Electronic Supplementary Material (ESI) for CrystEngComm

Synthesis and property investigation of two hexa-cobalt cluster based porous coordination polymers

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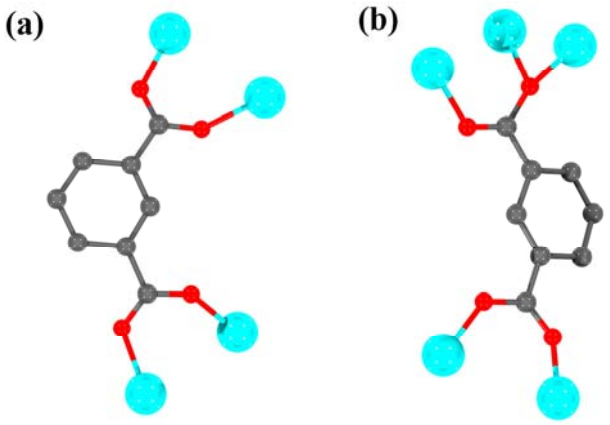

Fig. S1 The coordination modes of ip ligands in compound **1**.

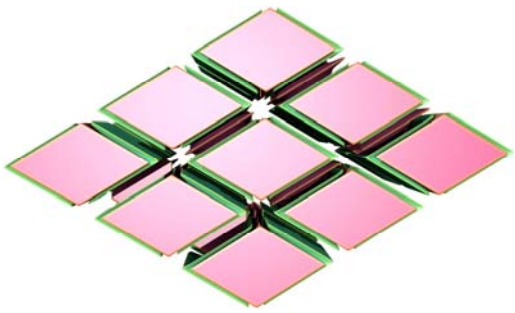

Fig. S2 The natural tiling of the network of **1**.

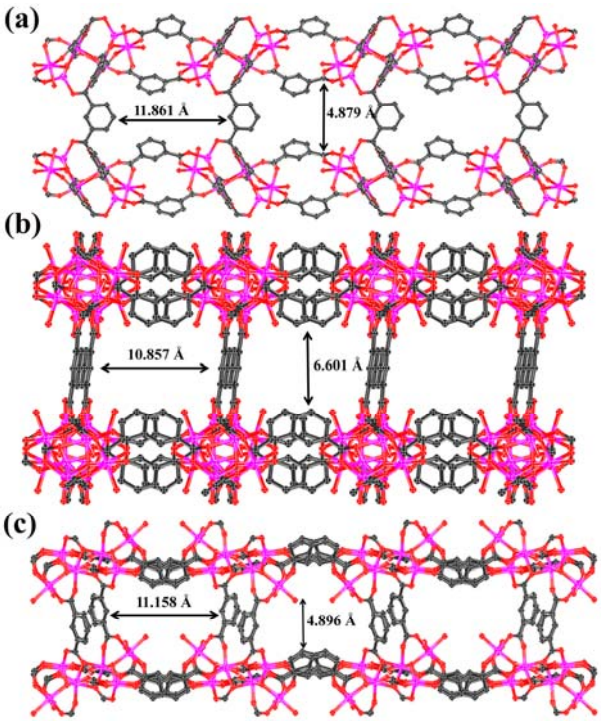

Fig. S3 The dimensions of channels along *a*, *b*, and *c* axes (up to down) in compound **1**.

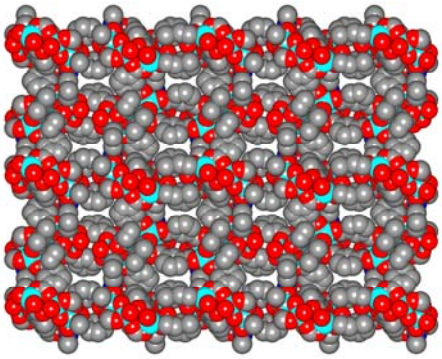

Fig. S4 The channel along the *c* direction in **2**. The hydrogen atoms of the ligands are omitted for clarity.

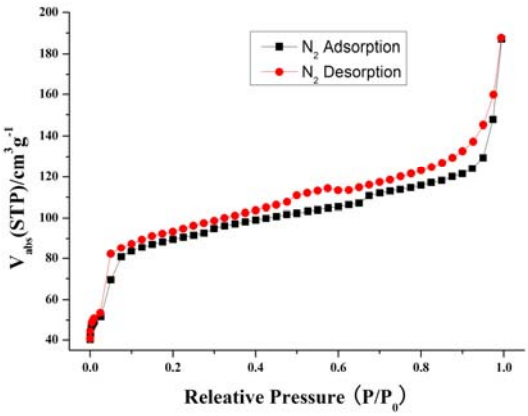

Fig. S5 N_2 sorption isotherms of **1**.

