Electronic Supplementary Information (ESI)

A unique Zn(II)-based MOF fluorescent probe for the dual detection of nitroaromatics and ketones in water

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Contents

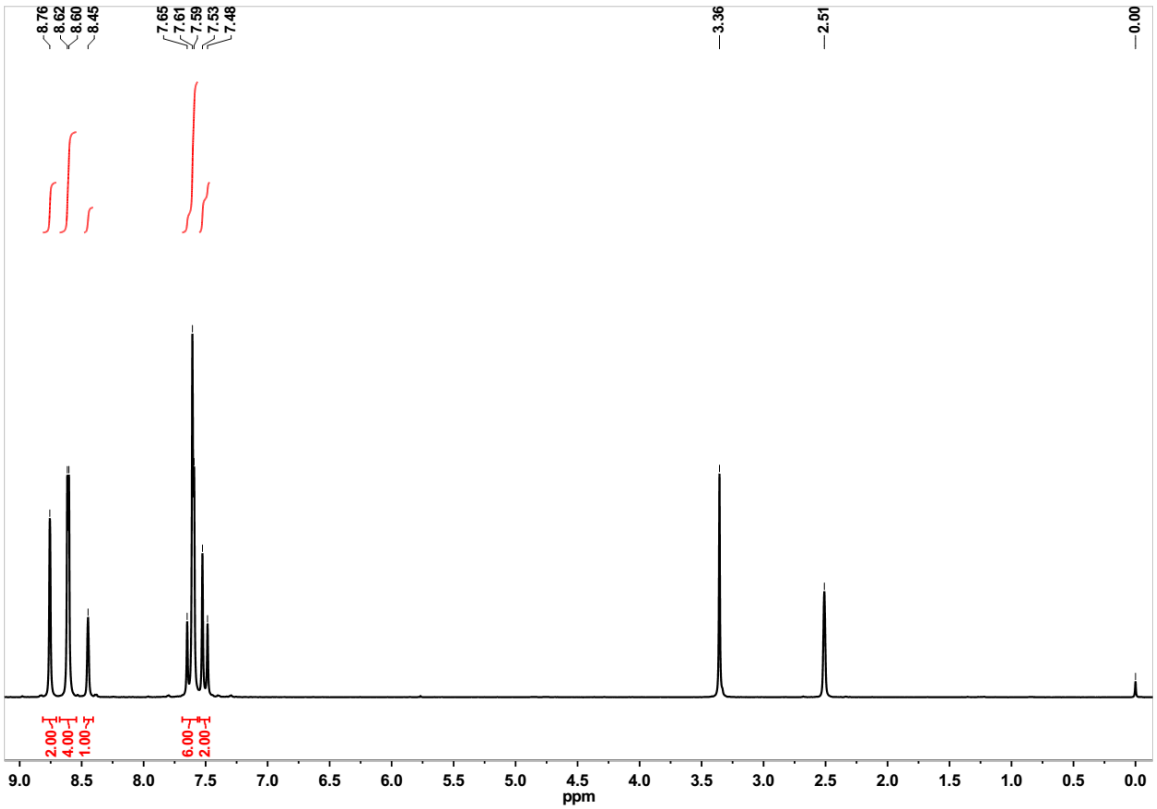

Fig. S1 The ^{1}H NMR spectrum of the bpvp ligand.

