Supporting Information

Two novel lead-based coordination polymers for luminescence sensing of anions, cations and small organic molecules

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Contents

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for compounds **1** and **2**.

Compound 1			
Bond	Distance/Å	Bond	Distance/Å
Pb(1)-O(1)	2.431(6)	Pb(1)-O(2)	2.521(6)
Pb(1)-O(5B)	2.525(6)	Pb(1)-O(4A)	2.622(7)
Pb(1)-O(6C)	2.674(6)	Pb(1)-O(3A)	2.678(6)
Pb(1)-O(4C)	2.8900(1)	Pb(1)-O(6B)	3.0537(1)
Angle	/°	Angle	/°
O(1)-Pb(1)-O(2)	52.2(2)	O(1)-Pb(1)-O(5B)	77.0(2)
O(2)-Pb(1)-O(5B)	80.4(2)	O(1)-Pb(1)-O(4A)	78.4(2)
O(2)-Pb(1)-O(4A)	115.0(2)	O(5B) -Pb(1)-O(4A)	131.1(2)
O(1)-Pb(1)-O(6C)	105.3(2)	O(2)-Pb(1)-O(6C)	76.41(19)
O(5B) -Pb(1)-O(6C)	147.4(2)	O(4A) -Pb(1)-O(6C)	80.1(2)
O(1)-Pb(1)-O(3A)	76.0(2)	O(2)-Pb(1)-O(3A)	127.9(2)
O(5B) -Pb(1)-O(3A)	83.3(2)	O(4A) -Pb(1)-O(3A)	49.8(2)
O(6C) -Pb(1)-O(3A)	129.15(17)	O(4C) -Pb(1)-O(6B)	70.044(1)
O(4C) -Pb(1)-O(5B)	92.611(2)	O(4C) -Pb(1)-O(2)	91.774(2)
O(4C) -Pb(1)-O(1)	143.321(2)	O(4C) -Pb(1)-O(3C)	138.262(2)
O(4C) -Pb(1)-O(4A)	130.323(2)	O(4C) -Pb(1)-O(6C)	65.713(2)
O(6B) -Pb(1)-O(6C)	133.302(2)	O(6B) -Pb(1)-O(4A)	120.448(1)
O(6B) -Pb(1)-O(3A)	78.001(1)	O(6B) -Pb(1)-O(1)	119.206(2)
O(6B) -Pb(1)-O(2)	119.762(2)	O(6B) -Pb(1)-O(5B)	45.652(1)
A, -x+1/2,y+1,z+1/2	B, -x+1/2,y+1,z-1/2	C, x-1/2,-y+1,z	

Compound 2			
Bond	Distance /Å	Bond	Distance /Å
Pb(1)-O(5C)	2.447(2)	Pb(1)-O(6C)	2.476(3)
Pb(1)-O(4A)	2.496(3)	Pb(1)-O(2B)	2.617(3)
Pb(1)-O(3A)	2.656(2)	Pb(1)-O(1)	2.685(3)
Pb(1)-O(2)	3.062(2)		
Angle	/°	Angle	/°
O(5C)-Pb(1)-O(6C)	52.88(8)	O(5C)-Pb(1)-O(4A)	86.02(10)
O(6C)-Pb(1)-O(4A)	90.52(10)	O(5C)-Pb(1)-O(2B)	79.70(9)
O(6C)-Pb(1)-O(2B)	108.95(10)	O(4A)-Pb(1)-O(2B)	140.35(9)
O(5C)-Pb(1)-O(A)	78.39(8)	O(6C)-Pb(1)-O(3A)	120.99(8)
O(4A)-Pb(1)-O(3A)	50.91(8)	O(2B)-Pb(1)-O(3A)	89.84(8)
O(5C) -Pb(1)-O(1)	122.65(9)	O(6C)-Pb(1)-O(1)	81.21(9)
O(4A)-Pb(1)-O(1)	131.60(9)	O(2B)-Pb(1)-O(1)	86.39(9)
O(3A)-Pb(1)-O(1)	157.36(8)	O(2)-Pb(1)-O(2B)	118.015(2)
O(2)-Pb(1)-O(3A)	120.027(2)	O(2)-Pb(1)-O(4A)	90.825(3)

O(2)-Pb(1)-O(5C)	152.308(4)	O(2)-Pb(1)-O(6C)	99.698(3)
O(2)-Pb(1)-O(1)	44.970(2)		

A, –x+1/2,y+1/2,-z+1/2 B, -x+1/2,y+1/2,-z+1/2 C, x-1,y+1,-z

Table S2. Comparison of sensing ability in terms of quenching coefficient (K_{sv}) and limit of detection (LOD) of compounds toward $Cr_2O_7^{2-}$, CrO_4^{2-} , Fe^{3+} and NB.

