

The effect of carboxylate and *N,N'*-ditopic ligand lengths on the structures of copper and zinc coordination polymers

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Supplementary information

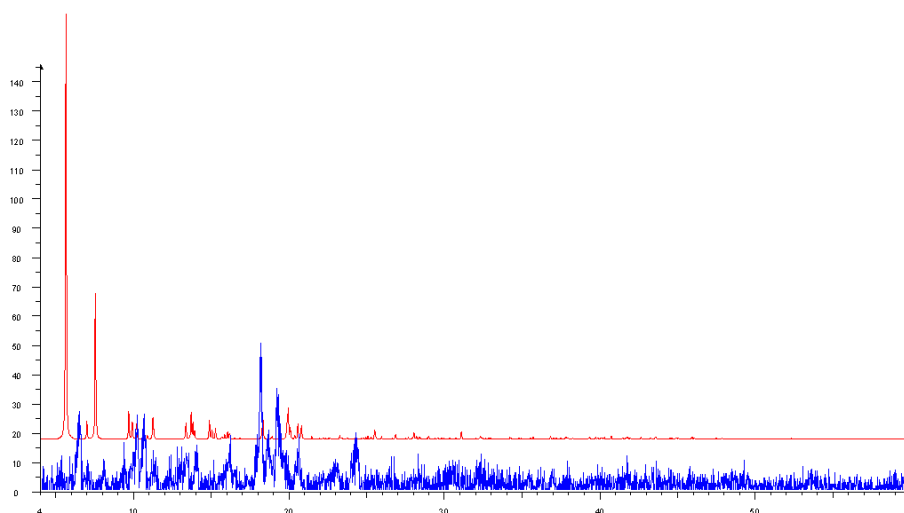


Fig. S1. The powder X-ray diffraction pattern for **1** (blue) in comparison with that simulated from the crystal structure (red).

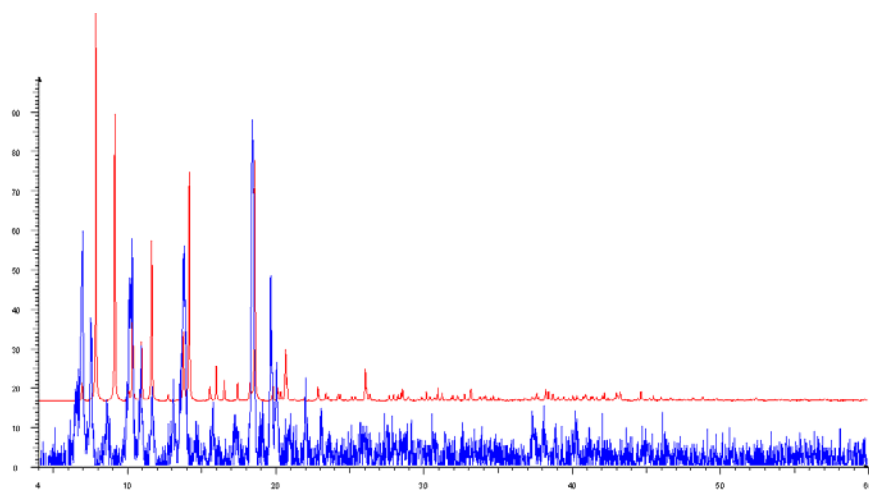


Fig. S2. The powder X-ray diffraction pattern for **2** (blue) in comparison with that simulated from the crystal structure (red).