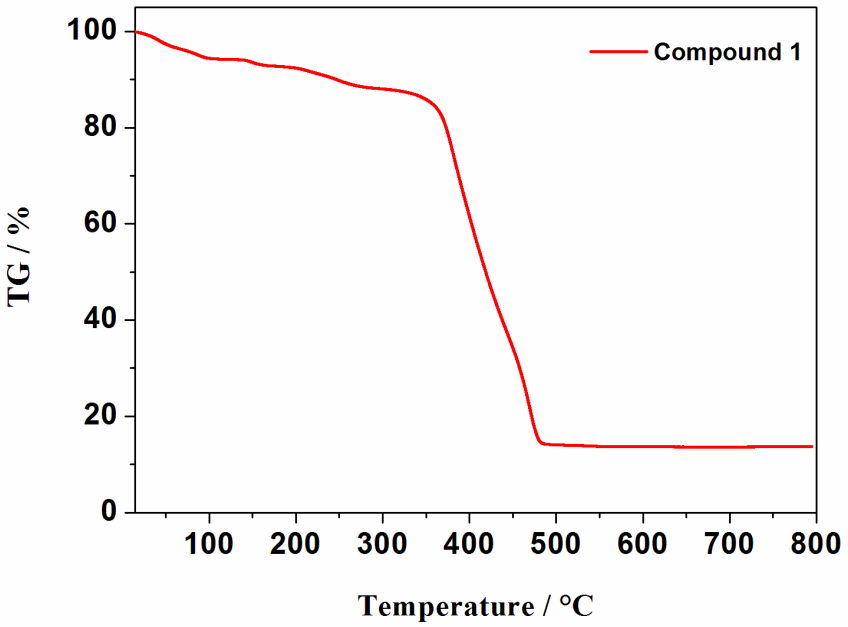

Fig. S2 The TGA curve of **1**.

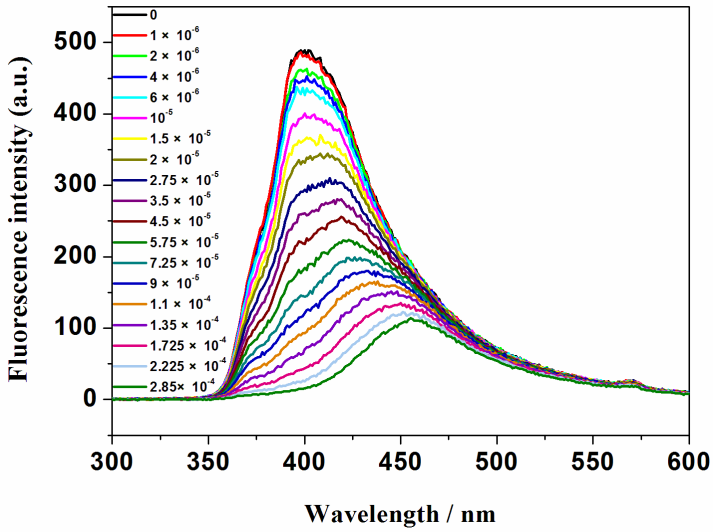

Fig. S3 The emission spectra of **1** in H_2O with the addition of different concentrations of 4-NA excited at 285 nm.

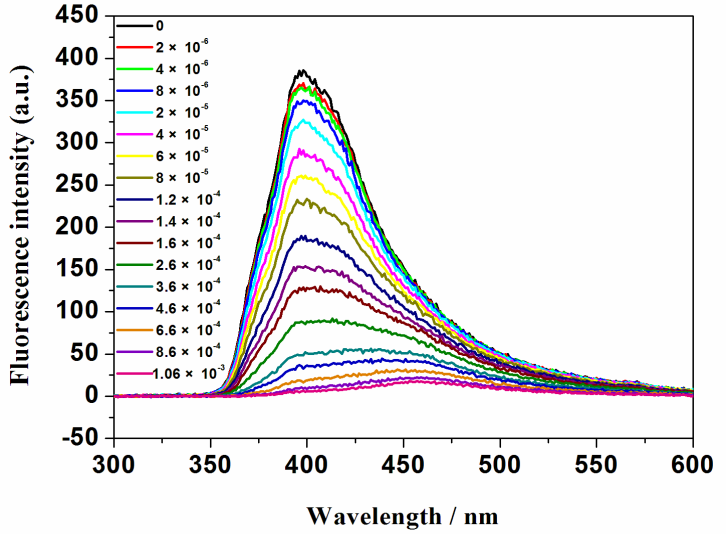

Fig. S4 The emission spectra of **1** in H_2O with the addition of different concentrations of 4-NP excited at 285 nm.