Compounds	Medium	Analytes	Quenching coefficient (K_{sv}, M^{-1})	Limit of detection (LOD, M)	Ref.
$[Pb(cbdcp)]\cdot 0.5H_2O\cdot 0.5CH_3OH$	H_2O	$Cr_2O_7^{2-}$	5.66×10^4	[a] 1.82×10^{-6}	This work
		CrO_4^{2-}	3.46×10^4	[a] 2.97×10^{-6}	
		Fe^{3+}	8.45×10^3	[a] 1.35×10^{-6}	
	DMF	NB	1.22×10^3	[a] 7.14×10^{-6}	
$[PbL_1)]$	H_2O	$Cr_2O_7^{2-}$	4.3×10^4	[a] 2.6×10^{-3}	62
[Pb(BPDP)]	H_2O	Fe^{3+}	2.2×10^4	—	63
$[Pb_3(BPDP)_{1.5}(OOCC_6H_4COOH)_3]$	H_2O	Fe^{3+}	2.23×10^4	—	63
$[Pb_3O_2L_2]$	H_2O	Fe^{3+}	7.8×10^3	[a] 7.85×10^{-6}	64
$[Pb_2(HL_3)(bib)_{1.5}(H_2O)]\cdot H_2O$	H_2O	$Cr_2O_7^{2-}$	2.8×10^4	—	65
		CrO_4^{2-}	7.4×10^3	—	
$[Tb_4L_4(NO_3)_2(Piv)_2]\cdot 2CH_3OH$	H_2O	$Cr_2O_7^{2-}$	7.44×10^3	[a] 2.7×10^{-5}	39
		CrO_4^{2-}	2.998×10^3	[a] 5.2×10^{-5}	
		Fe^{3+}	1.86×10^4	[a] 1×10^{-5}	
$[Zn_3(mtrb)_3(btc)_2]\cdot 3H_2O$	H_2O	$Cr_2O_7^{2-}$	4.62×10^3	[a] 2.83×10^{-3}	40
		CrO_4^{2-}	2.77×10^3	[a] 4.52×10^{-3}	
		Fe^{3+}	6.5×10^3	[a] 1.78×10^{-3}	
	MeOH	NB	2.875×10^3	—	
$[Eu(L_5)(HCOO)]\cdot H_2O$	H_2O	$Cr_2O_7^{2-}$	3.1×10^4	[b] 2×10^{-9}	41
		CrO_4^{2-}	2.0×10^4	[b] 1×10^{-9}	
		Fe^{3+}	4.76×10^3	[b] 1×10^{-9}	
$[Eu_2(L_6)_{1.5}(H_2O)_2\cdot EtOH]\cdot DMF$	DMF	$Cr_2O_7^{2-}$	1.53×10^3	[b] 1×10^{-5}	42
		Fe^{3+}	2.94×10^3	[b] 1×10^{-5}	
$[EuL_7]$	CH_3CN	$Cr_2O_7^{2-}$	1.06×10^4	[b] 1×10^{-6}	59
		Fe^{3+}	1.40×10^4	[b] 5×10^{-7}	
$[TbL_8]\cdot 2H_2O$	H_2O	$Cr_2O_7^{2-}$	2.31×10^4	[a] 5.94×10^{-6}	60
		Fe^{3+}	2.27×10^4	[a] 8.32×10^{-6}	
$[Eu(HL_9)(H_2O)_2(NO_3)]\cdot NO_3$	H_2O	$Cr_2O_7^{2-}$	7.52×10^4	[a] 1.7×10^{-5}	61
		Fe^{3+}	4.03×10^4	[a] 4.3×10^{-5}	
	DMF	NB	1.26×10^4	[a] 2.2×10^{-5}	
$[Tb(HL_9)(H_2O)_2(NO_3)]\cdot NO_3$	H_2O	$Cr_2O_7^{2-}$	4.99×10^4	[a] 2.5×10^{-5}	61
		Fe^{3+}	4.54×10^4	[a] 1.6×10^{-5}	
	DMF	NB	2.6×10^4	[a] 1.8×10^{-5}	
$[W_2(\mu_3\text{-}S)_6(\mu_4\text{-}S)_2Cu_8(CN)_4(3\text{-abpt})]\cdot CH_3CN\cdot H_2O$	CH_3CN	NB	3.94×10^4	[a] 1×10^{-3}	71
$[Zn_{24}(BDPO)_{12}(DMF)_{12}]\cdot 6DMF\cdot 52H_2O$	DMF	NB	9.1×10^2	—	72
$[Eu_4(INO)_5(\mu_3\text{-}OH)_2Cl_4(H_2O)]\cdot(NO_3)\cdot(H_2O)_5$	H_2O	NB	0.3×10^3	[b] 3×10^{-6}	26

[a] Detection limitation calculated by $3\delta/k$; [b] Detection limitation according to the experiment data.

