

Supporting Information

Porous coordination polymers with zeolite topologies constructed from 4-connected building units

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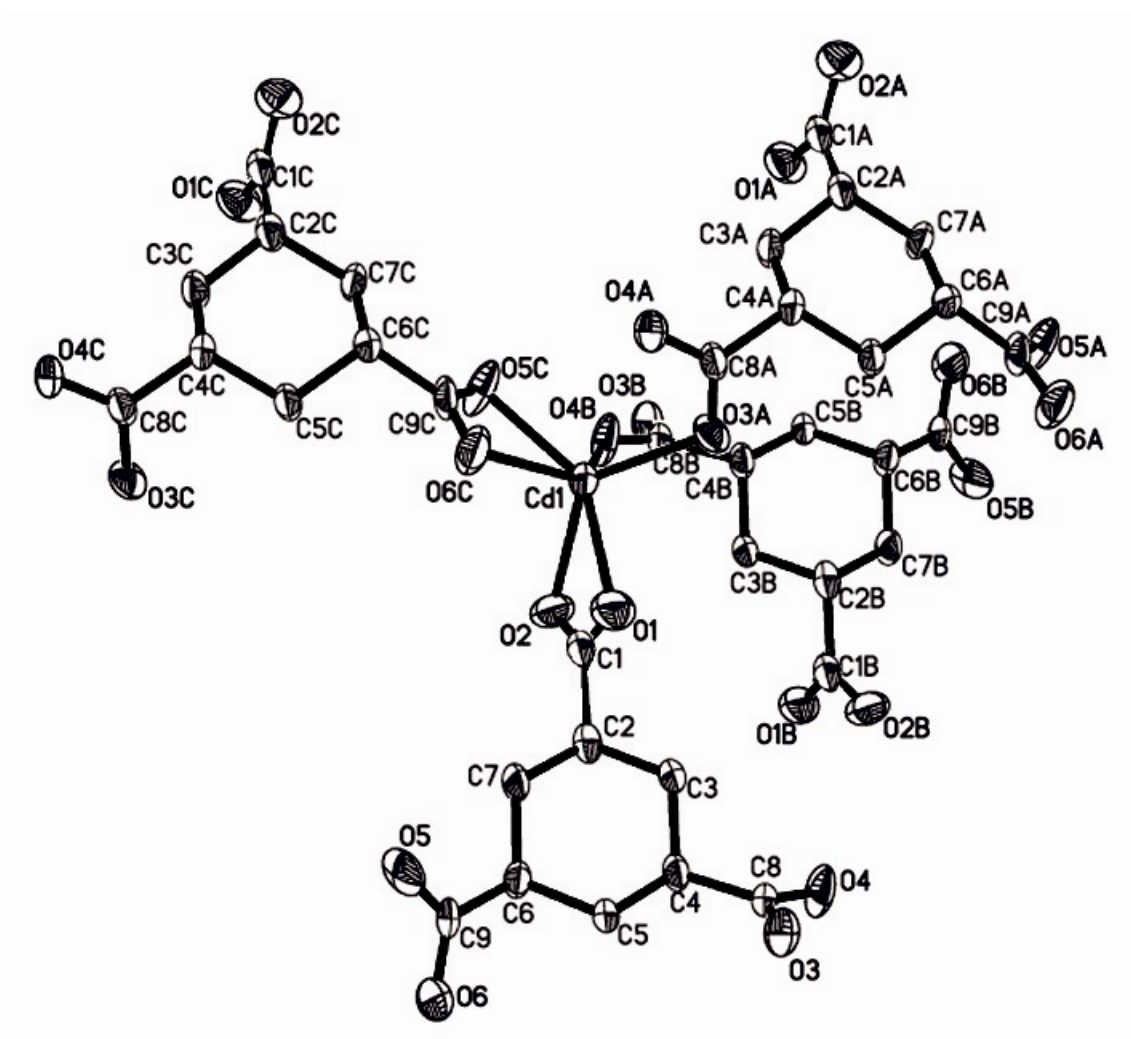


Fig. S2 ORTEP drawing (at 50% probability) of the coordination environment of cadmium ion in **2**. Hydrogen atoms have been omitted for clarity. Symmetry operations: A $-x+2, y-1/2, -z+1/2$; B $-x+1, y-1/2, -z+1/2$; C $-x+1, -y, -z$.

