Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information for:

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

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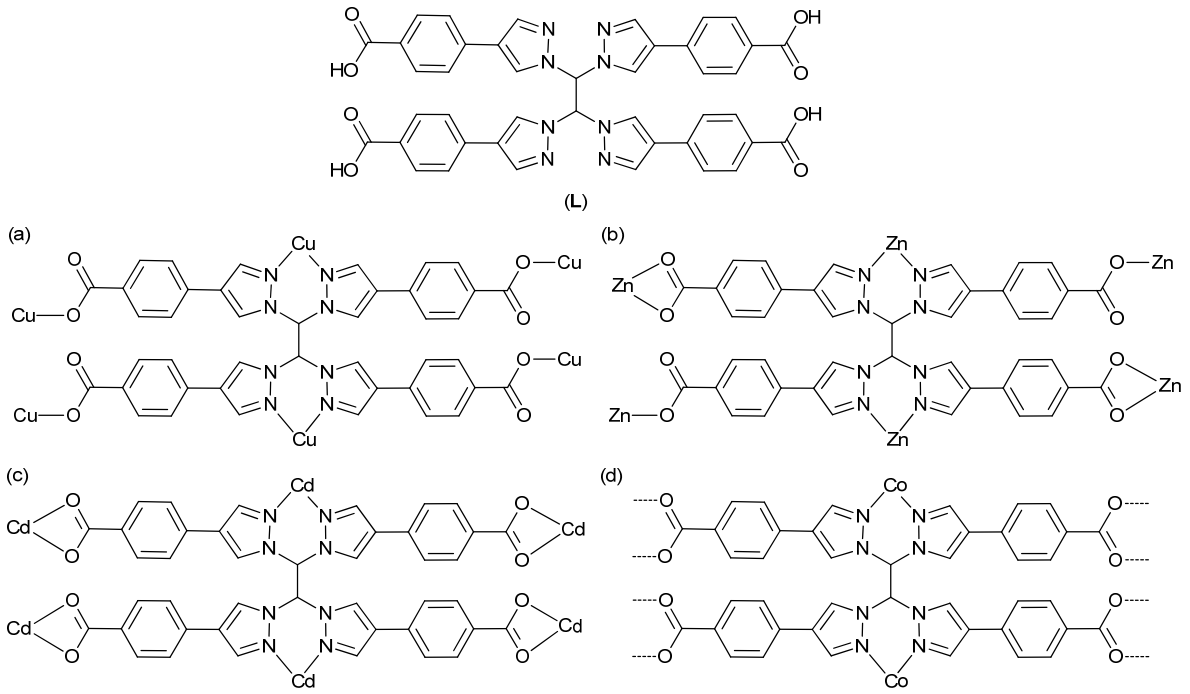

Chart 1. Coordination modes of **L** (top) in (a) $[Cu_2(\mathbf{L})(H_2O)_2]$, (b) $[Zn_2(\mathbf{L})]$, (c) $[Cd_2(\mathbf{L})]$ (Pink) and (d) $[Co_2(\mathbf{L})(H_2O)_6]$. The dashed bonds in (d) indicate hydrogen bonds with the carboxylate oxygen atoms acting as acceptors.

