Deliberate Design of a Neutral Heterometallic Organic Framework containing a Record 25-Fold Interpenetrating Diamondoid Network

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**Materials and Methods:** All chemicals were commercially purchased and used without further purification. The powder X-ray diffraction (PXRD) analyses were recorded on a Rigaku Dmax2500 diffractometer with Cu Kα radiation (λ = 1.54056 Å) with a step size of 0.05°. Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10 °C/min under an air atmosphere.

**Figure S1.** The TGA curve of 1.

**Figure S2.** XRPD patterns of simulated from the single-crystal data of 1 (black); as-synthesized 1 (red); activated at 250 °C (blue), activated at 300 °C (olive) and activated at 300 °C (pink).
TOPOS analysis results:

1: C H Cd Cu N O

Topology for Cd1

Atom Cd1 links by bridge ligands and has

<table>
<thead>
<tr>
<th>Common vertex with</th>
<th>R(A-A)</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd 1 -1.0000 -0.2500 -1.1250 (-1 0-1)</td>
<td>26.467A</td>
<td>1</td>
</tr>
<tr>
<td>Cd 1 1.0000 0.7500 -1.1250 ( 1 1-1)</td>
<td>26.467A</td>
<td>1</td>
</tr>
<tr>
<td>Cd 1 0.5000 -0.7500 1.3750 ( 0-1 1)</td>
<td>26.467A</td>
<td>1</td>
</tr>
<tr>
<td>Cd 1 -0.5000 1.2500 1.3750 (-1 1 1)</td>
<td>26.467A</td>
<td>1</td>
</tr>
</tbody>
</table>

Structural group analysis

Structural group No 1

Structure consists of 3D framework with CdCu2O8C52H32
There are 25 interpenetrating nets
PIV: Partial interpenetration vectors

[0,0,1] (13.20A) (5 nets [1,2,3,4,5])
[1/2,1/2,1/2] (14.66A) (5 nets [1,6,7,8,9])
[1/2,1/2,-1/2] (14.66A) (5 nets [1,10,11,12,13])
[1/2,-1/2,1/2] (14.66A) (5 nets [1,14,15,16,17])
[1/2,-1/2,-1/2] (14.66A) (5 nets [1,18,19,20,21])
[0,1,0] (18.51A) (5 nets [1,22,23,24,25])
PIC: [0,0,5][5/2,5/2,5/2][2,1,0] (PICVR=25)

Zt=25(5*5); Zn=1

Class Ib  Z=25(5*5)

Coordination sequences
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Cd1:  1  2  3  4   5   6   7   8   9  10
Num   4 12 24 42  64  92 124 162 204 252
Cum   5 17 41 83 147 239 363 525 729 981
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TD10=981

Vertex symbols for selected sublattice
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Cd1 Schlafli symbol:{6^6}
With circuits:[6(2).6(2).6(2).6(2).6(2).6(2)]
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Total Schlafli symbol: {6^6}
4-c net; uninodal net

Topological type: dia Diamond; 4/6/c1; sqc6  {6^6} - VS [6(2).6(2).6(2).6(2).6(2).6(2)]
(66853 types in 9 databases)