Supporting Information

Two mixed-ligand Cd(II)-organic frameworks with unique topologies: Selective luminescent sensing of TNP and Cu^{2+} ions with recyclable performances

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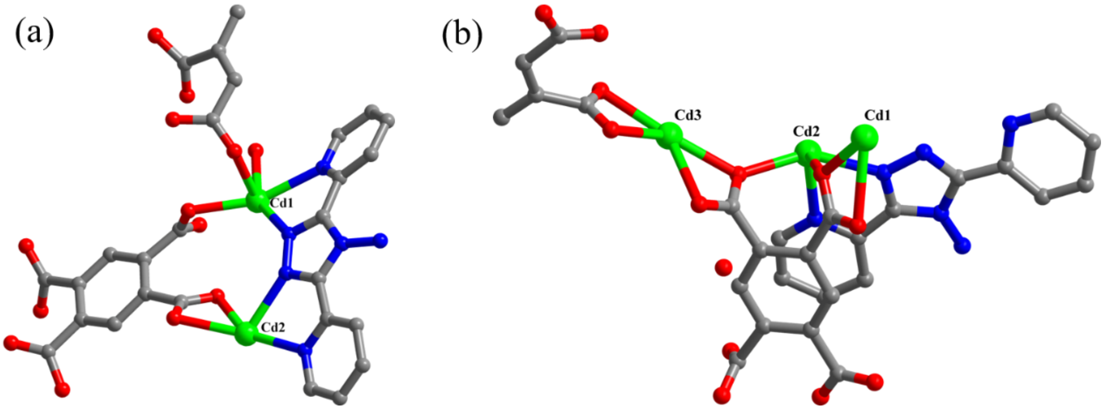

Fig. S1 The asymmetric unit of **1** (a) and **2** (b). All H atoms are omitted for clarity. Colour code: Cd green, C grey, O red, N blue.

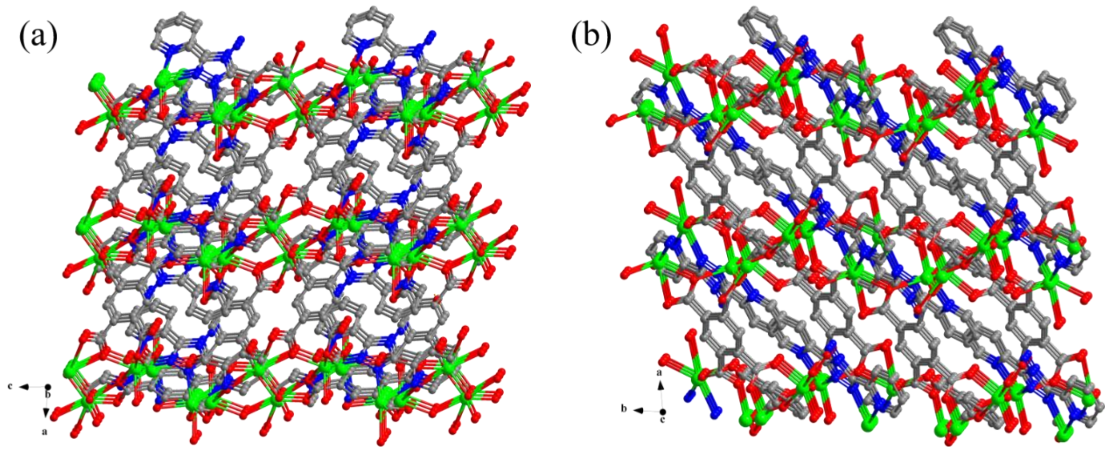

Fig. S2 3-D packing diagram of **2** viewed approximately along the *b* axis (a) and *c* axis (b). All H atoms are omitted for clarity. Colour code: Cd green, C grey, O red, N blue.

