Electronic Supplementary Material (ESI) for CrystEngComm
This journal is © The Royal Society of Chemistry 2012

Supporting Information

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

*Yan-Ping He, Yan-Xi Tan, Jian Zhang**

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, the Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China. E-mail: zhj@fjirsm.ac.cn.

This journal is © The Royal Society of Chemistry 2012

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.

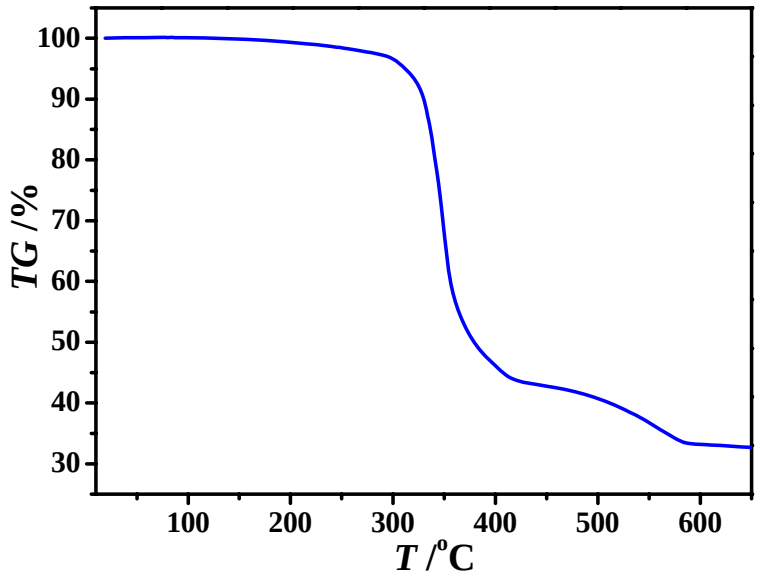

Figure S1. The TGA curve of **1**.

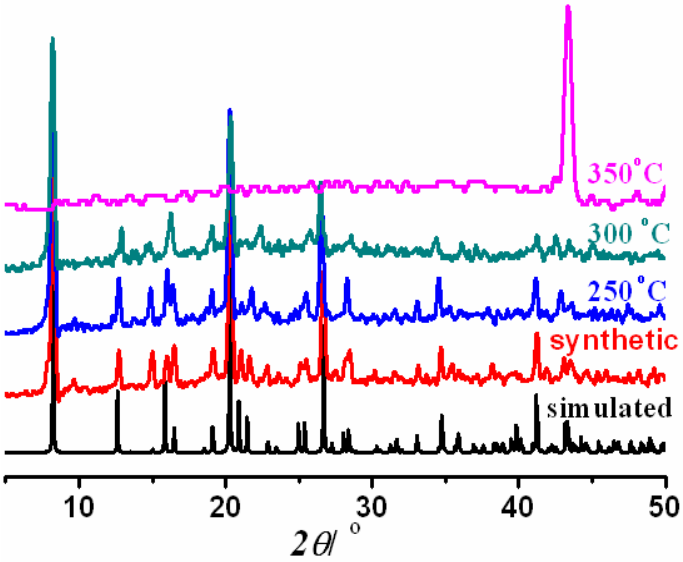

Figure S2. XRPD patterns of simulated from the single-crystal data of **1** (black); as-synthesized **1** (red); activated at 250 ºC (blue), activated at 300 ºC (olive) and activated at 300 ºC (pink).

This journal is © The Royal Society of Chemistry 2012

TOPOS analysis results:

################

1:C H Cd Cu N O

################

Topology for Cd1

Atom Cd1 links by bridge ligands and has

Common vertex with					R(A-A)	f
Cd 1	-1.0000	-0.2500	-1.1250	(-1 0-1)	26.467A	1
Cd 1	1.0000	0.7500	-1.1250	(1 1-1)	26.467A	1
Cd 1	0.5000	-0.7500	1.3750	(0-1 1)	26.467A	1
Cd 1	-0.5000	1.2500	1.3750	(-1 1 1)	26.467A	1

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])

This journal is © The Royal Society of Chemistry 2012

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

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

TD10=981

Vertex symbols for selected sublattice

Cd1 Schlafli symbol:{6^6}

With circuits:[6(2).6(2).6(2).6(2).6(2).6(2)]

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)