Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Luminescent MOF Material based on Cadmium(II) and Mixed Ligands: Application for Sensing Volatile Organic Solvent Molecules

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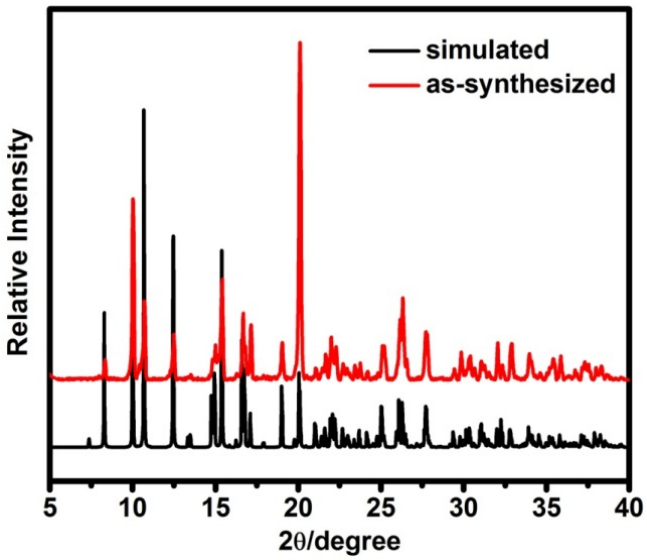

Fig. S1. Experimental and calculated power PXRD patterns for compound **1**, indicate the phase purity of the as-synthesized samples.

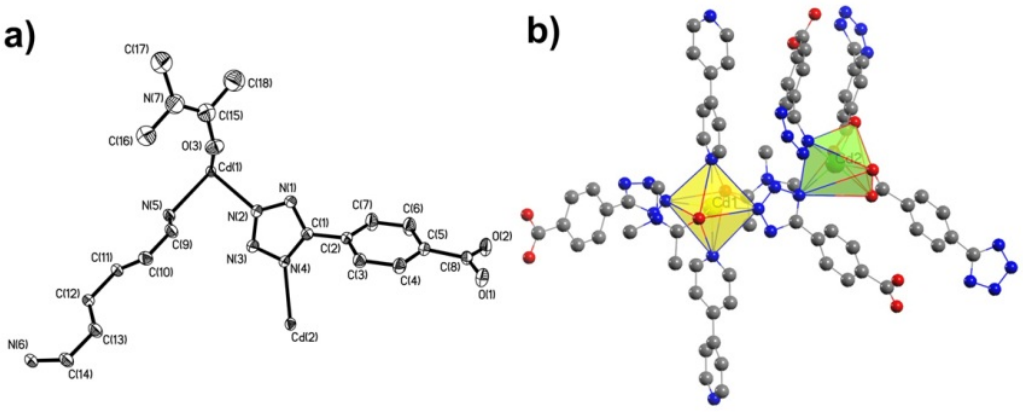

Fig. S2. a) The asymmetric unit of compound **1**; **b**) View of the coordination environment of Cd1 and Cd2 atoms in compound **1** (H atoms are omitted for clarity)**.**