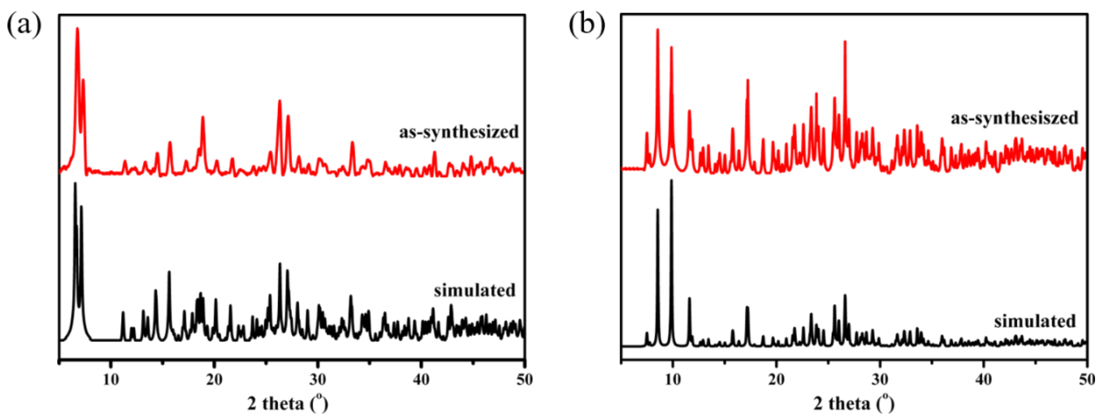

Fig. S3 The PXRD patterns of **1** (a) and **2** (b).

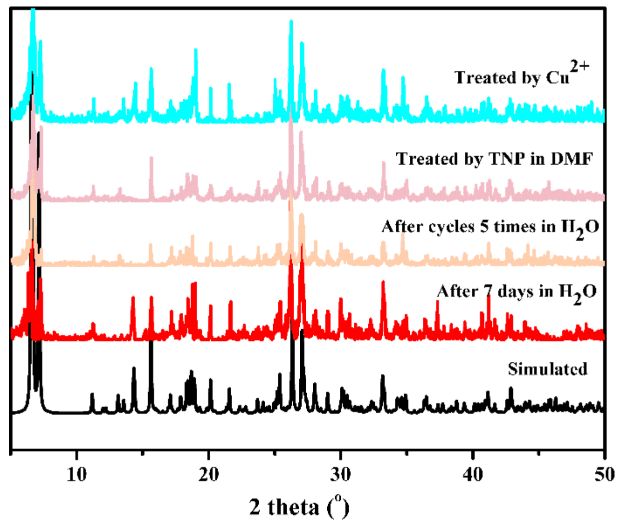

Fig. S4 PXRD patterns of **1** in different situations.

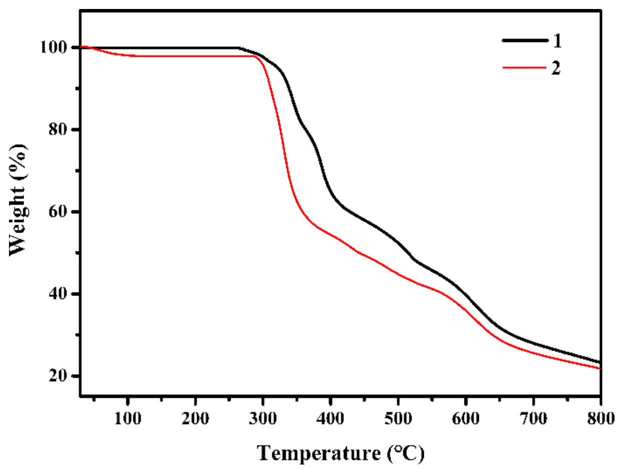

Fig. S5 Thermogravimetric analysis of **1** and **2**.

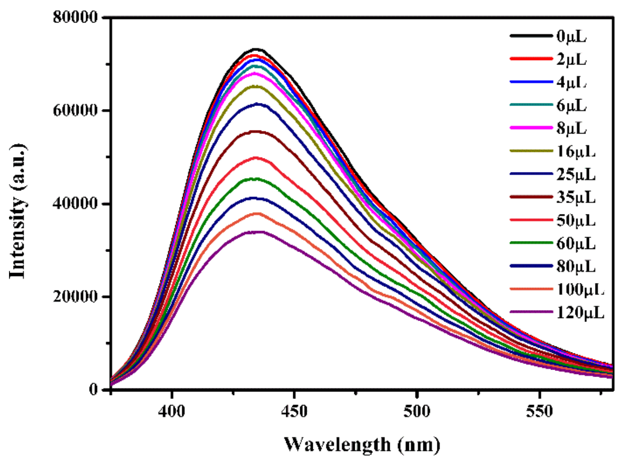

Fig. S6 Emission spectra of **1** dispersed in DMF with the addition of 4-NP solution (5 mM) (λ_{ex} = 357 nm).

