Supporting Information

A New Stable Luminescent Cd(II) Metal–Organic Framework with Fluorescent Sensing and Selective Dye Adsorption Properties

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Table S1. Selected bond lengths [Å] and angles [º] for complex **1**.

1			
Cd(1)-O(18)	2.172(10)	Cd(3)-O(3)#5	2.308(9)
Cd(1)-O(12)#1	2.223(9)	Cd(3)-O(7)	2.336(8)
Cd(1)-O(19)	2.290(13)	Cd(3)-O(9)	2.374(8)
Cd(1)-O(17)	2.321(13)	Cd(3)-O(4)#5	2.463(8)
Cd(1)-O(15)	2.336(9)	Cd(3)-O(8)	2.561(12)
Cd(1)-O(16)	2.388(9)	Cd(2)#3-O(5)	2.300(8)
Cd(2)-O(5)#2	2.299(8)	Cd(2)#2-O(13)	2.420(8)
Cd(2)-O(14)#3	2.324(8)	Cd(2)#2-O(14)	2.323(8)
Cd(2)-O(9)	2.409(8)	Cd(3)#5-O(11)	2.295(9)
Cd(2)-O(13)#3	2.421(8)	Cd(3)#4-O(4)	2.463(8)
Cd(2)-O(7)	2.426(9)	Cd(3)#4-O(3)	2.309(9)
Cd(2)-O(10)	2.427(9)	Cd(1)#6-O(12)	2.222(9)
Cd(3)-O(11)#4	2.295(9)	Cd(2)-N(1)#2	2.326(9)
N(1)-Cd(2)#3	2.326(9)	Cd(3)-N(4)#4	2.361(9)
O(18)-Cd(1)-O(19)	90.5(5)	N(4)-Cd(3)#5	2.361(9)
O(12)#1-Cd(1)-O(19)	83.9(6)	O(18)-Cd(1)-O(12)#1	131.8(4)
O(18)-Cd(1)-O(17)	94.1(5)	O(9)-Cd(2)-O(7)	76.9(3)
O(12)#1-Cd(1)-O(17)	88.4(5)	O(13)#3-Cd(2)-O(7)	90.4(3)
O(19)-Cd(1)-O(17)	172.3(5)	O(5)#2-Cd(2)-O(10)	130.8(3)
O(18)-Cd(1)-O(15)	80.3(3)	O(14)#3-Cd(2)-O(10)	78.8(3)
O(12)#1-Cd(1)-O(15)	146.8(3)	O(9)-Cd(2)-O(10)	53.3(3)
O(19)-Cd(1)-O(15)	88.5(5)	O(13)#3-Cd(2)-O(10)	131.3(3)
O(17)-Cd(1)-O(15)	98.4(4)	O(7)-Cd(2)-O(10)	102.5(3)
O(18)-Cd(1)-O(16)	136.6(4)	O(11)#4-Cd(3)-O(3)#5	144.6(3)

O(12)#1-Cd(1)-O(16)	90.8(3)	O(11)#4-Cd(3)-O(7)	92.3(3)
O(19)-Cd(1)-O(16)	85.8(4)	O(3)#5-Cd(3)-O(7)	122.9(3)
O(17)-Cd(1)-O(16)	95.0(5)	O(11)#4-Cd(3)-O(9)	94.0(3)
O(15)-Cd(1)-O(16)	56.3(3)	O(3)#5-Cd(3)-O(9)	96.0(3)
O(5)#2-Cd(2)-O(14)#3	147.8(3)	O(7)-Cd(3)-O(9)	79.3(3)
O(5)#2-Cd(2)-O(9)	89.2(3)	O(11)#4-Cd(3)-O(4)#5	91.3(3)
O(14)#3-Cd(2)-O(9)	122.5(3)	O(3)#5-Cd(3)-O(4)#5	54.9(3)
O(5)#2-Cd(2)-O(13)#3	92.6(3)	O(7)-Cd(3)-O(4)#5	169.3(3)
O(14)#3-Cd(2)-O(13)#3	55.2(3)	O(9)-Cd(3)-O(4)#5	90.3(3)
O(9)-Cd(2)-O(13)#3	167.3(3)	O(11)#4-Cd(3)-O(8)	134.4(4)
O(5)#2-Cd(2)-O(7)	97.2(3)	O(3)#5-Cd(3)-O(8)	75.1(3)
O(14)#3-Cd(2)-O(7)	86.0(3)	O(7)-Cd(3)-O(8)	52.3(3)
O(4)#5-Cd(3)-O(8)	129.2(3)	O(9)-Cd(3)-O(8)	104.3(4)

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

Table S2 Standard Deviation (δ) calculation for the detection of Fe^{3+} for **1**.