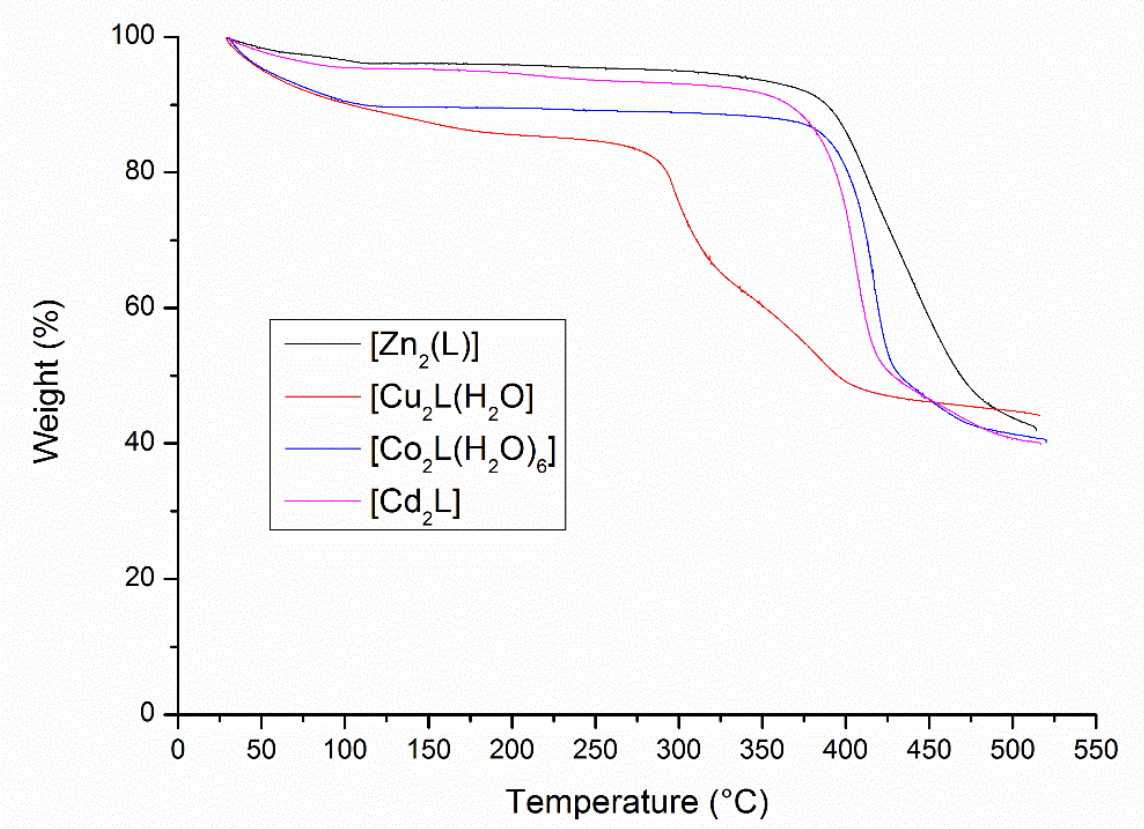

Figure SI 1. TGA traces of $[Cu_2(\mathbf{L})(H_2O)_2]$ (Red), $[Zn_2(\mathbf{L})]$ (Black), $[Cd_2(\mathbf{L})]$ (Pink) and $[Co_2(\mathbf{L})(H_2O)_6]$ (Blue) for the as-synthesised samples (washed in methanol). The small percentage of weight loss in the range 50-100°C is attributed to solvent removal (MeOH in the pores) before decomposition when the coordinated water molecules and ligands are lost.

