

Electronic Supplementary Information

New luminescent Cd(II)-MOF as highly selective chemical probe for Fe³⁺ in aqueous solution with mixed metal ions

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Table S1. Selected bond lengths [\AA] and angles [$^\circ$] for complex **1**.

Cd(1)-O(1)	2.201(5)	O(9)-Cd(1)-O(7)#2	111.0(2)
Cd(1)-O(2)#1	2.236(6)	O(1)-Cd(1)-O(5)	87.8(2)
Cd(1)-O(9)	2.344(6)	O(2)#1-Cd(1)-O(5)	83.6(2)
Cd(1)-O(7)#2	2.375(6)	O(9)-Cd(1)-O(5)	169.1(2)
Cd(1)-O(5)	2.399(6)	O(7)#2-Cd(1)-O(5)	79.2(2)
Cd(1)-O(8)#2	2.446(6)	O(1)-Cd(1)-O(8)#2	155.6(2)
O(1)-Cd(1)-O(2)#1	99.9(2)	O(2)#1-Cd(1)-O(8)#2	93.7(2)
O(1)-Cd(1)-O(9)	83.1(2)	O(9)-Cd(1)-O(8)#2	76.2(2)
O(2)#1-Cd(1)-O(9)	92.1(2)	O(7)#2-Cd(1)-O(8)#2	53.9(2)
O(1)-Cd(1)-O(7)#2	125.1(2)	O(5)-Cd(1)-O(8)#2	113.9(2)
O(2)#1-Cd(1)-O(7)#2	130.5(2)		

Symmetry codes: #1: $x+1, y, z$; #2: $-x+2, -y, -z+1$; #3: $x-1, y, z$; #4: $-x+1, -y, -z+2$; #5: $-x+2, -y-1, -z+1$.

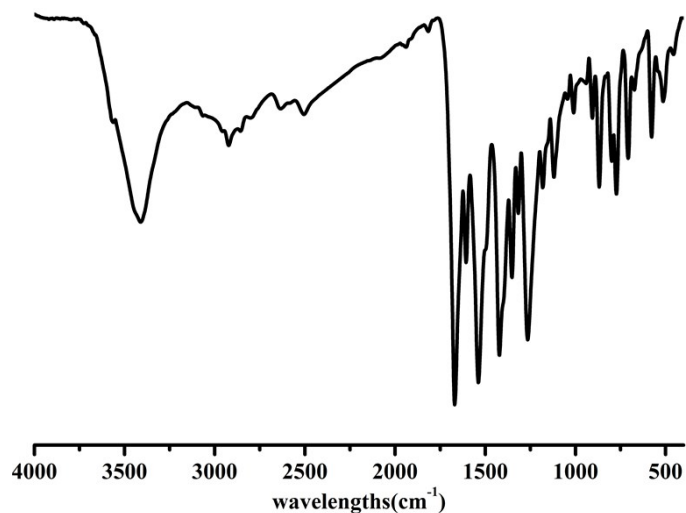


Fig. S1 The FT-IR spectra of complex **1**.

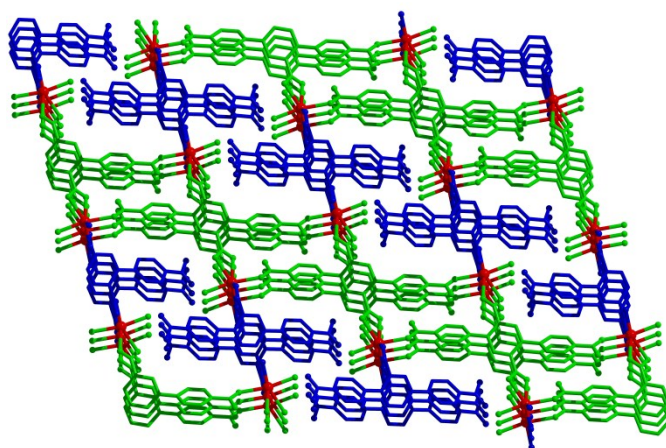
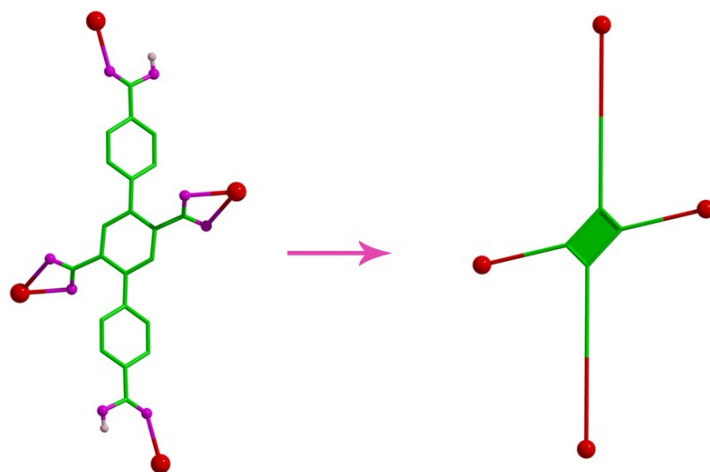
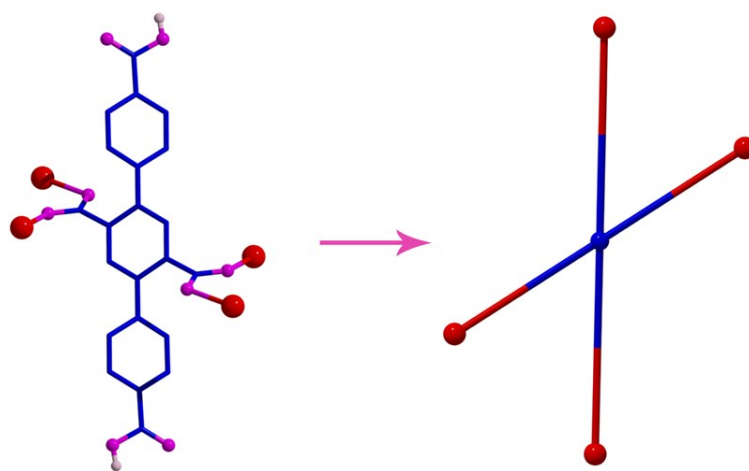