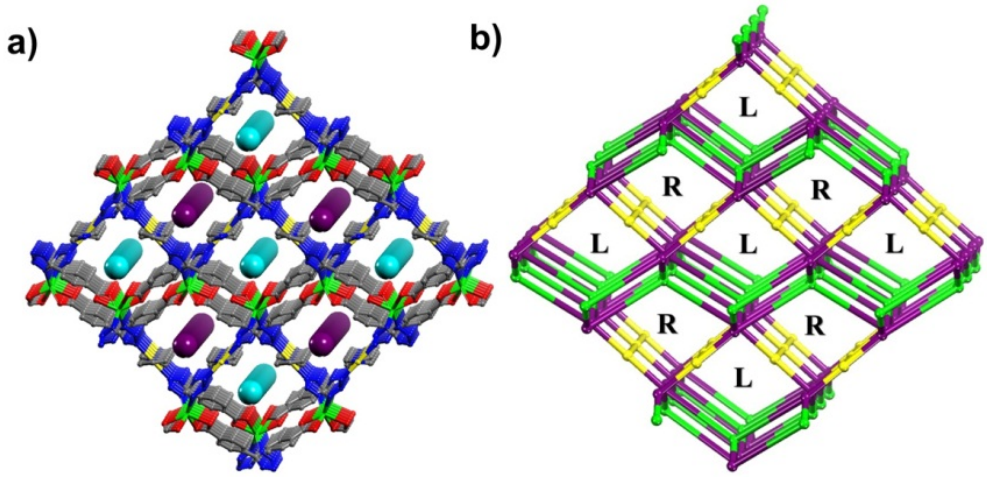

Fig. S3. a) and **b)** View of helical channels with opposite handedness along the [110] direction.

Table S1 The topological information for compound **1** (3,4,4)-c net calculated by *Topos 4.0* and *Systre*.

Vertex figure	**triangle + Square + Tetrahedron**										
Vertex	**CS1**	**CS2**	**CS3**	**CS4**	**CS5**	**CS6**	**CS7**	**CS8**	**CS9**	**CS10**	**Cum10**
V_1(triangle)	3	8	15	38	77	142	220	308	408	518	1737
V_2(square)	4	10	24	48	80	130	212	312	396	492	1708
V_3(tetrahedron)	4	6	16	38	82	152	226	304	418	538	1784

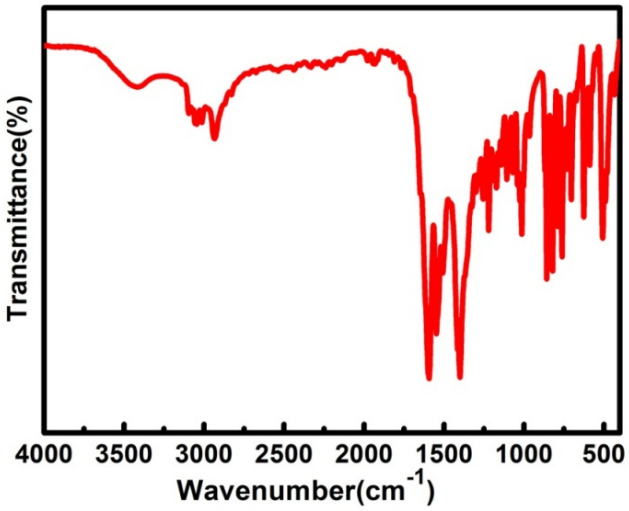

Fig. S4. Infrared spectrum for compound **1** (4000-400 cm^{-1}).

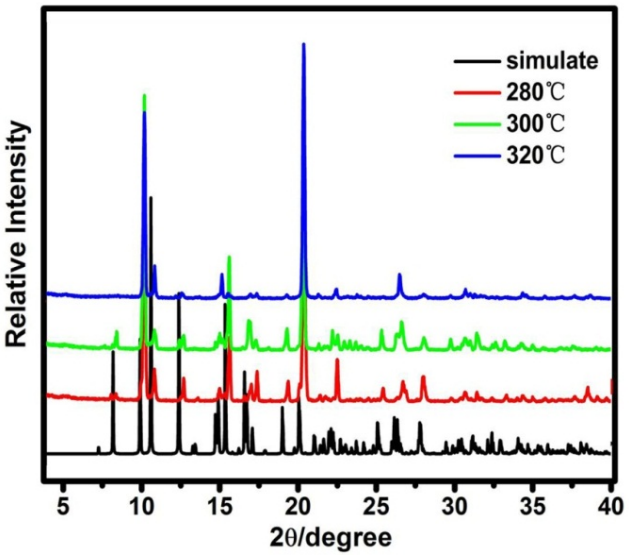

Fig. S5. The simulated and temperature-dependent powder XRD of compound **1**.