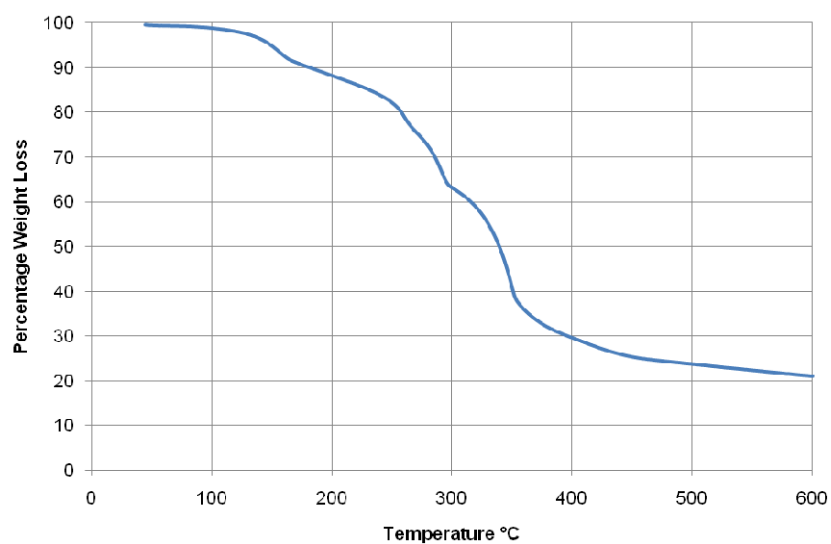


Fig. S3. The thermogravimetric analysis for crystals of **2**.

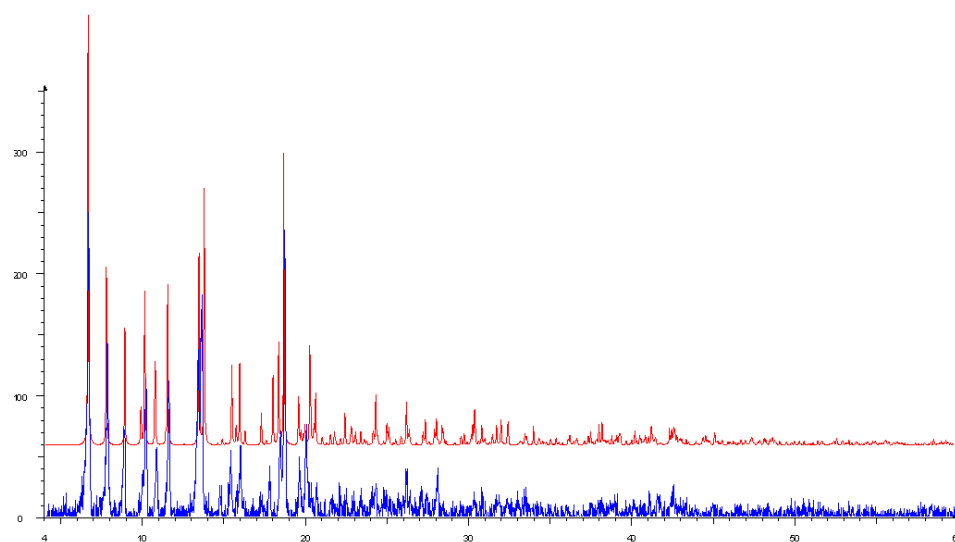


Fig. S4. The powder X-ray diffraction pattern for **3** (blue) in comparison with that simulated from the crystal structure (red).

