

Supporting information

A 3D pillared-layer metal-organic framework with fluorescence property for detection of nitroaromatic explosives

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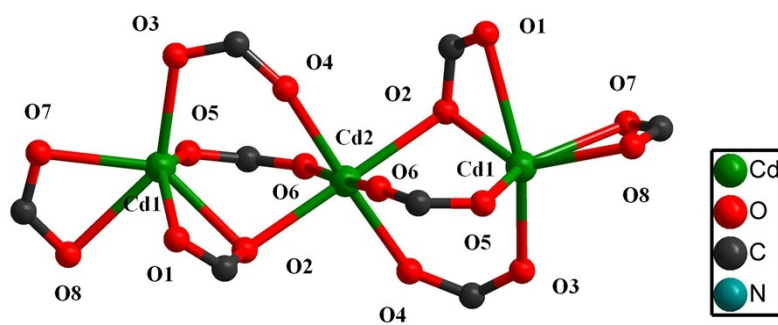


Fig. S1 The coordination environments around the Cd(II) ions.

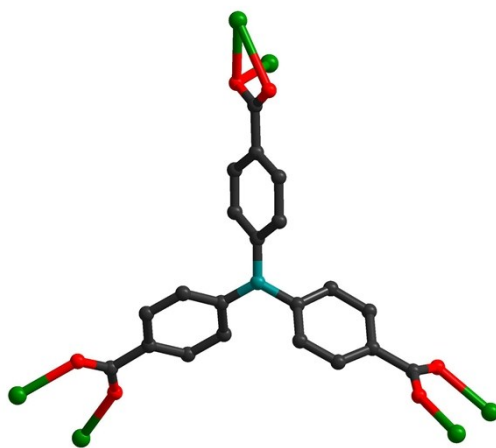


Fig. S2 The bridging coordination mode of NTB ligand.

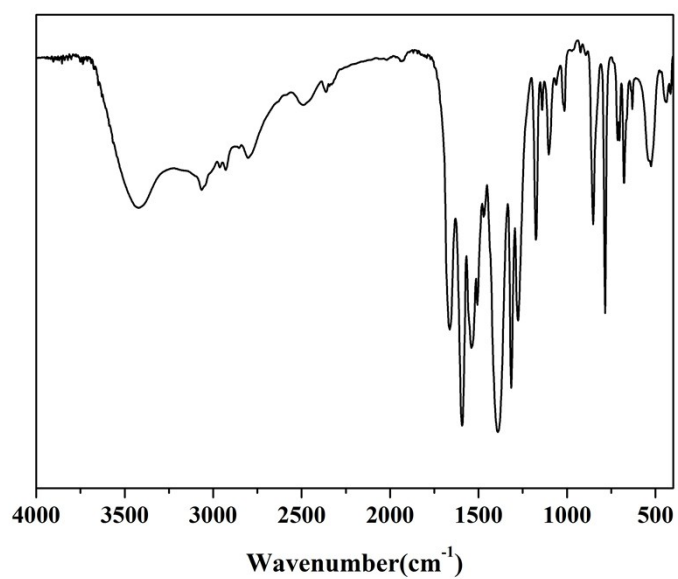


Fig. S3 FT-IR spectra of **1**.