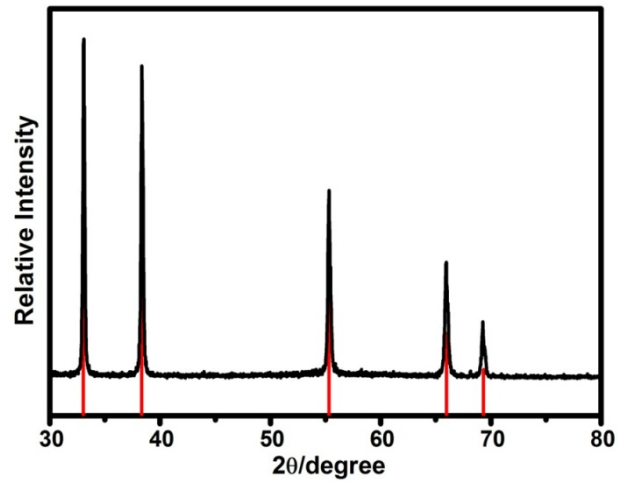

Fig. S6. Powder XRD studies indicate that compound **1** upon calcinations above 600 °C is a main phase of CdO (JCPDS: 05-0640).

Table S2 Selected bond lengths [Å] and angles [º] for compound **1**.

	compound **1**		
Cd(1)-N(2)	2.325(3)	Cd(2)-N(4)	2.298(3)
Cd(1)-N(2)#1	2.325(3)	Cd(2)-N(4)#3	2.298(3)
Cd(1)-O(3)#1	2.332(3)	Cd(2)-O(1)#4	2.349(3)
Cd(1)-O(3)	2.332(3)	Cd(2)-O(1)#5	2.349(3)
Cd(1)-N(5)	2.388(4)	Cd(2)-O(2)#4	2.368(3)
Cd(1)-N(6)#2	2.412(4)	Cd(2)-O(2)#5	2.368(3)
N(2)-Cd(1)-N(2)#1	174.19(17)	N(4)-Cd(2)-N(4)#3	85.87(18)
N(2)-Cd(1)-O(3)#1	92.46(12)	N(4)-Cd(2)-O(1)#4	96.40(12)
N(2)#1-Cd(1)-O(3)#1	87.22(12)	N(4)#3-Cd(2)-O(1)#4	144.19(11)
N(2)-Cd(1)-O(3)	87.22(12)	N(4)-Cd(2)-O(1)#5	144.19(11)
N(2)#1-Cd(1)-O(3)	92.46(12)	N(4)#3-Cd(2)-O(1)#5	96.40(12)
O(3)#1-Cd(1)-O(3)	173.81(17)	O(1)#4-Cd(2)-O(1)#5	101.91(17)
N(2)-Cd(1)-N(5)	87.09(8)	N(4)-Cd(2)-O(2)#4	122.09(11)
N(2)#1-Cd(1)-N(5)	87.09(8)	N(4)#3-Cd(2)-O(2)#4	93.07(11)
O(3)#1-Cd(1)-N(5)	86.91(8)	O(1)#4-Cd(2)-O(2)#4	55.59(11)
O(3)-Cd(1)-N(5)	86.91(8)	O(1)#5-Cd(2)-O(2)#4	93.56(11)
N(2)-Cd(1)-N(6)#2	92.91(8)	N(4)-Cd(2)-O(2)#5	93.07(11)
N(2)#1-Cd(1)-N(6)#2	92.91(8)	N(4)#3-Cd(2)-O(2)#5	122.09(11)
O(3)#1-Cd(1)-N(6)#2	93.09(8)	O(1)#4-Cd(2)-O(2)#5	93.56(11)
O(3)-Cd(1)-N(6)#2	93.09(8)	O(1)#5-Cd(2)-O(2)#5	55.59(10)
N(5)-Cd(1)-N(6)#2	180.0	O(2)#4-Cd(2)-O(2)#5	132.93(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y,z #2 x,y,z-1 #3 x,-y+1/2,-z+1/2

#4 -x+1,-y+1,-z #5 -x+1,y-1/2,z+1/2 #6 x,y,z+1