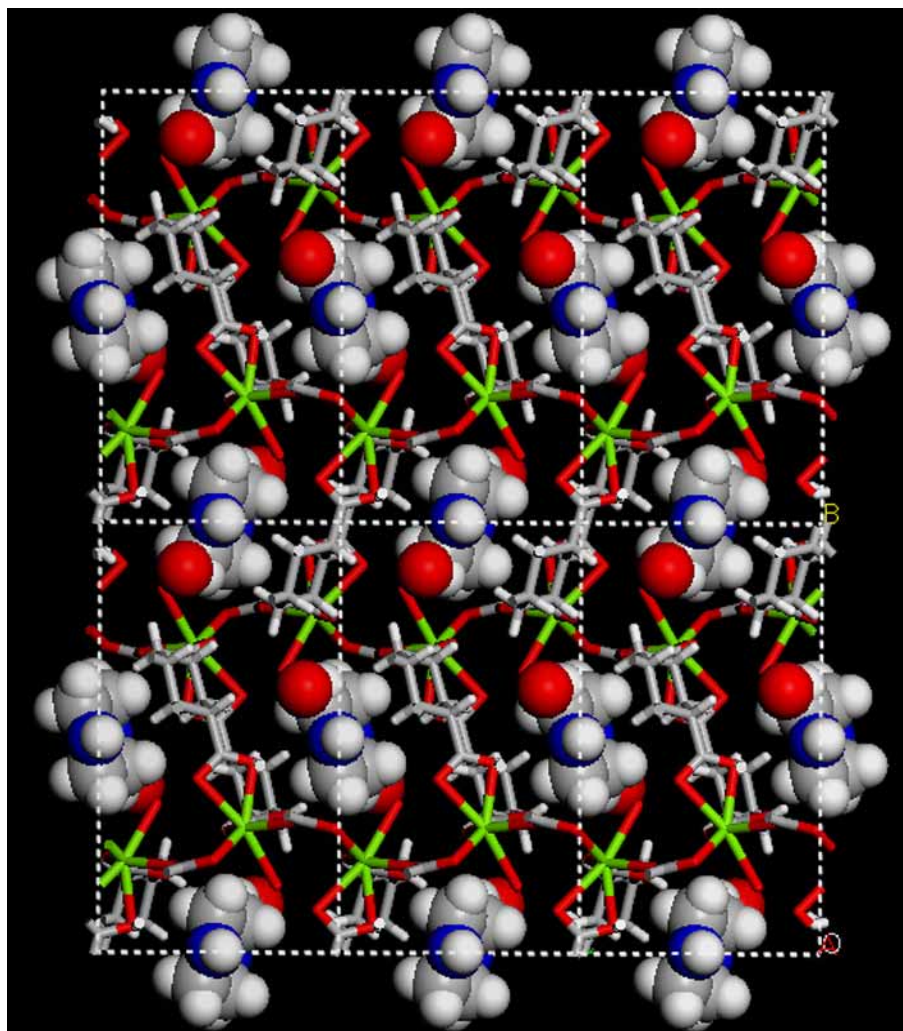


Fig. S3 Infinite three-dimensional coordination framework of **1** is shown along the [100] direction, where the vacancies are occupied by PIP and H₂O guest molecules (drawn in space-filling style). Color code: Cd green, C gray, H white, N blue, O red.

