Electronic Supplementary Information

for

Synthesis, structures and magnetic properties of isoreticular polyrotaxane-type two-dimensional coordination polymers

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X-ray Crystal Data:

Compound 1: Crystallized in orthorhombic space group Cmcm with Z = 4. The R(int) = 0.0771 shows that it is not a very good data set. The main structure was solved and refined without much of a problem. Further a lattice water molecule was found and the hydrogen atoms bonded to O atom were located. The atomic coordinates and isotropic thermal parameters were refined. However, the final agreement factors were relatively high. Despite several attempts, this data were found to be better than others and hence retained.

Compound 2: Crystallized in the monoclinic space group $P2_1/c$ with Z = 4. Initial refinements revealed that one of the pyridyl groups of bpe (C1a – C5a) was disordered. A common occupancy factor was refined to 0.78(2). Further one DMA and 1.5 water molecules were found in the voids. The DMA was disordered. Two orientations of the DMA molecules were successfully resolved and a common occupancy factor was refined to 0.52(1). Disordered water molecules were scattered in at least 4 different places in the voids with different occupancies. The final agreement factors are: R1 = 0.0641 for 5972 (Fo>4sig(F0) and 0.0937 for all 8502 data. The wR2 = 0.1595 for 690 parameters and GooF = 1.095. Since the thermal parameters of the atoms of the DMA molecule was not satisfactory, we have resorted to squeeze the electrons of the voids using SQUEEZE program. The final agreement factors were better and hence retained. In the squeezed structure, the common occupancy factor of the disordered pyridyl group was refined to 0.77(1). The final agreement factors are: R1 = 0.0602 for 6029 (Fo>4sig(F0) and 0.0829 for all 8502 data. The wR2 = 0.1540 for 560 parameters and GooF = 1.081.

PLATON shows solvent accessible void volume of 872.8 Ang^3 out of the cell volume, 4327.7(6) A^3 which is 20.17%.

Table S1 Crystal data for **1** and **2**

	1	**2**
formula	$C_{38}H_{28}Co_2N_2O_{14}S_2$	$C_{40}H_{26}Co_2N_2O_{12}S_2$
formula weight	918.60	908.61
crystal system	Orthorhombic	Monoclinic
space group	*Cmcm*	$P2_1/c$
a (Å)	12.7549(11)	15.9968(12)
b (Å)	13.7620(11)	22.1340(16)
c (Å)	21.742(2)	12.5998(9)
α (°)	90	90
β (°)	90	104.056(4)
γ (°)	90	90
V (Å^3)	3816.5(6)	4327.7(6)
Z	4	4
D_{calc} (g/cm^3)	1.599	1.395
μ (mm^{-1})	1.052	0.923
$2\theta_{max}$ (°)	52.00	52.00
reflections collected	22762	40331
independent reflections	2021 (R_{int} = 0.0771)	8502 (R_{int} = 0.0743)
goodness-of-fit on F^2	1.203	1.081
R_1, wR_2 [$I > 2\sigma(I)$]	0.1187, 0.2604	0.0602, 0.1459
R_1, wR_2 (all data)	0.1405, 0.2696	0.0829, 0.1540

