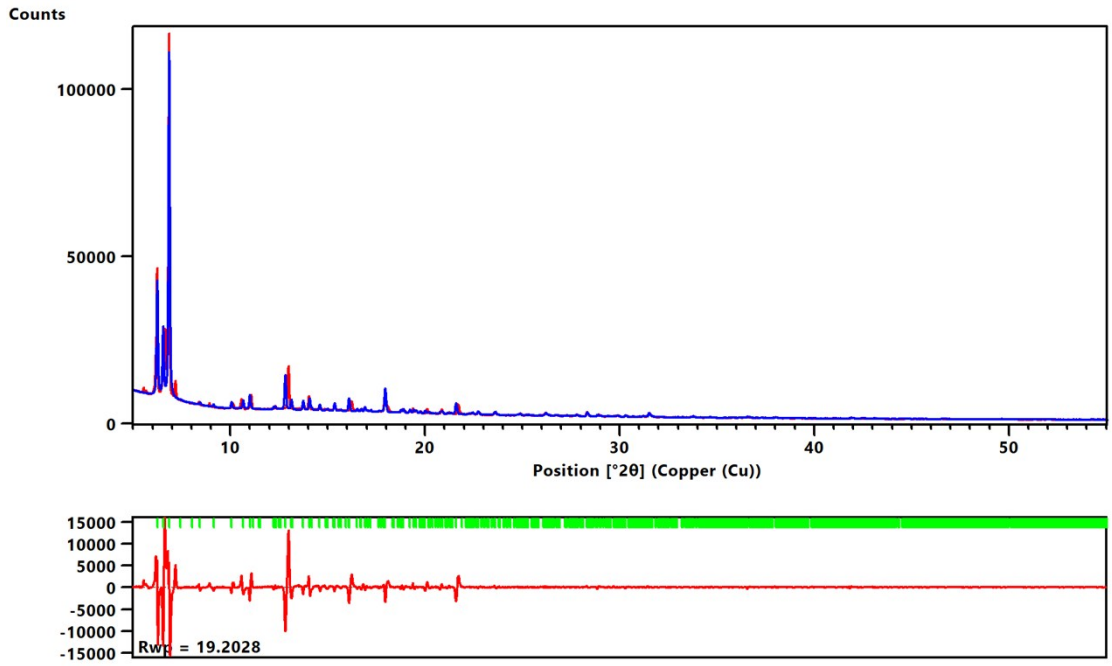

Fig. S8 LeBail fit of complex **3**. The top portion in the figure displays overlap of PXRD experimental pattern of the complex (in red) and the calculated pattern from the crystal structure (in blue). The plot below is the difference between the two patterns.

