

SUPPLEMENTARY MATERIAL

Tuning Packing, Structural Flexibility and Porosity in 2D Metal-Organic Frameworks by Metal Node Choice

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1. Additional Structural Information for β -ML1 and ML1 (M = Co(II) or Ni(II))

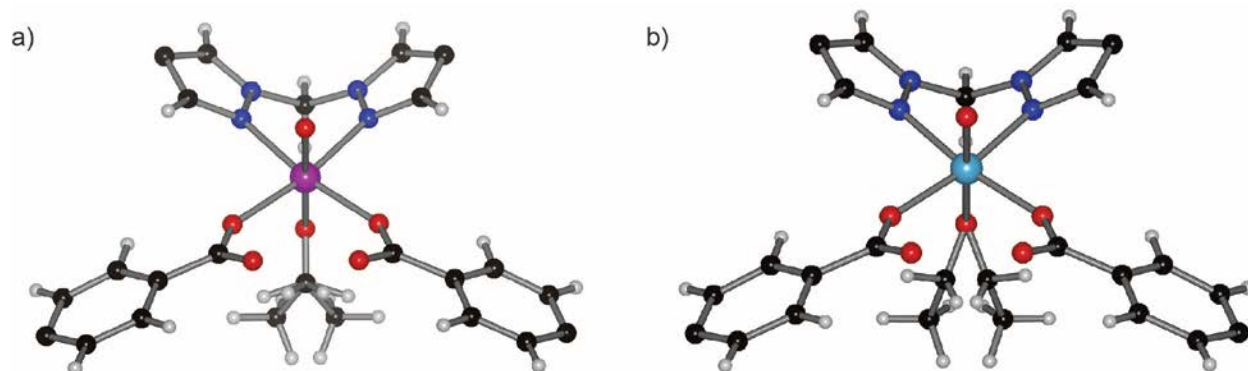


Figure S1. a) A view of the coordination sphere of the Co(II) and Ni(II) centres of (a) β -CoL1 and (b) β -NiL1 respectively. The hydrogen atoms of the water ligand could not be located in the difference map.

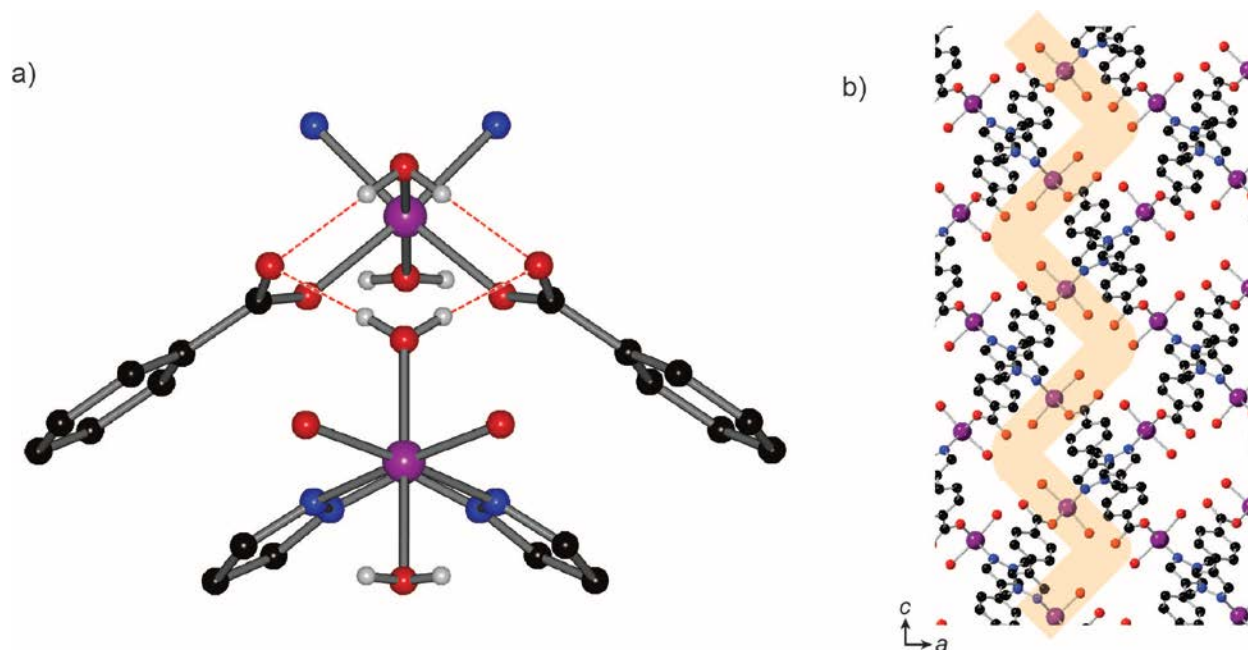


Figure S2. a) A view of the coordination sphere of the Co(II) centre of CoL1 highlighting the perpendicular relationship between the metal centres of two separate 2-D layers; b) the zig-zag conformation of the Co(II) metal centres viewed along the b axis (identical for NiL1).