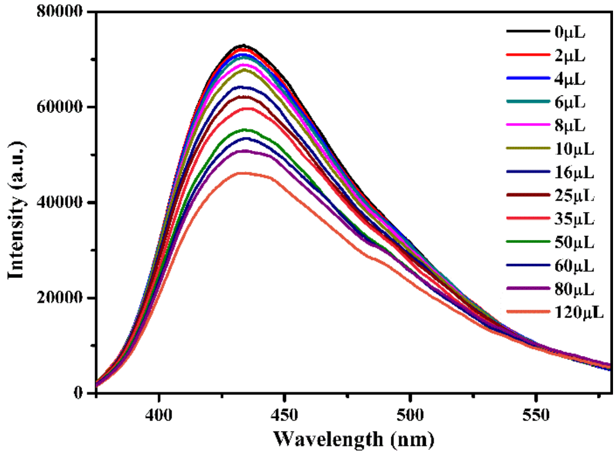

Fig. S7 Emission spectra of **1** dispersed in DMF with the addition of 2,4-DNT solution (5 mM) (λ_{ex} = 357 nm).

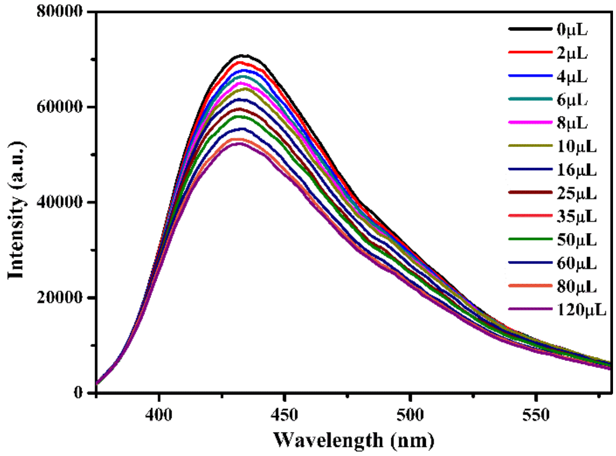

Fig. S8 Emission spectra of **1** dispersed in DMF with the addition of NB solution (5 mM) (λ_{ex} = 357 nm).

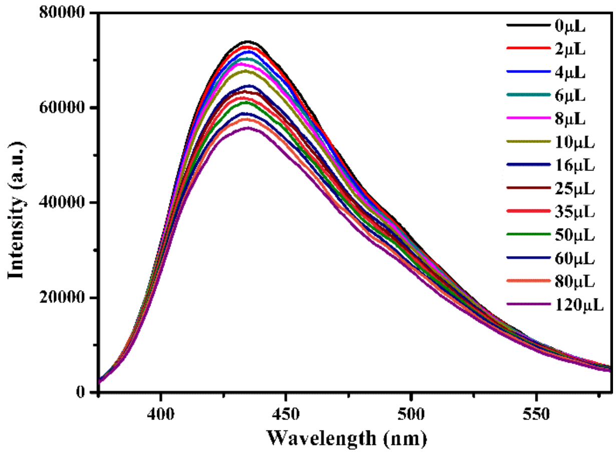

Fig. S9 Emission spectra of **1** dispersed in DMF with the addition of 4-NT solution (5 mM) (λ_{ex} = 357 nm).