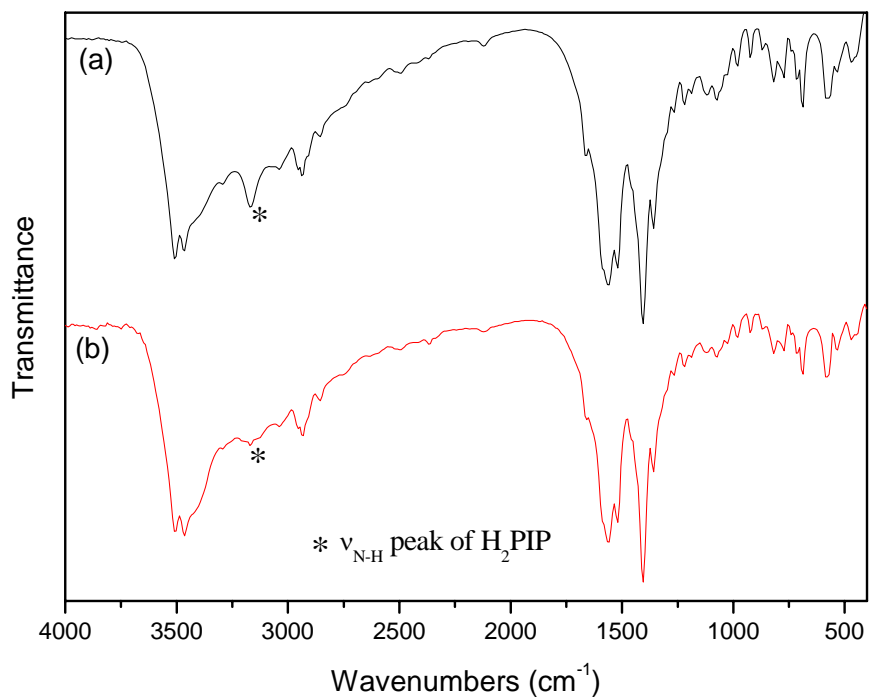


Fig. S4 IR spectra of the polymer **1**: (a) as-synthesized and (b) exchanged. FT-IR (KBr): $\bar{\nu} = 3509$ (m), 3463 (m), 3170 (m), 2939 (m), 1658 (w), 1558 (s), 1519 (m), 1404 (s), 1357 (m), 1218 (w), 1118 (w), 1072 (w), 979 (w), 925 (w), 817 (w), 771 (w), 686 (m), 578 (m), 470 (w) cm^{-1} .