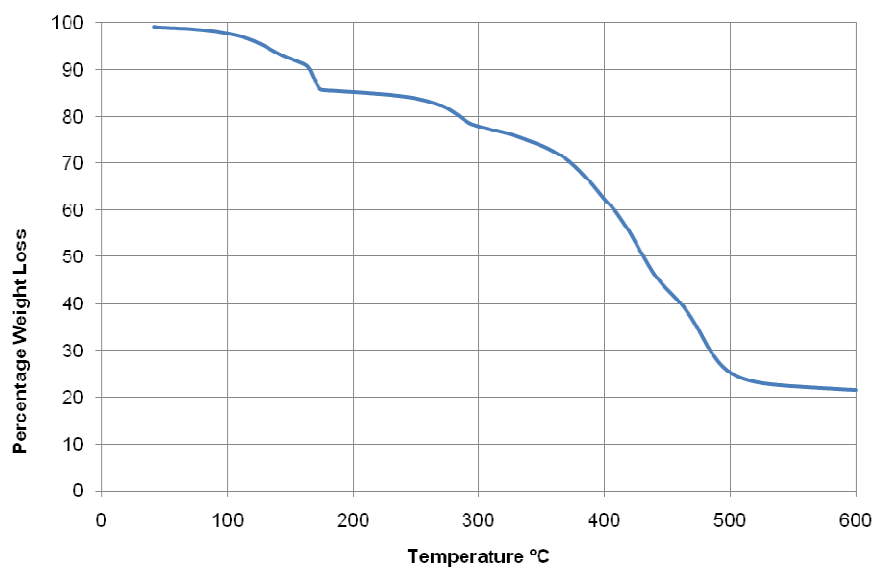


Fig. S5. The thermogravimetric analysis for **3**.

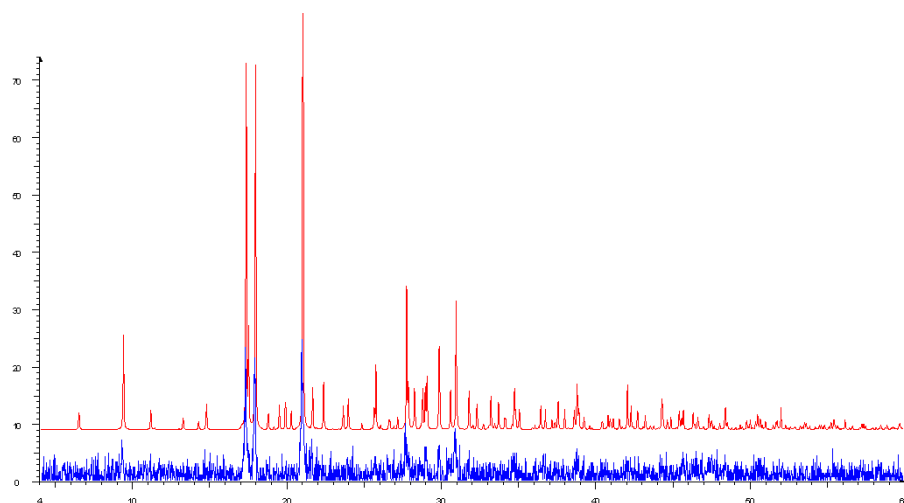


Fig. S6. The powder X-ray diffraction pattern for **4** (blue) in comparison with that simulated from the crystal structure (red).

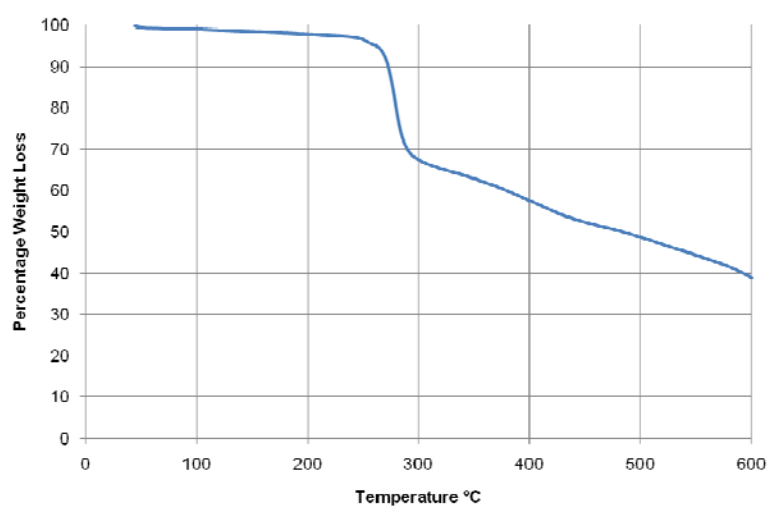


Fig. S7. The thermogravimetric analysis for **4**.