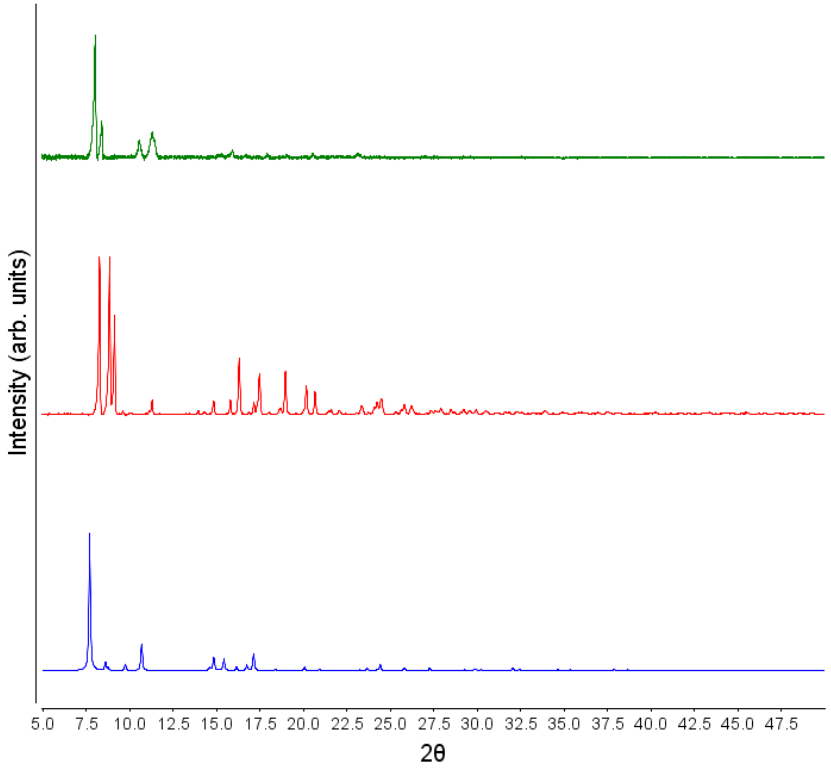

Figure SI 2. PXRD patterns for $[Cu_2(\mathbf{L})(H_2O)_2]$. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

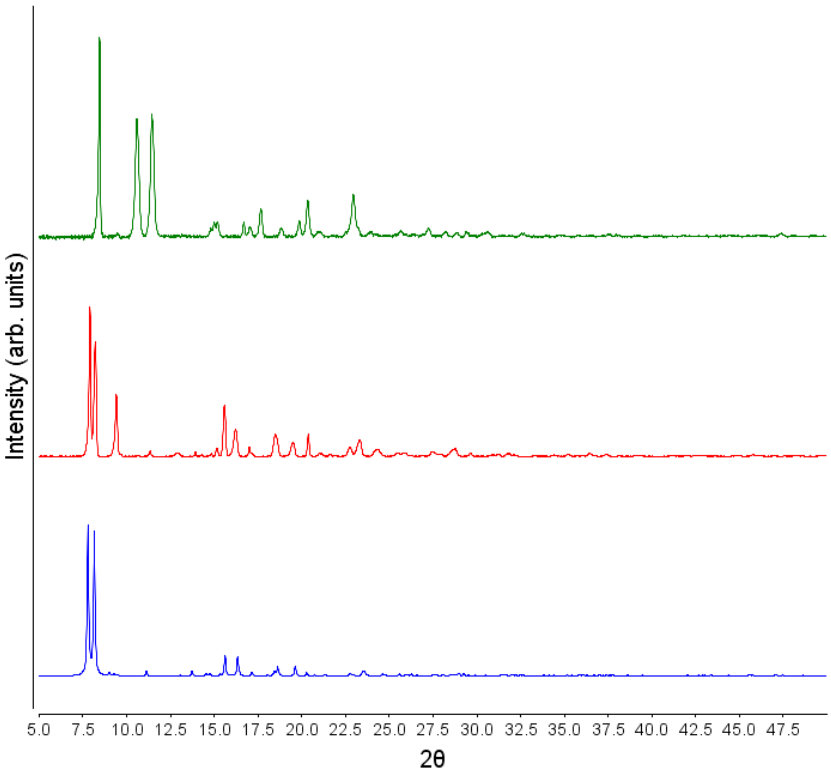

Figure SI 3. PXRD patterns for $[Zn_2(\mathbf{L})]$. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

