

Supporting Information

Luminescent metal-organic frameworks with 2-(4-pyridyl)-terephthalic acid ligand for detection of acetone

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Table S1 Selected bond lengths [Å] and bond angles [°] for **1-3**

Compound 1			
Zn(1)-O(1)	1.9576(17)	Zn(1)-O(1)W	1.991 (18)
Zn(1)-O(3)#2	1.9574(19)	Zn(1)-N(1)#1	2.041(2)
Zn(1)-C(8)#2	2.552(3)	N(1)-Zn(1)#3	2.041(2)
Zn(1)-O(4)	2.5306(20)	N(1)-C(11)	1.347(3)
N(1)-C(12)	1.344(3)	O(3)-Zn(1)#4	1.9575(19)
O(3)-C(8)	1.276(3)	O(2)-C(1)	1.245(3)
C(8)-Zn(1)#4	2.552(3)	O(4)-C(8)	1.238(4)
Zn(1)-Zn(1)	10.5561(5)	O(4)-C(5)	1.392(4)
O(1)-Zn(1)-O(1W)	101.81(8)	O(1)-Zn(1)-N(1)#1	100.89(8)
O(1)- Zn(1)-C(8)#2	134.32(8)	O(1W)-Zn(1)-N(1)#1	104.54(8)
O(1W)-Zn(1)-C(8)#2	106.31(8)	N(1)#1-Zn(1)-C(8)#2	105.85(8)
O(3)#2-Zn(1)-O(1)	105.20(8)	O(3)#2-Zn(1)-O(1W)	124.08(8)
O(3)#2-Zn(1)-N(1)#1	116.83(8)	O(3)#2-Zn(1)-C(8)#2	29.25(9)
C(1)-O(1)-Zn(1)	130.75(16)	C(11)-N(1)Zn(1)#3	118.37(17)
C(12)-N(1)-Zn(1)#3	123.58(17)	C(8)-O(3)-Zn(1)	102.19(17)
O(3)-C(8)-Zn(1)#4	48.56(13)	O(4)-C(8)-Zn(1)#4	74.93(15)
#1 3/2+x,1/2-y,1/2+z; #2 -1/2-x,1/2+y,1/2-z; #3 -3/2+x,1/2-y,-1/2+z; #4 -1/2-x,-1/2+y,1/2-z			
Compound 2			
Zn(1)-O(1)	2.579(3)	Zn(1)-O(2)	1.958(2)
Zn(1)-O(3)#1	1.976(2)	Zn(1)-O(4)#2	1.966(2)
Zn(1)-N(1)#3	2.065(3)	Zn(1)-C(1)	2.581(3)
O(1)-C(1)	1.227(5)	O(2)-C(1)	1.285(4)
O(3)-Zn(1)#4	1.976(2)	O(3)-C(8)	1.260(4)
O(4)-Zn(1)#2	1.996(2)	O(4)-C(8)	1.249(4)
N(1)-Zn(1)#5	2.065(3)	N(1)-C(11)	1.347(4)
N(1)-C(12)	1.337(5)	C(1)-C(2)	1.513(5)
Zn(1)-Zn (1)	4.7737(7)	C(2)-C(3)	1.387(5)
O(1)-Zn(1)-C(1)	27.51(10)	O(2)-Zn (1)-O(1)	56.37(9)
O(2)-Zn(1)-O(3)	125.07(10)	O(2)-Zn(1)-O(4)	124.54(10)
O(2)-Zn(1)-N(1)	102.61(11)	O(2)-Zn(1)-C(1)	28.94(12)
O(3)-Zn(1)-O(1)	104.26(9)	O(3)-Zn1)-N(1)	94.90(10)
O(3)-Zn(1)-C(1)	11.90(10)	O(4)-Zn(1)-O(1)	88.37(9)