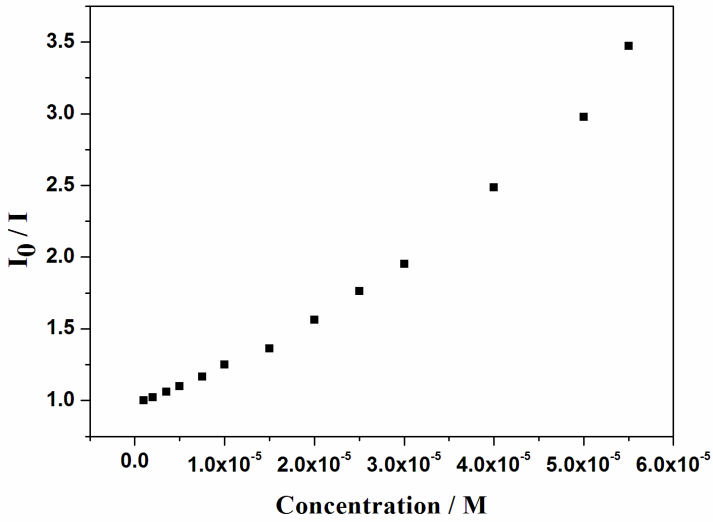

Fig. S5 The Stern-Volmer curve of **1** in H_2O with the addition of different concentrations of 2,4-DNP.

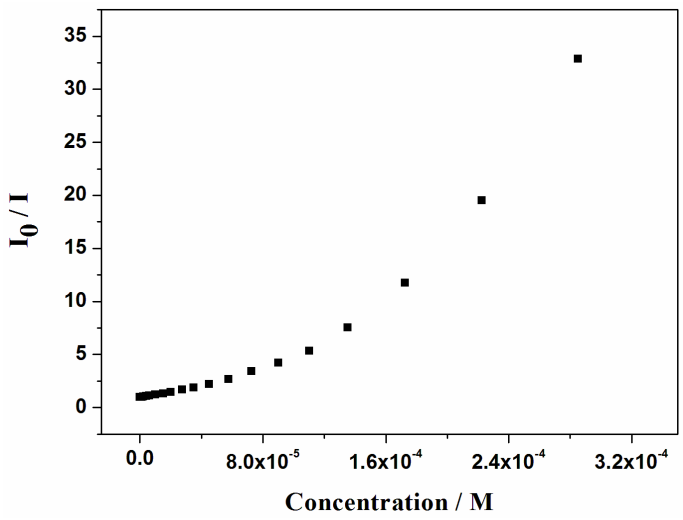

Fig. S6 The Stern-Volmer curve of **1** in H_2O with the addition of different concentrations of 4-NA.

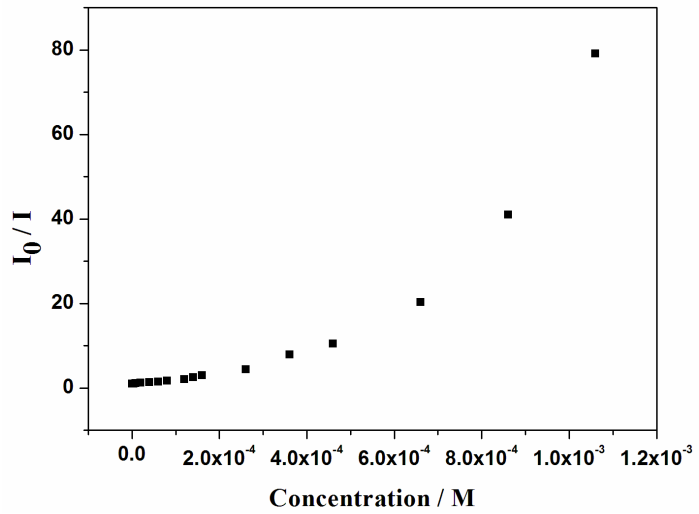

Fig. S7 The Stern-Volmer curve of **1** in H_2O with the addition of different concentrations of 4-NP.

