Electronic Supplementary Material (ESI) for Dalton Transactions.

Two isoreticular metal–organic frameworks with $CdSO_4$-like topology: selective gas sorption and drug delivery

Content

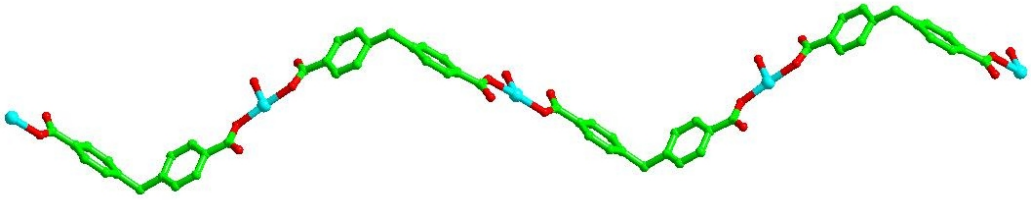

Fig. S1 A single $[Cu(L)]_n$ chain motif in **1.**

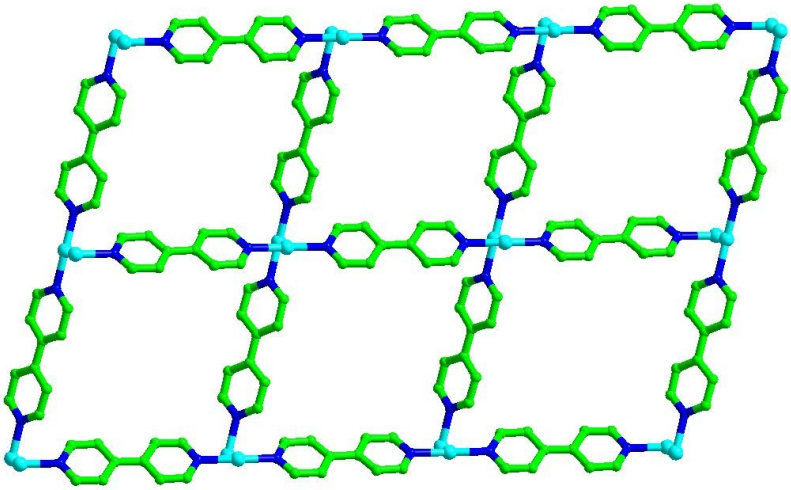

Fig. S2 Two mutually orthogonal sets the $[Cu(4,4'\text{-bipy})]_n$ in **1**

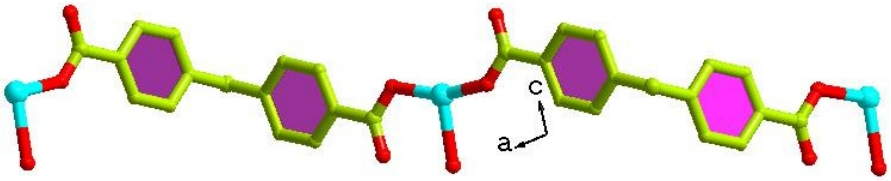

Fig. S3 View of the chain of $[Cu(H_2O)(L)]_n$

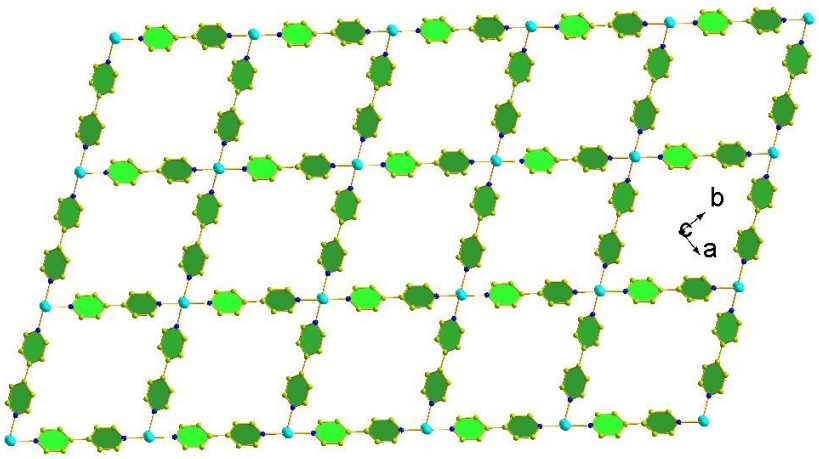

Fig. S4 Two mutually orthogonal sets the $[Cu(4,4'\text{-bipy})]_n$ in **2**