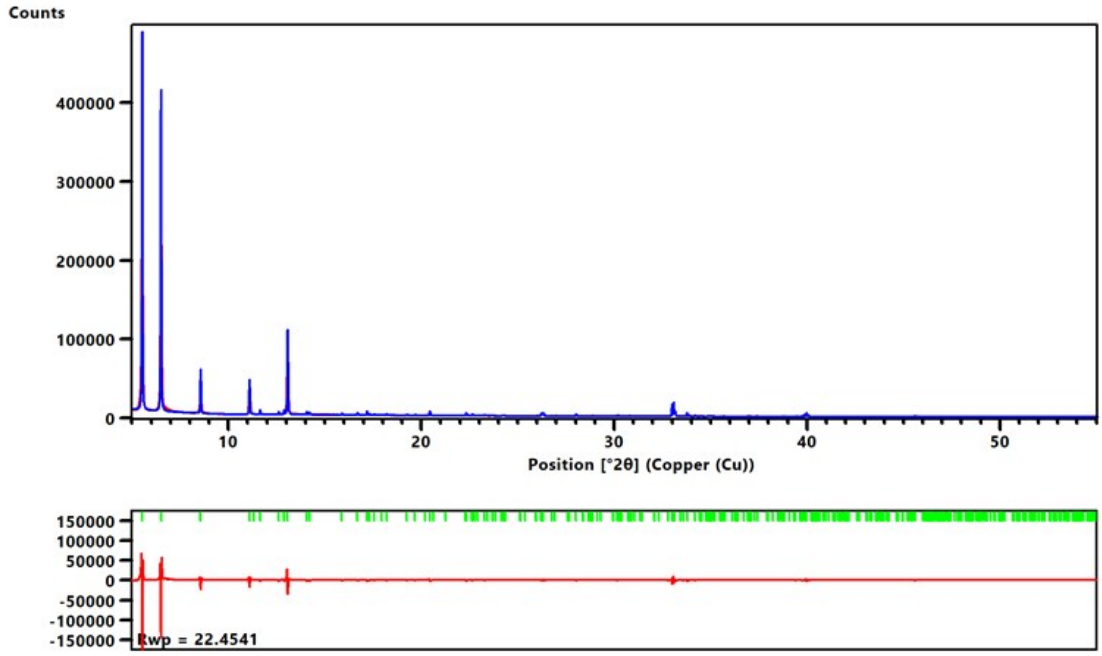

Fig. S9 LeBail fit of complex **4**. The top portion in the figure displays overlap of PXRD experimental pattern of the complex (in red) and the calculated pattern from the crystal structure (in blue). The plot below is the difference between the two patterns.

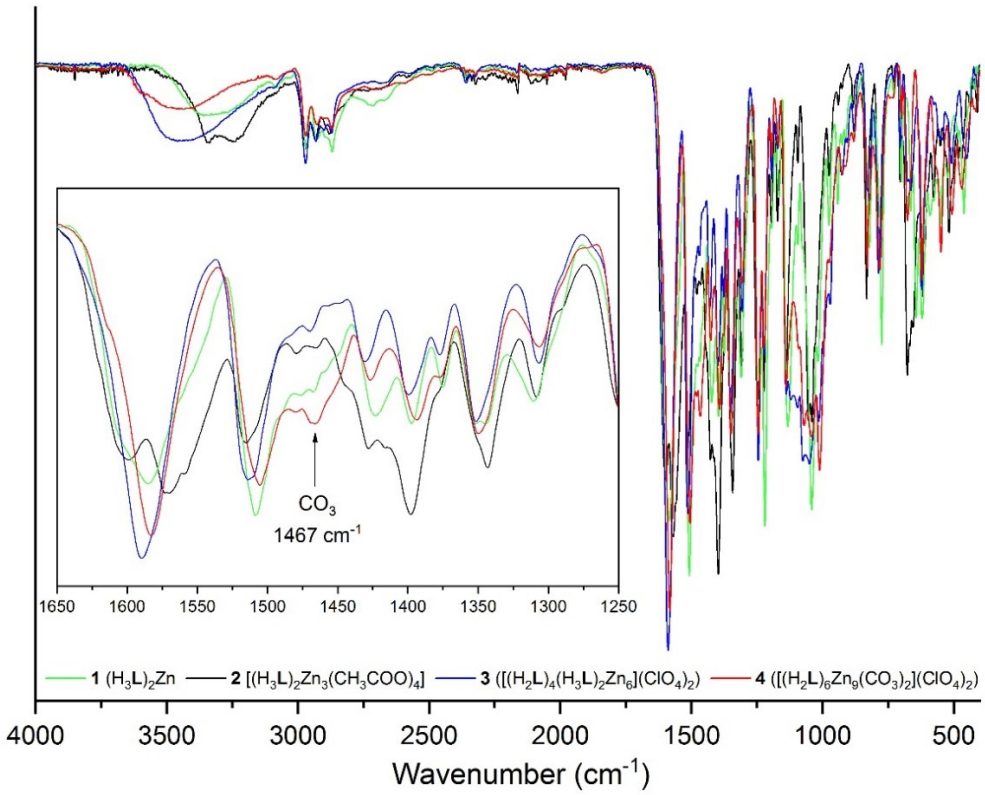

Fig. S10 FT-IR of Zn^{2+} complexes with H_4**L**. The presence of CO_3 in the architecture of **4** is supported by a peak at 1467 cm^{-1}.