Test	Fluorescence intensity (nm)
1	5408.519
2	5407.993
3	5407.633
4	5408.235
5	5408.432
6	5407.855
7	5407.944
8	5407.732
9	5408.439
10	5408.365
average	5408.115
Standard deviation (δ)	0.315

Table S3 Standard Deviation (δ) calculation for the detection of CrO_4^{2-} for **1**.

Test	Fluorescence intensity (nm)
1	5697.787
2	5696.832
3	5696.914
4	5696.798
5	5697.564
6	5697.643
7	5696.994
8	5697.441
9	5697.742
10	5697.698
average	5697.341
Standard deviation (δ)	0.408

Table S4 Standard Deviation (δ) calculation for the detection of $Cr_2O_7^{2-}$ for **1**.

Test	Fluorescence intensity (nm)
1	7681.412
2	7682.102
3	7682.094
4	7682.111
5	7681.564
6	7681.643
7	7682.204
8	7681.441
9	7681.742
10	7681.698
average	7681.801
Standard deviation (δ)	0.901

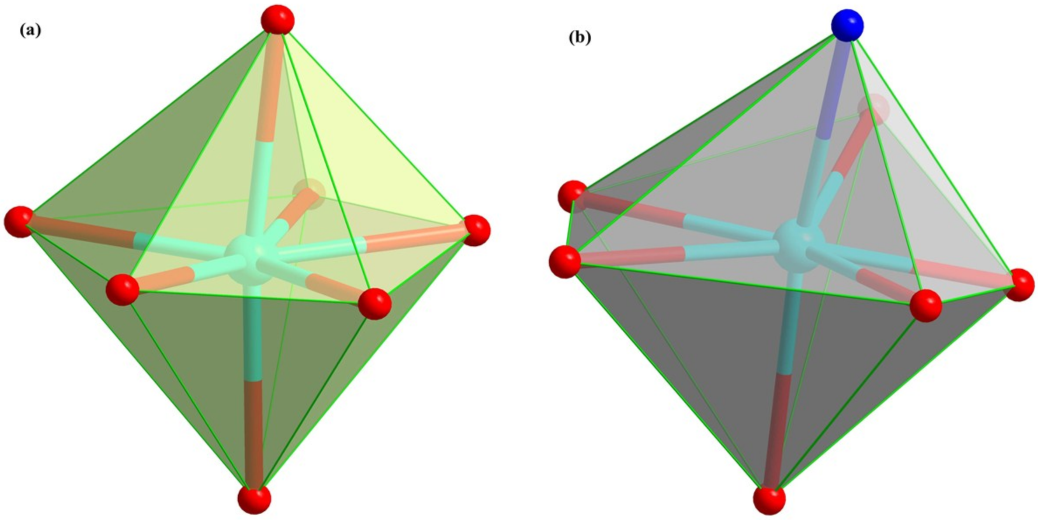


Fig. S1 Coordination arrangement of Cd^{2+}1 (a) and Cd^{2+}2, Cd^{2+}3 (b) ions could be described as a distorted pentagonal bipyramid.

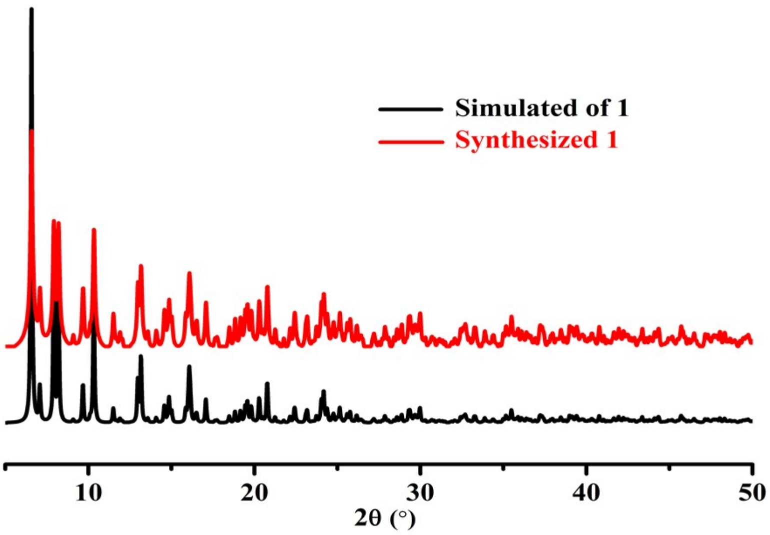


Fig. S2 PXRD patterns of complex **1** simulated from the X-ray single-crystal data and as-synthesized products.