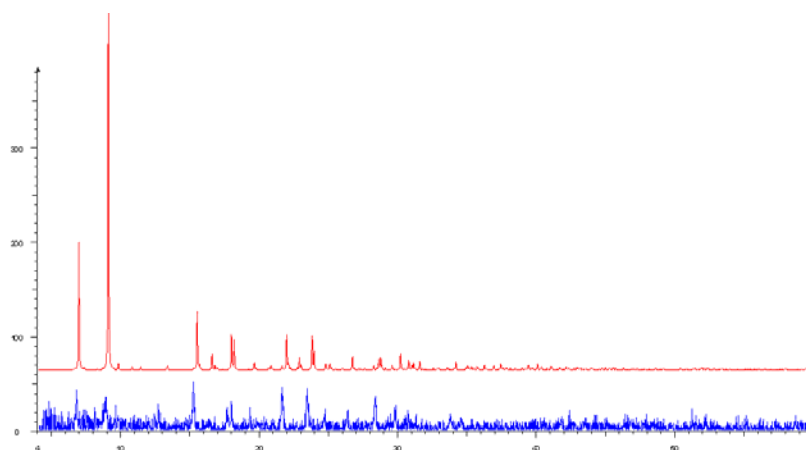


Fig. S8. The powder X-ray diffraction pattern for **5** (blue) in comparison with that simulated from the crystal structure (red).

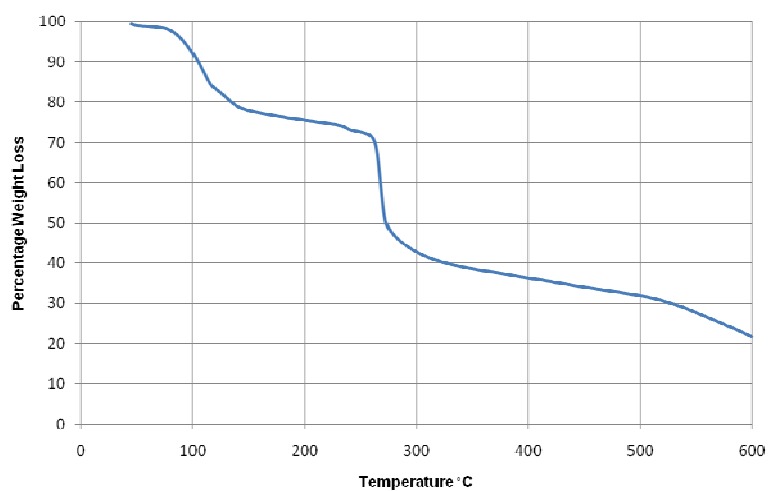


Fig. S9. The thermogravimetric analysis for **5**.

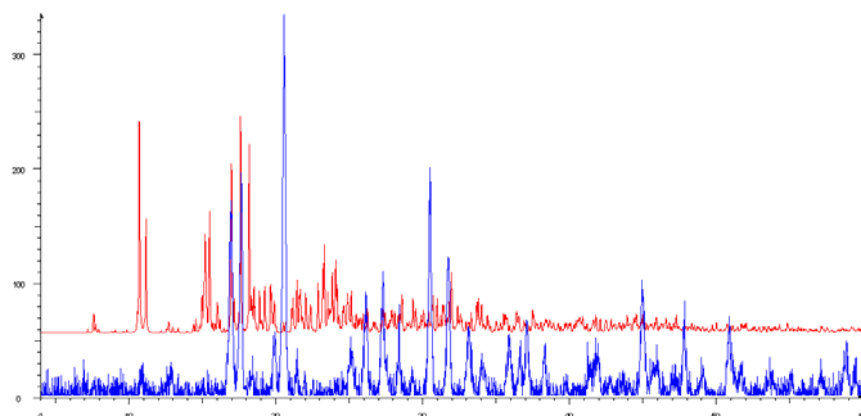


Fig. S10. The powder X-ray diffraction pattern for **6** (blue) in comparison with that simulated from the crystal structure (red).