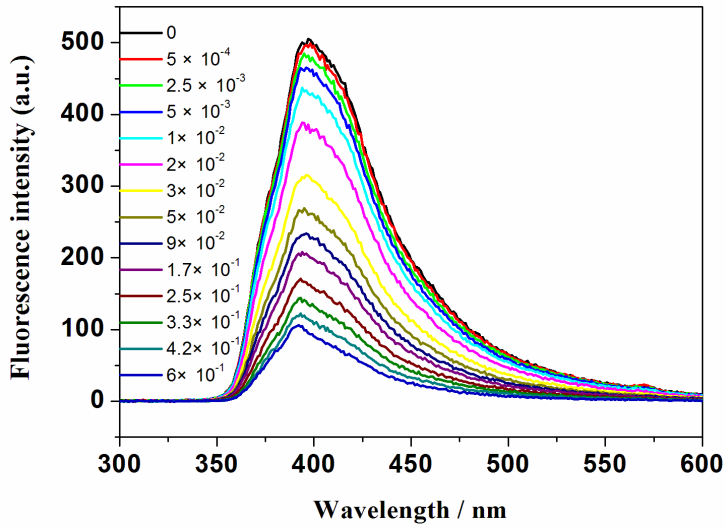

Fig. S8 The emission spectra of **1** in H_2O with the addition of different concentrations of acetone excited at 285 nm.

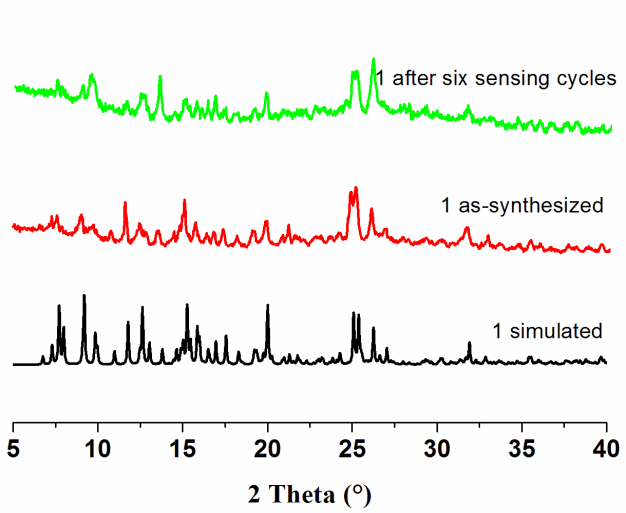

Fig. S9 The PXRD patterns of **1** after six cycles experiment for the detection of 2,4-DNP.

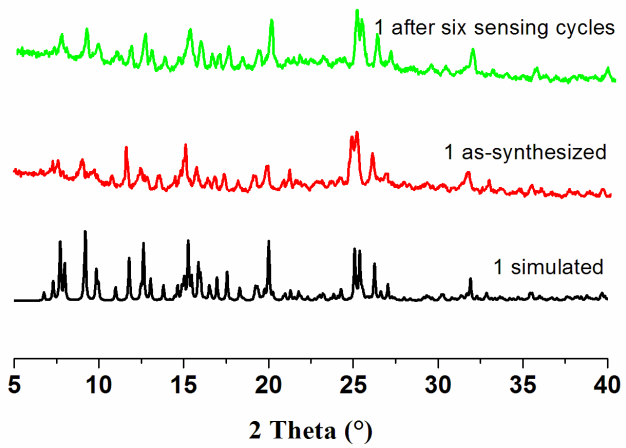

Fig. S10 The PXRD patterns of **1** after six cycles experiment for the detection of *p*-BQ.

