Supporting Information for

Self-adaptation of a conformationally flexible yet restricted "piperazine-pyrazine" building block toward the design of coordination polymers

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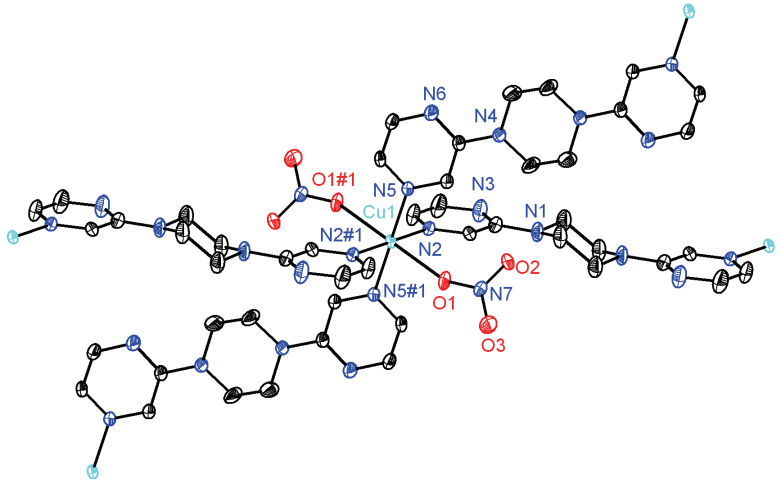

Fig. S1 ORTEP plot of the coordination environment around Cu^{2+} ion in **1** with 50% thermal ellipsoid probability. Symmetric code: #1 –x, –y+2, –z+1.

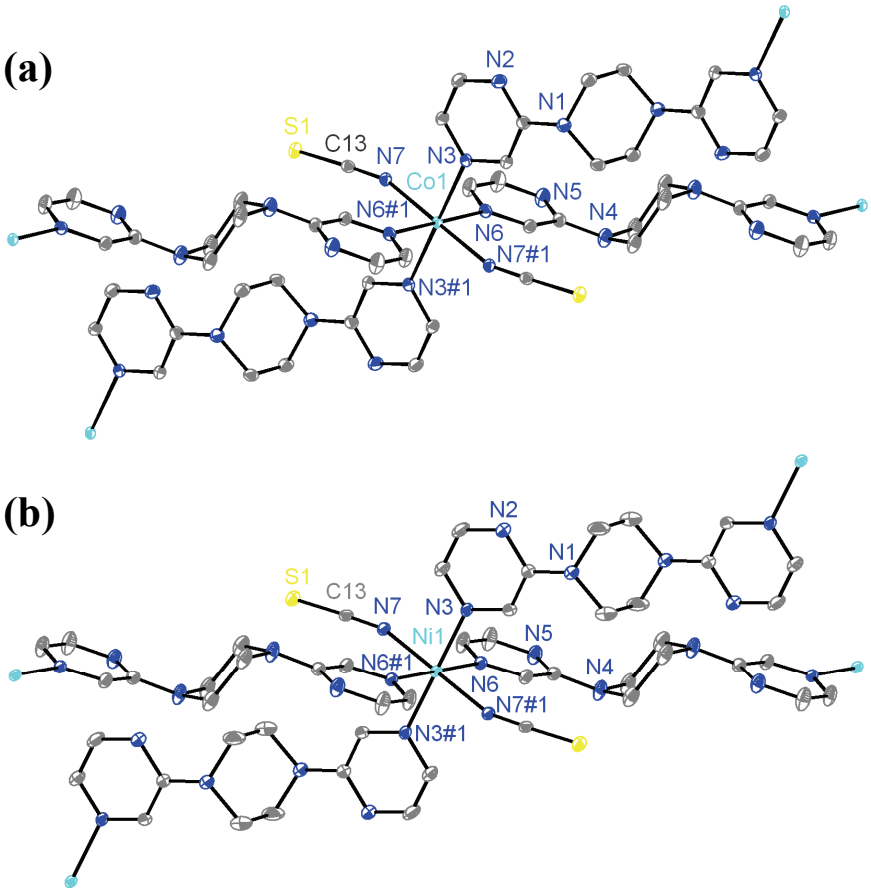

Fig. S2 (a) ORTEP plot of the coordination environment around Co^{2+} ion in **2** with 30% thermal ellipsoid probability. Symmetric code: #1 –x+1/2, –y+3/2, –z. (b) ORTEP plot of the coordination environment around Ni^{2+} ion in **3** with 15% thermal ellipsoid probability. Symmetric code: #1 –x+1/2, –y+3/2, –z.