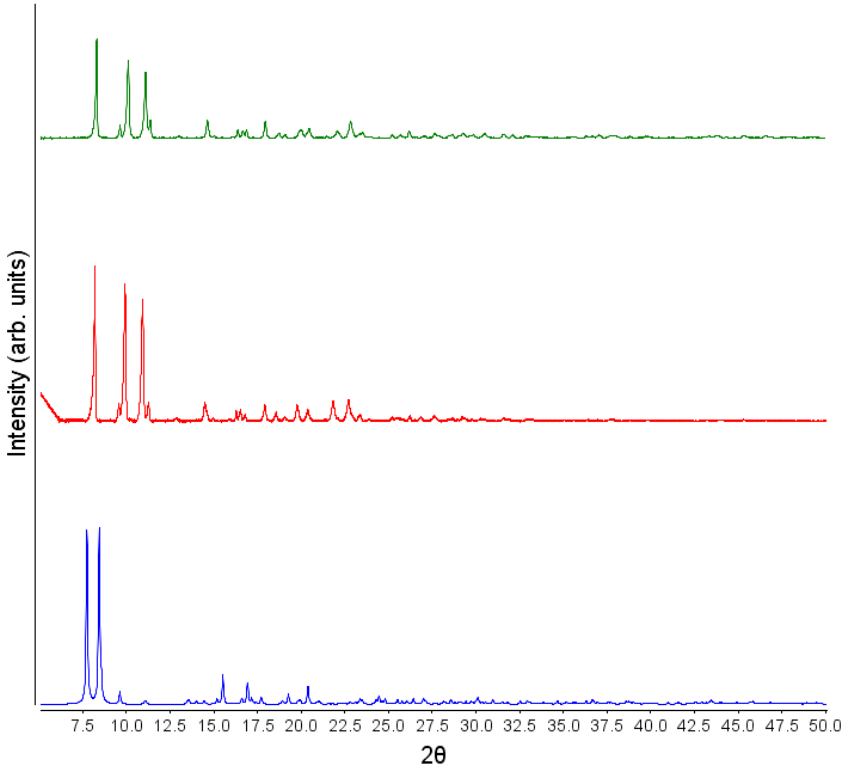

Figure SI 4. PXRD patterns for [Cd_2(**L**)]. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

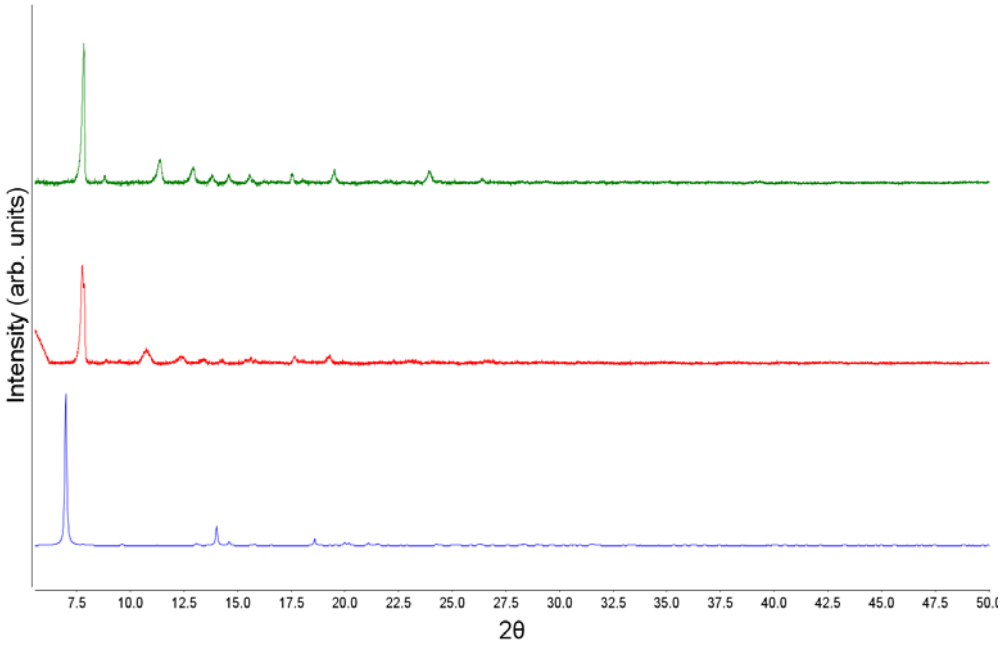

Figure SI 5. PXRD patterns for [Co_2(**L**)(H_2O)$_6$]. Simulated pattern (Blue), sample washed in DMF and MeOH (Red), and activated sample (Green).

