Supporting information for

Three porous metal-organic frameworks based on azobenzenetricarboxylate ligand: synthesis, structures, and magnetic property

Miao Meng, Di-Chang Zhong* and Tong-Bu Lu*

Table S1 Selected bond distances (Å) and angles (°) for **1-3**

1

Cd(1)-O(8)	2.245(4)	Cd(1)-O(7)	2.316(4)	Cd(1)-O(5)#1	2.353(3)
Cd(1)-O(3)#2	2.360(3)	Cd(1)- O(1)	2.366(3)	Cd(1)-O(4)#2-	2.377(3)
Cd(1)-O(6)#1	2.442(3)	Cd(1)-O(8)	2.245(4)		
C(1)-O1	1.223(6)	C(1)-O2	1.315(6)		
O(8)-Cd(1)-O(7)	176.55(13)	O(8)-Cd(1)-O(5)#1	95.56(14)	O(7)-Cd(1)-O(5)#1	84.77(13)
O(8)-Cd(1)-O(3)#2	92.01(13)	O(7)-Cd(1)-O(3)#2	88.96(13)	O(5)#1-Cd(1)-O(3)#2	156.96(12)
O(8)-Cd(1)-O(1)	90.55(14)	O(7)-Cd(1)-O(1)	92.88(13)	O(5)#1-Cd(1)-O(1)	78.36(11)
O(3)#2-Cd(1)-O(1)	79.84(12)	O(8)-Cd(1)-O(4)#2	95.05(14)	O(7)-Cd(1)-O(4)#2	82.78(13)
O(5)#1-Cd(1)-O(4)#2	144.72(13)	O(3)#2-Cd(1)-O(4)#2	55.44(12)	O(1)-Cd(1)-O(4)#2	135.04(12)
O(8)-Cd(1)-O(6)#1	85.79(14)	O(7)-Cd(1)-O(6)#1	91.64(13)	O(5)#1-Cd(1)-O(6)#1	54.17(11)
O(3)#2-Cd(1)-O(6)#1	148.41(12)	O(1)-Cd(1)-O(6)#1	131.63(11)	O(4)#2-Cd(1)-O(6)#1	93.30(12)

2

Cd(1)-O(4)#1	2.256(5)	Cd(1)-O(9)	2.289(6)	Cd(1)-O(8)	2.299(5)
Cd(1)-O(2)	2.312(5)	Cd(1)-O(7)	2.315(5)	Cd(1)-O(1)	2.537(5)
Cd(1)-O(3)#1	2.575(5)	Cd(2)-O(6)	2.236(4)	Cd(2)-O(6)#2	2.236(4)
Cd(2)-O(10)	2.243(9)	Cd(2)-O(11)	2.275(5)	Cd(2)-O(11)#2	2.275(5)
O(4)#1-Cd(1)-O(9)	89.5(2)	O(4)#1-Cd(1)-O(8)	139.32(17)	O(9)-Cd(1)-O(8)	95.7(2)
O(4)#1-Cd(1)-O(2)	83.84(17)	O(9)-Cd(1)-O(2)	87.1(2)	O(8)-Cd(1)-O(2)	136.60(17)
O(4)#1-Cd(1)-O(7)	93.5(2)	O(9)-Cd(1)-O(7)	174.27(19)	O(8)-Cd(1)-O(7)	85.20(19)
O(2)-Cd(1)-O(7)	88.3(2)	O(4)#1-Cd(1)-O(1)	137.28(16)	O(9)-Cd(1)-O(1)	84.57(18)
O(8)-Cd(1)-O(1)	83.40(16)	O(2)-Cd(1)-O(1)	53.68(15)	O(7)-Cd(1)-O(1)	89.92(17)
O(4)#1-Cd(1)-O(3)#1	53.72(16)	O(9)-Cd(1)-O(3)#1	88.88(19)	O(8)-Cd(1)-O(3)#1	85.98(16)
O(2)-Cd(1)-O(3)#1	137.41(16)	O(7)-Cd(1)-O(3)#1	96.83(18)	O(1)-Cd(1)-O(3)#1	166.90(14)
O(6)-Cd(2)-O(6)#2	172.8(3)	O(6)-Cd(2)-O(10)	86.39(16)	O(6)#2-Cd(2)-O(10)	86.39(16)
O(6)-Cd(2)-O(11)	79.48(19)	O(6)#2-Cd(2)-O(11)	105.46(19)	O(10)-Cd(2)-O(11)	131.77(16)
O(6)-Cd(2)-O(11)#2	105.46(19)	O(6)#2-Cd(2)-O(11)#2	79.48(19)	O(10)-Cd(2)-O(11)#2	131.77(16)
O(11)-Cd(2)-O(11)#2	96.5(3)				