(H_2L_1=6,6′-(perfluoropropane-2,2-diyl)bis(2,3-dihydrophthalazine-1,4-dione);

H_2BPDP = 4,4′-biphenyldiphosphonate(monoethyl ester);

H_2L_2 = 4-(1H-tetrazol-5-yl)phenol;

H_5L_3 = 3,5-di(2′,4′-dicarboxylphenyl)benozoic acid;

bib = 1,4-bis(imidazol-1-yl) benzene;

H_2L_4 = 2-(((2-hydroxy-3-methoxybenzyl)imino)methyl)-6-methoxyphenol;

piv = pivalic acid;

mtrb = 1,3-bis(1,2,4-triazole-4-ylmethyl)benzene;

btc = 1,3,5-benzenetricarboxylate;

H_2L_5 = 5-((pyridin-3-yloxy)methyl)isophthalic acid;

L_6 = 5,5'-(carbonylbis(azanediyl))diisophthalic acid;

L_7 = 3-bis(3-carboxyphenyl)imidazolium;

H_2L_9 = 4-(3,5-dicarboxylphenyl)-2-methylpyridine;

3-abpt = 4-amino-3,5-bis(3-pyridyl)-1,2,4-triazole;

H_4BDPO = 2,4-Bis(3,5-dicarboxyphenylamino)-6-ol triazine;

HINO = isonicotinic acid N-oxide.)

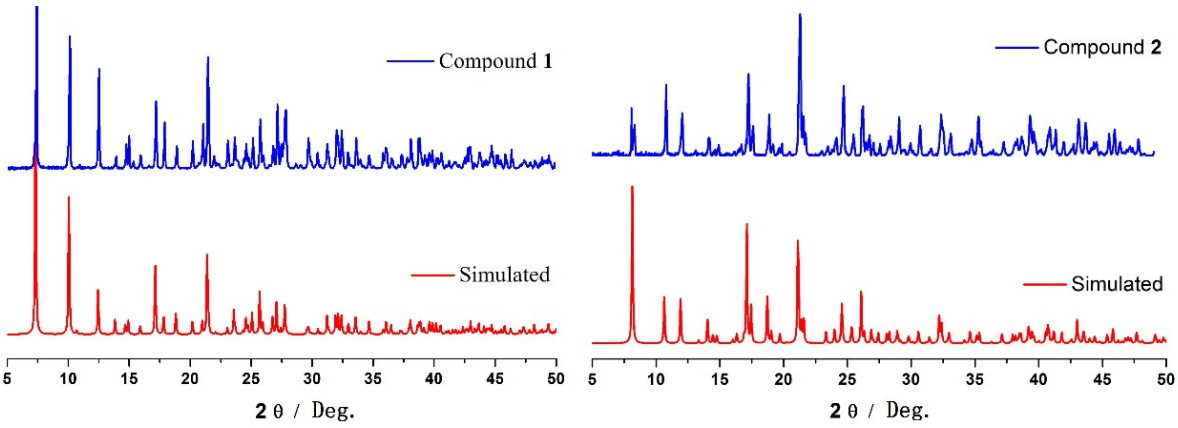

Fig. S1 PXRD patterns of simulated and as-synthesized compounds **1** and **2**.

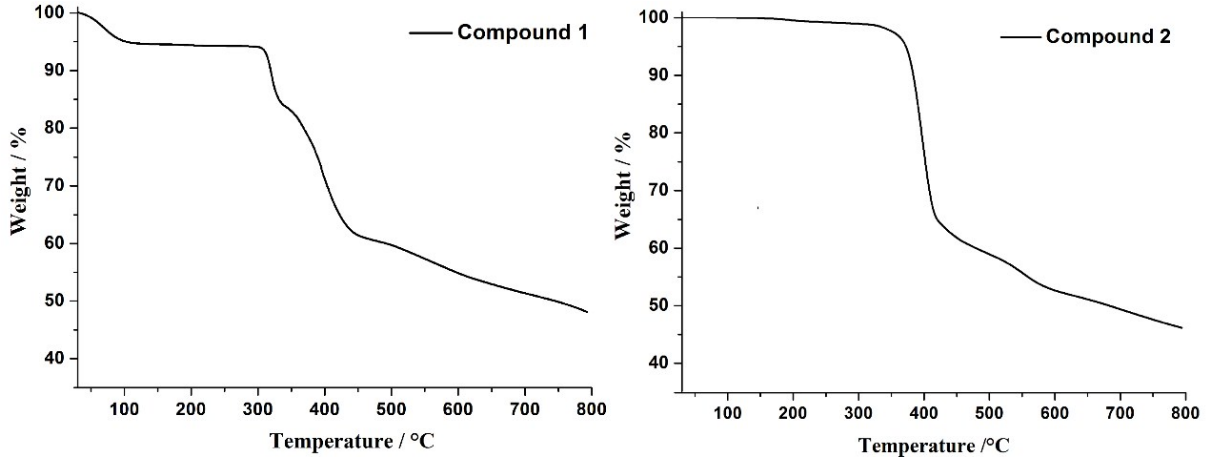

Fig. S2 TGA diagrams of as-synthesized compounds **1** and **2**.