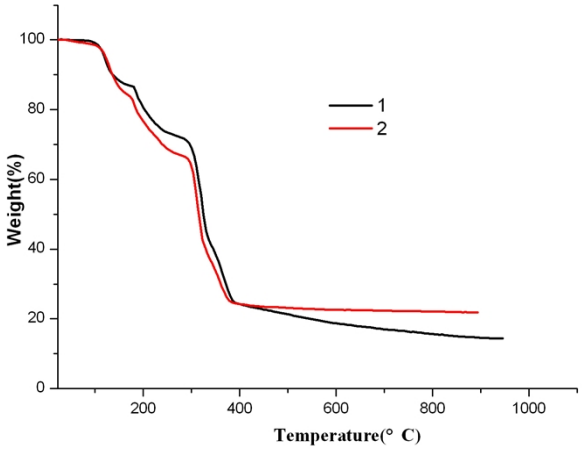

Fig. S5 view of TGA in compounds **1-2**.

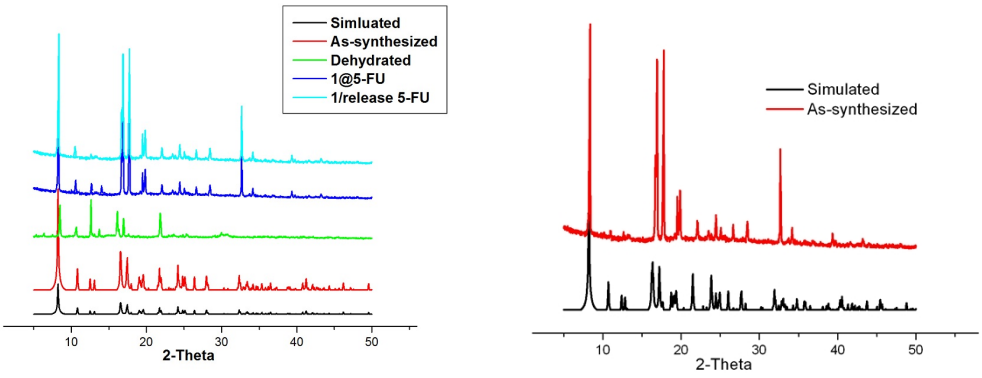

Fig. S6 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized product, desolvated sample, 5-FU containing sample and after 5-Fu release sample in compound **1** and Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product in **2**.

Table S1 different calculated potential gas adsorption feature in **1**

Probe sphere radius (Å)	Guest molecule	potential porosity ($m^2.g^{-1}$)
1.3	He	1773(9)
1.45	H_2	1700(7)
1.65	CO_2	1680(20)
1.7	Ar	1657(20)
1.8	N_2	1586(15)
1.9	CO	1541(13)