3

Mn(1)-O(9)#1	2.094(5)	Mn(1)-O(12)#2	2.109(5)	Mn(1)-O(14)	2.168(6)
Mn(1)-O(1)	2.183(5)	Mn(1)-O(4)#3	2.259(5)	Mn(1)-O(13)	2.297(5)
Mn(2)-O(7)	2.133(5)	Mn(2)-O(10)#1	2.148(5)	Mn(2)-O(3)#3	2.158(5)
Mn(2)-O(15)	2.165(5)	Mn(2)-O(6)#4	2.166(5)	Mn(2)-O(13)	2.323(5)
Mn(3)-O(11)#2	2.106(5)	Mn(3)-O(5)#5	2.131(5)	Mn(3)-O(16)	2.168(5)
Mn(3)-O(17)	2.201(5)	Mn(3)-O(8)	2.254(5)	Mn(3)-O(2)#6	2.265(5)
O(9)#1-Mn(1)-O(12)#2	170.3(2)	O(9)#1-Mn(1)-O(14)	89.3(2)	O(12)#2-Mn(1)-O(14)	94.0(2)
O(9)#1-Mn(1)-O(1)	91.0(2)	O(12)#2-Mn(1)-O(1)	98.11(19)	O(14)-M n(1)-O(1)	90.5(2)
O(9)#1-Mn(1)-O(4)#3	86.44(18)	O(12)#2-Mn(1)-O(4)#3	84.34(16)	O(14)-Mn(1)-O(4)#3	92.1(2)
O(1)-Mn(1)-O(4)#3	176.25(19)	O(9)#1-Mn(1)-O(13)	89.4(2)	O(12)#2-Mn(1)-O(13)	87.82(19)
O(14)-Mn(1)-O(13)	176.4(2)	O(1)-Mn(1)-O(13)	86.18(18)	O(4)#3-Mn(1)-O(13)	91.09(18)
O(7)-Mn(2)-O(10)#1	179.5(2)	O(7)-Mn(2)-O(3)#3	90.2(2)	O(10)#1-Mn(2)-O(3)#3	90.2(2)
O(7)-Mn(2)-O(15)	89.4(2)	O(10)#1-Mn(2)-O(15)	90.9(2)	O(3)#3-Mn(2)-O(15)	91.7(2)
O(7)-Mn(2)-O(6)#4	94.7(2)	O(10)#1-Mn(2)-O(6)#4	84.84(19)	O(3)#3-Mn(2)-O(6)#4	173.4(2)
O(15)-Mn(2)-O(6)#4	92.8(2)	O(7)-Mn(2)-O(13)	86.28(18)	O(10)#1-Mn(2)-O(13)	93.40(19)
O(3)#3-Mn(2)-O(13)	89.65(18)	O(15)-Mn(2)-O(13)	175.5(2)	O(6)#4-Mn(2)-O(13)	86.25(18)
O(11)#2-Mn(3)-O(5)#5	163.3(2)	O(11)#2-Mn(3)-O(16)	99.0(2)	O(5)#5-Mn(3)-O(16)	97.8(2)
O(11)#2-Mn(3)-O(17)	82.3(2)	O(5)#5-Mn(3)-O(17)	81.0(2)	O(16)-Mn(3)-O(17)	178.7(2)
O(11)#2-Mn(3)-O(8)	84.4(2)	O(5)#5-Mn(3)-O(8)	97.4(2)	O(16)-Mn(3)-O(8)	85.1(2)
O(17)-Mn(3)-O(8)	94.7(2)	O(11)#2-Mn(3)-O(2)#6	95.16(19)	O(5)#5-Mn(3)-O(2)#6	86.7(2)
O(16)-Mn(3)-O(2)#6	82.3(2)	O(17)-Mn(3)-O(2)#6	97.9(2)	O(8)-Mn(3)-O(2)#6	167.18(19)

Symmetry codes for **1**: #1 = x-1, y, z+1; #2 = -x+2, y+1/2, -z+3/2; #3 = -x+2, y-1/2, -z+3/2; #4 = x+1, y, z-1; **2**: #1 = x-1/2, y+1/2, z; #2 = -x+1, y, -z; #3 = x+1/2, y-1/2, z; #4 = -x+1, y, -z+1; **3**: #1 = x+1/2, -y+3/2, z+1/2; #2 = x+1/2, y-1/2, z; #3 = x, -y+1, z+1/2; #4 = x-1/2, y+1/2, z; #5 = x-1/2, y+3/2, z; #6 = x, y+1, z; #7 = x, y-1, z; #8 = x, -y+1, z-1/2; #9 = x+1/2, y-3/2, z; #10 = x-1/2, -y+3/2, z-1/2.