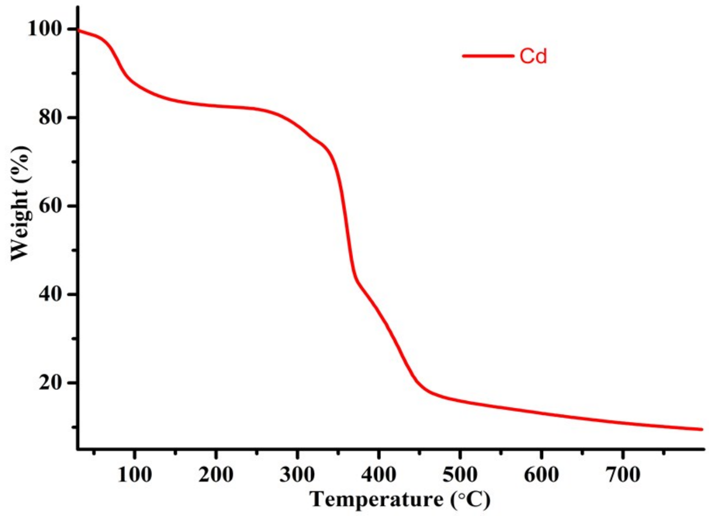


Fig. S3 The TGA curve of complex **1**.

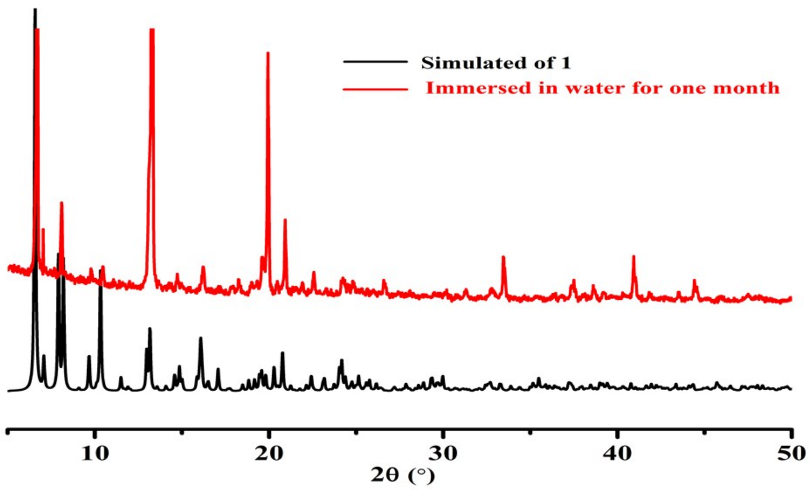


Fig. S4 PXRD patterns of **1** immersed in water at room temperature for one month.