Fig. S2 The 3D framework of **1**.



(a)



(b)

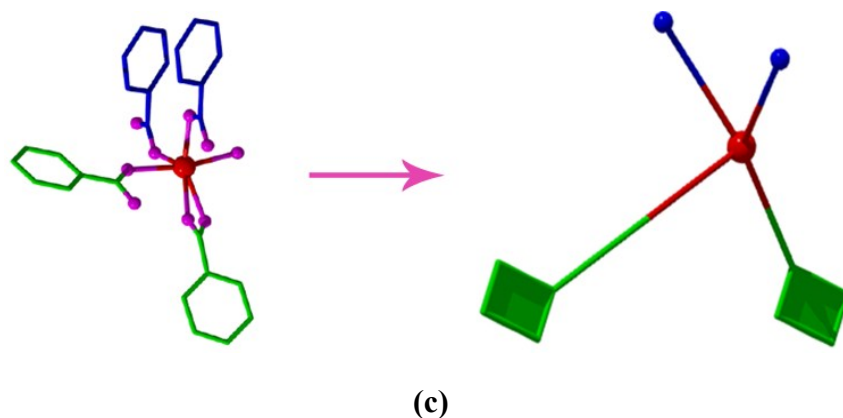


Fig. S3 The ligands of $H_2L_a^{2-}$ (a), $H_2L_b^{2-}$ (b) and $Cd(II)$ ions (c) simplified as four-connected nodes, respectively.

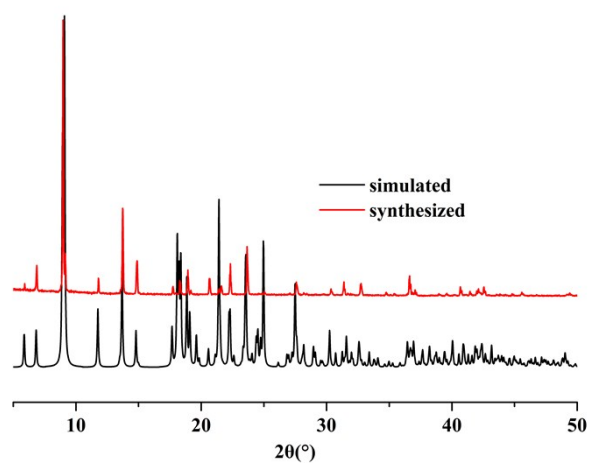


Fig. S4 PXRD patterns of complex **1** simulated from the X-ray single-crystal data and as-synthesized products.

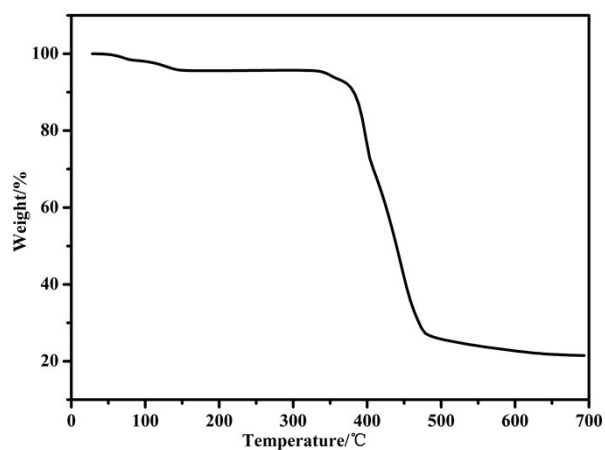


Fig. S5 The TGA curve of complex **1**.