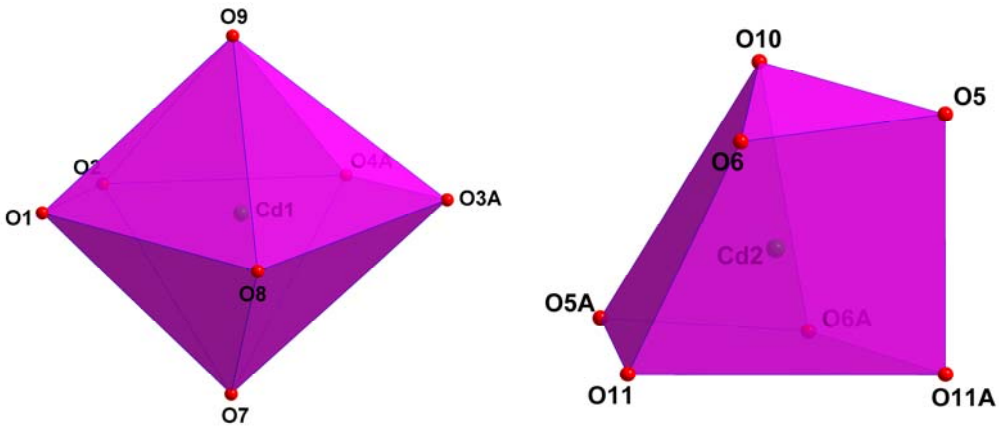

Fig. S1 The coordination geometries of Cd1 and Cd2 in **2**.

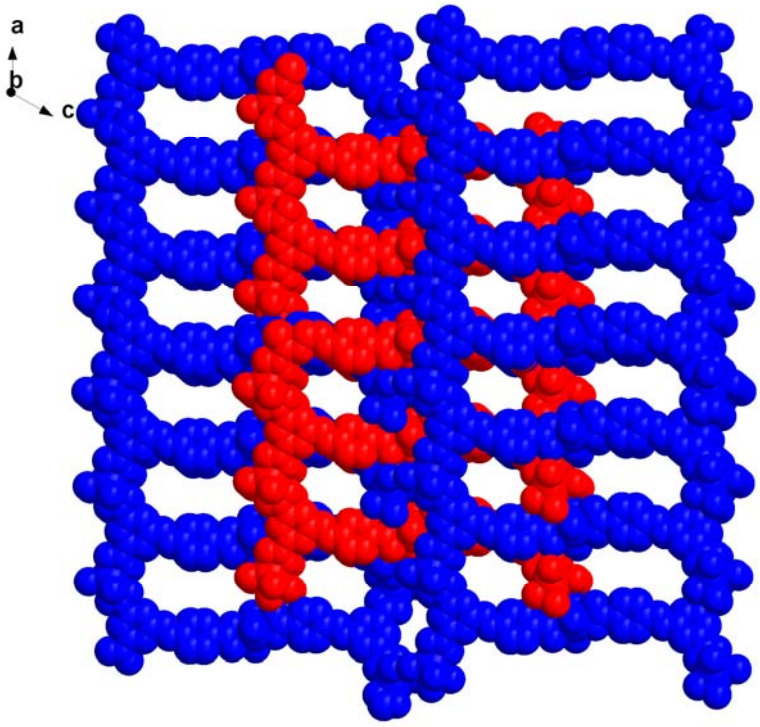

Fig. S2 The 3D porous structure of **2**.

Topological Analysis for 1 and 2 by TOPOS 4.0.

{[Cd(HABTC)(H_2O)$_2$]·3H_2O}$_n$ (1)

Topology for C1 ($HABTC^{2-}$)

The links to Atom C1

Cd1	0.3886	-0.2853	0.3094	(1-1 0)	6.418 Å
Cd1	0.6114	0.2147	0.1906	(0 0 0)	6.489 Å
Cd1	-0.3886	0.2147	1.1906	(-1 0 1)	10.568 Å

Topology for Cd1

The links to Atom Cd1

C1	0.7622	0.5233	-0.0252	(1 0 0)	6.418 Å
C1	0.2378	0.0233	0.5252	(0 0 0)	6.489 Å
C1	1.2378	0.0233	-0.4748	(1 0 -1)	10.568 Å

Vertex symbols for selected sublattice

C1 Point (Schlafli) symbol: {6^3}
Extended point symbol: [6.6.6]

Cd1 Point (Schlafli) symbol: {6^3}
Extended point symbol: [6.6.6]

Point (Schlafli) symbol for net: {6^3}

3,3-c net; uninodal net

Topological type: hcb; Shubnikov hexagonal plane net/(6,3) (topos&RCSR.ttd) {6^3}

- VS [6.6.6] (67358 types in 9 databases)

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{[Cd_3($ABTC$)$_2$(H_2O)$_9$]·CH_3OH·DMF·2H_2O}$_n$ (2)

Topology for Sc1 ($ABTC^{3-}$)

The links to Atom Sc1

Sc1	0.3276	0.9647	0.7267	(-1 0 0)	10.165 Å
Sc1	1.3276	-0.0353	0.7267	(0-1 0)	10.165 Å
Sc1	0.1724	0.4647	-0.7267	(1 0 0)	23.778 Å

Vertex symbols for selected sublattice

Sc1 Point (Schlafli) symbol: {8^2.10}
Extended point symbol: [8(2).8(2).10(2)]

Point (Schlafli) symbol for net: {8^2.10}

3-c net; uninodal net

Topological type: 2(3)2/2-plane minimal net; plane SP KIa (topos&RCSR.ttd) {8^2.10} - VS [8(2).8(2).*] (67358 types in 9 databases)

Elapsed time: 2.83 sec.