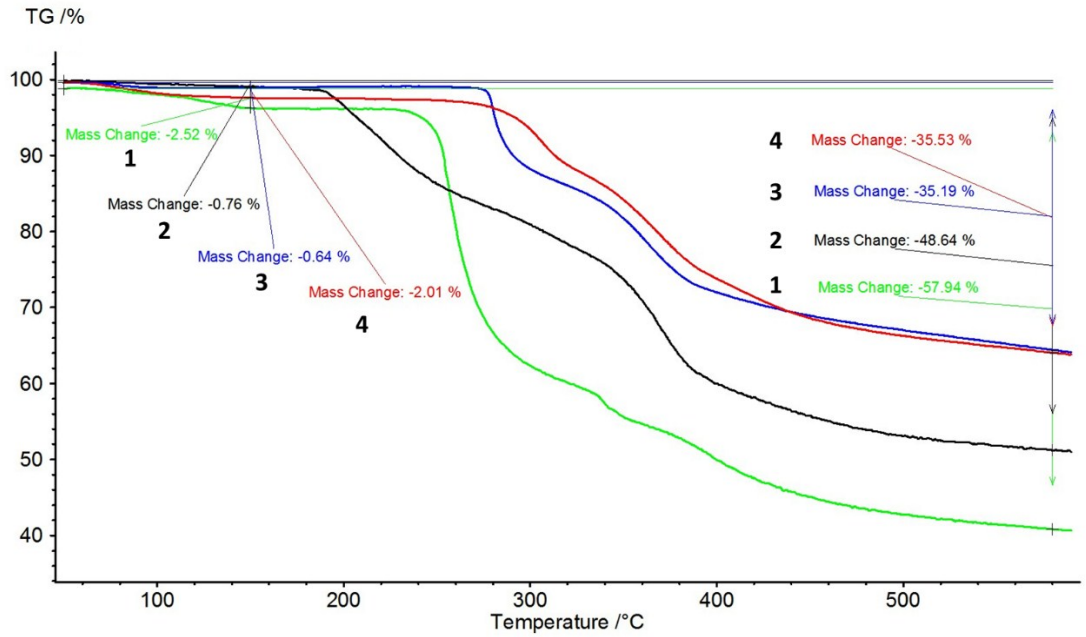

Fig. S11 TGA spectra of Zn^{2+} complexes under argon gas measured from 50-590 ˚C at 10 ˚C per/min. The first mass loss evet calculated is from 50-150 ˚C and accounts for solvent loss, while the second is calculated from 50-590 ˚C.

Crystallographic information

Complex 1

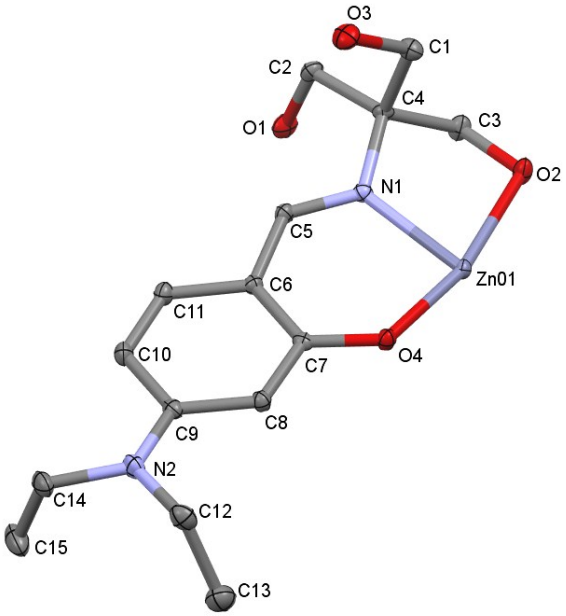

Fig. S12 Asymmetric unit of **1** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, solvent molecules and anions omitted for clarity.

Complex 2

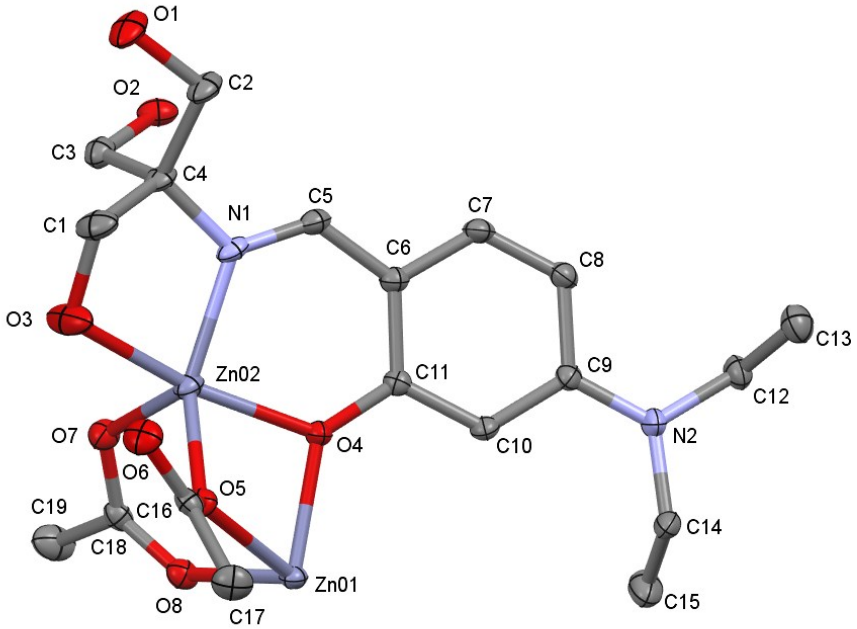

Fig. S13 Asymmetric unit of **2** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, solvent molecules and anions omitted for clarity.