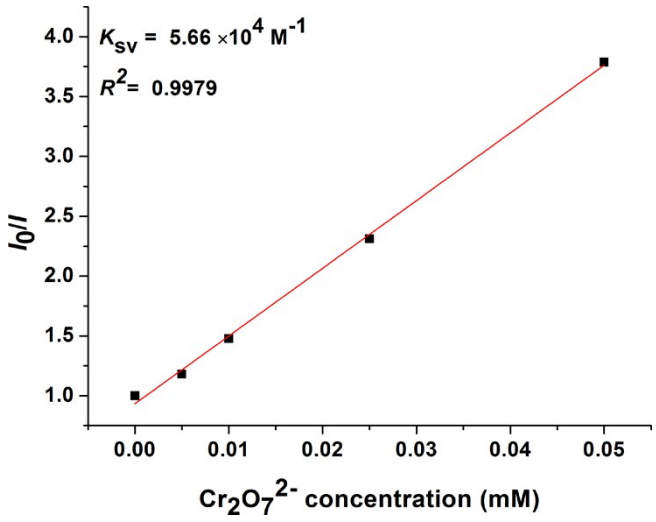

Fig. S3 I_0/I versus concentration of $Cr_2O_7^{2-}$ plotted according to Stern-Volmer equation.

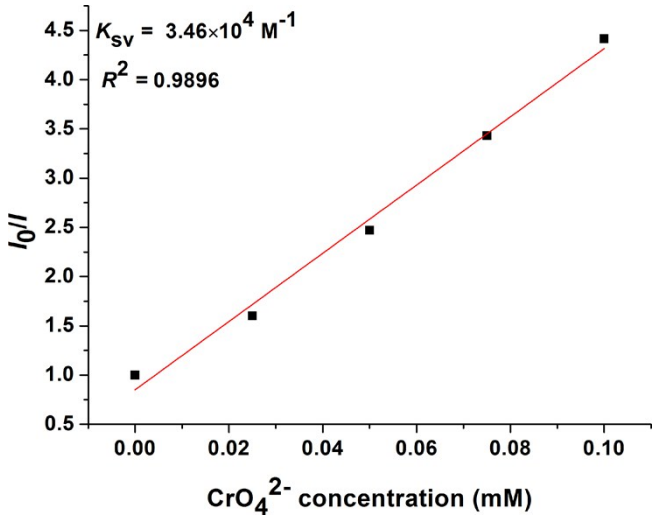

Fig. S4 I_0/I versus concentration of CrO_4^{2-} plotted according to Stern-Volmer equation.

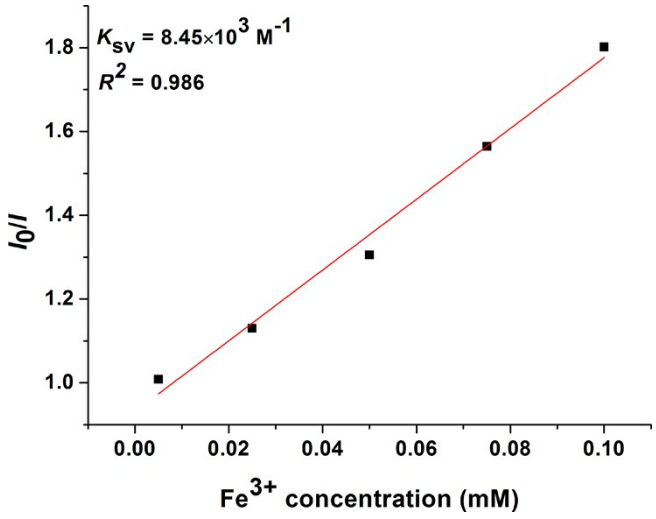

Fig. S5 I_0/I versus concentration of Fe^{3+} plotted according to Stern-Volmer equation.

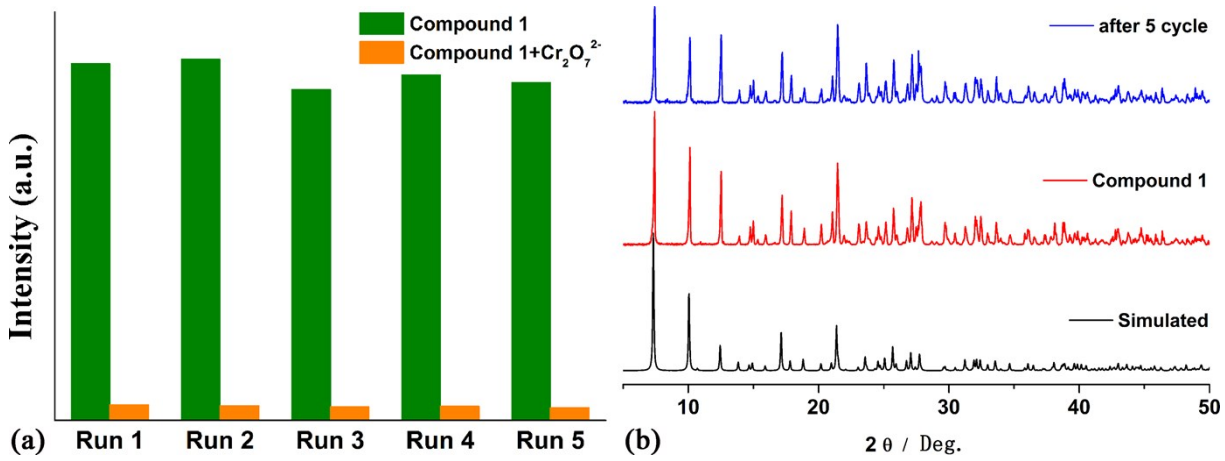

Fig. S6 (a) Luminescent intensity of compound **1** and sensing $Cr_2O_7^{2-}$ (0.5 mM) during 5 times recycling experiments; (b) PXRD patterns of simulation, before and after 5 times recycling experiments.