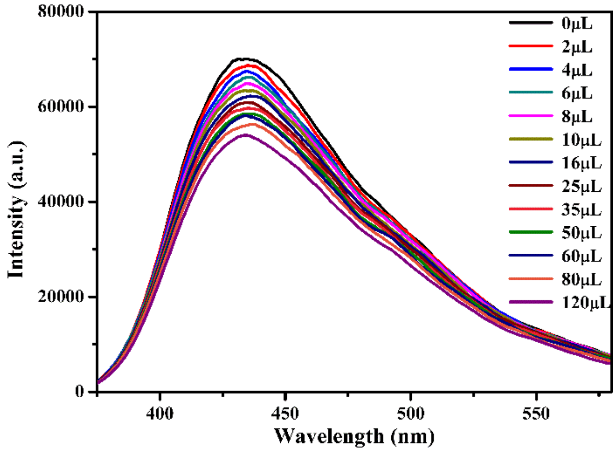

Fig. S10 Emission spectra of **1** dispersed in DMF with the addition of 1,3-DNB solution (5 mM) (λ_{ex} = 357 nm).

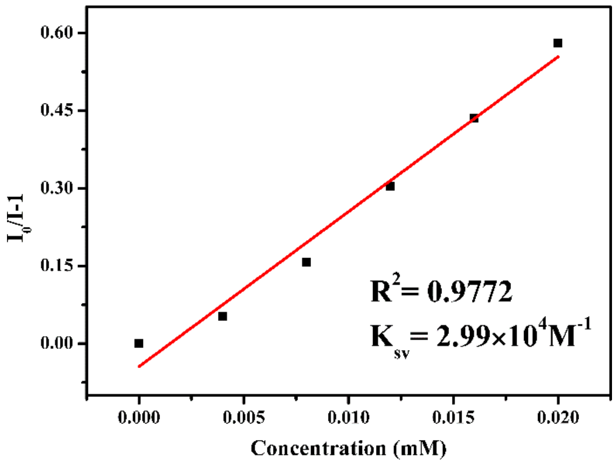

Fig. S11 Stern-Volmer plot for TNP of **1** in DMF suspension at the low concentration (0-0.020 mM).

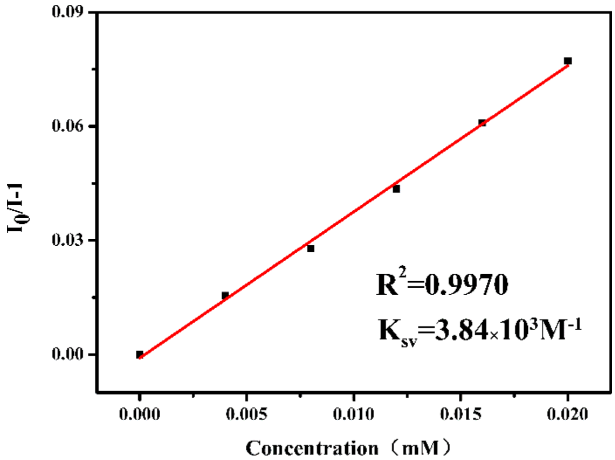

Fig. S12 Stern-Volmer plot for 4-NP of **1** in DMF suspension at the low concentration (0-0.020 mM).

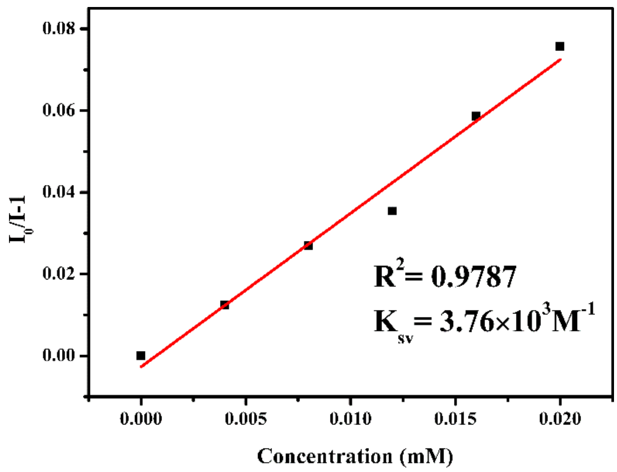

Fig. S13 Stern-Volmer plot for 2,4-DNT of **1** in DMF suspension at the low concentration (0-0.020 mM).