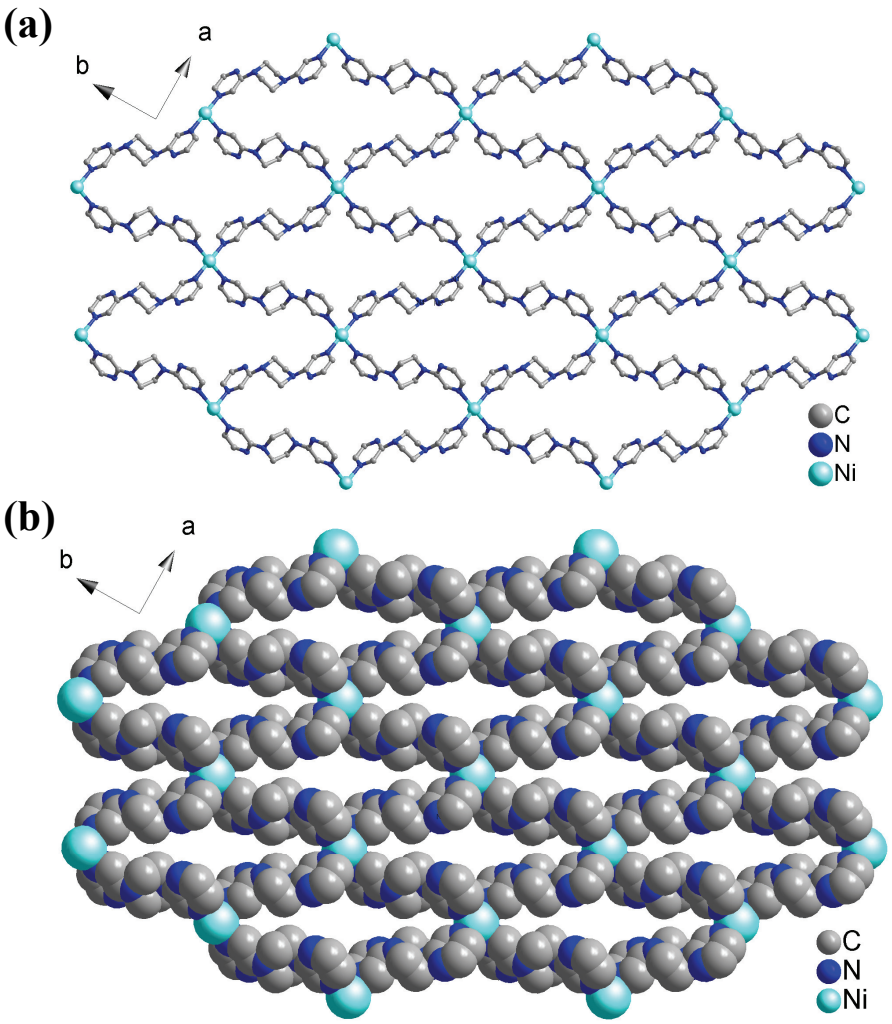

Fig. S3 (a) Ball-and-stick and (b) space-filling representations of the Ni(bpzp)-based topologically (4,4)-layer structure with each metal center as a four-connected node and each bpzp ligand as a 2-connected linear linkage in **3**. Thiocynate anions and hydrogen atoms are omitted for clarity.