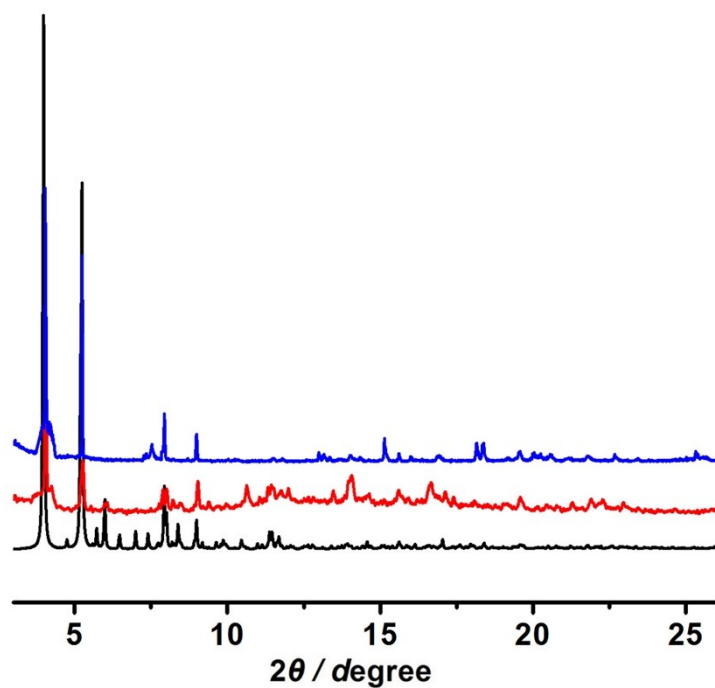


Fig. S4 X-ray powder diffraction patterns of **1**: simulated (black), as-synthesized (red) and after luminescent quenching of PA(blue).

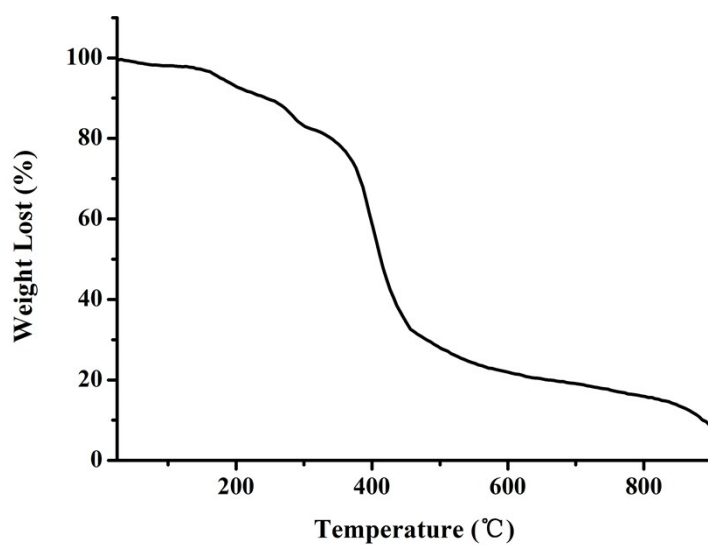


Fig. S5 TG curves of **1**.

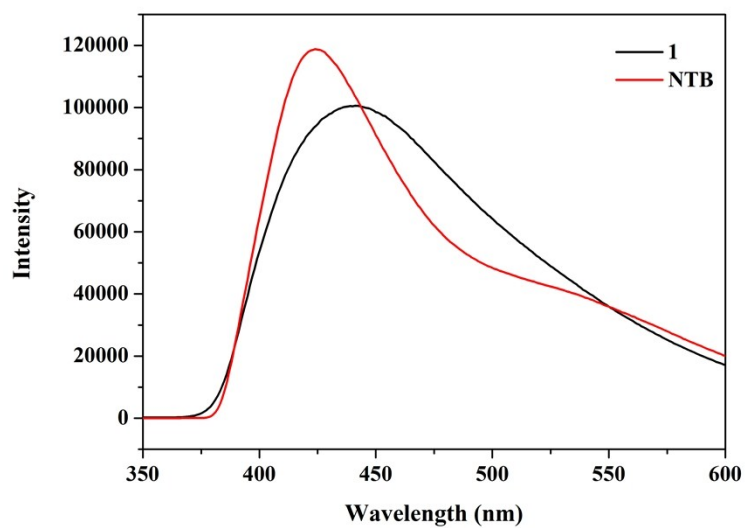


Fig. S6 Photoluminescence spectra of NTB and **1** treated in DMF.