O(4)-Zn(1)-O(3)	102.68(10)	O(4)-Zn(1)-N(1)	99.24(11)
O(4)-Zn(1)-C(1)	106.14(10)	N(1)-Zn(1)-O(1)	157.35(9)
N(1)-Zn(1)-C(1)	130.70(11)	C(1)-O(1)-Zn(1)	76.3(2)

#1 -1/2+x,1/2-y,-1/2+z; #2 -x,-y,1-z; #3 -1/2+x,-1/2+y,+z; #4 1/2+x,1/2-y,1/2+z; #5 1/2+x,1/2+y,+z

Compound 3

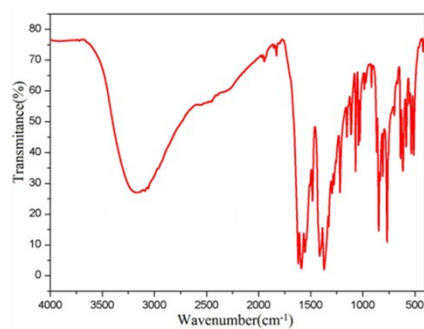
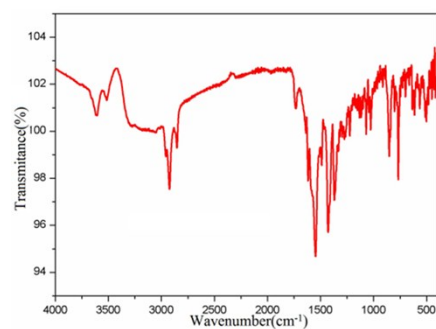
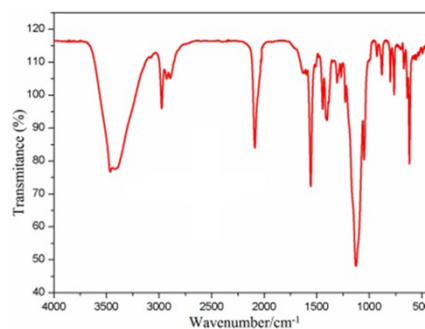
N(1)-C(11)	1.335(3)	N(1)-C(12)	1.352(3)
N(1)-Cd(1)#1	2.297(2)	Cd(1)-O(4)#2	2.2897(18)
Cd(1)-N(1)#2	2.297(2)	Cd(1)-O(1A)#4	2.3107(18)
Cd(1)-O(3)#2	2.3299(18)	Cd(1)-O(1)	2.3436(19)
Cd(1)-O(2B)#5	2.4878(18)	Cd(1)-O(2)#4	2.5774(19)
Cd(1)-C(8)#2	2.641(3)	O(1A)-Cd(1)#6	2.3107(18)
C(1)-O(2)	1.246(3)	C(1)-O(1)	1.275(3)
C(11)-N(1)-Cd(1)#1	126.67(18)	C(12)-N(1)-Cd(1)#1	115.64(17)
O(4)#2-Cd(1)-N(1)#2	148.17(7)	O(4)#2-Cd(1)-O(1)#4	120.19(6)
N(1)#3-Cd(1)-O(1)#4	85.87(7)	O(4)#2-Cd(1)-O(3)#2	57.28(6)
N(1)#3-Cd(1)-O(3)#2	90.97(7)	O(1)#4-Cd(1)-O(3)#2	150.67(6)
O(4)#2-Cd(1)-O(1)	90.32(6)	N(1)#3-Cd(1)-O(1)	91.43(7)
O(1)#4-Cd(1)-O(1)	120.00(5)	O(3)#2-Cd(1)-O(1)	89.19(6)
O(4)#2-Cd(1)-O(2)#5	84.66(6)	N(1)#5-Cd(1)-O(2)#5	88.32(7)
O(1)#4-Cd(1)-O(2)#5	69.97(6)	O(3)#2-Cd(1)-O(2)#5	80.80(6)
O(1)-Cd(1)-O(2)#5	169.98(6)	O(4)#2-Cd(1)-O(2)#4	115.80(6)
N(1)#5-Cd(1)-O(2)#4	94.17(7)	O(1)#4-Cd(1)-O(2)#4	52.65(6)
O(3)#2-Cd(1)-O(2)#4	156.61(6)	O(1)-Cd(1)-O(2)#4	67.90(6)
O(2)#5-Cd(1)-O(2)#4	122.11(5)	O(4)#2-Cd(1)-C(8)#2	28.95(7)
N(1)#5-Cd(1)-C(8)#2	119.27(8)	O(1)#4-Cd(1)-C(8)#2	141.79(7)
O(3)#2-Cd(1)-C(8)#2	28.32(7)	O(1)-Cd(1)-C(8)#2	89.65(7)
O(2)#5-Cd(1)-C(8)#2	81.75(7)	O(2)#4-Cd(1)-C(8)#2	140.63(7)