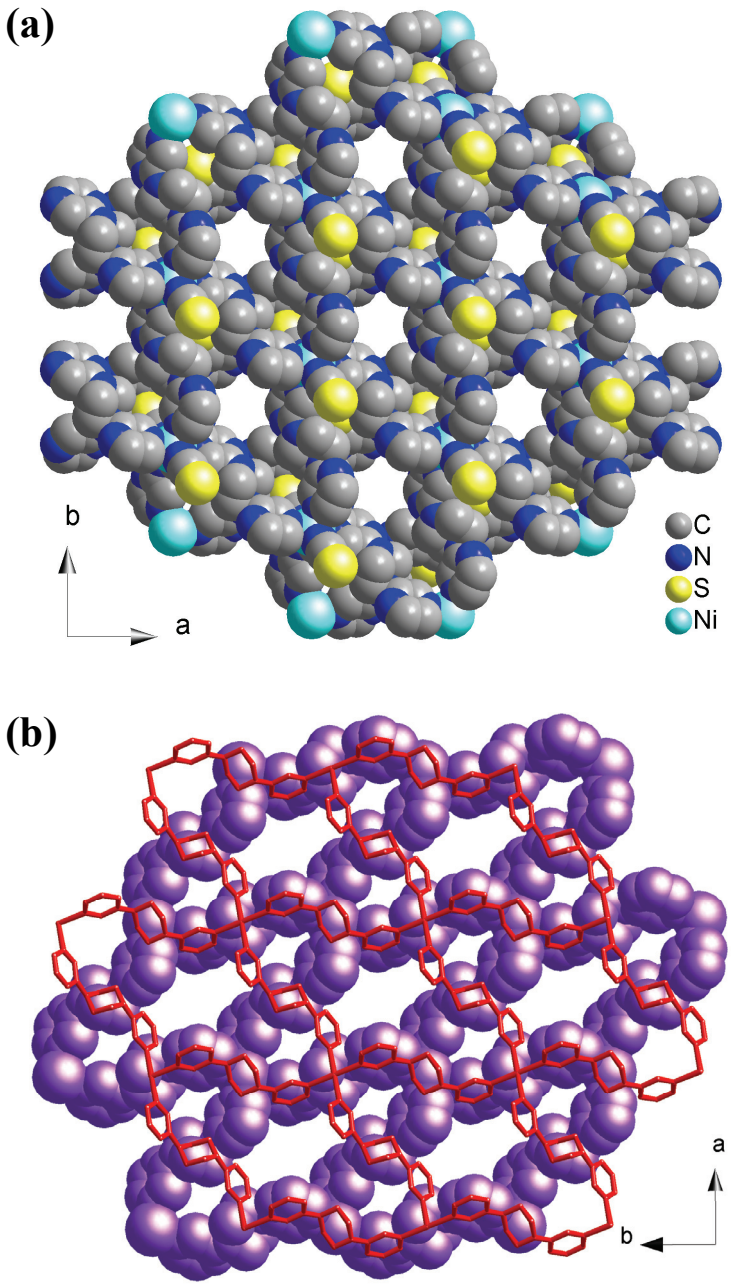

Fig. S4 Packing diagrams of **3**: (a) Space-filling model showing hexagonal-shaped channel openings along the crystallographic *c*-axis. (b) Highlighting the ABAB layer-stacking with a rotation angle of 60° between the two neighboring layers.

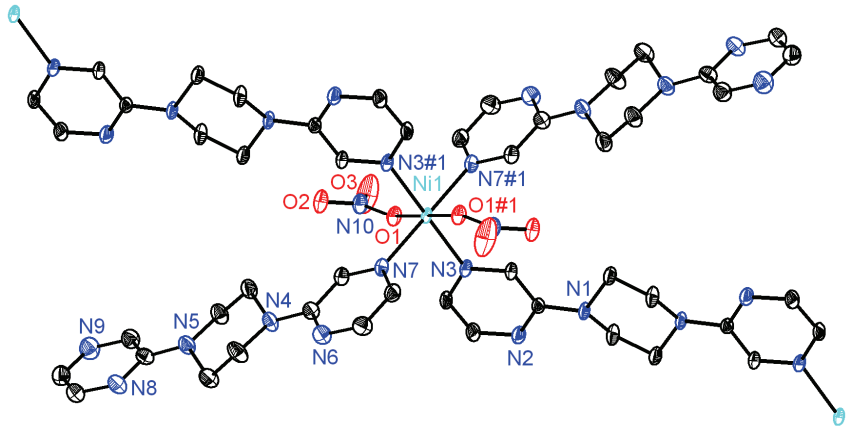

Fig. S5 ORTEP plot of the coordination environment around Ni^{2+} ion in **4** with 50% thermal ellipsoid probability. Symmetric code: #1 –x+1, –y+1, –z+1.