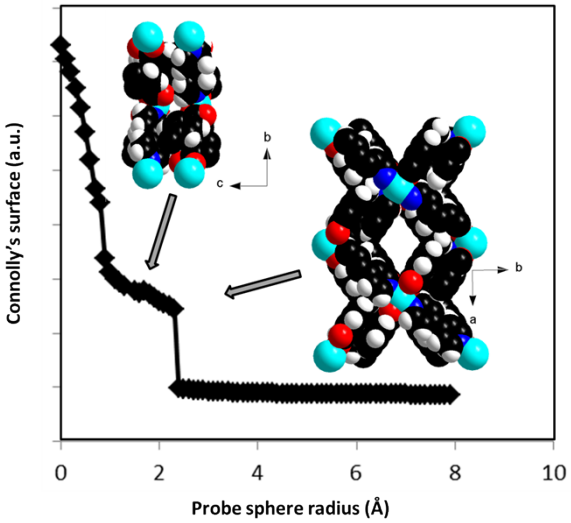

Fig S7. Porosity profile for the compound **1**

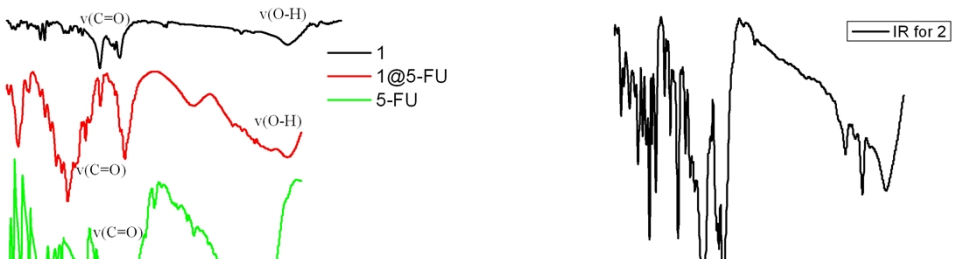

Fig S8 IR spectra of 5-FU (green), **1** loaded with 5-FU (red) and **1** (black) and the IR spectra of **2**(right).

Drug Loading

To load 5-fluorouracil (5-FU) into the pores of **1**, dehydrated **1** (10 mg) was dispersed in a 5-FU (20 mg) containing ethanol solution (5 mL) and stirred for 5 days yielding homogenous light solution, followed by centrifugation and washing extensively with DMSO to obtain the drug-loaded **1**. The adsorbed amount of 5-Fu into the porous solids was estimated by HPLC, and FTIR.

Determination of the 5-Fluorouracil Content

Optimisation of 5-Fu adsorption

Table S2. Estimated f-Fu content = f(several impregnation parameters).

Table S2 5-FU drug loading rate of MOFs

m(MOFs)/	Drug content m(5-FU)/m(MOFs)			
m(5-FU)	1d	3d	5d	7d
1:1	0.201 ± 0.011	0.217 ± 0.014	0.259 ± 0.013	0.223 ± 0.016
1:2	0.180 ± 0.031	0.239 ± 0.011	0.275 ± 0.017	0.229 ± 0.014
1:3	0.193 ± 0.019	0.211 ± 0.013	0.221 ± 0.012	0.215 ± 0.029

Drug Release

The release of 5-FU from 5-FU-loaded **1** was evaluated using a semi-permeable dialysis bag diffusion technique right after the 5-FU loading. The as-prepared 5-FU-loaded **1** was dispersed in 500 mL PBS (pH 7.4). The release mediums was placed into pretreated semi permeable dialysis bags and then immersed into 5 mL PBS at 37 °C with gentle shaking. At certain time intervals, 5-FU concentration moved out of semi-premeable dialysis dag into water was measured by HPLC.