#1 5/2-x,1/2+y,1/2-z; #2 2-x,1-y,1-z; #3 5/2-x,-1/2+y,1/2-z; #4 3/2-x,-1/2+y,1/2-z; #5 +x,-1+y,+z; #6 3/2-x,1/2+y,1/2-z; #7 +X,1+Y,+Z

#7 +x,1+y,+z

Table S2 Detection limits of some MOFs used for fluorescent sensing of acetone.

Compound	Detection limit	References
$[\text{Zn}(\text{L})(\text{bpdc})] \cdot 1.6\text{H}_2\text{O}$	0.0478 vol% (478 ppm)	32
$[\text{Cd}_2(\text{L})(\text{Hbptc})_2]$	0.0465 vol% (465 ppm)	32
$[\text{Cd}(\text{Tipb})(\text{mta})] \cdot (\text{DMF})_x(\text{H}_2\text{O})_y$	0.075 vol% (750 ppm)	33
$\{[\text{Cd}_3(\text{L})(\text{H}_2\text{O})_2(\text{DMF})_2]\}_n$	1.0 vol% (10000 ppm)	34
$\{[\text{Cd}_3(\text{L})(\text{dib})]\}_n$	2.0 vol% (20000 ppm)	34
$[\text{Eu}_2(\text{m}_2\text{-pzdc})(\text{m}_4\text{-pzdc})(\text{m}_2\text{-ox})(\text{H}_2\text{O})_4]$	5.75 vol% (57500 ppm)	35
$[\text{Cd}_3(\text{L}^1)_2(\text{BTB})_2(\text{H}_2\text{O})] \cdot \text{DMF} \cdot \text{H}_2\text{O}$	0.122 vol% (1220 ppm)	36
$[\text{Zn}_2(\text{TPC4A})(\text{DMF})(\text{H}_2\text{O})_4] \cdot 3\text{H}_2\text{O}$	5 vol% (50000 ppm)	37
$[\text{Zn}(2,5\text{-PDC})(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$	0.0055 vol% (55 ppm)	38
$[\text{Eu}(\text{BTB})(\text{H}_2\text{O})_2 \cdot \text{solvent}]_n$	0.3 vol% (3000 ppm)	39
$\{[\text{Cd}(\text{pta})] \cdot \text{H}_2\text{O}\}_n$	0.0825 vol% (825 ppm)	This work