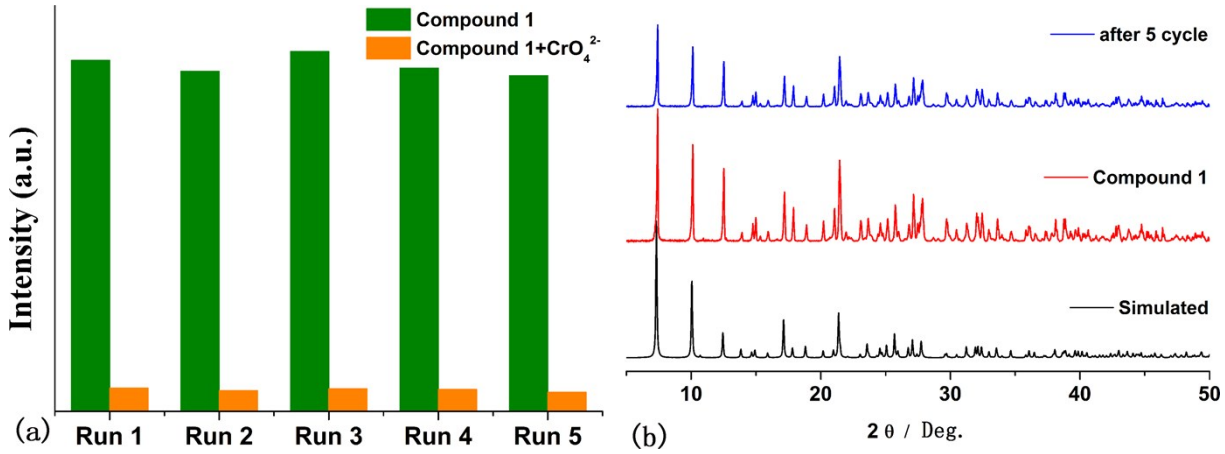

Fig. S7 (a) Luminescent intensity of compound **1** and sensing CrO_4^{2-} (0.5 mM) during 5 times recycling experiments; (b) PXRD patterns of simulation, before and after 5 times recycling experiments.

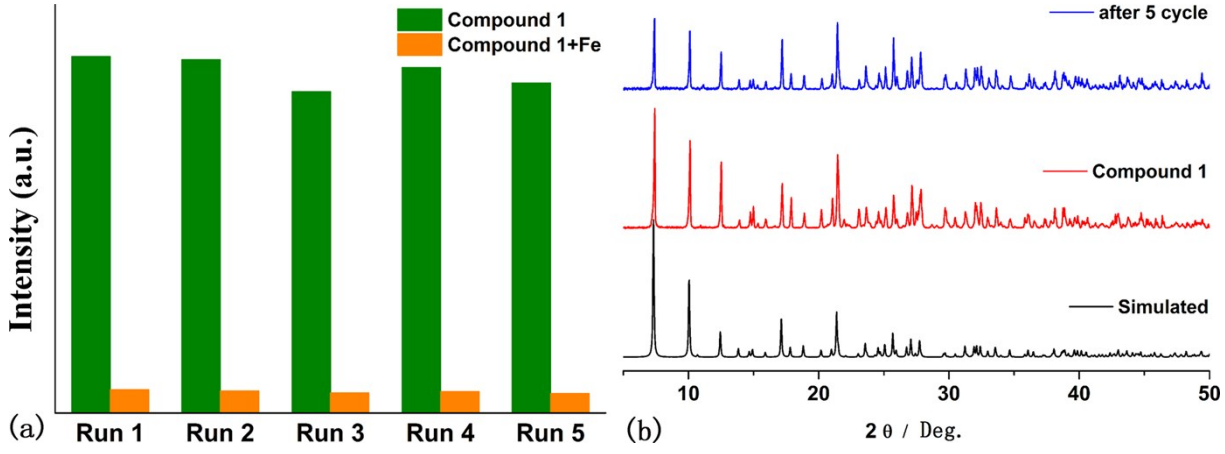

Fig. S8 (a) Luminescent intensity of compound **1** and sensing Fe^{3+} (1.5 mM) during 5 times recycling experiments; (b) PXRD patterns of simulation, before and after 5 times recycling experiments.

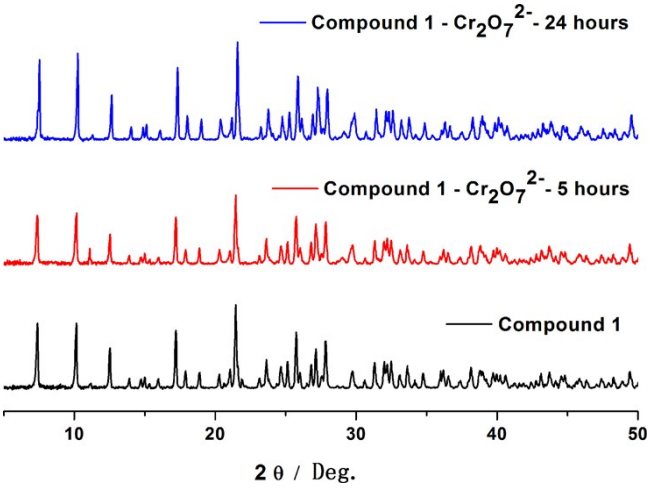

Fig. S9 The PXRD patterns of compound **1** before and after immersing in $Cr_2O_7^{2-}$ aqueous solution for 5 hours and 24 hours.