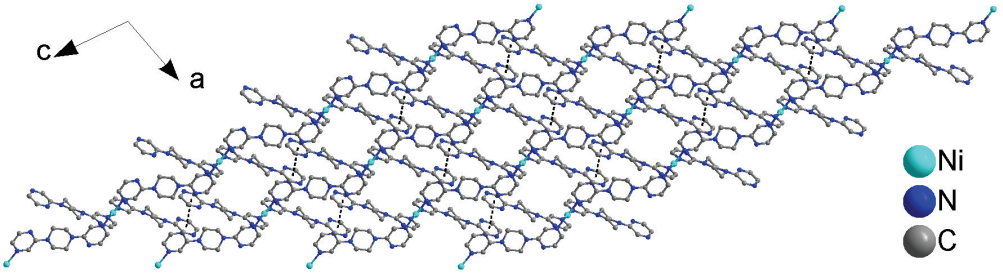

Fig. S6 Weak π–π interactions (dashed lines) assisted 2D supramolecular layer structure in **4** viewed down the crystallographic *b*-axis. Nitrate anions and hydrogen atoms are omitted for clarity.

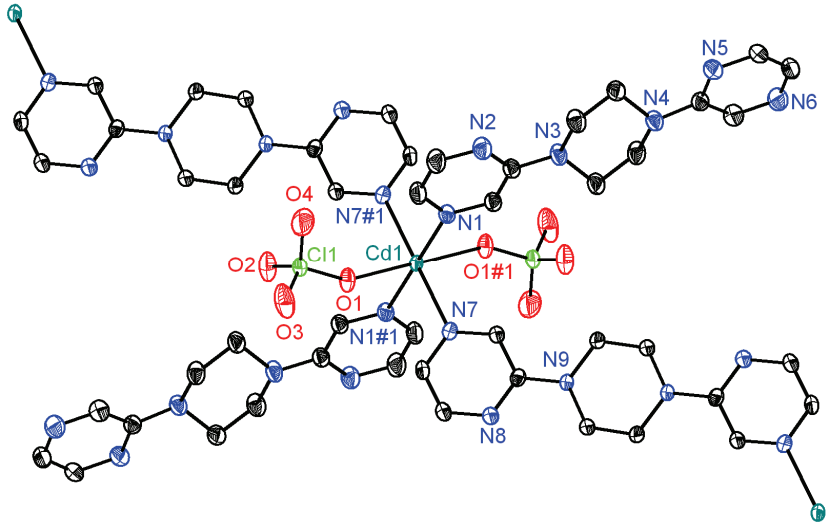

Fig. S7 ORTEP plot of the coordination environment around Cd^{2+} ion in **5** with 50% thermal ellipsoid probability. Symmetric code: #1 –x+2, –y, –z+1.

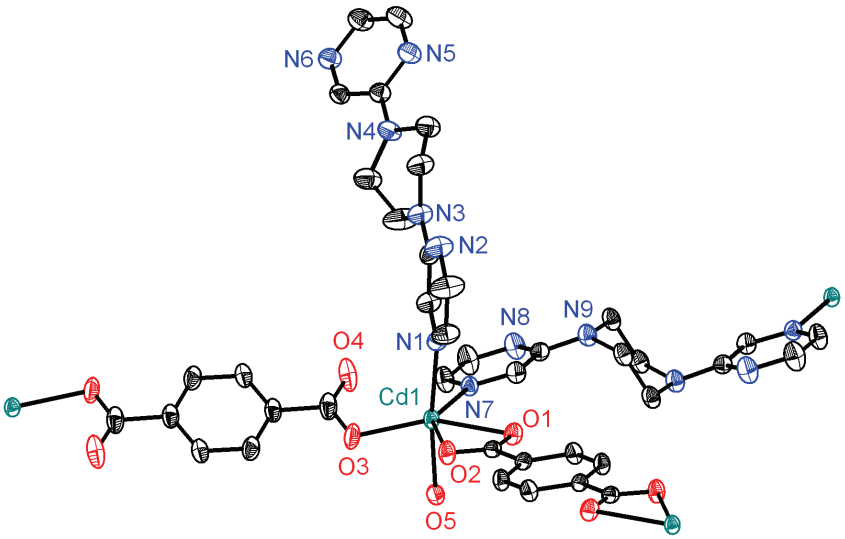

Fig. S8 ORTEP plot of the coordination environment around the Cd^{2+} ion in **6** with 50% thermal ellipsoid probability. The hydrogen atoms are omitted for clarity.