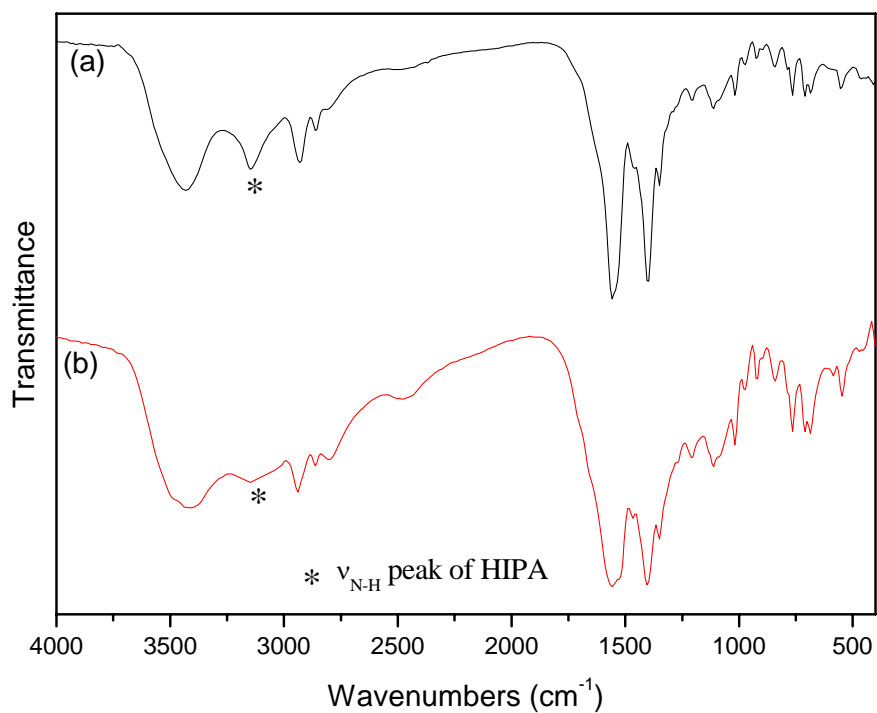


Fig. S5 IR spectra of the polymer **2**: (a) as-synthesized and (b) exchanged. FT-IR (KBr): $\bar{\nu} = 3432$ (m), 3147 (m), 2931 (m), 2861 (w), 1558 (s), 1396 (s), 1349 (w), 1203 (w), 1111 (m), 1018 (w), 971 (w), 925 (w), 848 (w), 763 (m), 709 (w), 686 (w), 547 (w) cm⁻¹.

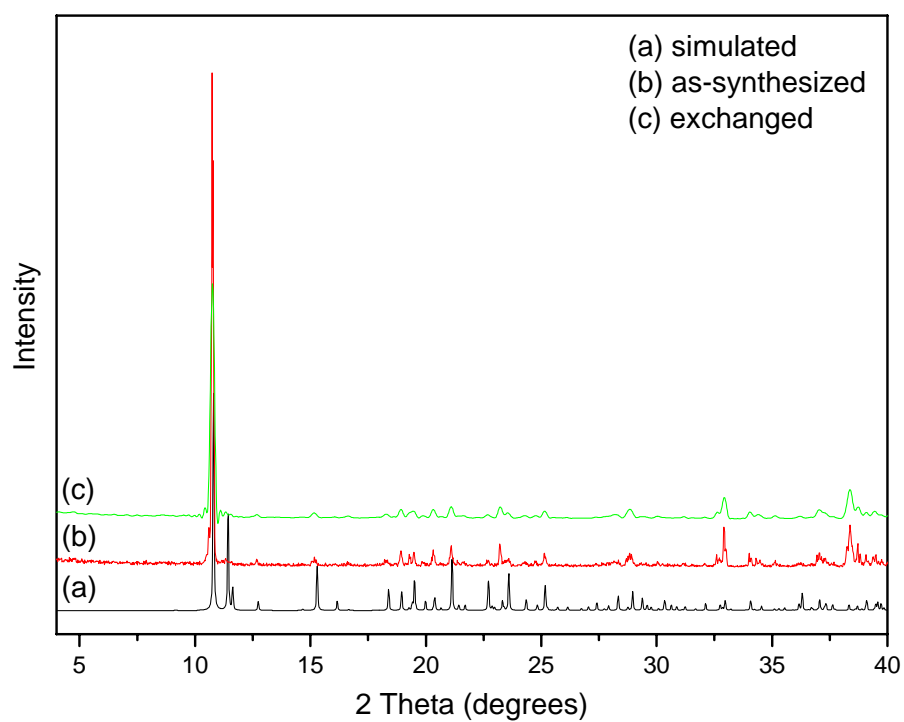


Fig. S6 Power XRD patterns of the polymer **1**: (a) simulated, (b) as-synthesized and (c) exchanged.