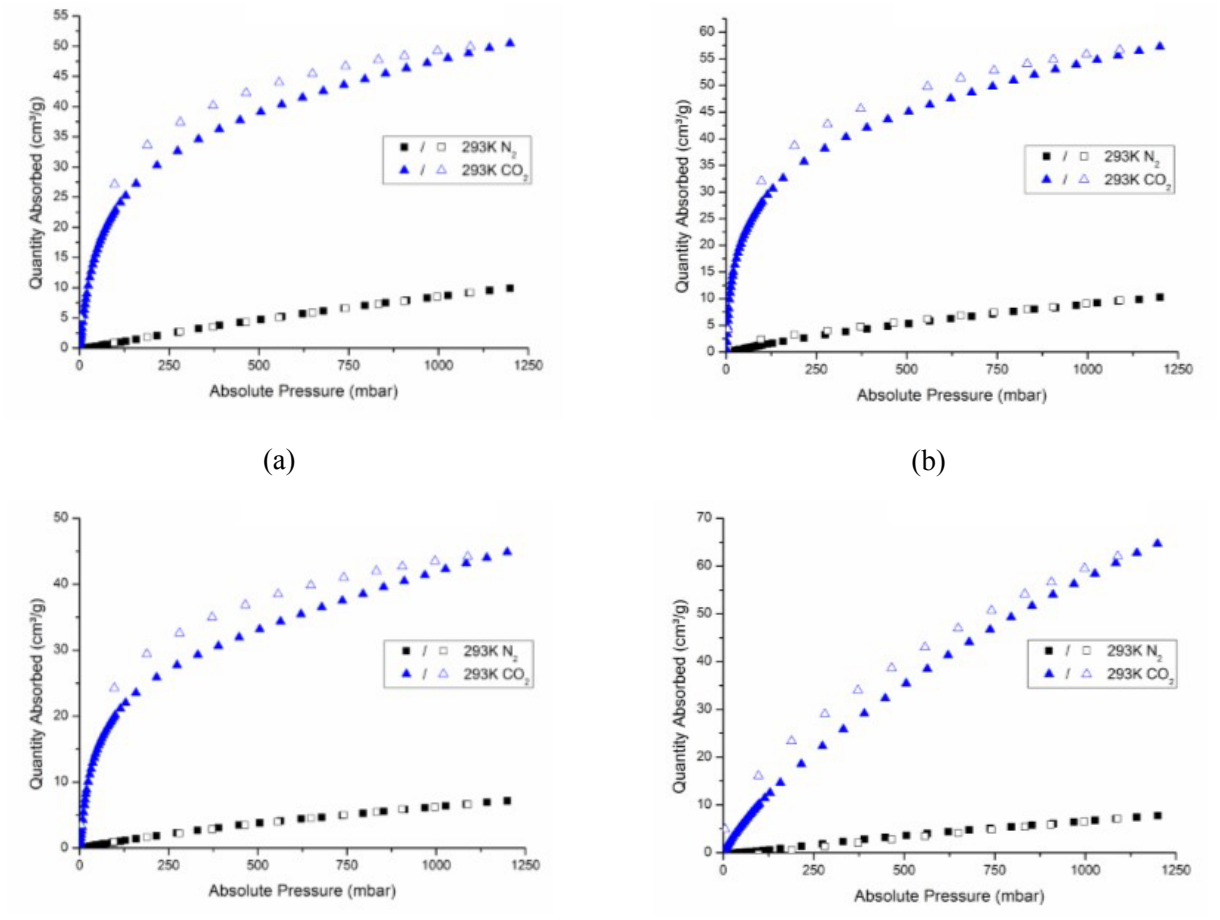

Figure SI 6. CO_2 and N_2 isotherms at 293 K for (a) $[Cu_2(\mathbf{L})(H_2O)_2]$, (b) $[Zn_2(\mathbf{L})]$, (c) $[Cd_2(\mathbf{L})]$ and (d) $[Co_2(\mathbf{L})(H_2O)_6]$.