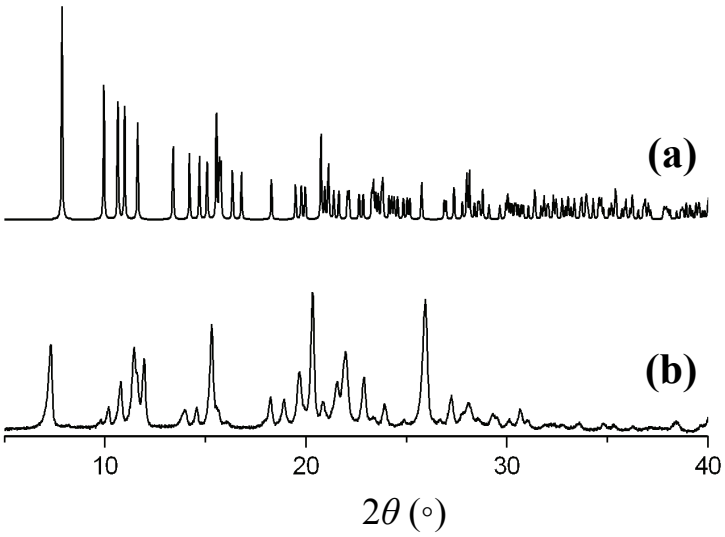

Fig. S9 Powder X-ray diffraction patterns of **1**·3H_2O. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

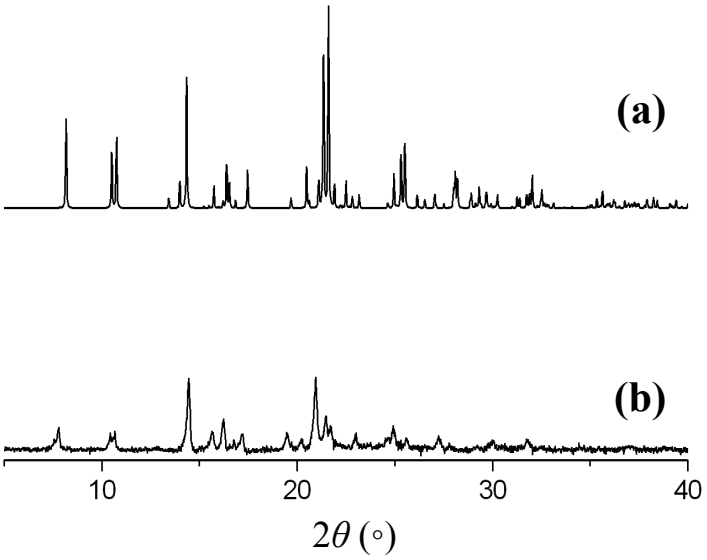

Fig. S10 Powder X-ray diffraction patterns of **2**·CH_2Cl_2·2CH_3OH. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

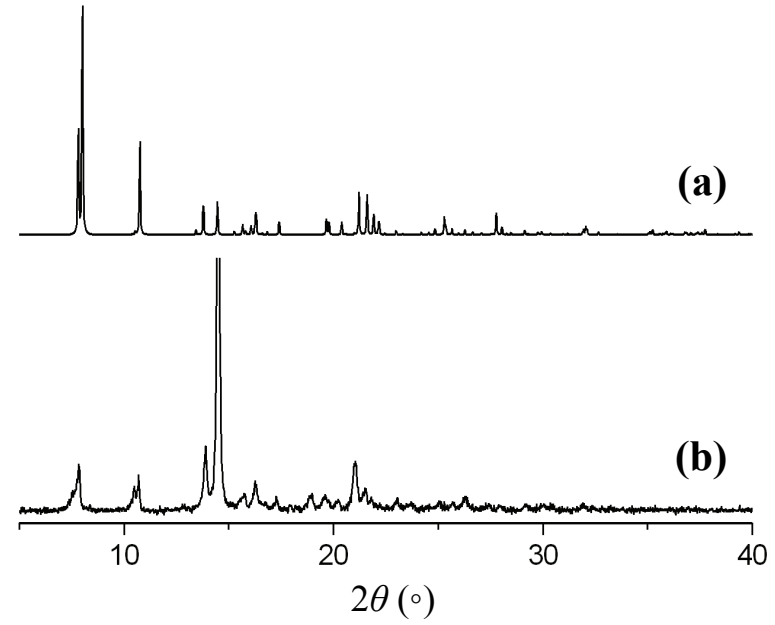

Fig. S11 Powder X-ray diffraction patterns of **3**·4CH_3OH. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