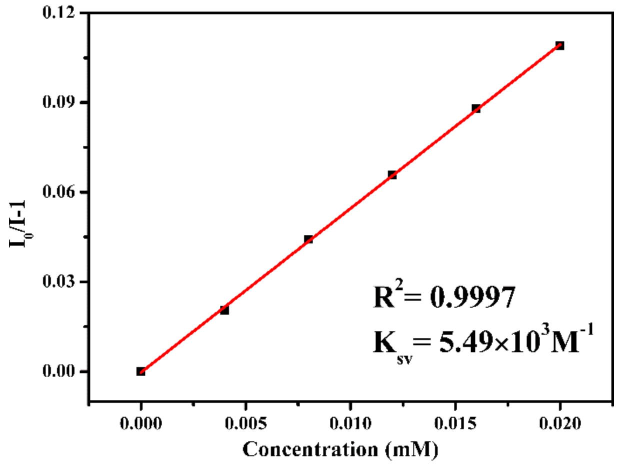

Fig. S14 Stern-Volmer plot for NB of **1** in DMF suspension at the low concentration (0-0.020 mM).

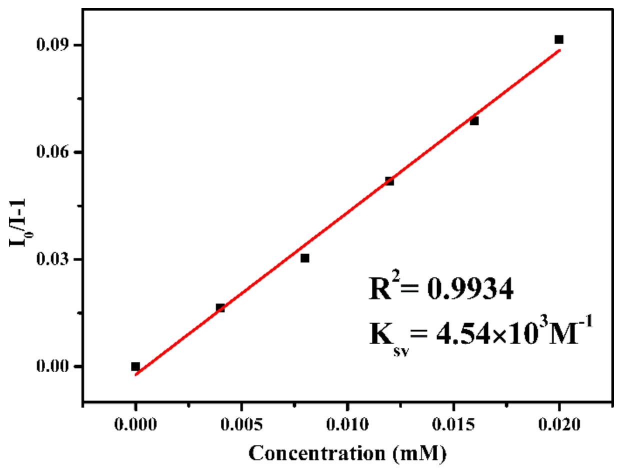

Fig. S15 Stern-Volmer plot for 4-NT of **1** in DMF suspension at the low concentration

(0-0.020 mM).

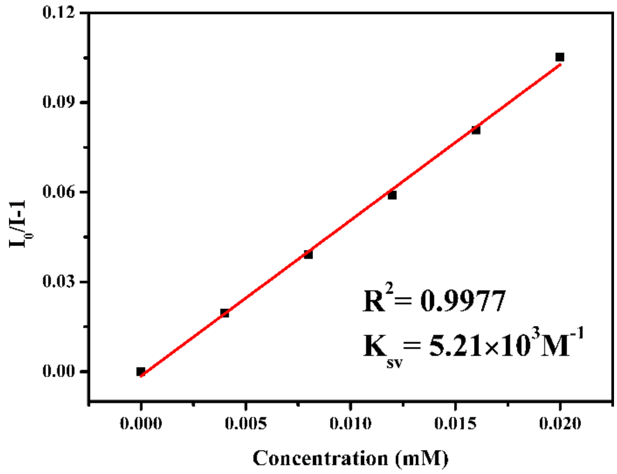

Fig. S16 Stern-Volmer plot for 1,3-DNB of **1** in DMF suspension at the low concentration (0-0.020 mM).