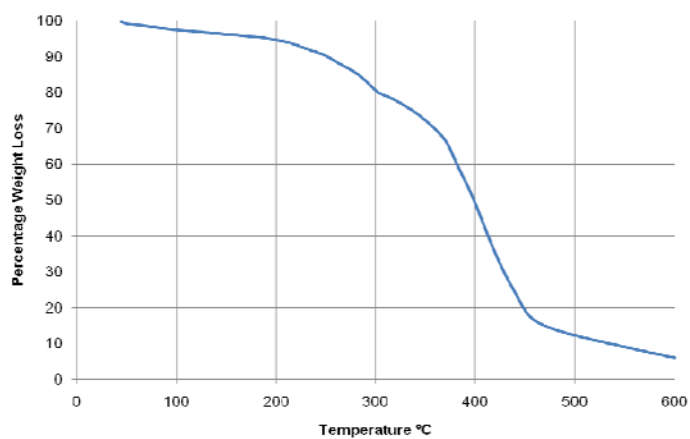


Fig. S11. The thermogravimetric analysis for **6**.

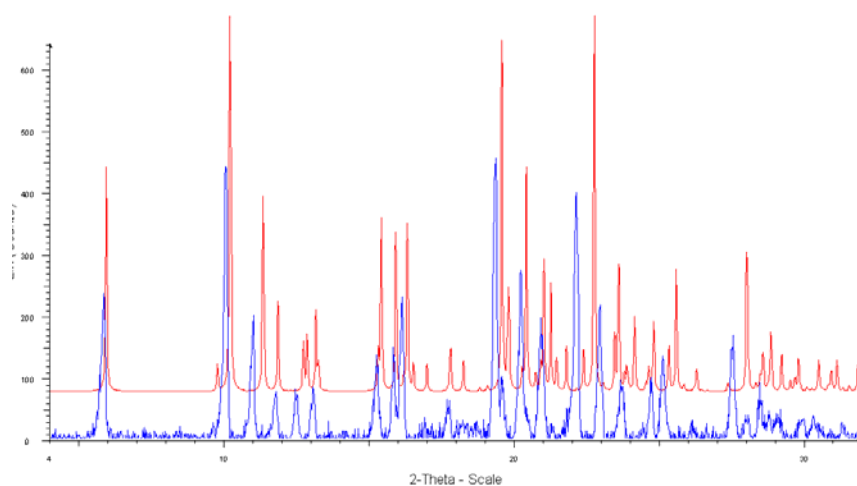


Fig. S12. The powder X-ray diffraction pattern for **7** (blue) in comparison with that simulated from the crystal structure (red).

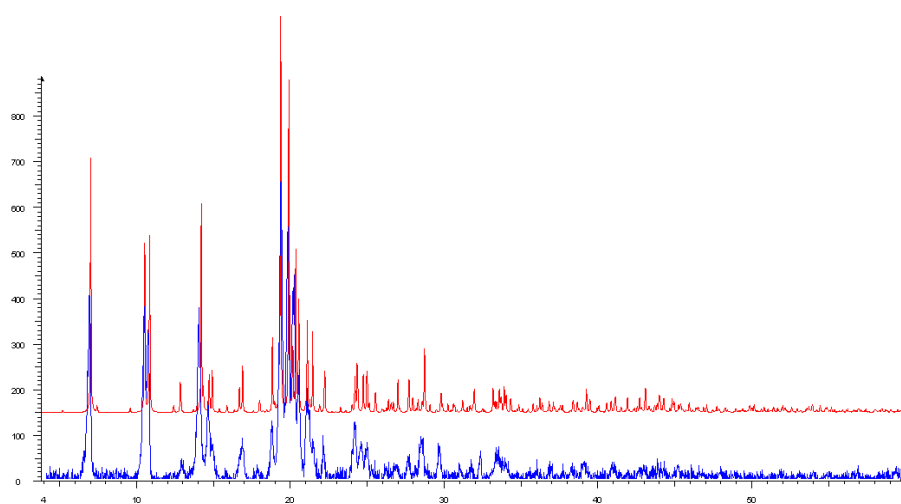


Fig. S13. The powder X-ray diffraction pattern for **8** (blue) in comparison with that simulated from the crystal structure (red).