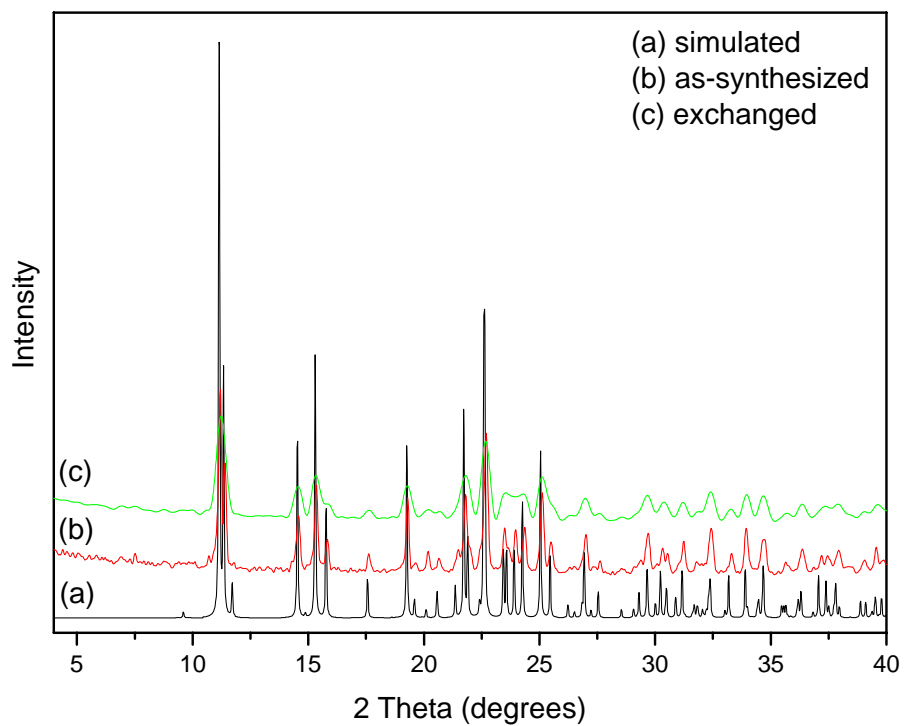


Fig. S7 Power XRD patterns of the polymer **2**: (a) simulated, (b) as-synthesized and (c) exchanged.