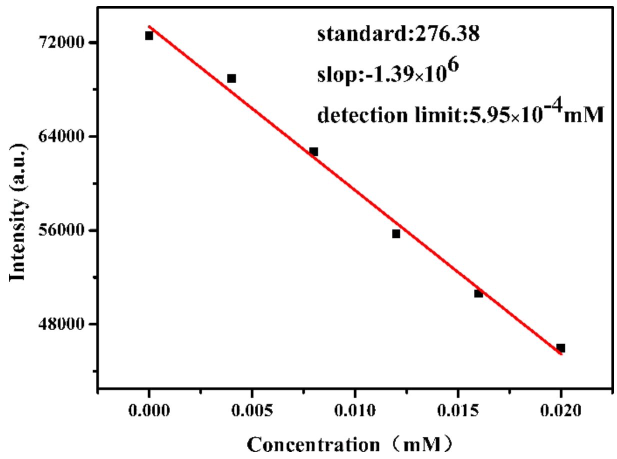

Fig. S17 The LOD for TNP of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

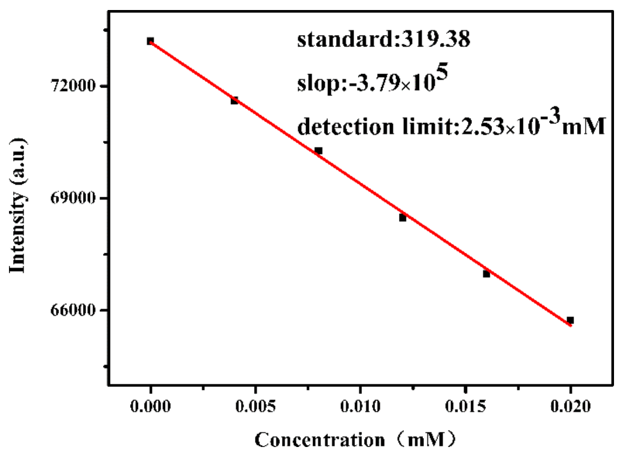

Fig. S18 The LOD for 4-NP of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

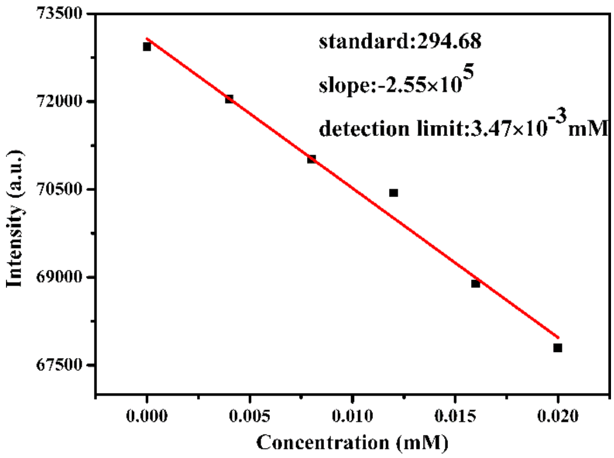

Fig. S19 The LOD for 2,4-DNT of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

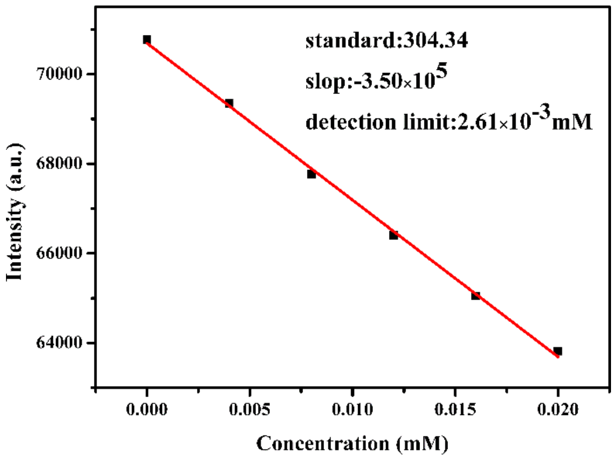

Fig. S20 The LOD for NB of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

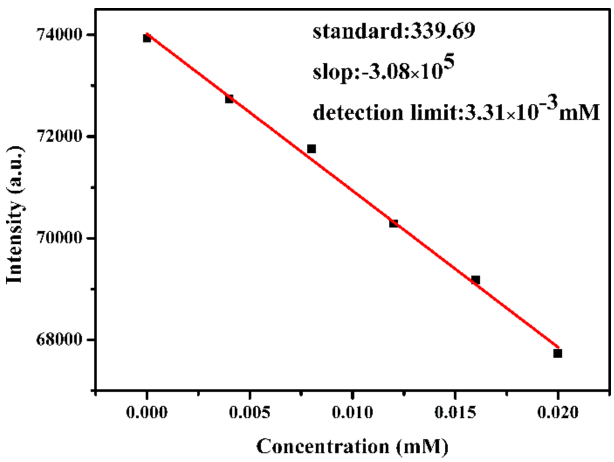

Fig. S21 The LOD for 4-NT of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