2. Unit Cell Parameters for the Solvent Exchanged Forms of NiL1

Table S1. Unit cell parameters for the various solvent exchanged forms of NiL1.

Sample	Treatment	a (Å)	b (Å)	c (Å)	V (Å ³)
NiL1· xS	as-synthesised	11.2054(2)	20.1664(4)	13.3065(3)	3006.90(11)
NiL1·EtOH	ethanol exchanged	10.6799(2)	20.3654(3)	13.2980(3)	2892.32(9)
NiL1·MeOH	methanol exchanged	11.409(2)	20.322(4)	13.065(3)	3029.2(11)
NiL1·Tol	toluene exchanged	10.933(2)	20.875(4)	11.989(2)	2736.2(10)

3. Powder X-ray Diffraction

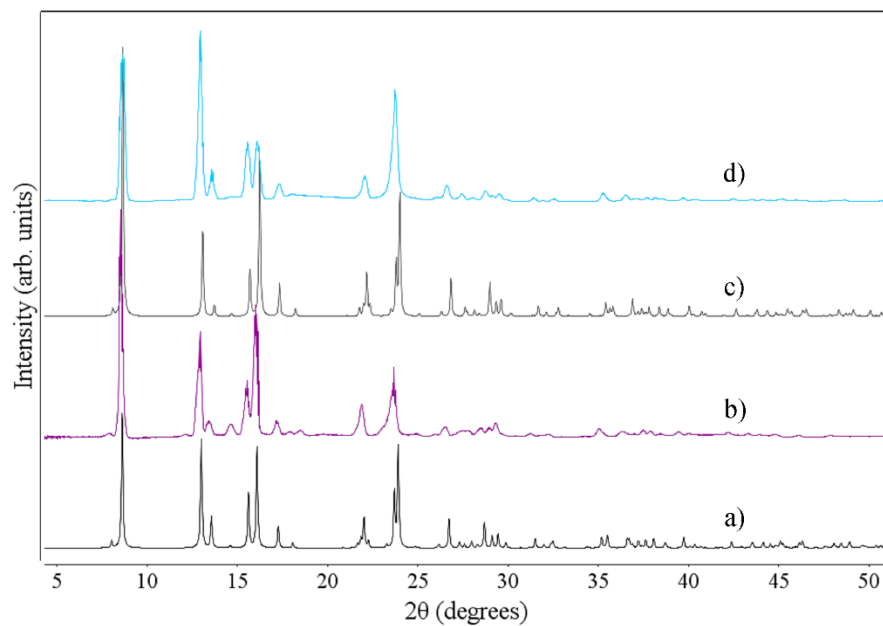


Figure S3. a) PXRD patterns of a) β -CoL1 simulated; b) β -CoL1 as-synthesised; c) β -NiL1 simulated; d) β -NiL1 as-synthesised.

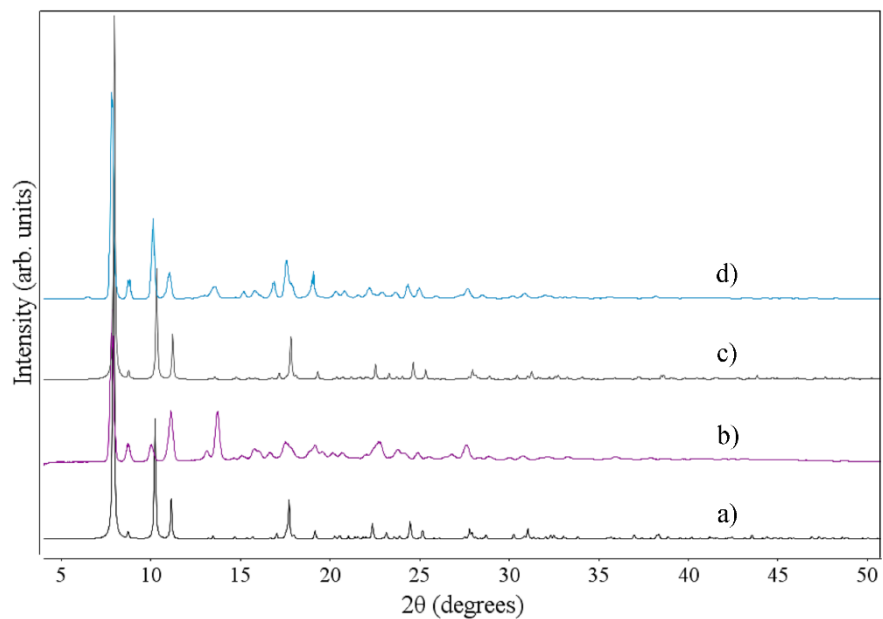


Figure S4. a) PXRD patterns of a) CoL1 simulated; b) CoL1 as-synthesised; c) NiL1 simulated; d) NiL1 as-synthesised.