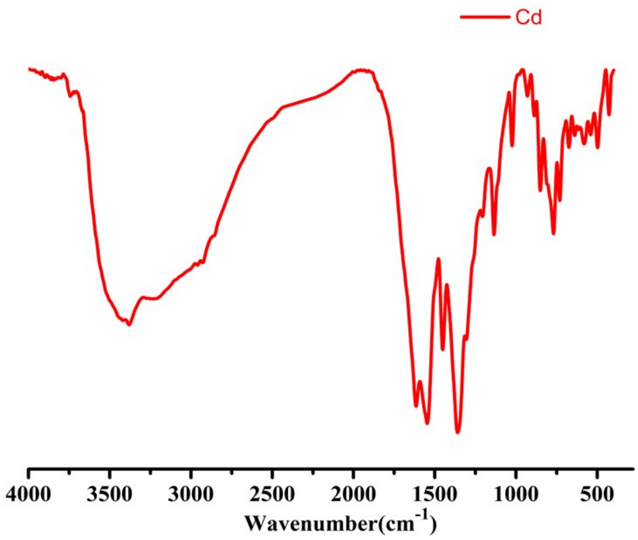
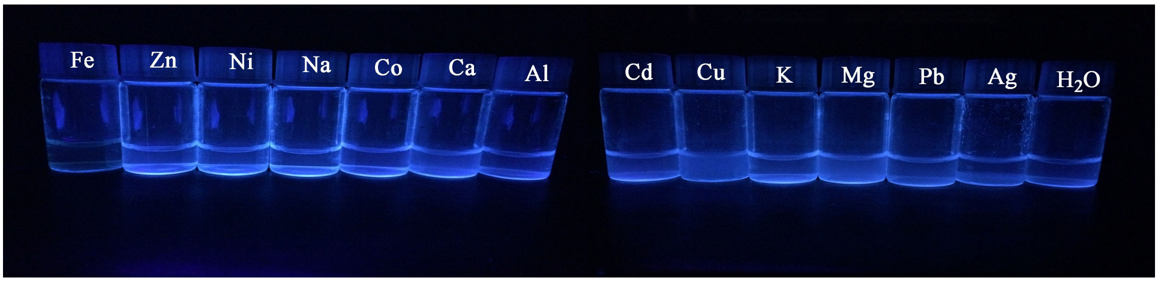
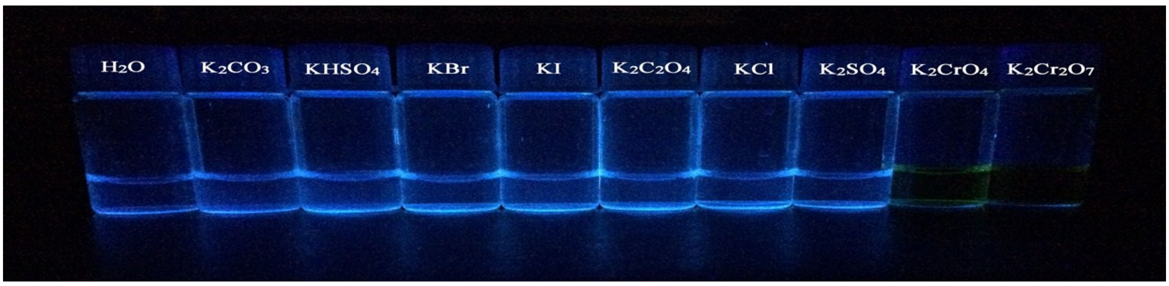


Fig. S5 The FT-IR spectra of complex **1**.

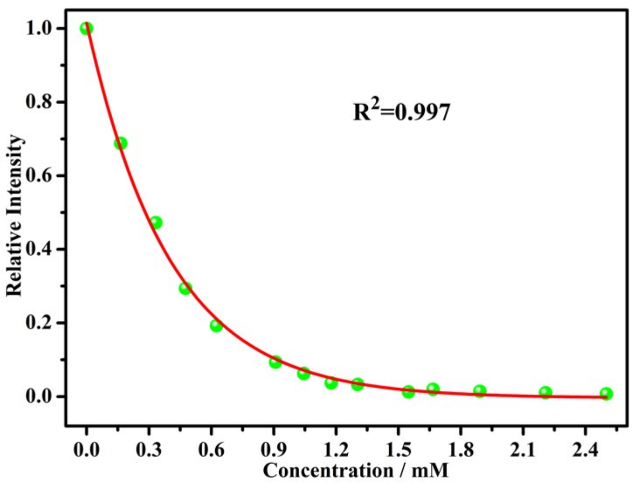


(a)

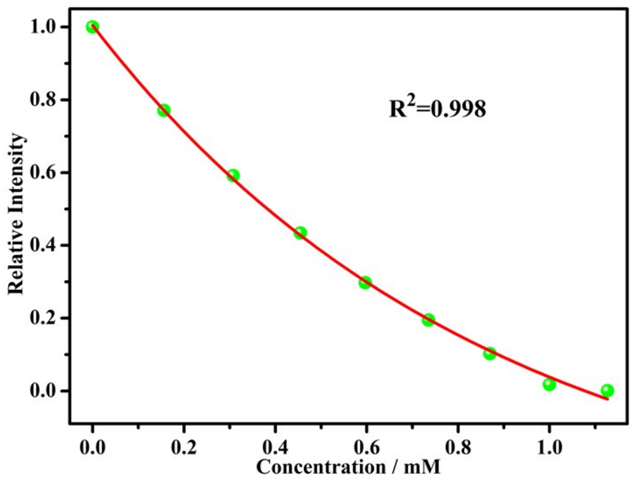


(b)