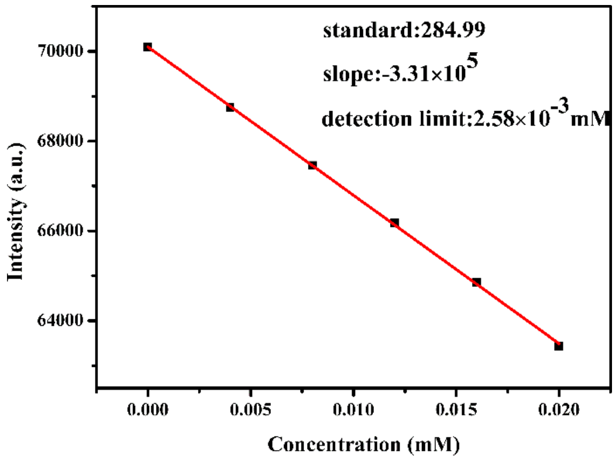

Fig. S22 The LOD for 1,3-DNB of **1** in DMF suspension was calculated with 3σ/k (k: slope, σ: standard) at the low concentration (0-0.020 mM).

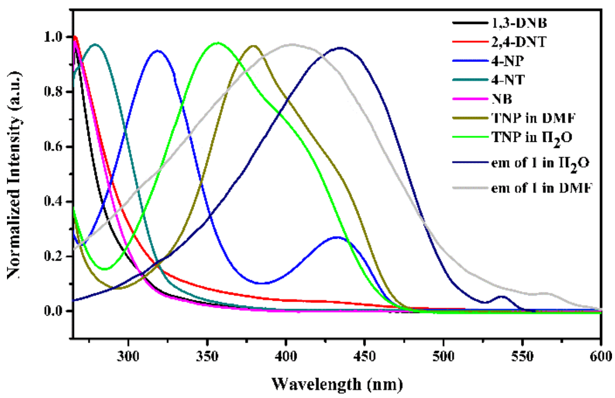

Fig. S23 Spectral overlap between the absorption spectra of 1,3-DNB, 2,4-DNT, 4-NP, 4-NT, NB, TNP and the emission spectra of **1** in DMF and H_2O media.

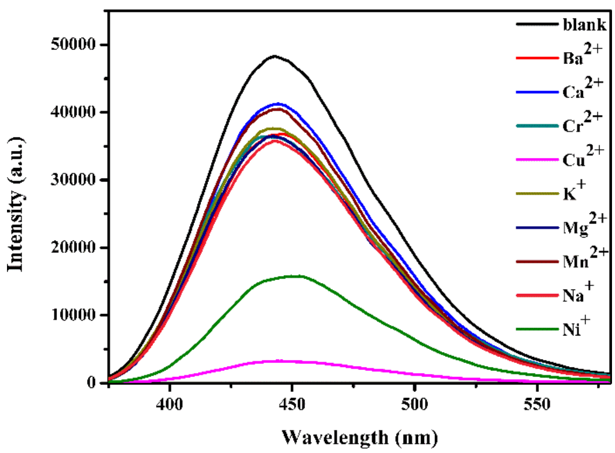

Fig. S24 Emission spectra of **1** in aqueous solutions of different cations (λ_{ex} = 357 nm).

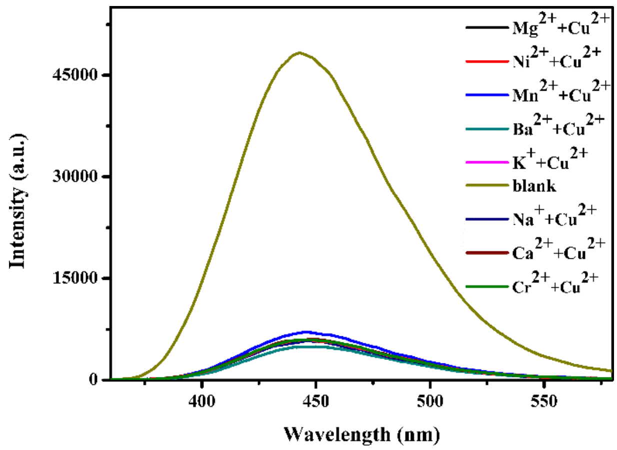

Fig. S25 Emission spectra of **1** in aqueous solutions of mixed cations. The concentrations of Cu^{2+} and other anions were 2 mM, respectively (λ_{ex} = 357 nm).