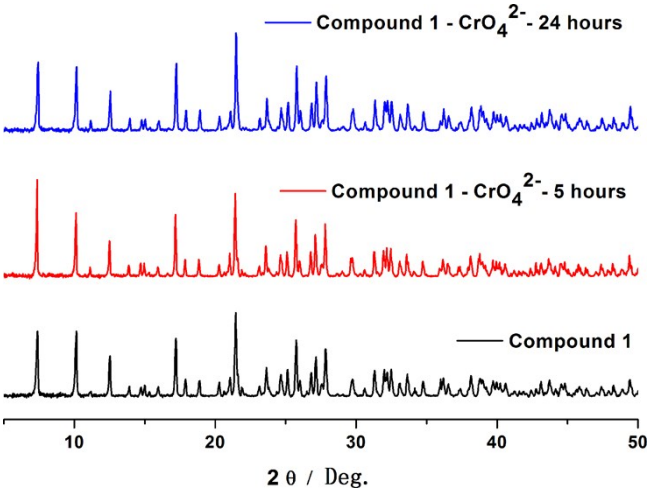

Fig. S10 The PXRD patterns of compound **1** before and after immersing in CrO_4^{2-} aqueous solution for 5 hours and 24 hours.

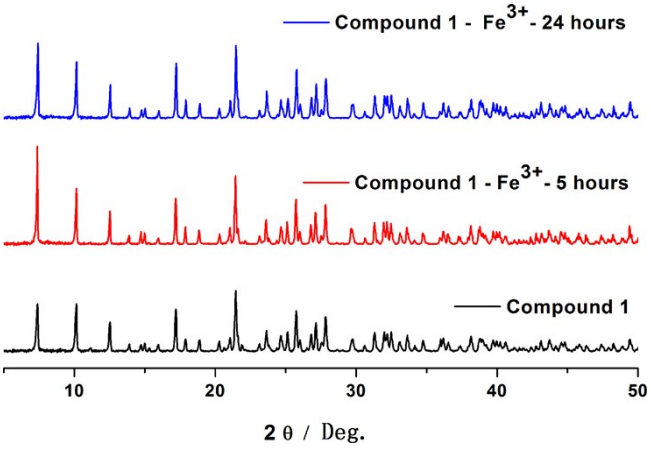

Fig. S11 The PXRD patterns of compound **1** before and after immersing in Fe^{3+} aqueous solution for 5 hours and 24 hours.

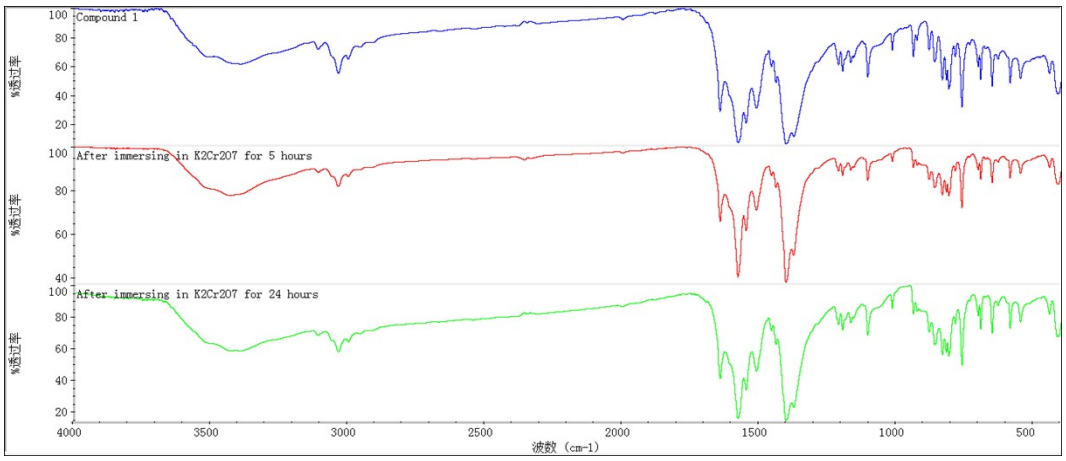

Fig. S12 The IR diagrams of compound **1**before and after immersing in $Cr_2O_7^{2-}$ aqueous solution for 5 hours and 24 hours.