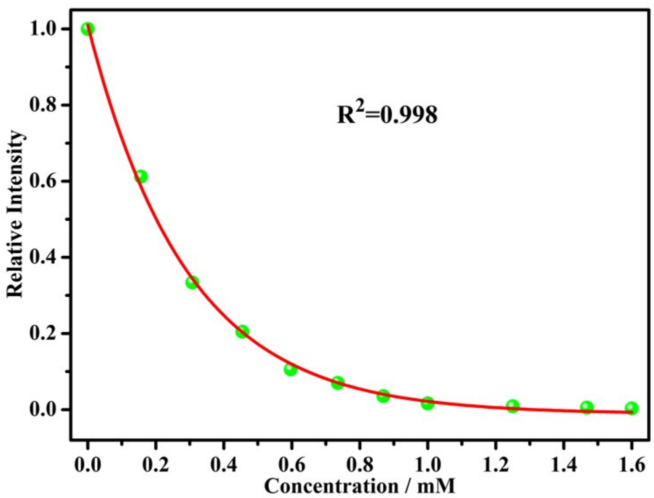
Fig. S6 (a) Pictures of different Mn+@**1** solutions (M = Cu^{2+}, Mg^{2+}, Al^{3+}, Cd^{2+}, Pb^{2+}, Co^{2+}, Ca^{2+}, Zn^{2+}, Na^{+}, K^{+}, Ni^{2+}, Ag^{+} and Fe^{3+} respectively); (b) Pictures of different **1**@A^{n-} solutions (A = $Cr_2O_7^{2-}$, CrO_4^{2-}, HSO_4^{-}, CO_3^{2-}, Br^{-}, Cl^{-}, I^{-}, $C_2O_4^{2-}$ and SO_4^{2-} respectively).



(a) Fe^{3+}

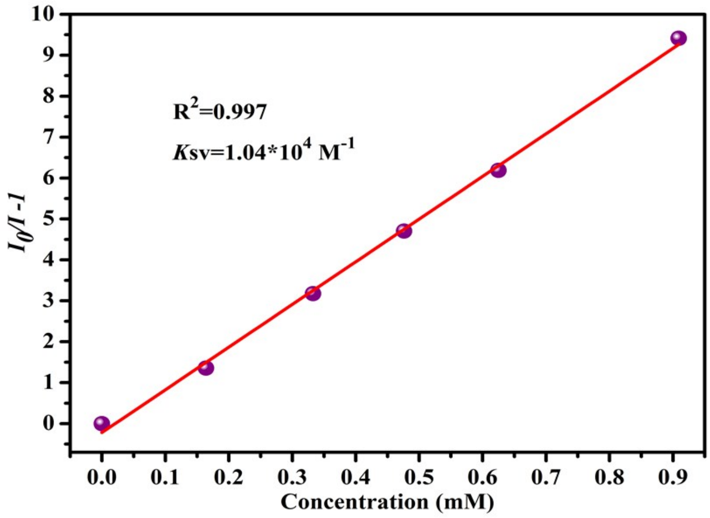


(b) $Cr_2O_7^{2-}$

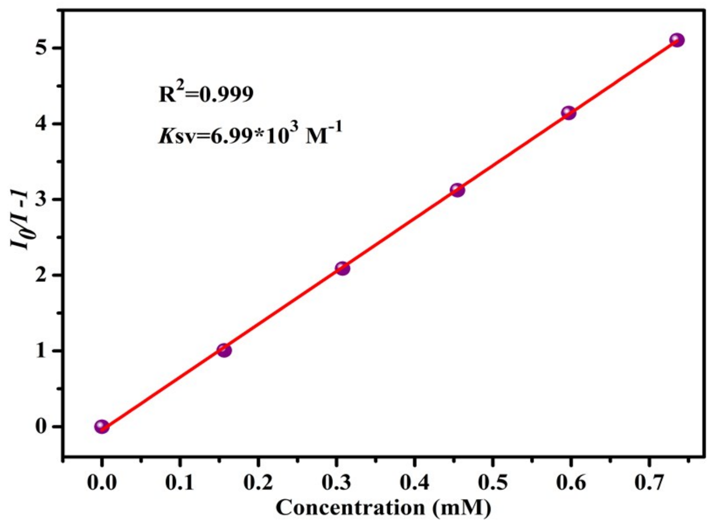


(c) CrO_4^{2-}

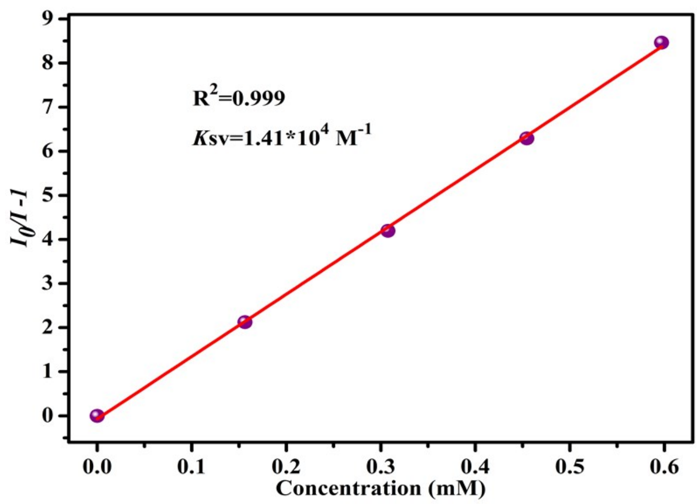
Figure S7 The linear correlation for the plot of I_0/I vs concentration of Fe^{3+} (a), $Cr_2O_7^{2-}$ (b) and CrO_4^{2-} (c) ions, respectively, in low concentration range.