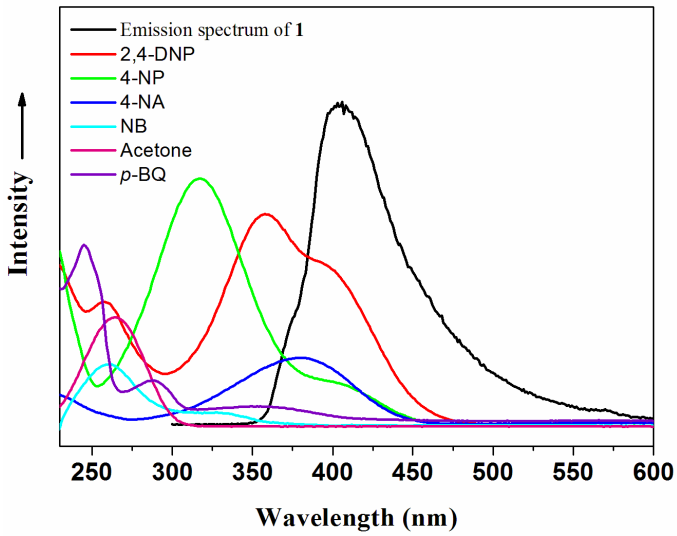

Fig. S11 Spectral overlap between the absorption spectrum of nitroaromatics or ketones (2×10^{-5} mol Ł$^{-1}$) in water and the emission spectrum of **1** (2 mg) in 2 mL of water.

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

Zn(1)-O(7)	2.005(3)
Zn(1)-O(13)	2.021(3)
Zn(1)-N(1)	2.031(3)
Zn(1)-O(1)	2.055(3)
Zn(1)-Zn(2)	3.0093(7)
Zn(2)-O(8)	2.025(3)
Zn(2)-N(4)#1	2.033(3)
Zn(2)-O(2)	2.034(3)
Zn(2)-O(14)	2.045(3)
Zn(3)-O(1W)	2.047(3)
Zn(3)-N(5)	2.092(4)
Zn(3)-O(4)	2.259(3)
Zn(3)-O(17)#2	2.276(3)
Zn(4)-O(5)#1	1.986(3)
Zn(4)-O(9)	2.023(3)
Zn(4)-O(2W)	2.027(3)
Zn(4)-N(2)#3	2.077(3)
Zn(4)-O(10)	2.387(3)
O(7)-Zn(1)-O(13)	158.65(12)
O(7)-Zn(1)-N(1)	100.08(13)
O(13)-Zn(1)-O(1)	87.53(14)
N(1)-Zn(1)-O(1)	99.60(14)
O(7)-Zn(1)-Zn(2)	82.65(8)
O(8)-Zn(2)-N(4)#1	101.75(13)
O(8)-Zn(2)-O(2)	88.58(15)
O(2)-Zn(2)-O(14)	84.67(15)
N(4)#1-Zn(2)-O(20)	105.72(13)
O(2)-Zn(2)-O(20)	156.76(12)
O(1W)-Zn(3)-O(18)#2	95.12(13)
O(1W)-Zn(3)-N(5)	101.70(13)
O(1W)-Zn(3)-O(4)	156.79(11)
N(5)-Zn(3)-O(4)	87.09(13)
N(5)-Zn(3)-O(17)#2	96.23(12)
O(5)#1-Zn(4)-O(2W)	100.40(12)
O(2W)-Zn(4)-N(2)#3	98.58(13)
O(9)-Zn(4)-O(10)	58.80(11)
O(2W)-Zn(4)-O(10)	90.55(11)
N(2)#3-Zn(4)-O(10)	95.95(11)

Symmetry transformations used to generate equivalent atoms for **1**: #1: $-x + 7/2, y + 1/2, -z + 1/2$; #2: $-x + 5/2, y - 1/2, -z + 1/2$; #3: $x + 1, y$, z; #4: $-x + 7/2, y - 1/2, -z + 1/2$; #5: $-x + 5/2, y + 1/2, -z + 1/2$; #6: $x - 1, y, z$.

Table S2. The hydrogen bonding with the protonated pyridyl end in the Hbpvp ligand [Å and °].

D-H...A	d(D-H)	d(D...A)	<(DHA)
N(3)-H(3N)...O(16)[a]	0.92(2)	2.578(5)	163(6)
N(6)-H(6N)...O(12)[b]	0.91(2)	2.651(5)	151(5)

Symmetry transformations used to generate equivalent atoms: a: $x - 1, y, z - 1$; b: $-x + 5/2$, y – 1/2, –z – 1/2.