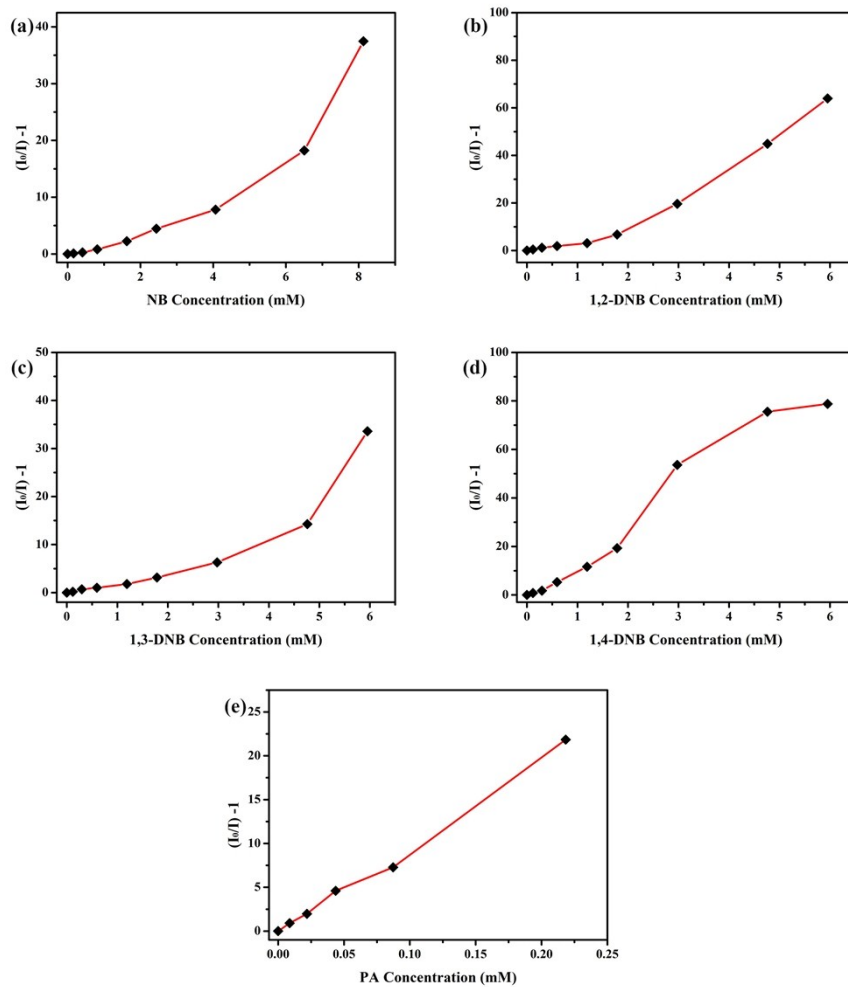


Fig. S7 Corresponding Stern-Volmer plots of (a) NB, (b) 1,2-DNB, (c) 1,3-DNB, (d) 1,4-DNB and (e) PA.

Table S1 Crystal data and structure refinements for **1**

	1
Formula	C ₆₆ H ₇₂ N ₈ O ₂₀ Cd ₃
Formula weight	1634.20
Crystal system	orthorhombic
Space group	<i>Cmca</i>
<i>a</i> (Å)	35.549(5)
<i>b</i> (Å)	27.181(5)
<i>c</i> (Å)	23.930(5)
α (°)	90.000(5)
β (°)	90.000(5)
γ (°)	90.000(5)
<i>V</i> (Å ³)	23123(7)
<i>Z</i>	8
<i>D</i> _{calcd.} [gcm ⁻³]	0.718
<i>F</i> (000)	4912
Reflections collected	65424/10446
<i>R</i> (int)	0.0583
Goodness-of-fit on <i>F</i> ²	1.068
<i>R</i> ₁ ^a [<i>I</i> > 2σ (<i>I</i>)]	0.0399
<i>wR</i> ₂ ^b	0.1229

Table S2 Selected bond lengths [Å] for **1**.