(a) Fe^{3+}



(b) $Cr_2O_7^{2-}$



(c) CrO_4^{2-}

Fig. S8 Quenching efficiency defined by the Stern–Volmer relationship for Fe^{3+}, $Cr_2O_7^{2-}$ and CrO_4^{2-} ions.

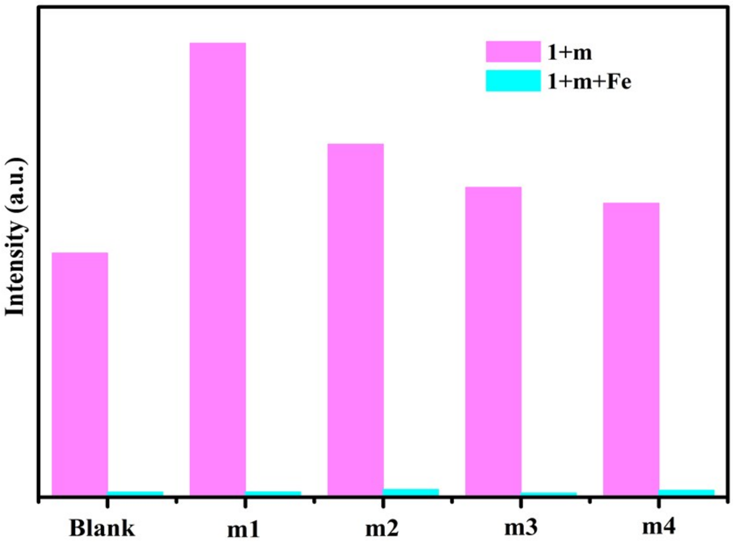


Fig. S9 Luminescence intensity at 406 nm of **1** dispersed in water with addition of different mixed ions (10^{-2}M) mixed solution added Fe^{3+} ions (10^{-2} M) (m1: Ag^{2+}/Pb^{2+}; m2: $Cu^{+}/K^{+}/Mg^{2+}$; m3: $Al^{3+}/Cd^{2+}/Ca^{2+}/Co^{2+}$; m4: $Na^{+}/Ni^{2+}/Zn^{2+}$).

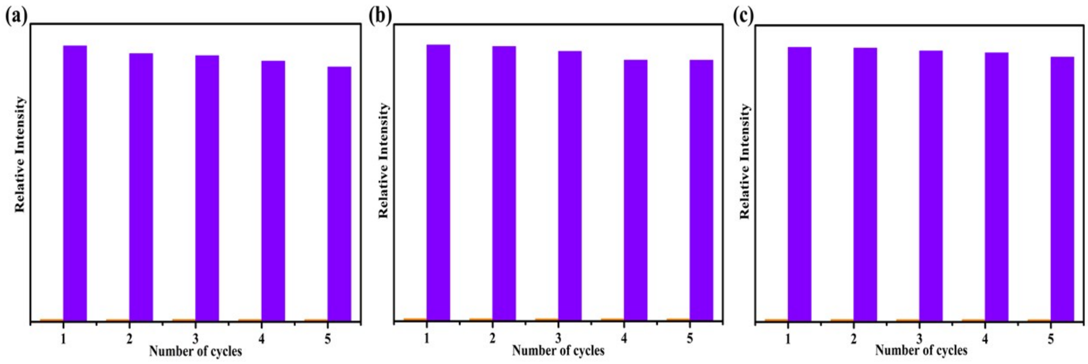


Fig. S10 Luminescent intensity at 406 nm of **1** after five recycles in Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$ solutions (10^{-2} M).