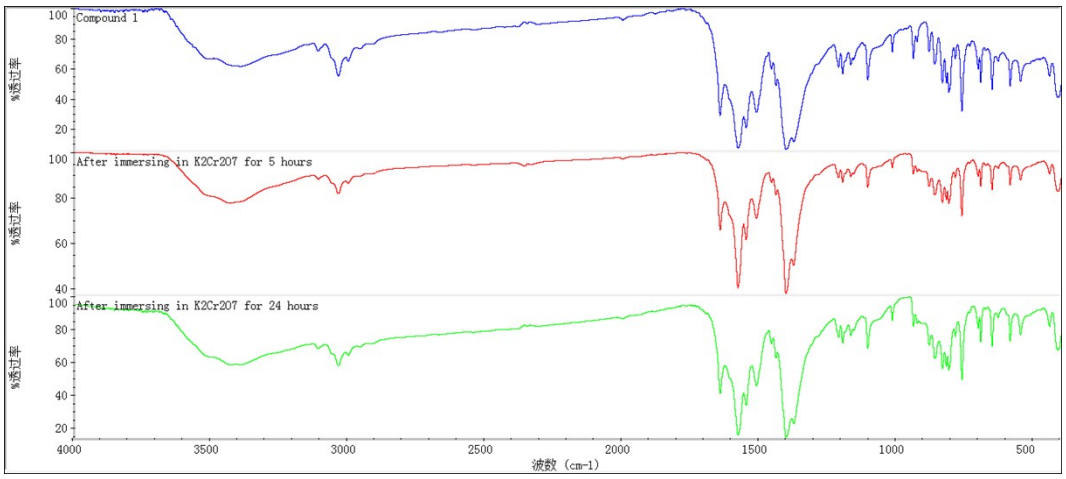

Fig. S13 The IR diagrams of compound **1**before and after immersing in CrO_4^{2-} aqueous solution for 5 hours and 24 hours.

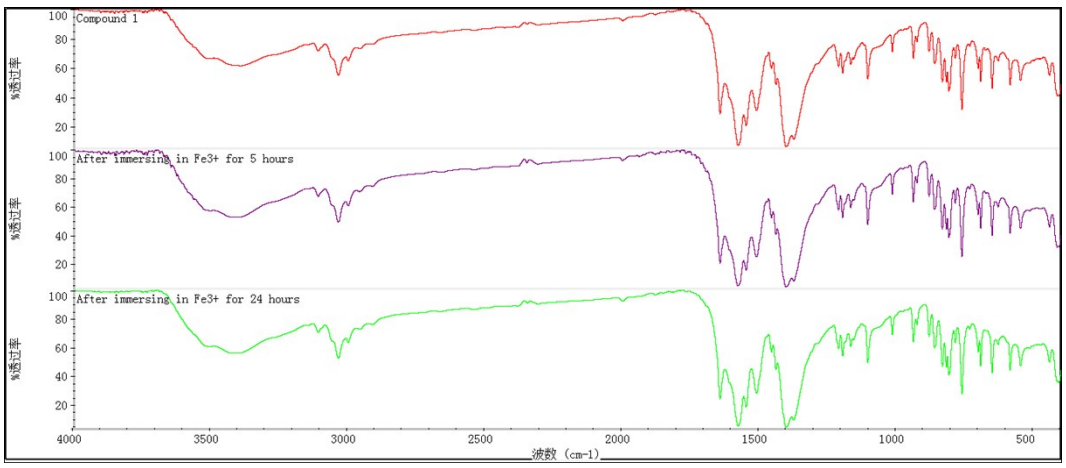

Fig. S14 The IR diagrams of compound **1**before and after immersing in Fe^{3+} aqueous solution for 5 hours and 24 hours.

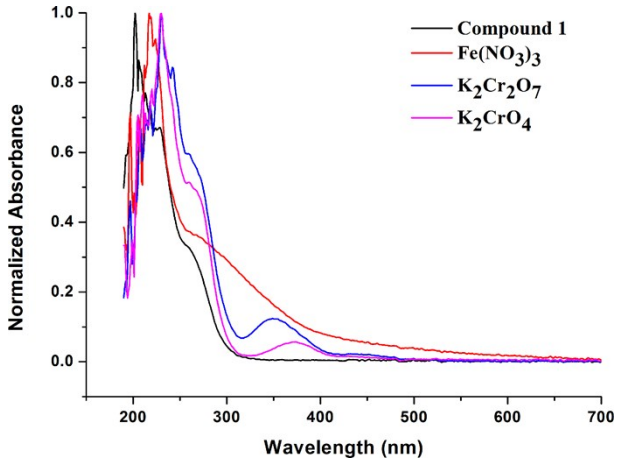

Fig. S15 The UV-vis absorption spectra of compound **1** and $Cr_2O_7^{2-}$, CrO_4^{2-} and Fe^{3+} aqueous solution (1.5mM).

