Supporting information for:

Utilising Hinged Ligands in MOF Synthesis: A Covalent Linking Strategy for Forming 3D MOFs

Campbell J. Coghlan, a Christian J. Doonan a and Christopher J. Sumby a

a. Centre for Advanced Nanomaterials, School of Chemistry and Physics, University of Adelaide, Adelaide, Australia

Contact details:

CJD: Tel: +61 8 8313 5770; Fax: +61 8 8313 4358; E-mail: christian.doonan@adelaide.edu.au,
CJS: Tel: +61 8 8313 7406. Fax. +61 8 8313 4358. E-mail: christopher.sumby@adelaide.edu.au
Chart 1. Coordination modes of L (top) in (a) [Cu₂(L)(H₂O)₂], (b) [Zn₂(L)], (c) [Cd₂(L)] (Pink) and (d) [Co₂(L)(H₂O)₆]. The dashed bonds in (d) indicate hydrogen bonds with the carboxylate oxygen atoms acting as acceptors.
**Figure SI 1.** TGA traces of $[\text{Cu}_2(\text{L})(\text{H}_2\text{O})_2]$ (Red), $[\text{Zn}_2(\text{L})]$ (Black), $[\text{Cd}_2(\text{L})]$ (Pink) and $[\text{Co}_2(\text{L})(\text{H}_2\text{O})_6]$ (Blue) for the as-synthesised samples (washed in methanol). The small percentage of weight loss in the range 50-100°C is attributed to solvent removal (MeOH in the pores) before decomposition when the coordinated water molecules and ligands are lost.
Figure SI 2. PXRD patterns for \([\text{Cu}_2(\text{L})(\text{H}_2\text{O})_2]\). Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

Figure SI 3. PXRD patterns for \([\text{Zn}_4(\text{L})]\). Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).
Figure SI 4. PXRD patterns for $[\text{Cd}_2(L)]$. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

Figure SI 5. PXRD patterns for $[\text{Co}_2(L)(\text{H}_2\text{O})_6]$. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).
Figure SI 6. CO₂ and N₂ isotherms at 293 K for (a) \([\text{Cu}_2(L)(\text{H}_2\text{O})_2]\), (b) \([\text{Zn}_2(L)]\), (c) \([\text{Cd}_2(L)]\) and (d) \([\text{Co}_2(L)(\text{H}_2\text{O})_6]\).

Figure SI 7. (a) 77 K N₂ adsorption isotherms for \([\text{Cu}_2(L)(\text{H}_2\text{O})_2]\), \([\text{Zn}_2(L)]\), \([\text{Cd}_2(L)]\) and \([\text{Co}_2(L)(\text{H}_2\text{O})_6]\). (b) Enlargements of the low pressure region of the 77 K N₂ adsorption isotherms.
Figure SI 8. Pore size distribution calculated from the 77 K N2 adsorption isotherms for [Cu2(L)(H2O)2], [Zn2(L)], [Cd2(L)] and [Co2(L)(H2O)6]. The green trace shows the pore size distribution for a sample of [Zn2(L)] that had been soaked in water and reactivated from methanol (see Figure 5 in the manuscript for PXRD data.)