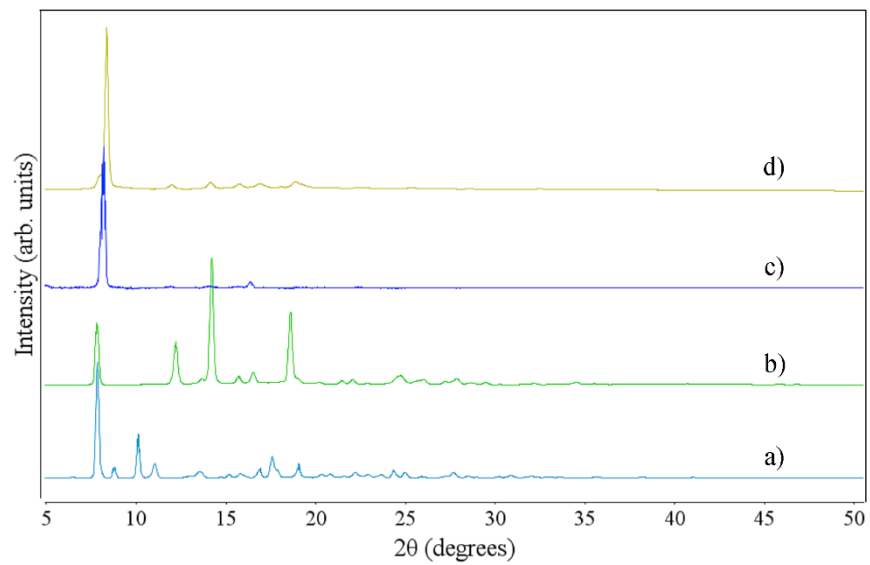


Figure S5. a) PXRD patterns of a) **NiL1** as-synthesised; b) **NiL1·xCH₃OH** heated to 100 °C; c) **CoL1** treated at 260 °C; d) **NiL1** treated at 260 °C.

4. Gas Adsorption

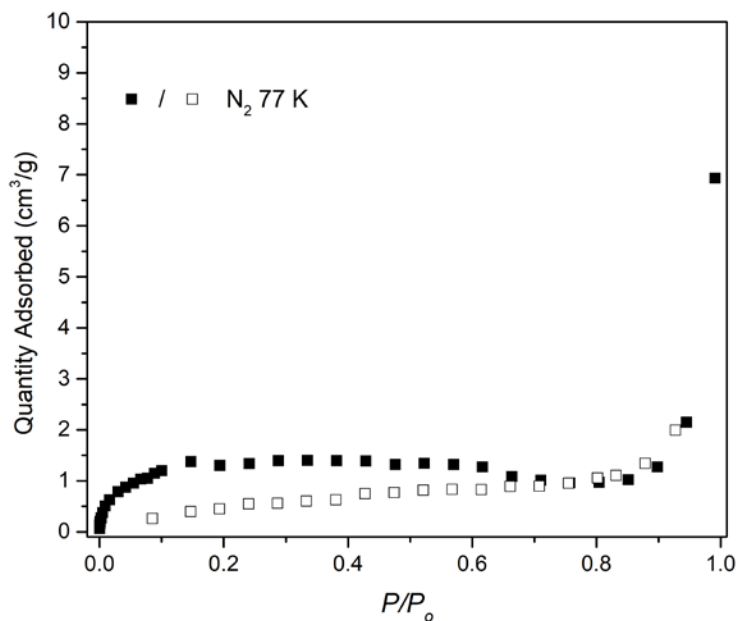


Figure S6. a) N₂ isotherm of NiL1-*ac* measured at 77 K. Filled and empty symbols represent the adsorption and desorption processes respectively.

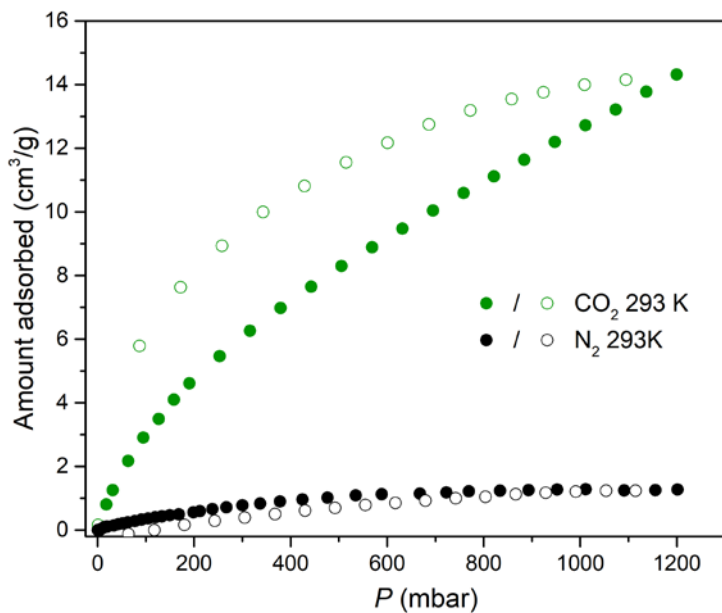


Figure S7. a) 293 K CO₂ and N₂ isotherms of NiL1-*ac*. Filled and empty symbols represent the adsorption and desorption processes respectively.