**(a)****(b)****(c)****Fig. S1** IR spectra of 1 (a), 2 (b) and 3 (c).

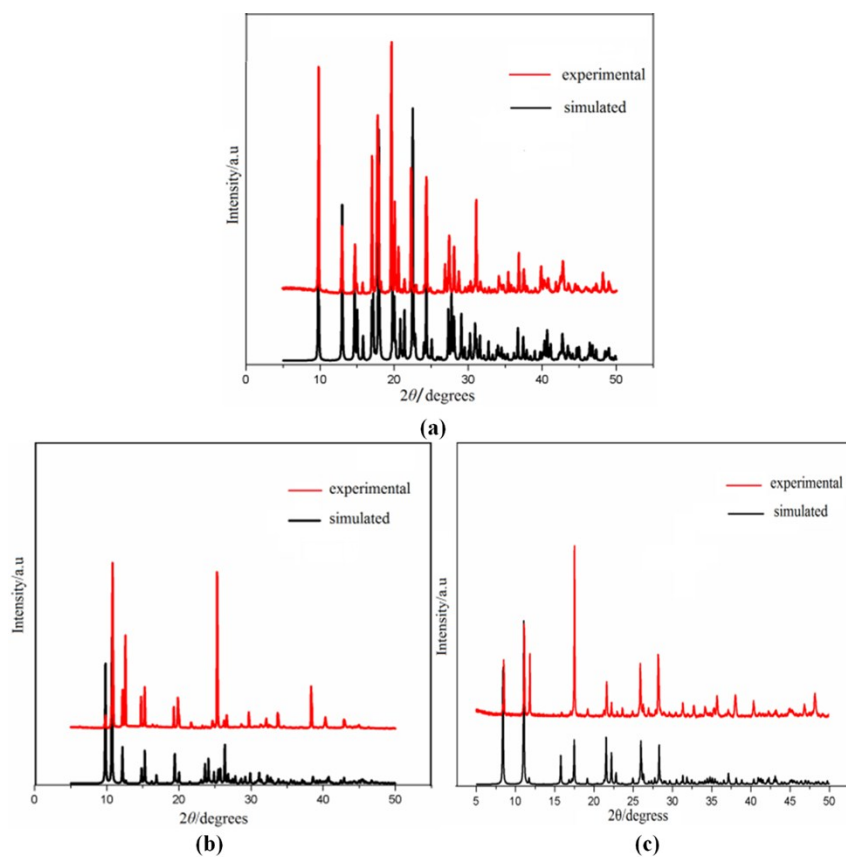


Fig. S2 PXRD patterns of **1** (a), **2** (b) and **3** (c).

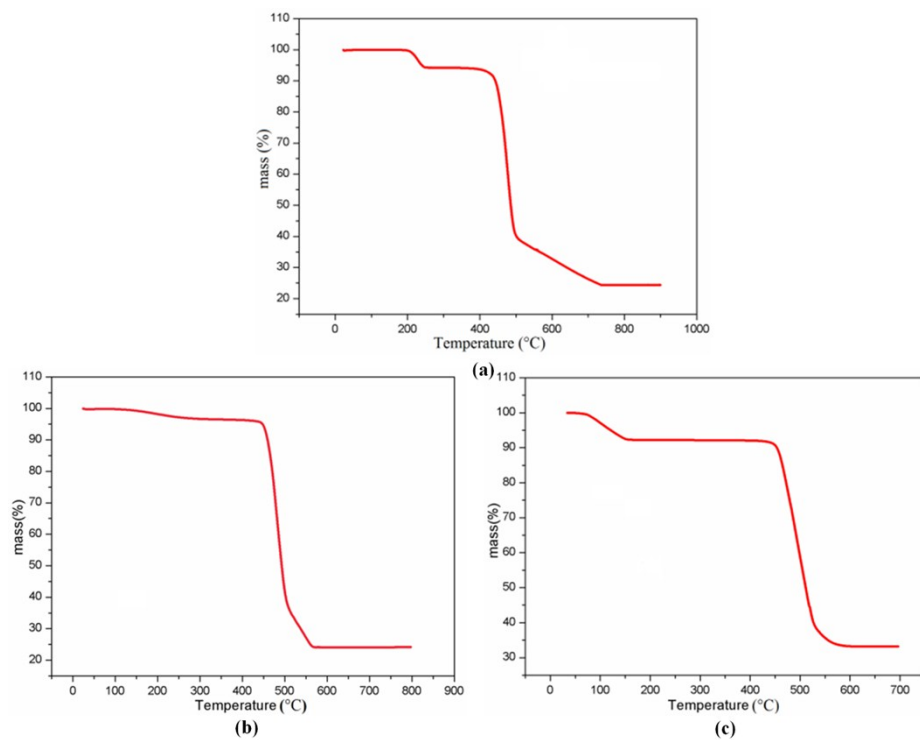


Fig. S3 TG curves for **1** (a), **2** (b) and **3** (c).