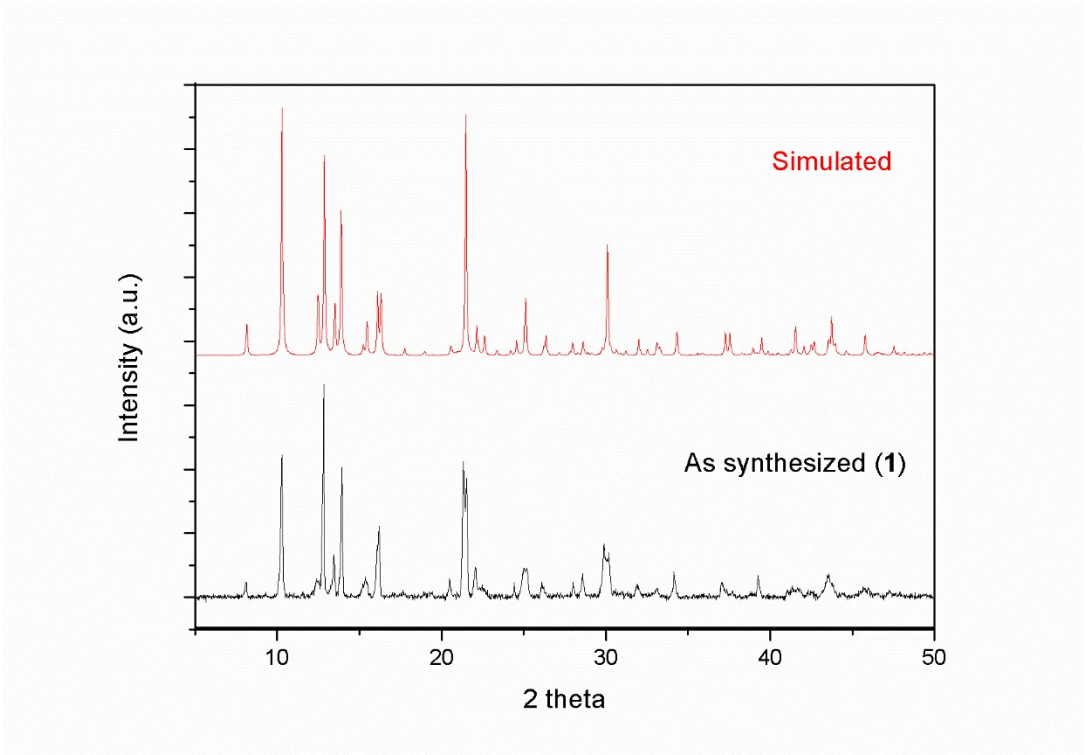

Fig. S1 Comparison of PXRD patterns for **1**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data.

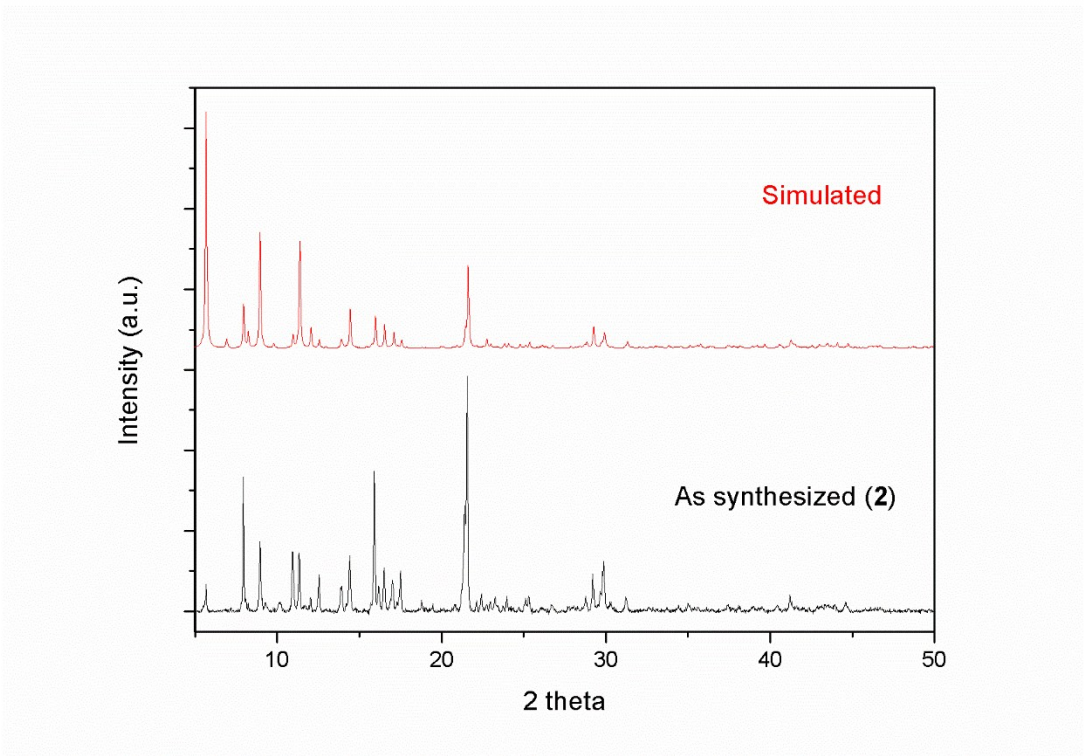

Fig. S2 Comparison of PXRD patterns for **2**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data. The difference in the intensities may be attributed to the preferred orientations of the powdered sample as compared to that generated from the single crystal data.

