Supporting Information

A luminescent metal-organic framework as an ideal chemosensor for nitroaromatic compounds

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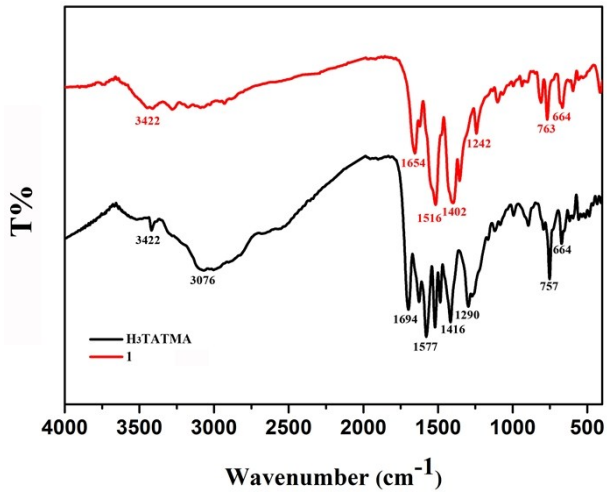

Fig. S1 The FT-IR spectra of H_3TATMA (black) and **1** (red).

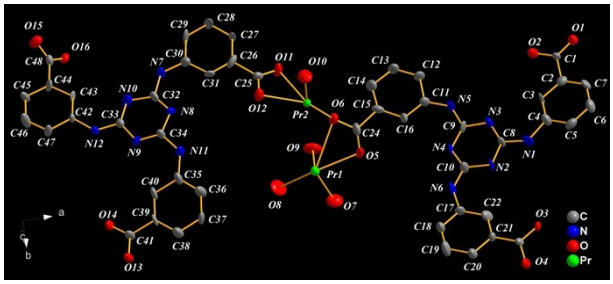

Fig. S2 The asymmetric unit of **1**.

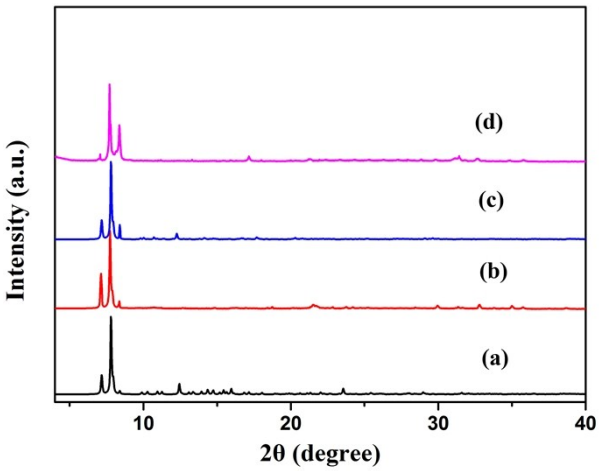

Fig. S3 The PXRD patterns of simulated (a), the as-synthesized 1 (b), **1** immersed in DMF after one week (c), and **1** dispersed in DMF with NB of 600 ppm after repeated five times (d).

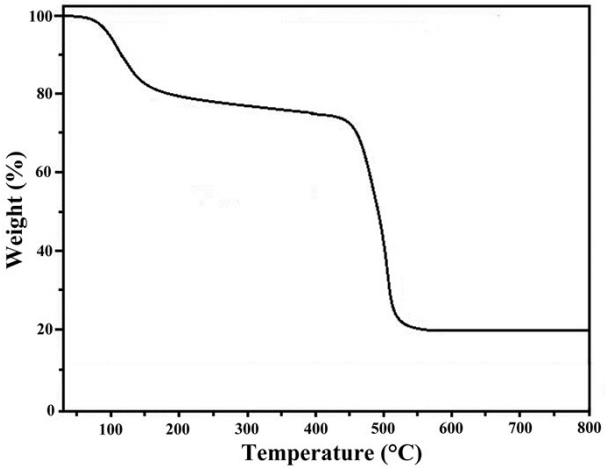

Fig. S4 The TGA plots of **1** in air condition.