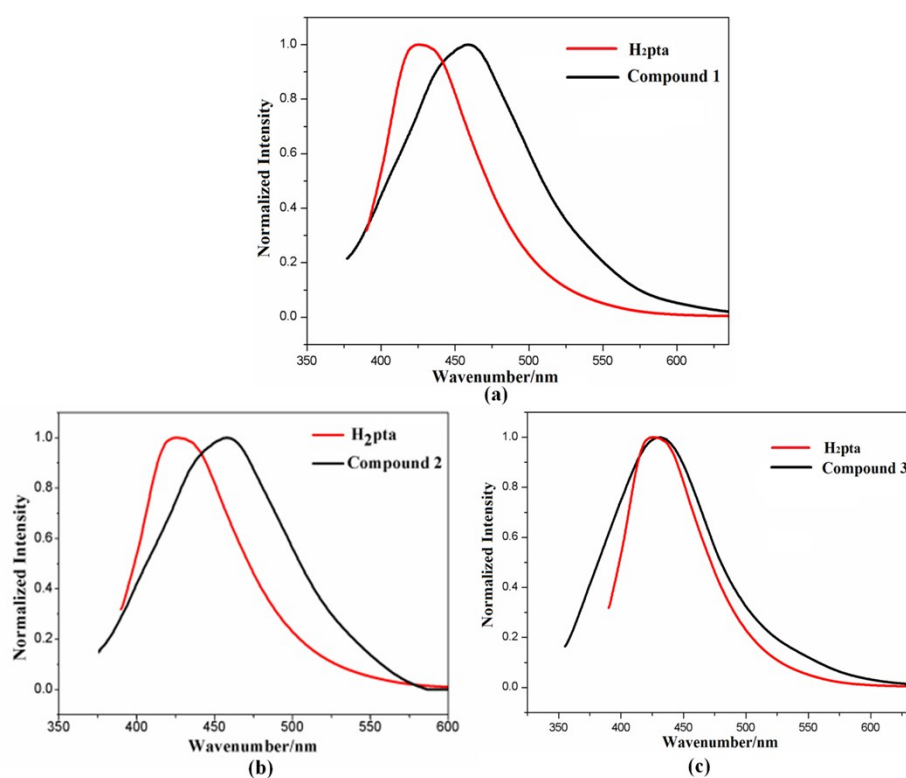


Fig. S4 Solid-state fluorescence spectra of H₂pta and compounds **1** (a), **2** (b) and **3** (c)

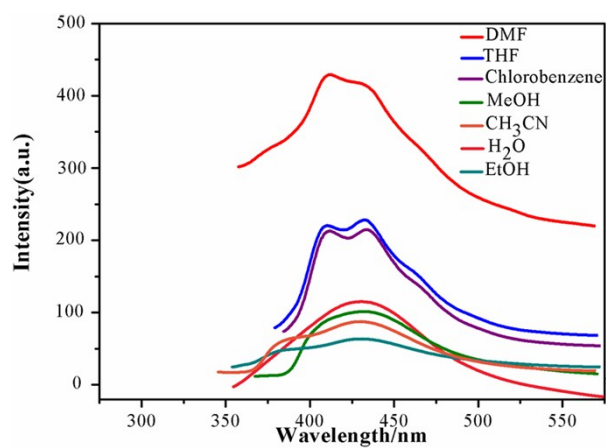


Fig. S5 Fluorescent intensities ($\lambda_{\text{ex}} = 277 \text{ nm}$) of **3** upon the solutions of acetone and different normal solvents (1mL solvents : 1mL acetone)