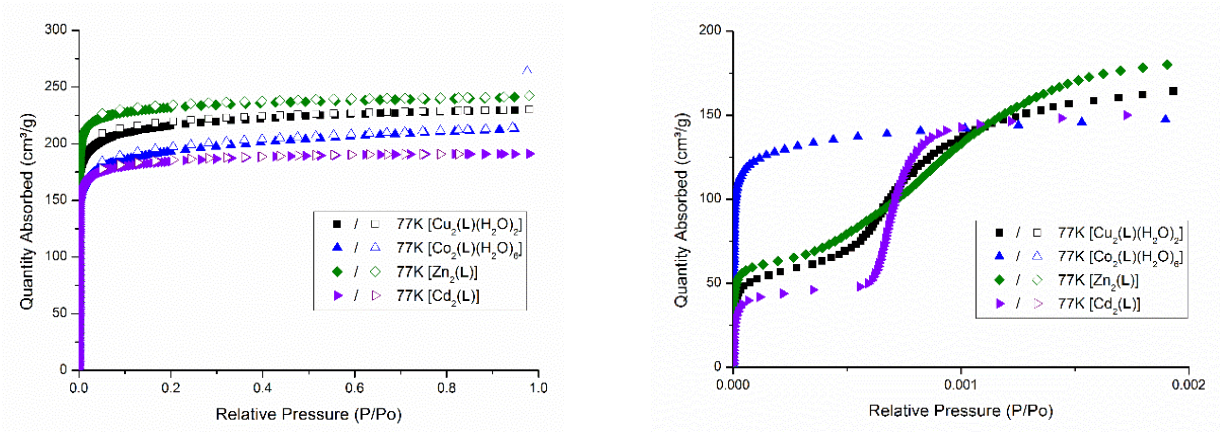

Figure SI 7. (a) 77 K N_2 adsorption isotherms for $[Cu_2(\mathbf{L})(H_2O)_2]$, $[Zn_2(\mathbf{L})]$, $[Cd_2(\mathbf{L})]$ and $[Co_2(\mathbf{L})(H_2O)_6]$. (b) Enlargements of the low pressure region of the 77 K N_2 adsorption isotherms.

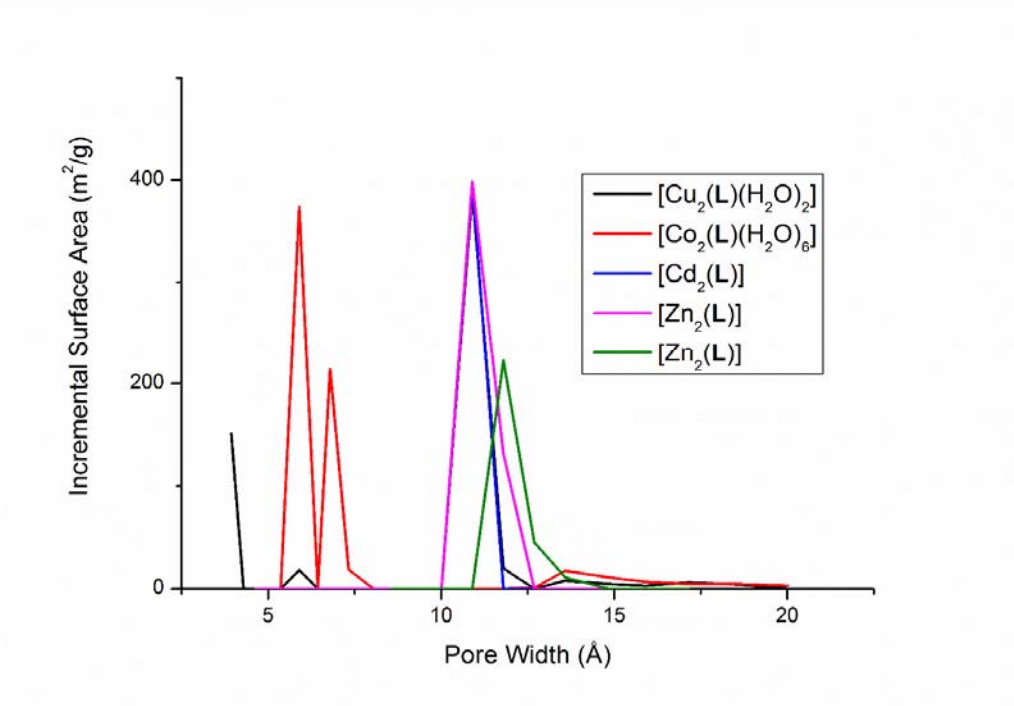

Figure SI 8. Pore size distribution calculated from the 77 K N_2 adsorption isotherms for $[Cu_2(\mathbf{L})(H_2O)_2]$, $[Zn_2(\mathbf{L})]$, $[Cd_2(\mathbf{L})]$ and $[Co_2(\mathbf{L})(H_2O)_6]$. The green trace shows the pore size distribution for a sample of $[Zn_2(\mathbf{L})]$ that had been soaked in water and reactivated from methanol (see Figure 5 in the manuscript for PXRD data.