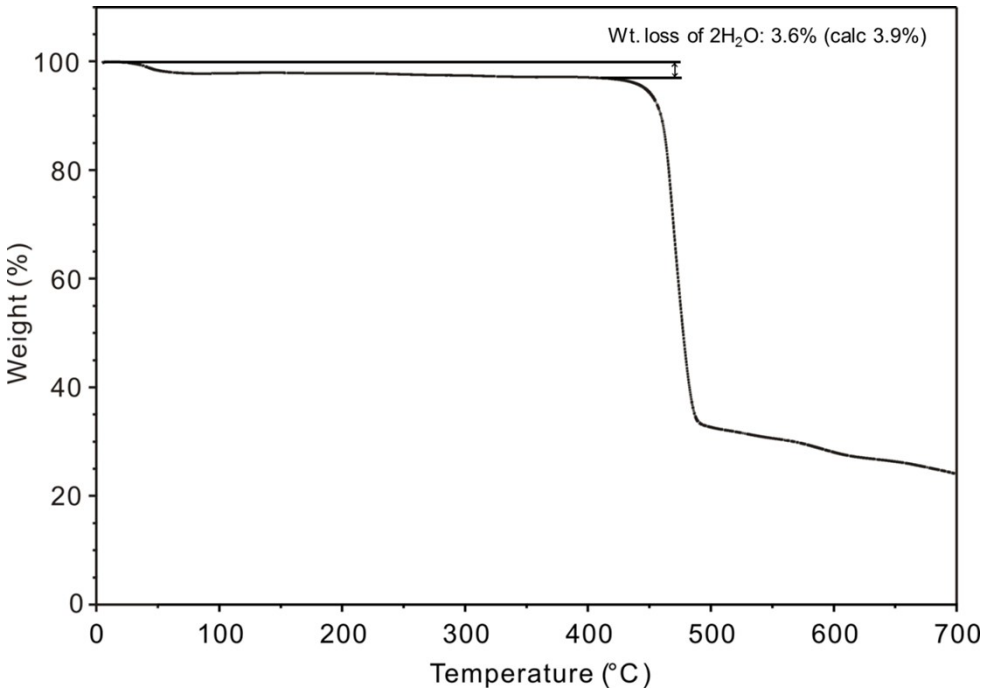

Figure S3. TGA curve of **1** with heating rate of 5 °C·min^{-1} under N_2 flow. The desolvated MOF is stable up to 440 °C.

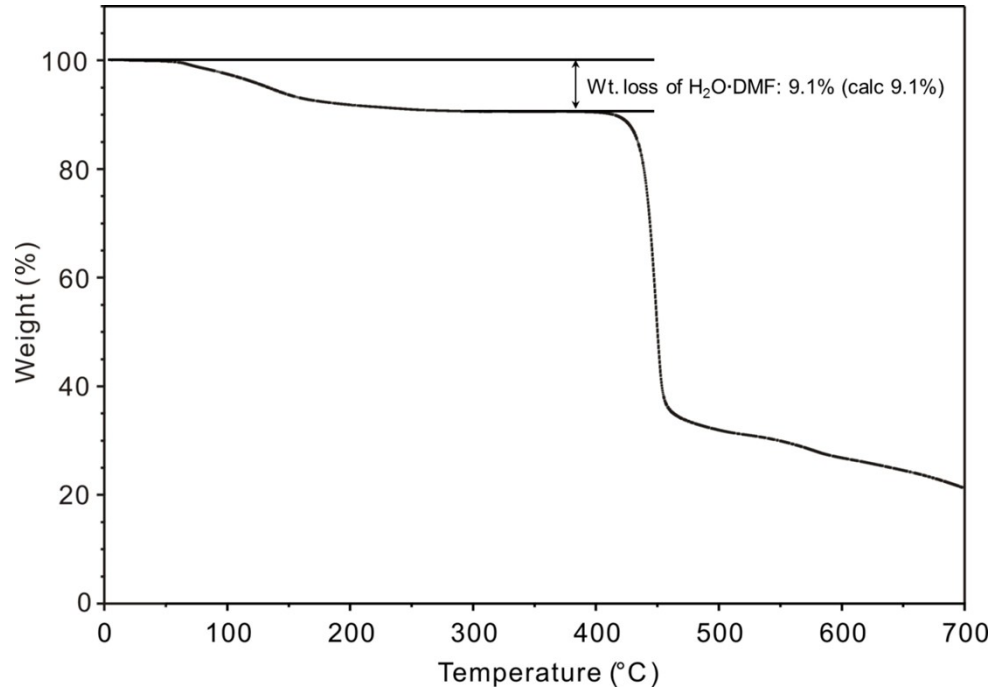

Figure S4. TGA curve of **2** with heating rate of 5 °C·min^{-1} under N_2 flow. The desolvated MOF is stable up to 420 °C.