N_2 sorption measurement The synthesized crystals were allowed to stand at room temperature for a duration of 7 days. Approximately every 24 h, the solution was decanted, and the crystals were washed with CH_2Cl_2 (3×10 mL) before fresh CH_2Cl_2 (10 mL) was added. This process was repeated three times. At the end, the CH_2Cl_2 solution was decanted, and the crystals were washed with CH_2Cl_2 (2×10 mL) and soaked in pure CH_2Cl_2 (10 mL) for four days until needed.

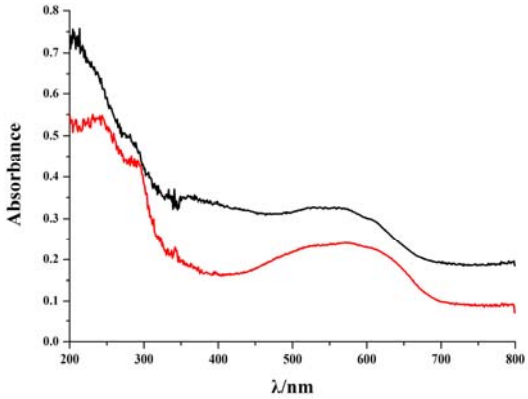

Fig. S6 The diffuse reflectance UV-Vis absorption spectra of the purple and blue crystals of **1**.

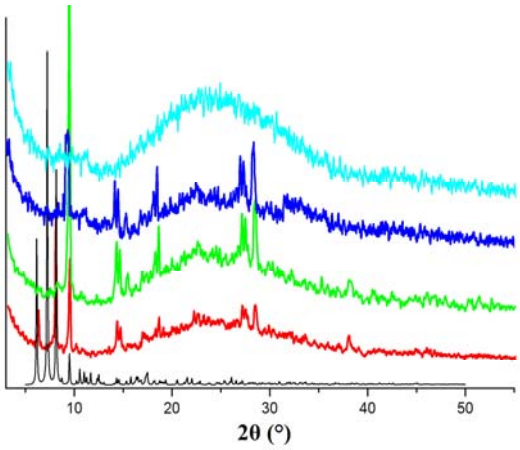

Fig. S7 Experimental and simulated powder X-Ray diffraction patterns for **1** (black: simulated; red: experimental; green: desolvated; blue: upon heating; cyan: upon water vapor).

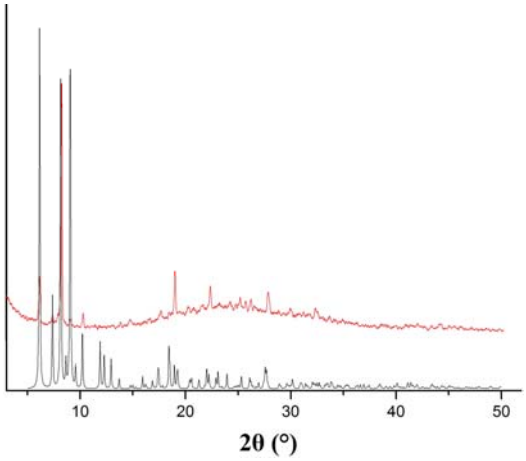

Fig. S8 Experimental and simulated powder X-Ray diffraction patterns for **2** (black: simulated; red: experimental).

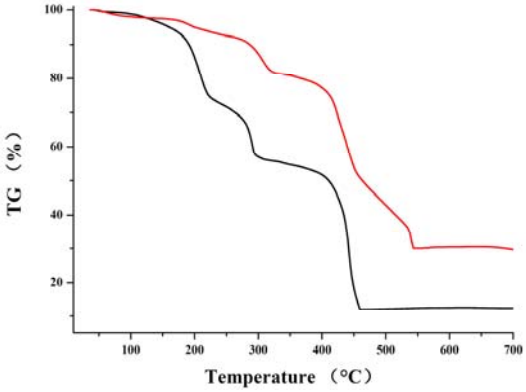

Fig. S9 TG profile of **1** (black) and evacuated **1** (red).

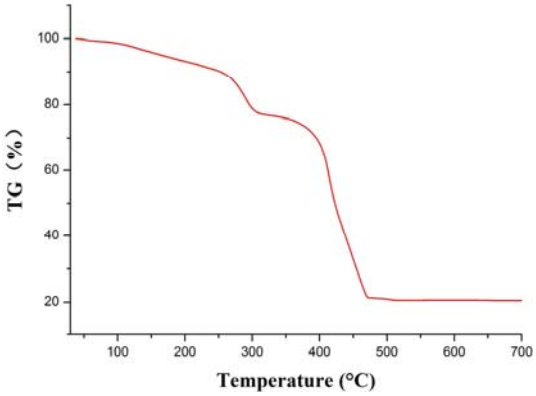

Fig. S10 TG profile of **2**.