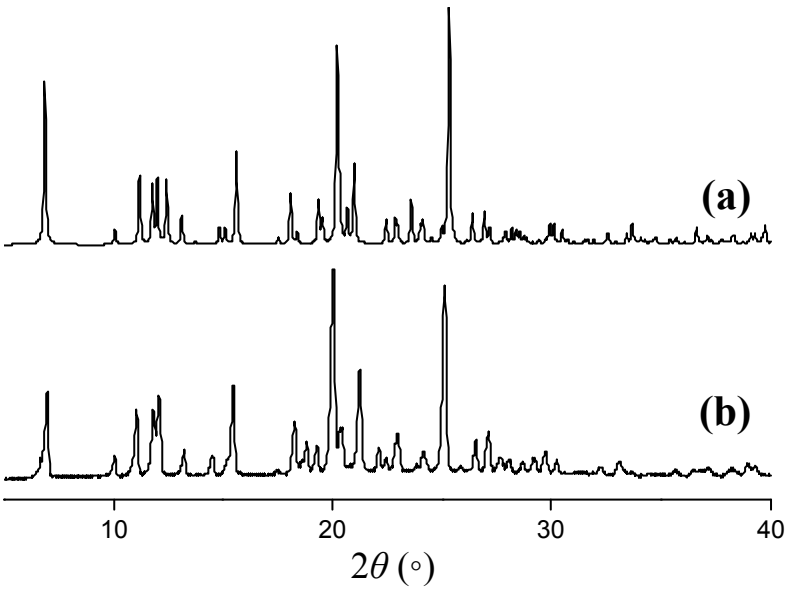

Fig. S12 Powder X-ray diffraction patterns of **4**. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

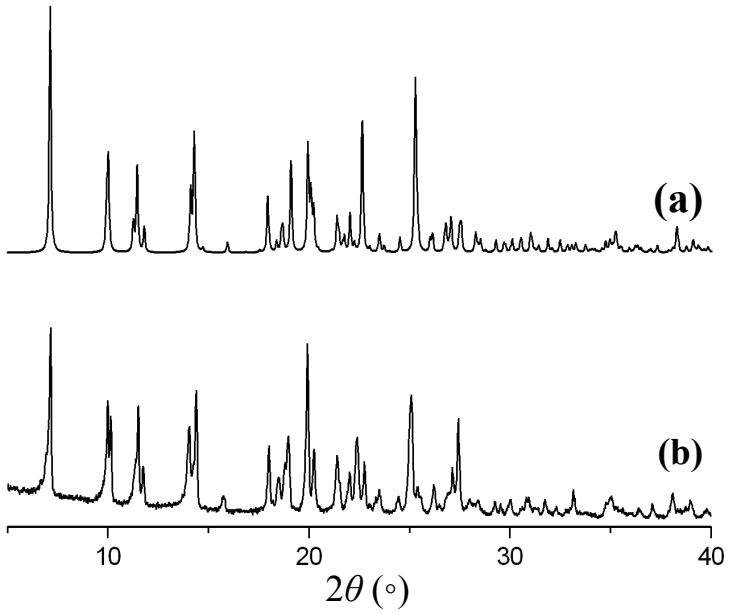

Fig. S13 Powder X-ray diffraction patterns of **5**. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

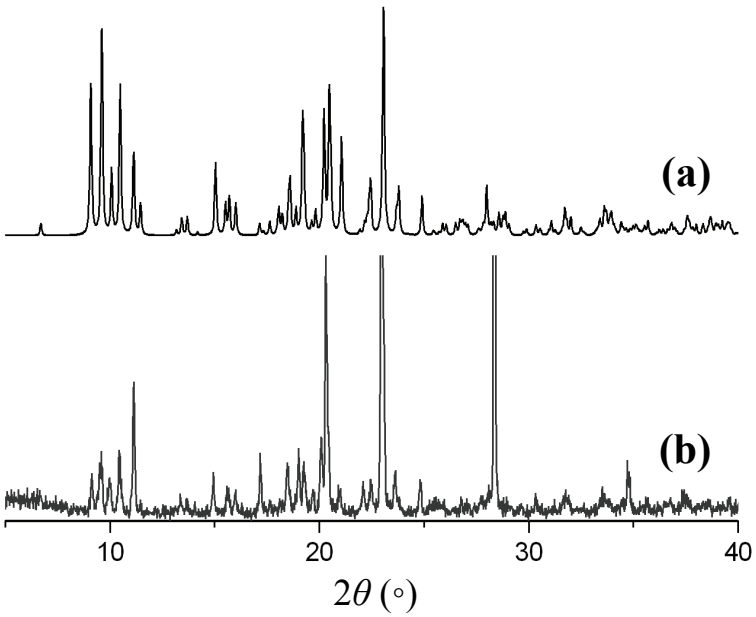

Fig. S14 Powder X-ray diffraction patterns of **6**·H_2O. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