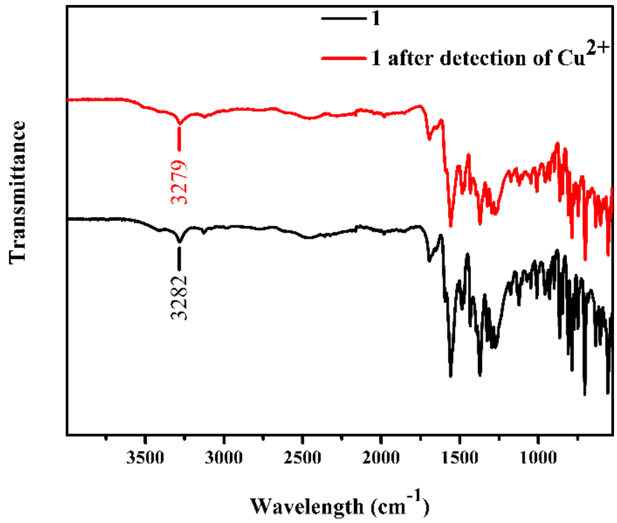

Fig. S26 The IR spectra of **1** before and after detection of Cu^{2+}.

Table S1 Selected bond lengths (Å) and angles (deg) for **1** and **2**.

Bond	Lengths (Å)	Bond	Angles (°)
		1	
Cd(1)-N(2)	2.314(2)	N(2)-Cd(1)-O(6)	153.10(8)
Cd(1)-O(6)	2.354(2)	N(2)-Cd(1)-O(4)	87.95(7)
Cd(2)-O(3)	2.293(2)	O(13)#1-Cd(1)-N(2)	87.30(8)
Cd(2)-O(1)	2.410(2)	O(1)-Cd(1)-O(13)#1	105.50(7)
Cd(1)-N(1)	2.410(2)	O(1)-Cd(1)-O(4)	79.67(7)
Cd(1)-O(4)	2.3176(19)	O(1)-Cd(1)-O(6)	91.52(7)
Cd(1)-O(1)	2.2496(19)	O(4)-Cd(1)-O(6)	89.80(7)
Cd(1)-O(13)#1	2.2868(19)	N(2)-Cd(1)-N(1)	70.32(8)
O(1)-Cd(1)-N(1)	159.92(8)	O(1)-Cd(1)-N(2)	114.38(8)
		2	
O(4)-Cd(3)#4	2.467(4)	N(5B)#1-Cd(1)-O(1)	139.2(7)
Cd(1)-O(5)#2	2.262(4)	N(4A)-Cd(2)-N(1A)	71.0(2)
O(1)-Cd(2)	2.440(4)	O(3)-Cd(2)-O(9)#5	82.86(14)
Cd(2)-N(4A)	2.208(6)	O(1)-Cd(1)-O(2)	52.15(13)
Cd(2)-O(9)#5	2.335(4)	O(5)#2-Cd(1)-O(2)	79.95(17)
O(8)-Cd(3)	2.155(4)	O(12)#3-Cd(1)-O(1)	127.02(16)
Cd(1)-O(2)	2.623(5)	O(5)#2-Cd(1)-O(1)	97.00(15)
O(9)-Cd(3)	2.374(4)	N(6B)#1-Cd(1)-O(1)	76.9(5)
Cd(2)-O(3)	2.229(4)	O(12)#3-Cd(1)-O(2)	82.19(15)
Cd(1)-O(12)#3	2.304(5)	O(3)-Cd(2)-N(1B)	104.0(5)
Cd(1)-O(1)	2.336(4)	O(3)-Cd(2)-N(1A)	92.4(2)

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

Table S2 The ICP results of **1@CuCl$_2$** (50 mg compound soaked in 2 mL of 2 mM $CuCl_2$ for 24 hours).

Sample	Concentration/(mg/kg)	Determined ion
1@CuCl$_2$	175424	Cd^{2+}
1@CuCl$_2$	176271	Cd^{2+}
1@CuCl$_2$	1864	Cu^{2+}
1@CuCl$_2$	1856	Cu^{2+}

Results analysis:

the ratio of Cd^{2+} : Cu^{2+} in **1@CuCl$_2$** : [(175424+176271)/2] : [(1864+1856)/2] = 94.54 : 1