Specific details:

One of the ethyl groups is disordered over two positions and modelled with occupancies of 0.75 and 0.25 respectively. There is also a disordered methanol solvent molecule present in the lattice, which is modelled over three positions. A number of the solvent methyl hydrogens give rise to close contacts with ligand hydrogen atoms. Attempts to model the solvent with the O/C positions swapped did not give satisfactory results.

Complex 3

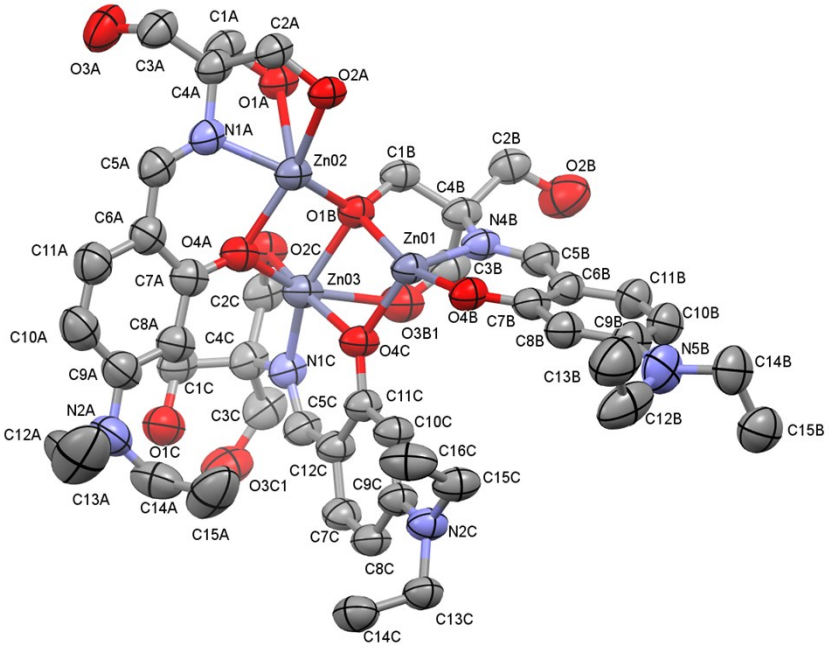

Fig. S14 Asymmetric unit of **3** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, solvent molecules and anions omitted for clarity.

Specific details:

One of the ethyl groups and two of the methoxy groups are disordered over two positions. In addition the perchlorate anions are significantly disordered and instead of modelling them, this region of the structure was treated with the solvent masking routine of OLEX2. A number of restraints and constraints were required to facilitate realistic modelling.

Complex 4

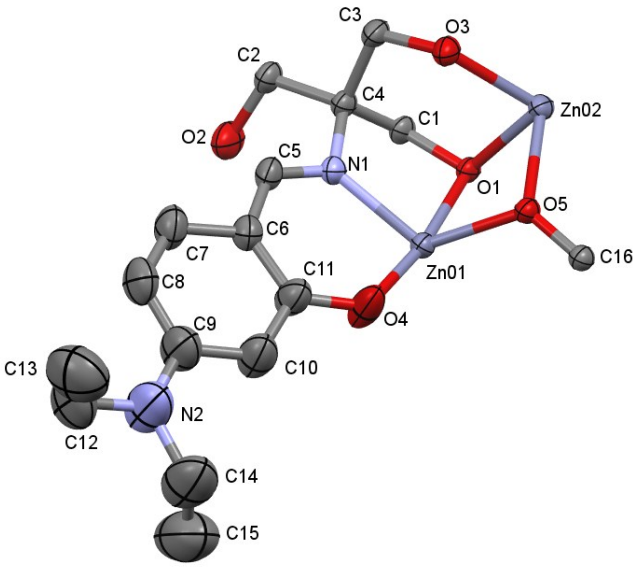

Fig. S15 Asymmetric unit of **4** with thermal ellipsoids drawn at 50% probability. Hydrogen atoms, solvent molecules and anions omitted for clarity.

Specific details:

The ligand is disordered over two positions (occupancy 0.75 and 0.25, respectively). In addition one solvent position is a mixture of methanol (0.75) and water (0.25). A number of restraints and constraints were required to facilitate realistic modelling.