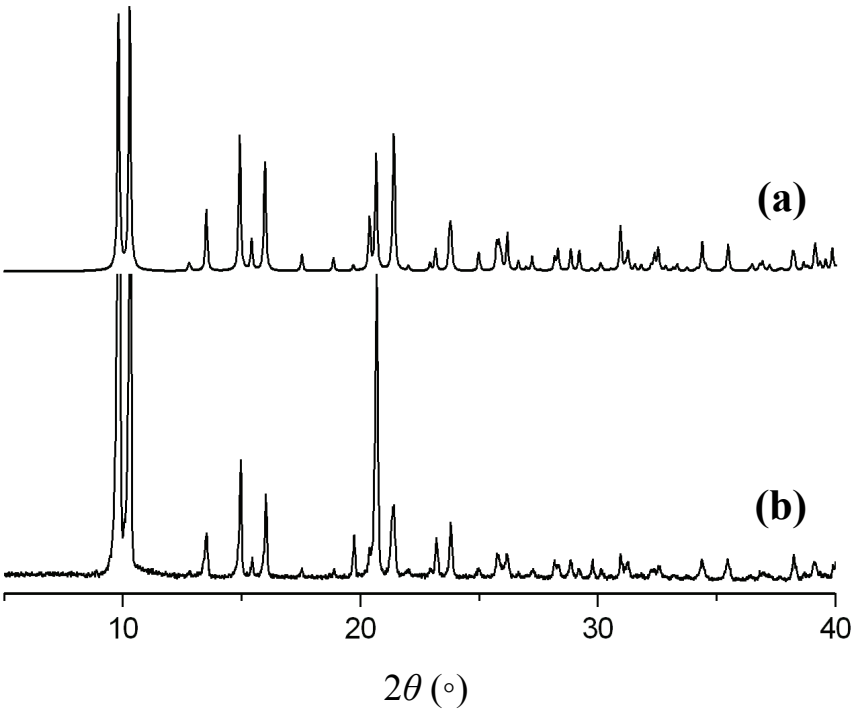

Fig. S15 Powder X-ray diffraction patterns of **7**. (a) Simulated from the single-crystal data. (b) A freshly grounded sample at room temperature.

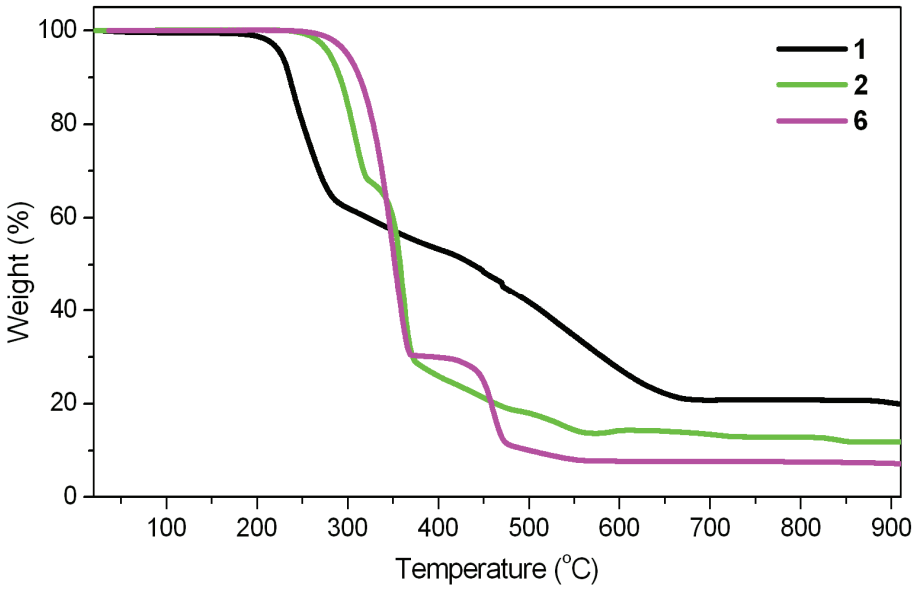

Fig. S16 Thermal stabilities of the evacuated materials of **1**·2H_2O, **2**·2CH_3OH, and **6**·H_2O.