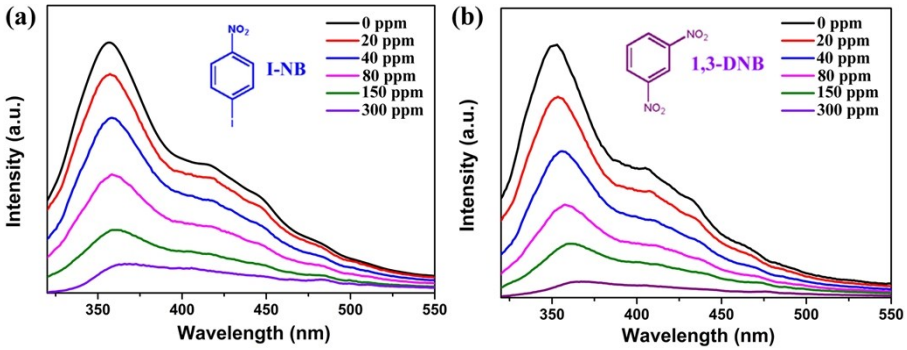

Fig. S5 Emission spectra of 1 titrated with I-DB (a) and 1, 3-DNB (b) in DMF about 2 minutes, respectively.

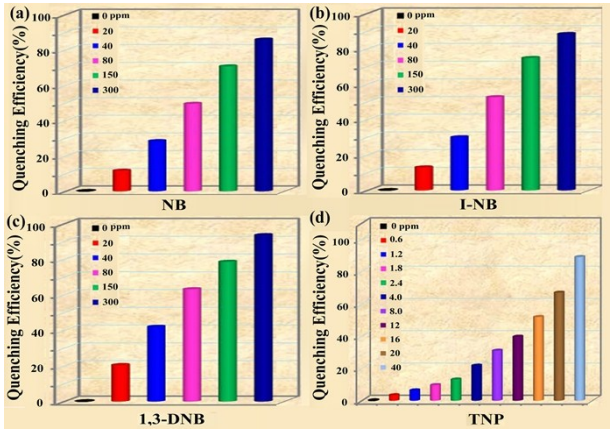

Fig. S6 The corresponding quenching efficiency of **1** titrated with NB (a), I-NB (b), 1,3-DNB (c) and TNP (d) in DMF, respectively. The quenching efficiency (%) was estimated using the formula $(I_0 - I)/I_0 \times 100\%$, where I_0 is the maximum luminescent intensity of **1** before exposure to the analyte and I is the luminescent intensity for any given concentration of quencher.

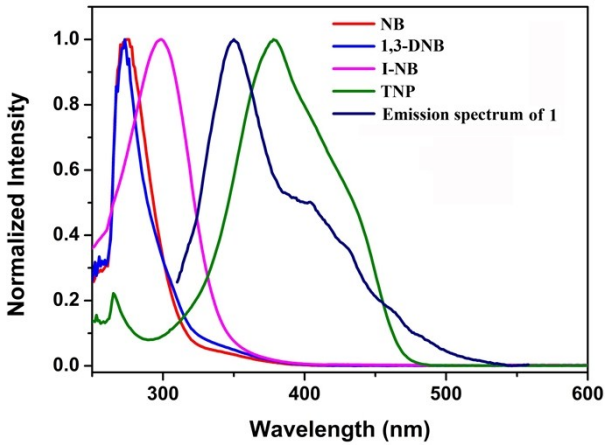

Fig. S7 The spectral overlap between the absorption spectra of analytes and the emission spectrum of **1**.

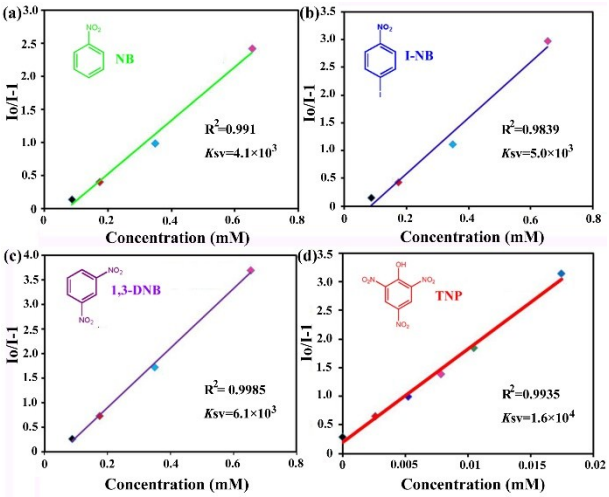

Fig. S8 The Stern-Volmer plots for 1 with NB (a), I-NB (b), 1,3-DNB (c) and TNP (d) at low concentrations, respectively. The solid lines fit to the concentration-resolved data using Stern-Volmer equation.