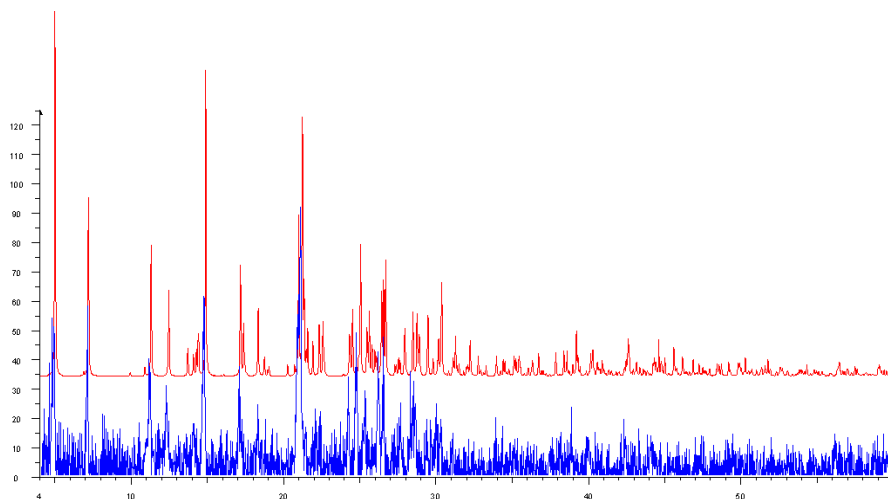


Fig. S14. The powder X-ray diffraction pattern for **9** (blue) in comparison with that simulated from the crystal structure (red).

Crystallography

X-ray data for compounds **1**, **5** and **7-9** were collected on a Nonius Kappa CCD diffractometer using Mo-K α radiation, while those for compound **2** were measured on a Bruker APEX II diffractometer using synchrotron radiation ($\lambda = 0.69450$ Å) at Station 9.8 of the SRS Daresbury Laboratory. A Bruker Apex II diffractometer using synchrotron radiation ($\lambda = 0.7749$ Å) at Station 11.3.1 of the ALS Lawrence Berkeley National Laboratory was used to collect the single crystal data for compounds **3** and **6**. X-ray data for compound **4** was collected on an Oxford Diffraction Gemini diffractometer fitted with an Atlas CCD detector, using Mo-K α radiation. Unless noted, all non-hydrogen atoms were refined anisotropically in the final least squares run, and hydrogen atoms were included at calculated positions. The structures were solved using SHELXS-97 and refined using full-matrix least squares in SHELXL-97.

Refinements were generally straightforward with the following exceptions and points of note. For **1**, the oxygen of the benzyl alcohol solvent moiety was disordered equally over two proximate sites. The associated hydrogens could not be reliably located so were omitted from the final refinement. Compound **3** contained a solvent DMF molecule which was disordered over two sites (55:45). The dabco CH₂ groups were equally disordered due to the nitrogen atoms being located on a crystallographic 2-fold rotation axis. Due to the poor diffracting ability of the crystal at higher Bragg angles, the data was truncated at 20°. The crystallographic data for **5** were poor, as the intensity of the reflections dropped off above

Bragg angles of 14° . Nonetheless, an unambiguous structural model was still obtained. The asymmetric unit for compound **6** contained six full occupancy DMF molecules, and an additional half molecule of DMF located on an inversion centre. Some distance restraints were applied to the solvent molecules, and atomic displacement parameter restraints were applied to the dabco carbon atoms. All fragments with less than 50 % occupancy were treated isotropically. Large atomic displacement parameters were observed for the chelating carboxylate groups attached to Zn(1) in **8**. There is also residual electron density positioned here in the Fourier map. This indicates some disorder, however attempts to refine a sensible model where the carboxylate is disordered between monodentate and bidentate coordination were unsuccessful.