

Supporting Materials

An unusual (4,4)-connected 3D porous cadmium metal-organic framework as a luminescent sensor for detection of nitrobenzene

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Table S1 Selected bond lengths and angles for **1** (Å and °).

1			
Cd(1)-O(3)#1	2.266(6)	Cd(1)-O(5)	2.275(6)
Cd(1)-N(6)#2	2.287(7)	Cd(1)-N(3)	2.304(7)
Cd(1)-O(2)	2.344(6)	Cd(1)-O(1)	2.405(5)
O(3)#1-Cd(1)-O(5)	123.7(2)	O(3)#1-Cd(1)-N(6)#2	89.3(2)
O(5)-Cd(1)-N(6)#2	85.9(2)	O(3)#1-Cd(1)-N(3)	81.7(2)
O(5)-Cd(1)-N(3)	87.6(2)	N(6)#2-Cd(1)-N(3)	163.6(3)
O(3)#1-Cd(1)-O(2)	90.6(2)	O(5)-Cd(1)-O(2)	145.7(2)
N(6)#2-Cd(1)-O(2)	93.9(2)	N(3)-Cd(1)-O(2)	99.9(2)
O(3)#1-Cd(1)-O(1)	140.1(2)	O(5)-Cd(1)-O(1)	93.1(2)
N(6)#2-Cd(1)-O(1)	110.2(2)	N(3)-Cd(1)-O(1)	85.2(2)
O(2)-Cd(1)-O(1)	54.84(18)		

Symmetry transformations used to generate equivalent atoms: #1 $-x+1/2, y-1/2, -z+1/2$; #2 $x+1/2, -y+3/2, z+1/2$.

Table S2 Hydrogen bonds for **1** (Å and °).

D-H...A	d(D-H)	d(H...A)	D(D...A)	<(DHA)
O(5)-H(5A)...O(6) ⁱ	0.89(2)	1.80(2)	2.694(10)	177(7)
O(5)-H(5B)...O(1) ⁱⁱ	0.89(2)	1.94(5)	2.712(8)	143(8)
O(6)-H(6A)...O(4)	0.90(2)	2.04(6)	2.820(9)	143(6)
O(6)-H(6B)...O(3) ⁱ	0.900(19)	2.05(2)	2.822(9)	143(4)
O(7)-H(7C)...O(4)	0.90(2)	2.05(2)	2.875(19)	150(6)
O(7)-H(7D)...O(8) ⁱⁱ	0.90(2)	2.07(4)	2.97(4)	178(8)
O(8)-H(8C)...O(6) ⁱ	0.90(2)	2.20(2)	2.89(2)	133(3)
O(8)-H(8D)...O(7) ⁱⁱ	0.90(2)	2.40(2)	2.97(4)	124(4)

Symmetry transformations used to generate equivalent atoms: i $-x+1/2, y-1/2, -z+1/2$; ii $-x+1/2, -y+3/2, -z$.