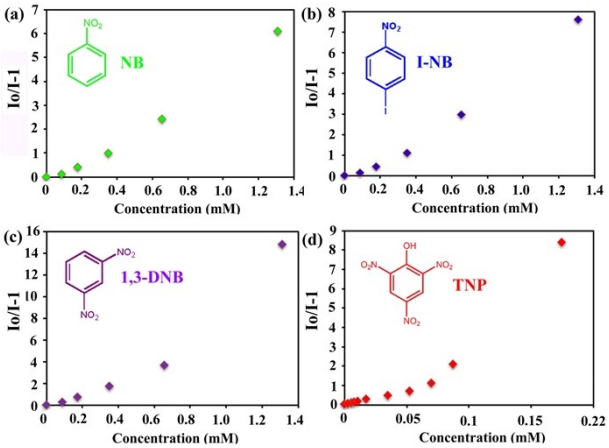

Fig. S9 The Stern-Volmer plot for NB (a), I-NB (b), 1,3-DNB (c) and TNP (d) in full concentration region, respectively.

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

1			
O(1)-Pr(1)#1	2.598(8)	O(2)-Pr(1)#1	2.494(8)
O(3)-Pr(2)#2	2.564(8)	O(3)-Pr(1)#2	2.649(7)

O(4)-Pr(1)#2	2.676(8)	O(5)-Pr(1)	2.499(8)
O(6)-Pr(2)	2.479(7)	O(6)-Pr(1)	2.807(8)
O(7)-Pr(1)	2.513(11)	O(8)-Pr(1)	2.524(11)
O(9)-Pr(1)	2.528(9)	O(10)-Pr(2)	2.480(10)
O(11)-Pr(2)	2.450(9)	O(12)-Pr(2)	2.515(8)
O(13)-Pr(2)#3	2.527(8)	O(14)-Pr(2)#3	2.496(7)
O(15)-Pr(2)#4	2.517(8)	O(16)-Pr(1)#4	2.520(8)
O(16)-Pr(2)#4	2.648(8)	Pr(1)-O(2)#3	2.494(8)
Pr(1)-O(16)#2	2.520(8)	Pr(1)-O(1)#3	2.598(9)
Pr(1)-O(3)#4	2.649(7)	Pr(1)-O(4)#4	2.676(8)
Pr(2)-O(14)#1	2.496(7)	Pr(2)-O(15)#2	2.517(8)
Pr(2)-O(13)#1	2.527(8)	Pr(2)-O(3)#4	2.564(8)
Pr(2)-O(16)#2	2.648(8)		
O(2)#3-Pr(1)-O(5)	120.6(3)	O(2)#3-Pr(1)-O(16)#2	89.5(3)
O(5)-Pr(1)-O(16)#2	78.1(3)	O(2)#3-Pr(1)-O(7)	78.2(3)
O(5)-Pr(1)-O(7)	78.6(3)	O(16)#2-Pr(1)-O(7)	143.0(3)
O(2)#3-Pr(1)-O(9)	140.4(3)	O(5)-Pr(1)-O(9)	78.8(3)
O(16)#2-Pr(1)-O(9)	129.8(3)	O(7)-Pr(1)-O(9)	72.1(3)
O(2)#3-Pr(1)-O(8)	78.1(3)	O(5)-Pr(1)-O(8)	142.0(3)
O(16)#2-Pr(1)-O(8)	138.4(3)	O(7)-Pr(1)-O(8)	73.3(4)
O(9)-Pr(1)-O(8)	68.6(3)	O(2)#3-Pr(1)-O(1)#3	50.4(3)
O(5)-Pr(1)-O(1)#3	70.5(3)	O(16)#2-Pr(1)-O(1)#3	73.5(3)
O(7)-Pr(1)-O(1)#3	71.8(3)	O(9)-Pr(1)-O(1)#3	136.2(3)
O(8)-Pr(1)-O(1)#3	122.0(3)	O(2)#3-Pr(1)-O(3)#4	120.7(2)
O(5)-Pr(1)-O(3)#4	110.2(2)	O(16)#2-Pr(1)-O(3)#4	72.3(2)
O(7)-Pr(1)-O(3)#4	143.5(3)	O(9)-Pr(1)-O(3)#4	75.0(3)
O(8)-Pr(1)-O(3)#4	80.3(3)	O(1)#3-Pr(1)-O(3)#4	144.7(3)
