Electronic Supplementary Information (ESI) for

Direction of unusual mixed-ligand metal-organic frameworks: a new type of 3-D polythreading involving 1-D and 2-D structural motifs and a 2-fold interpenetrating porous network

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Experimental

Materials and general methods. With the exception of the ligand bis(4-pyridyl)-4-amino-1,2,4-triazole (bpt), which was prepared according to the literature procedure (F. Bentiss, M. Lagrenee, M. Traisnel, B. Mernari and H. Elattari, *J. Heterocycl. Chem.,* 1999, **36**, 149–152), all of the starting materials and solvents were obtained commercially and used as received. Fourier transform (FT)-IR spectra (KBr pellets) were taken on an AVA-TAR-370 (Nicolet) spectrometer. Elemental (Carbon, Hydrogen and Nitrogen) analyses were performed on a CE-440 (Leemanlabs) analyzer. Thermogravimetric analysis (TGA) experiments were performed on a Dupont thermal analyzer in the temperature range of 25 – 800 °C under nitrogen atmosphere at a heating rate of 10 °C/min. Powder X-ray diffraction (PXRD) patterns were recorded on a Rigaku RU200 diffractometer at 60 kV, 300 mA for Cu Kα radiation (λ = 1.5406 Å), with a scan speed of 2 deg/min and a step size of 0.02° in 2θ. The calculated patterns were produced using the SHELXTL-XPOW program and single-crystal reflection data.

Single-Crystal X-ray Diffraction Determination and Refinement. Semi-empirical absorption corrections were applied using SADABS and the program SAINT was used for integration of the diffraction profiles. The structures were solved by direct methods using the SHELXS program of the SHELXTL package and refined with SHELXL. The final refinement was performed by full-matrix least-squares methods on F^2 with anisotropic thermal parameters for all the non-H atoms. H atoms bonded to C/N were placed geomet-

rically and allowed to ride during subsequent refinement with an isotropic displacement parameter fixed at 1.2 times U_{eq} of the parent atoms. With the exception of H atoms of the lattice water O13 in **2**, which cannot be located, all H atoms of aqua molecules were first found in difference electron density maps, and then placed in the calculated sites. In the refinement of the structure of **2**, 29 restraints were used for both DMF molecules applying DFIX instruction (details: DFIX 1.2 0.01 C43 O11 O12 C45; DFIX 1.45 0.01 N13 C41 N13 C42 N13 C43 N14 C44 N14 C45 N14 C46; and DFIX 2.45 0.02 C44 C45 C44 C46 C45 C46).
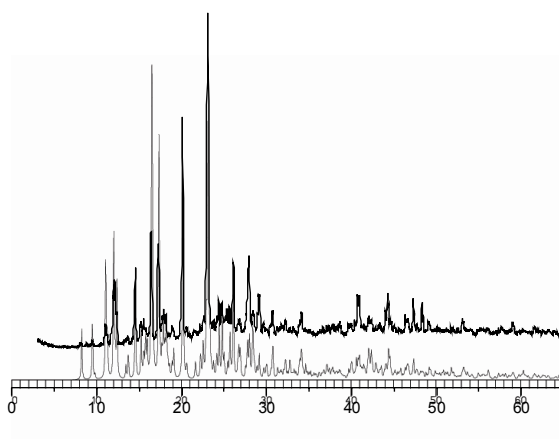

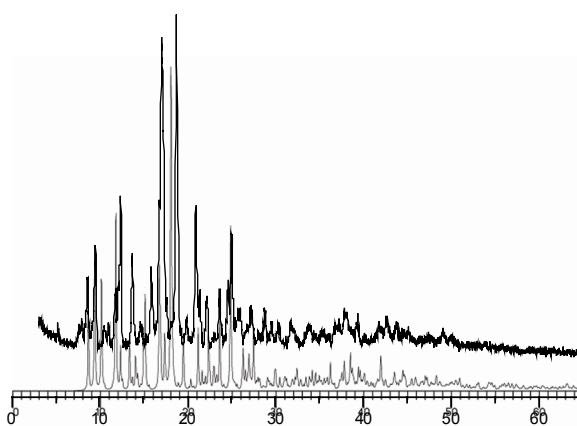**Fig. S1. PXRD patterns for MOF 1 (grey) calculated; (black) as-synthesized**