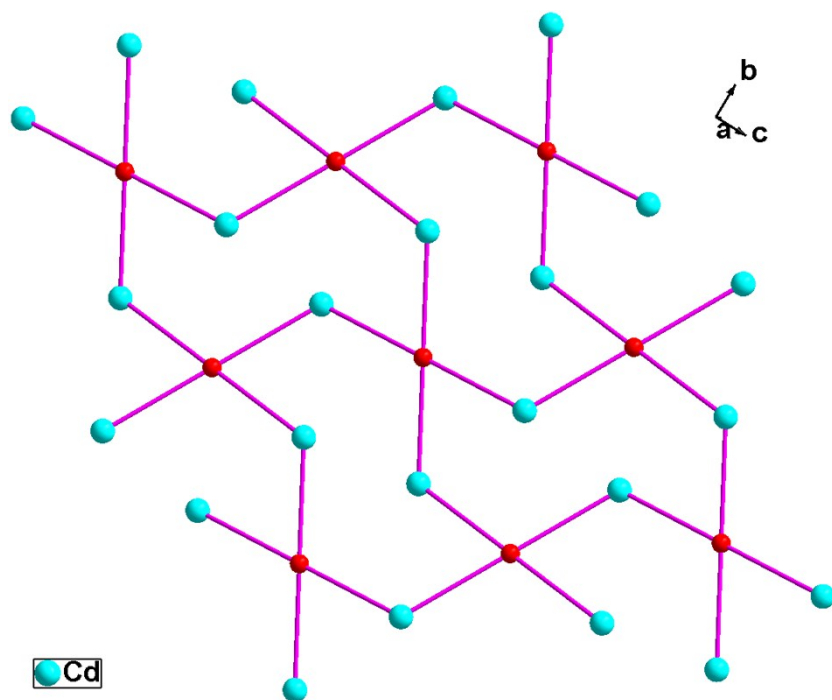


Fig. S1 Schematic depiction of the $[\text{Cd}_2(\text{btec})]_n$ 2D network of **1**. The red balls present the 4-connected btec ligands.

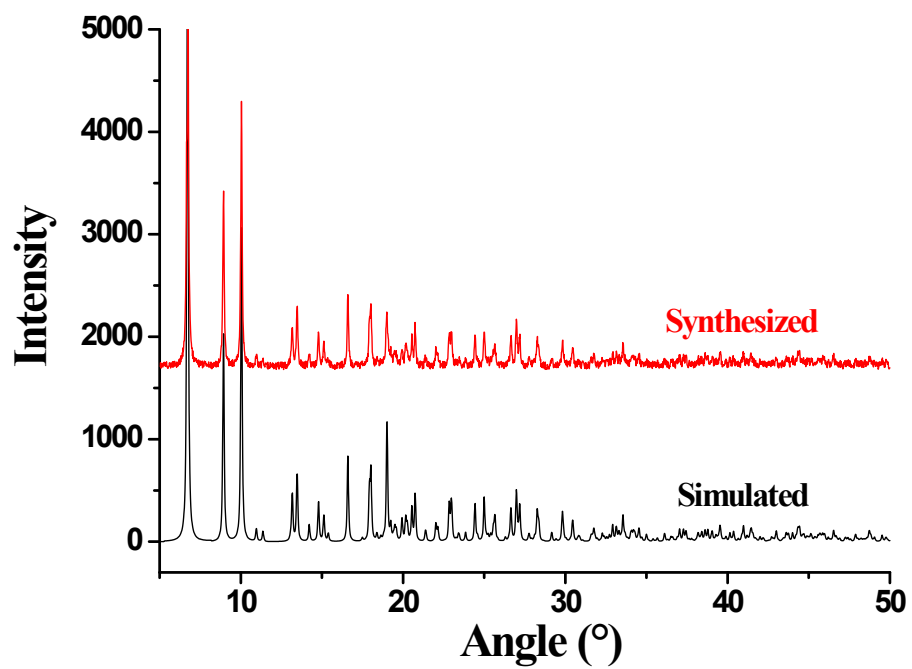


Fig. S2 PXRD patterns of the measured and simulated of **1**.

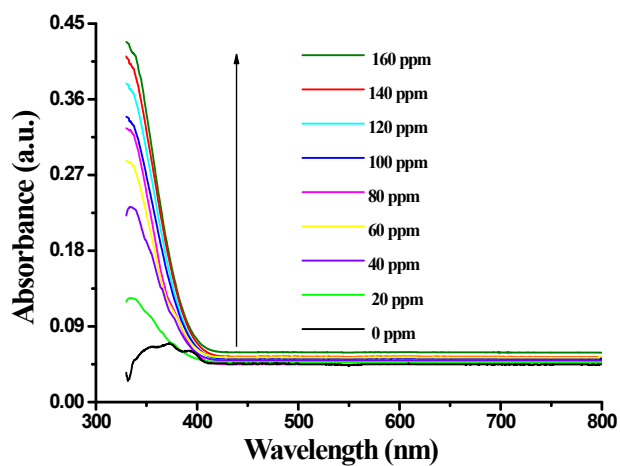


Fig. S3 UV-vis absorption spectra of **1** dispersed in acetone solvent (**1@NBZ@acetone**) in presence of different concentration of nitrobenzene (NBZ).