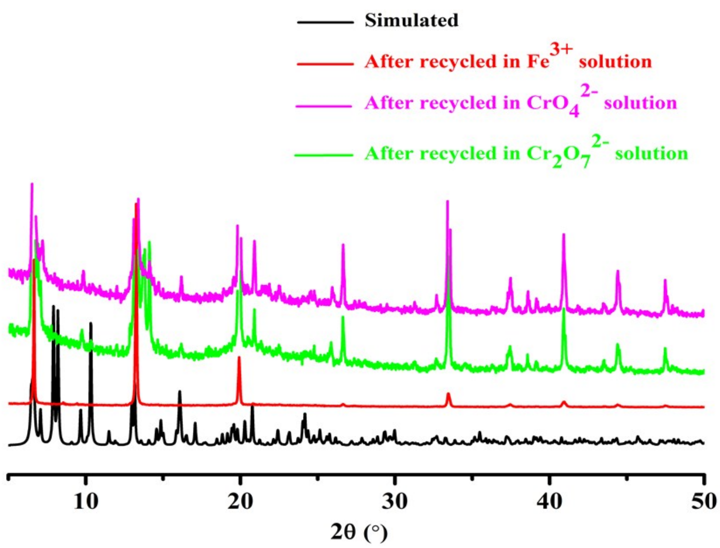


Fig. S11 The PXRD patterns of **1** treated by Fe^{3+}, CrO_4^{2-} and $Cr_2O_7^{2-}$ aqueous solutions.

Sample	Concentration of Cd^{2+} (ug/mL)
Blank sample (H_2O)	0.0196
Initial solution after immersing in H_2O	0.0228
Final solution after recycle sensing experiment for Fe^{3+}	0.0212
Final solution after recycle sensing experiment for CrO_4^{2-}	0.0201
Final solution after recycle sensing experiment for $Cr_2O_7^{2-}$	0.0199

Fig. S12 ICP experiments of **1** after immersing in different solution.

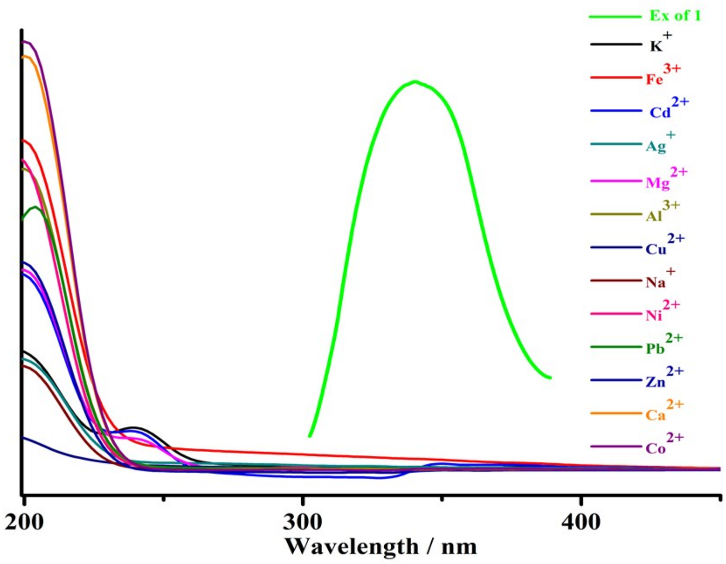


Fig. S13 UV-Vis adsorption spectrum of $M(NO_3)_n$ aqueous solution and the excitation spectrum of **1**.