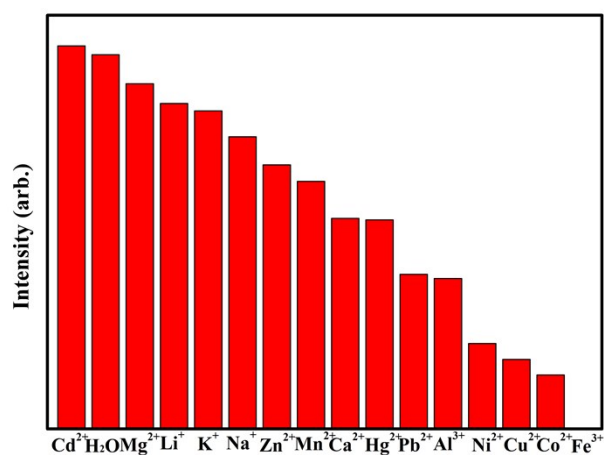


Fig. S6 The comparison of the luminescent intensities with different metal ions in aqueous solution.

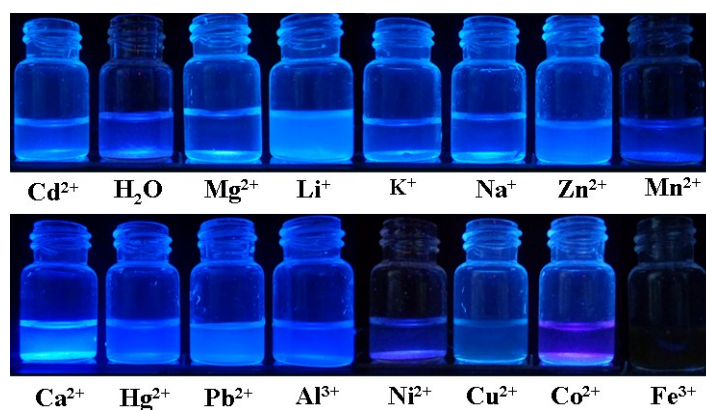


Fig. S7 The visible color change of in aqueous solution containing the product of **1** and different metal ions.

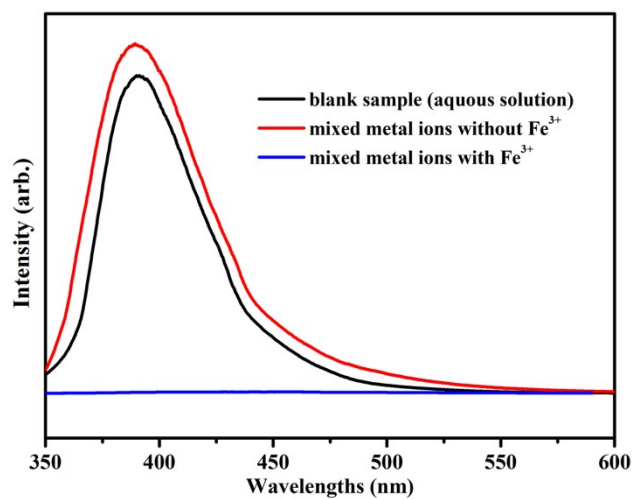


Fig. S8 Emission spectra of **1** in aqueous solution with mixed metal ions.

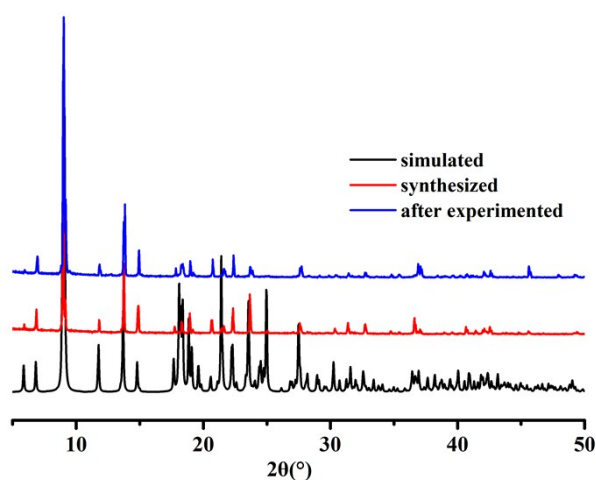


Fig. S9 The PXRD patterns of complex **1** after series of sensing experiments.

Sample	Concentration of Cd^{2+} (ug/mL)
Blank sample (H_2O)	0.1951
Initial solution after immersing in H_2O	0.2035
Final solution after sensing experiment for Fe^{3+}	0.1853

Linear equation: $y = 0.02917x + 0.0019$ ($y = \text{Abs}$; $x = \text{Concentration}$); $R^2 = 0.9979$

Fig. S10 ICP experiments of **1** after immersing in different solution (The concentration of complex **1** in solution for the ICP was 1000 ug/mL. The initial solution was the aqueous solution after **1** immersed for almost one week. And the final solution was the original solution after sensing experiment for Fe^{3+} , and the product of **1** was immersed for almost one month).