Fig. S2. PXRD patterns for MOF 2 (grey) calculated; (black) as-synthesized
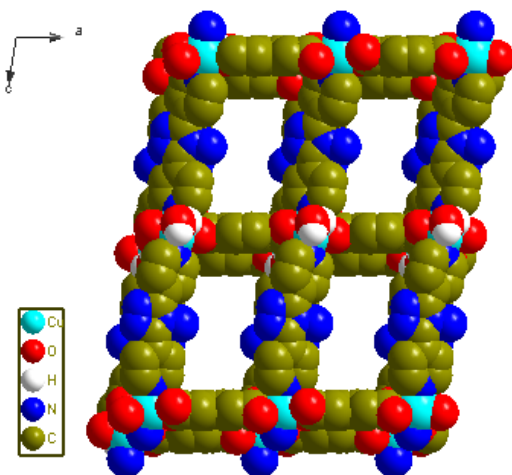
Fig. S3. Packing diagram of the 2-D layered motifs in 1: space-filling model of the hydrogen-bonded 3-D supramolecular framework with channels
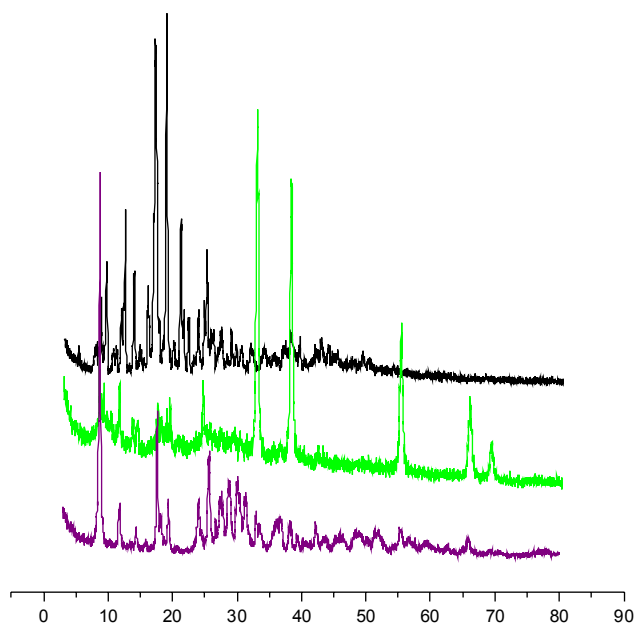

Fig. S4. PXRD patterns for MOF 2 (black) taken at room temperature; (green) after removal of the guest solvates; (c) after reintroduction of the guest molecules

Table S1 Possible hydrogen bond geometries in the crystal structures of **1** and **2**

Complex	D–H···A	D···A (Å)	H···A (Å)	D–H···A (°)
1	O7–H7A···O8	3.010(4)	2.16	179
	O7–H7B···O2^a	2.741(4)	1.90	173
	C12–H12···O3^b	3.087(4)	2.42	129
	N5–H5A···O6^c	3.215(3)	2.33	156
	N5–H5B···N11^a	3.038(4)	2.11	168
	N5–H5B···N10^a	3.132(4)	2.37	138
	N9–H9A···N3^d	2.975(4)	2.07	163
	N9–H9B···O3	3.176(4)	2.30	155
	O8–H8A···O6^e	2.891(4)	2.13	146
	O8–H8B···O1	2.817(4)	1.99	159
2	O5–H5C···O8^f	2.899(4)	2.00	173
	O5–H5D···N2^g	2.988(4)	2.11	169
	O10–H10A···O11^h	2.699(4)	1.85	157
	O10–H10B···O2^i	2.752(4)	1.87	165
	N5–H5A···O9^h	2.872(4)	2.10	144
	N5–H5B···N8	3.006(5)	2.16	157
	N11–H11A···O1^j	3.031(4)	2.18	158
	N11–H11B···O13	2.944(4)	2.14	148

^{a} –x + 2, y – 1/2, –z + 1/2. ^{b} –x + 1, y – 1/2, –z + 1/2. ^{c} x + 1, –y + 3/2, z + 1/2. ^{d} –x + 1, y + 1/2, –z + 1/2. ^{e} –x + 1, –y + 1, –z. ^{f} –x + 3/2, y – 1/2, –z + 1/2. ^{g} –x + 2, –y, –z + 1. ^{h} –x + 1, –y + 1, –z + 1. ^{i} x – 1, y, z. ^{j} x – 1/2, –y + 1/2, z – 1/2.