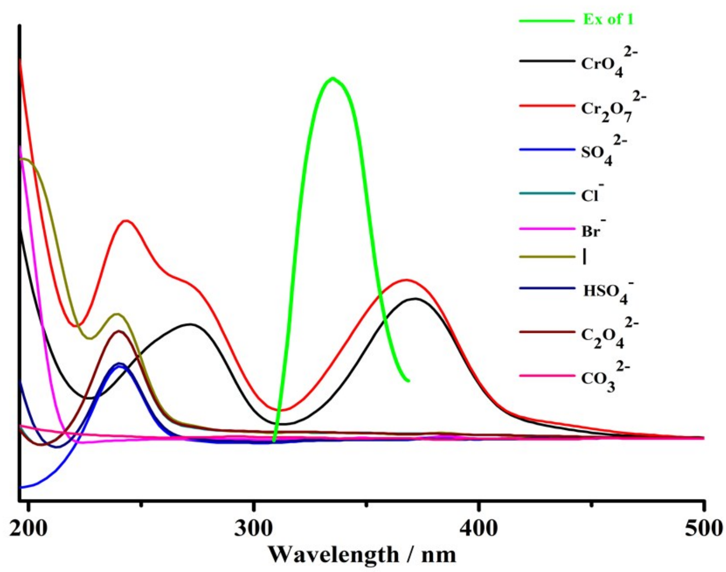
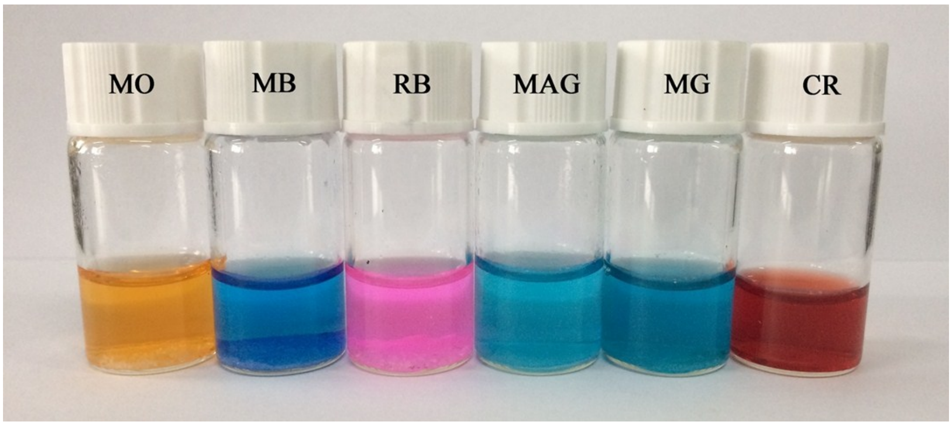
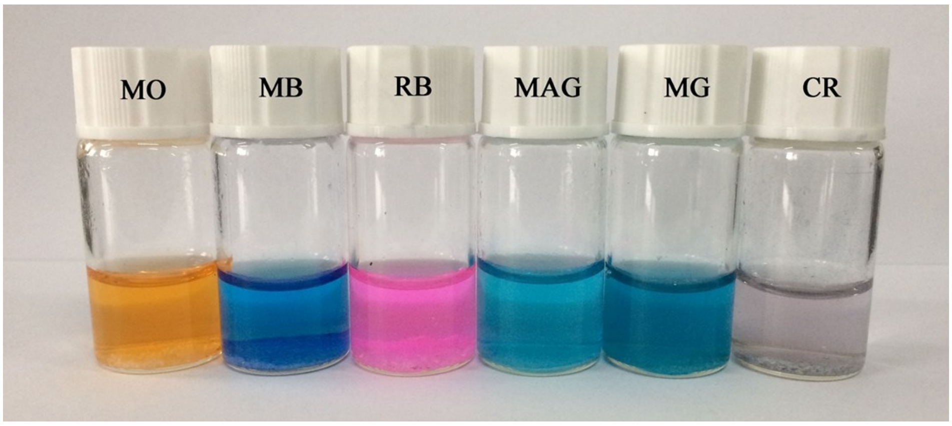


Fig. S14 UV-Vis adsorption spectrum of $K_n(A)$ aqueous solution and the excitation spectrum of **1**.



(a)



(b)

Fig. S15 Selective adsorption of CR with addition of **1** before (a) and after (b).

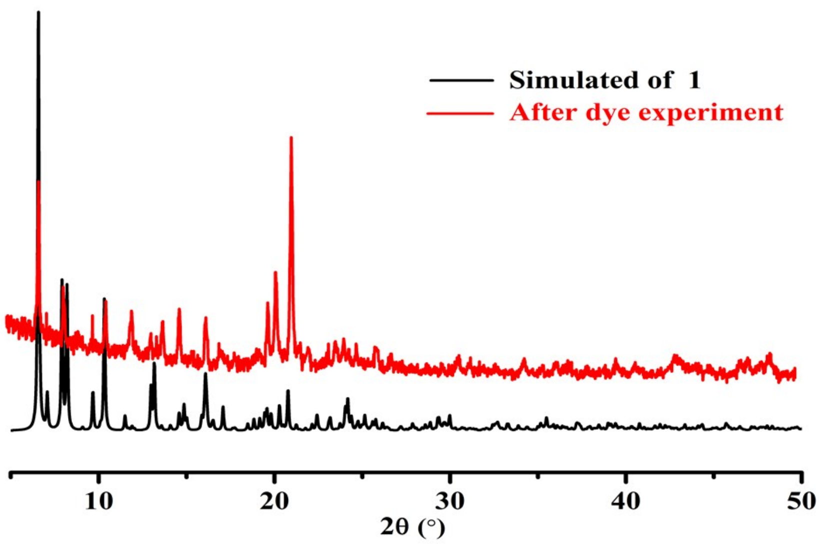


Fig. S16 PXRD powder diffraction patterns of **1** after dye experiment.