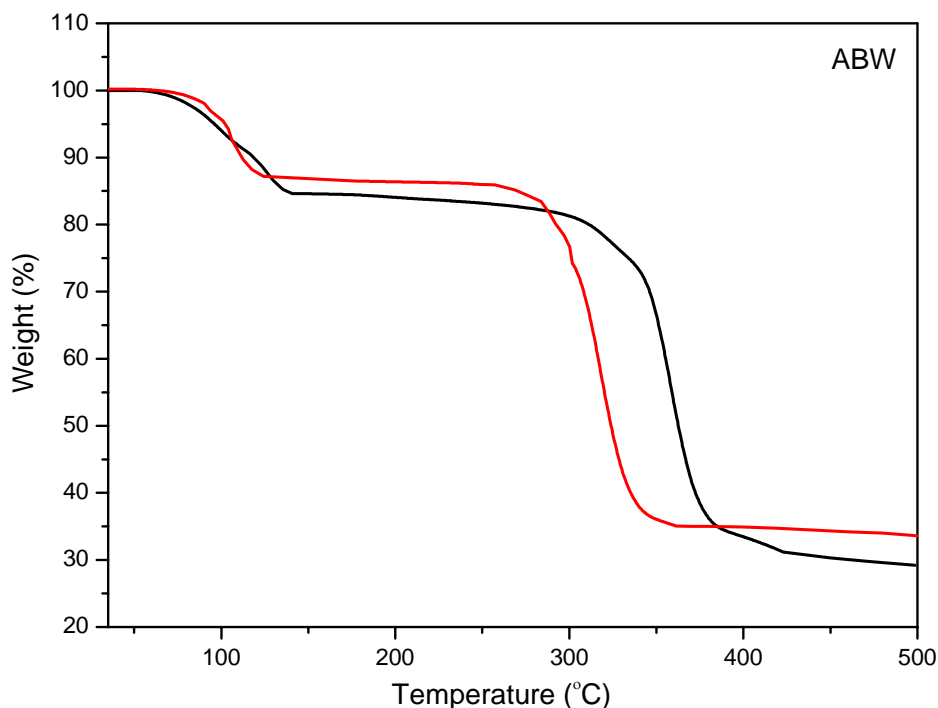


Fig. S8 The thermogravimetric analysis (TGA) curves of **1** in air: as-synthesized (black line) and exchanged (red line). The TGA curve of as-synthesized **1** shows that the weight loss of 15.37 % between 50 and 140 °C corresponds to the loss of a guest H₂O and 0.5 guest PIP (calculated 15.30 %). Decomposition of **1** began above 300 °C. The residue was CdO (experimental: 31.60 % and calculated: 31.65 %). Elemental analysis and inductively coupled plasma (ICP) analysis: C 32.51, H 4.92, N 3.39, Cd 27.66 % (calcd: C 32.57, H 4.72, N 3.45, Cd 27.71 %). The TGA curve of exchanged **1** shows that the weight loss of 13.20 % between 70 and 125 °C corresponds to the loss of 0.38 guest PIP and a coordinated H₂O (calculated 13.49 %). Decomposition of exchanged **1** began above 260 °C. The residue was CdO and K₂O (experimental: 35.06 % and calculated: 35.11 %). Elemental analysis and ICP analysis for Cd(CTC)(H₂O) · (H₂PIP)_{0.32} · K_{0.18}: C 32.51, H 3.86, N 2.31, Cd 29.61, K 1.80 % (Calcd: C 32.59, H 3.95, N 2.37, Cd 29.67, K 1.86 %).

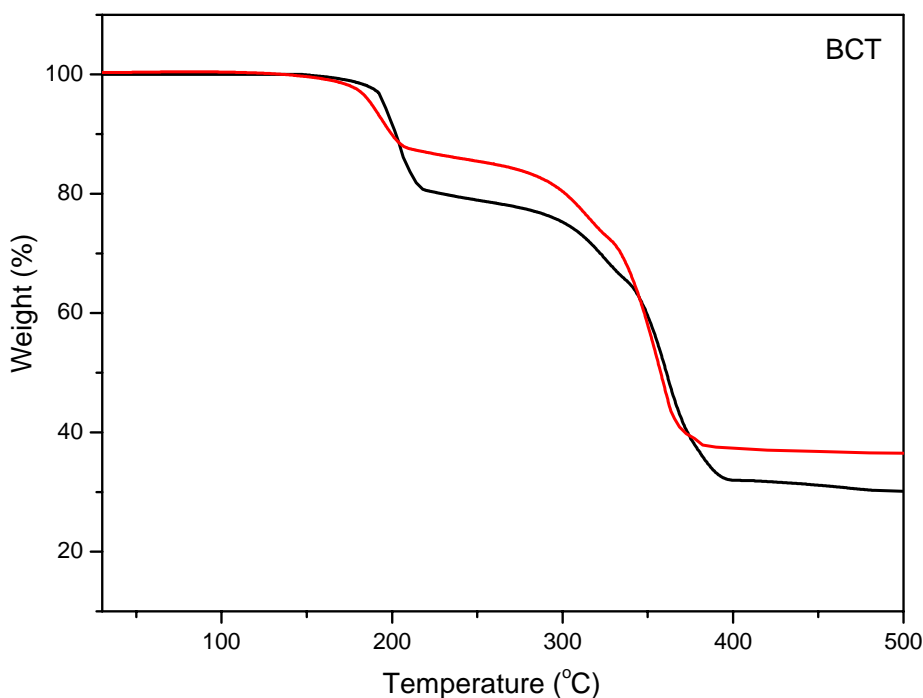


Fig. S9 The thermogravimetric analysis (TGA) curves of **2** in air: as-synthesized (black line) and exchanged (red line). The TGA curve of **2** shows that the weight loss of 19.15 % from 150 to 218 °C is attributed to the loss of a guest IPA (calculated 18.95 %). Decomposition of **2** began about 300 °C. The residue was CdO (experimental: 32.12 % and calculated: 31.97 %). Elemental analysis and ICP analysis: C 35.82, H 4.52, N 3.36, Cd 27.91 % (calcd: C 35.88, H 4.77, N 3.49, Cd 27.98 %). The TGA curve of exchanged **2** shows that the weight loss of 11.66 % between 140 and 205 °C corresponds to the loss of 0.59 guest HIPA (calculated 11.62 %). Decomposition of exchanged **2** began above 270 °C. The residue was CdO and K₂O (experimental: 38.01 % and calculated: 38.22 %). Elemental analysis and ICP analysis for Cd(CTC) · (HIPA)_{0.59} · K_{0.41}: C 33.39, H 3.94, N 2.11, Cd 29.11, K 4.18 % (Calcd: C 33.47, H 3.89, N 2.14, Cd 29.08, K 4.15 %).