Two isoreticular metal–organic frameworks with CdSO$_4$-like topology: selective gas sorption and drug delivery

Content

Detailed structural description of 1 and 2

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

Fig. S2 Two mutually orthogonal sets the [Cu(4,4'-bipy)]$_n$ in 1
Fig. S3 View of the chain of \([\text{Cu(H}_2\text{O})(\text{L})]_n\)

Fig. S4 Two mutually orthogonal sets the \([\text{Cu(4,4’-bipy)}]_n\) 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

<table>
<thead>
<tr>
<th>Probe sphere radius (Å)</th>
<th>Guest molecule</th>
<th>potential porosity (m².g⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.3</td>
<td>He</td>
<td>1773(9)</td>
</tr>
<tr>
<td>1.45</td>
<td>H₂</td>
<td>1700(7)</td>
</tr>
<tr>
<td>1.65</td>
<td>CO₂</td>
<td>1680(20)</td>
</tr>
<tr>
<td>1.7</td>
<td>Ar</td>
<td>1657(20)</td>
</tr>
<tr>
<td>1.8</td>
<td>N₂</td>
<td>1586(15)</td>
</tr>
<tr>
<td>1.9</td>
<td>CO</td>
<td>1541(13)</td>
</tr>
</tbody>
</table>

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>
<thead>
<tr>
<th>m(MOFs)/m(5-FU)</th>
<th>1d</th>
<th>3d</th>
<th>5d</th>
<th>7d</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:1</td>
<td>0.201 ± 0.011</td>
<td>0.217 ± 0.014</td>
<td>0.259 ± 0.013</td>
<td>0.223 ± 0.016</td>
</tr>
<tr>
<td>1:2</td>
<td>0.180 ± 0.031</td>
<td>0.239 ± 0.011</td>
<td>0.275 ± 0.017</td>
<td>0.229 ± 0.014</td>
</tr>
<tr>
<td>1:3</td>
<td>0.193 ± 0.019</td>
<td>0.211 ± 0.013</td>
<td>0.221 ± 0.012</td>
<td>0.215 ± 0.029</td>
</tr>
</tbody>
</table>

**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**
1: C100 H4 N8 O28

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(H2O)(C10H8N2)(C15H10O4)], 4H2O

Topology for 2
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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
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Structural group analysis
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Structural group No 1
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Structure consists of 3D framework with CuO4N2C25H17
Coordination sequences
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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)
Elapsed time: 8.99 sec.