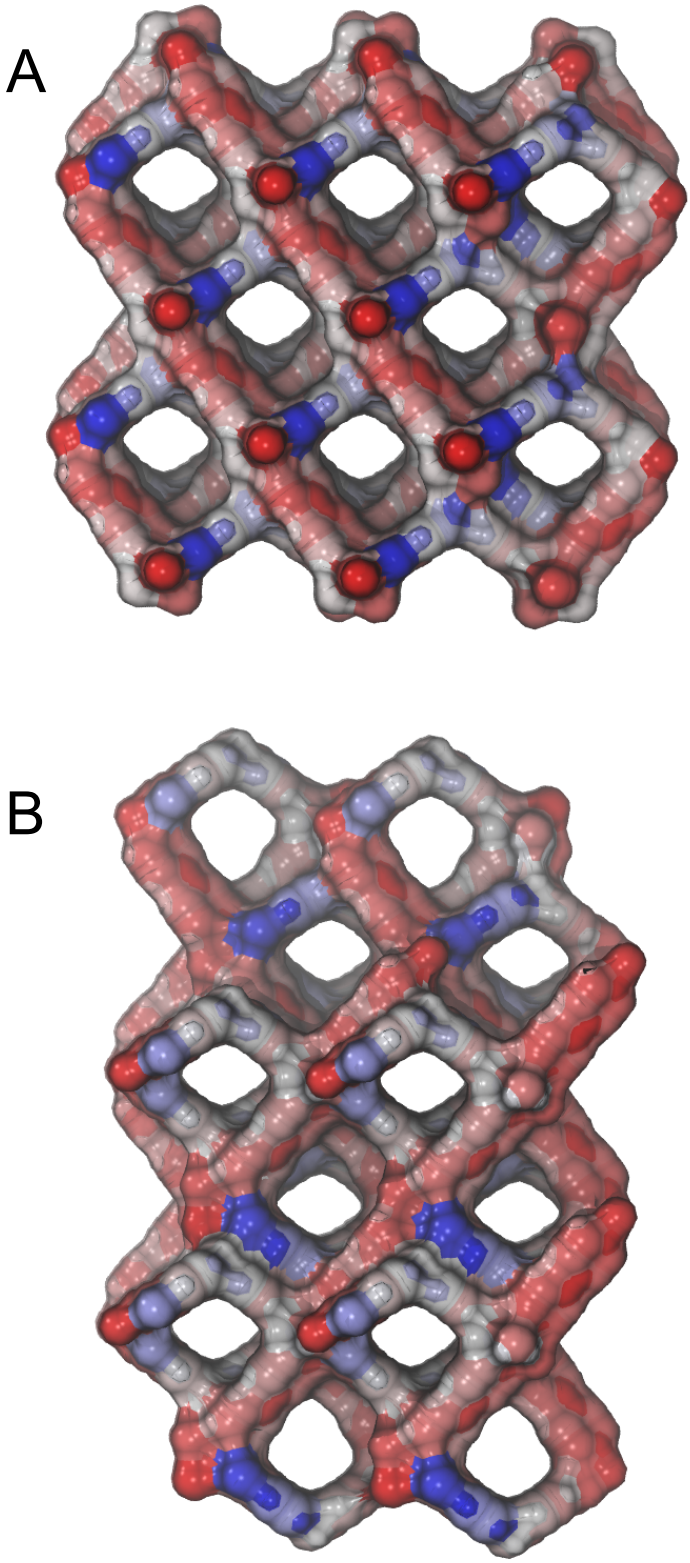

Fig. S9 Structural comparison of metal-organic frameworks **1** (A) and **2** (B) with respect to pore dimensions and charge distribution derived from the chemical environment of the pores.

The detailed **topological analysis**
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1:C100 H Cu4 N8 O28
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Topology for 1

Atom Cu1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Cu 1	0.2526	0.7480	1.0399	(1 1 2)	11.163A	1
Cu 1	1.2526	-0.2520	1.0399	(2 0 2)	11.170A	1
Cu 1	-0.2526	0.2480	0.4601	(-1 0-1)	13.873A	1
Cu 1	1.7474	0.2480	1.4601	(1 0 0)	13.873A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with CuO4N2C25H18

Coordination sequences

Cu1:	1	2	3	4	5	6	7	8	9	10
Num	4	12	30	58	94	138	190	250	318	394
Cum	5	17	47	105	199	337	527	777	1095	1489

TD10=1489

Vertex symbols for selected sublattice

Cu1 Point symbol:{6^5.8}
Extended point symbol:[6.6.6.6.6(2).8(2)]

Point symbol for net: {6^5.8}
4-c net; uninodal net

Topological type: cds CdSO4; 4/6/t4; sqc5 (topos&RCSR.ttd) {6^5.8} - VS [6.6.6.6.6(2).*] (71801 types in 11 databases)

Non-equivalent circuits

Circuit No 1; Type=6a; Centroid: (0.000,0.500,0.000)

##
2:[Cu (H2 O) (C10 H8 N2) (C15 H10 O4)], 4H2 O
##

Topology for 2

Atom Cu1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Cu 1	1.0000	1.0000	0.5000	(1 1 1)	11.276A	1
Cu 1	0.0000	0.0000	0.5000	(0 0 1)	11.276A	1
Cu 1	1.5000	0.5000	1.0000	(2 0 1)	13.840A	1
Cu 1	-0.5000	0.5000	0.0000	(0 0 0)	13.840A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with CuO4N2C25H17

Coordination sequences

Cu1:	1	2	3	4	5	6	7	8	9	10
Num	4	12	30	58	94	138	190	250	318	394
Cum	5	17	47	105	199	337	527	777	1095	1489

TD10=1489

Vertex symbols for selected sublattice

Cu1 Point symbol:{6^5.8}
Extended point symbol:[6.6.6.6.6(2).8(2)]

Point symbol for net: {6^5.8}
4-c net; uninodal net

Topological type: cds CdSO4; 4/6/t4; sqc5 (topos&RCSR.ttd) {6^5.8} - VS [6.6.6.6.6(2).*] (73010 types in 11 databases)
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