Cd(1)-O(2)	2.282(3)
Cd(1)-O(1)	2.572(3)
Cd(1)-O(5)	2.212(3)
Cd(1)-O(3)	2.212(3)
Cd(1)-O(8)	2.402(4)
Cd(1)-O(7)	2.296(4)

Cd(2)-O(2)	2.308(3)
Cd(2)-O(2)#1	2.308(3)
Cd(2)-O(4)#1	2.187(3)
Cd(2)-O(4)	2.187(3)
Cd(2)-O(6)	2.245(3)
Cd(2)-O(6)#1	2.245(3)

Table S3 Selected angles [°] for **1**.

O(2)-Cd(1)-O(1)	53.19(10)
O(2)-Cd(1)-O(8)	95.06(14)
O(2)-Cd(1)-O(7)	139.02(16)
O(5)-Cd(1)-O(2)	120.09(11)
O(5)-Cd(1)-O(1)	102.35(12)
O(5)-Cd(1)-O(8)	141.10(15)
O(5)-Cd(1)-O(7)	88.08(16)
O(3)-Cd(1)-O(2)	95.58(11)
O(3)-Cd(1)-O(1)	148.01(11)
O(3)-Cd(1)-O(5)	99.81(13)
O(3)-Cd(1)-O(23)	101.40(16)
O(3)-Cd(1)-O(8)	92.16(16)
O(3)-Cd(1)-O(7)	109.08(18)
O(8)-Cd(1)-O(1)	84.90(15)
O(7)-Cd(1)-O(1)	94.51(17)
O(7)-Cd(1)-O(8)	53.08(17)
O(2)-Cd(2)-O(2)#1	179.11(15)
O(4)#1-Cd(2)-O(2)#1	86.40(11)
O(4)#1-Cd(2)-O(2)	94.23(11)
O(4)-Cd(2)-O(2)	86.40(11)

O(4)-Cd(2)-O(2)#1	94.23(11)
O(4)-Cd(2)-O(4)#1	89.53(19)
O(4)#1-Cd(2)-O(6)#1	95.97(14)
O(4)#1-Cd(2)-O(6)	174.38(13)
O(4)-Cd(2)-O(6)#1	174.38(13)
O(4)-Cd(2)-O(6)	95.97(14)
O(6)#1-Cd(2)-O(2)#1	87.28(12)
O(6)#1-Cd(2)-O(2)	92.02(12)
O(6)-Cd(2)-O(2)	87.28(12)
O(6)-Cd(2)-O(2)#1	92.03(12)
O(6)#1-Cd(2)-O(6)	78.56(19)

Table S4 The fluorescence quenching efficiency (K_{sv}) of some previously reported MOF sensors.

MOF	K_{sv} (M^{-1})	References
$[(CH_3)_2NH_2]_2[Cd_3(NTB)_2(BDC)] \cdot 4DMF$ (1)	9.65×10^4	This work
$[Tb_2(H_2L)_3(H_2O)_2] \cdot 21H_2O$	9.20×10^3	[1]
$[Zn_2(L)_2(bpy)]$	1.53×10^4	[2]
$[Zn_2(L)_2(azp)]$	3.11×10^4	[2]
$[NH_2(CH_3)_2][Zn_4O(bpt)_2(bdc)_{0.5}]$	1.69×10^4	[3]
$[NH_2(CH_3)_2][Zn_4O(bpt)_2(bdc-NH_2)_{0.5}]$	6.19×10^4	[3]
$[Zn_3(L)_2(bipy)(\mu_3-OH)_2] \cdot 3H_2O$	2.30×10^4	[4]
$[Cd(5-BrIP)(TIB)]_n$	2.68×10^4	[5]
$[Li]_4[Cd_3Li_2(BDC)_6]$	7.83×10^4	[6]

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