O(2)#3-Pr(1)-O(4)#4	72.4(2)	O(5)-Pr(1)-O(4)#4	147.3(3)
O(16)#2-Pr(1)-O(4)#4	71.9(2)	O(7)-Pr(1)-O(4)#4	133.9(3)
O(9)-Pr(1)-O(4)#4	111.0(3)	O(8)-Pr(1)-O(4)#4	66.5(3)
O(1)#3-Pr(1)-O(4)#4	111.8(2)	O(3)#4-Pr(1)-O(4)#4	48.3(2)
O(2)#3-Pr(1)-O(6)	153.7(3)	O(5)-Pr(1)-O(6)	48.3(2)
O(16)#2-Pr(1)-O(6)	65.8(2)	O(7)-Pr(1)-O(6)	115.9(3)
O(9)-Pr(1)-O(6)	65.5(3)	O(8)-Pr(1)-O(6)	126.1(3)
O(1)#3-Pr(1)-O(6)	110.6(3)	O(3)#4-Pr(1)-O(6)	61.9(2)
O(4)#4-Pr(1)-O(6)	105.8(2)	O(11)-Pr(2)-O(6)	104.1(3)
O(11)-Pr(2)-O(10)	87.0(3)	O(6)-Pr(2)-O(10)	148.6(3)
O(11)-Pr(2)-O(14)#1	74.5(3)	O(6)-Pr(2)-O(14)#1	81.2(3)
O(10)-Pr(2)-O(14)#1	73.6(3)	O(11)-Pr(2)-O(12)	52.3(3)
O(6)-Pr(2)-O(12)	136.8(3)	O(10)-Pr(2)-O(12)	72.9(3)
O(14)#1-Pr(2)-O(12)	117.2(3)	O(11)-Pr(2)-O(15)#2	124.6(3)
O(6)-Pr(2)-O(15)#2	118.5(3)	O(10)-Pr(2)-O(15)#2	74.9(3)
O(14)#1-Pr(2)-O(15)#2	141.8(3)	O(12)-Pr(2)-O(15)#2	72.4(3)
O(11)-Pr(2)-O(13)#1	125.7(3)	O(6)-Pr(2)-O(13)#1	74.6(3)

O(10)-Pr(2)-O(13)#1	75.1(3)	O(14)#1-Pr(2)-O(13)#1	51.4(2)
O(12)-Pr(2)-O(13)#1	148.0(3)	O(15)#2-Pr(2)-O(13)#1	99.7(3)
O(11)-Pr(2)-O(3)#4	80.5(3)	O(6)-Pr(2)-O(3)#4	67.7(3)
O(10)-Pr(2)-O(3)#4	143.7(3)	O(14)#1-Pr(2)-O(3)#4	133.5(3)
O(12)-Pr(2)-O(3)#4	72.5(3)	O(15)#2-Pr(2)-O(3)#4	84.5(3)
O(13)#1-Pr(2)-O(3)#4	138.8(3)	O(11)-Pr(2)-O(16)#2	151.9(3)
O(6)-Pr(2)-O(16)#2	68.9(2)	O(10)-Pr(2)-O(16)#2	113.4(3)
O(14)#1-Pr(2)-O(16)#2	128.3(2)	O(12)-Pr(2)-O(16)#2	113.4(2)
O(15)#2-Pr(2)-O(16)#2	50.2(3)	O(13)#1-Pr(2)-O(16)#2	79.9(2)
O(3)#4-Pr(2)-O(16)#2	71.6(2)		

Symmetry transformations used to generate equivalent atoms:

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