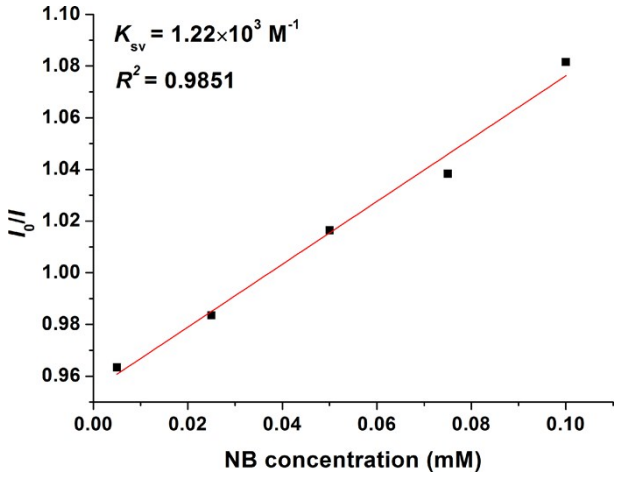

Fig. S16 I_0/I versus concentration of NB plotted according to Stern-Volmer equation.

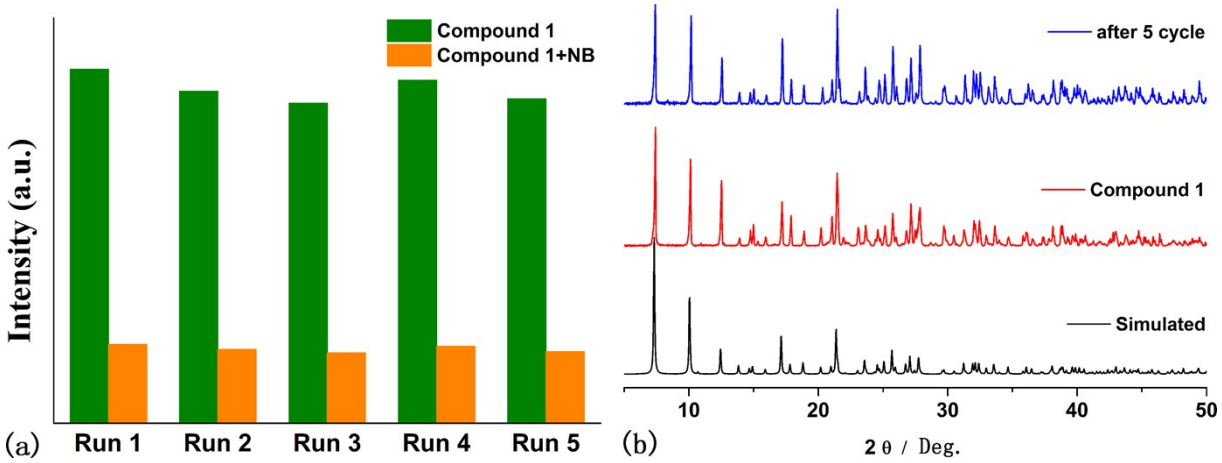

Fig. S17 (a) Luminescent intensity of compound **1** and sensing NB during 5 times recycling experiments; (b) PXRD patterns of simulation, before and after 5 times recycling experiments.

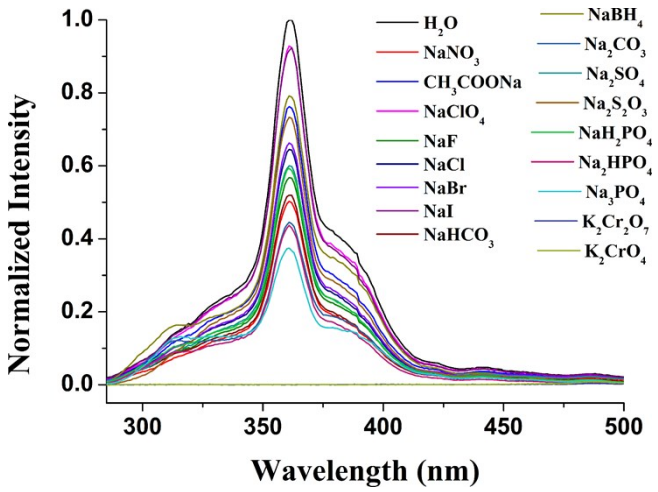

Fig. S18 Normalized luminescent intensities of compound **1** dispersed in inorganic anion aqueous solution.

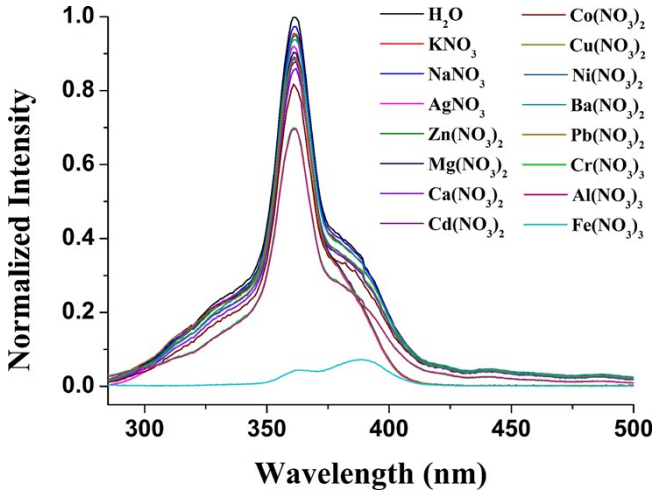

Fig. S19 Normalized luminescent intensities of compound **1** dispersed in metal cations aqueous solution.

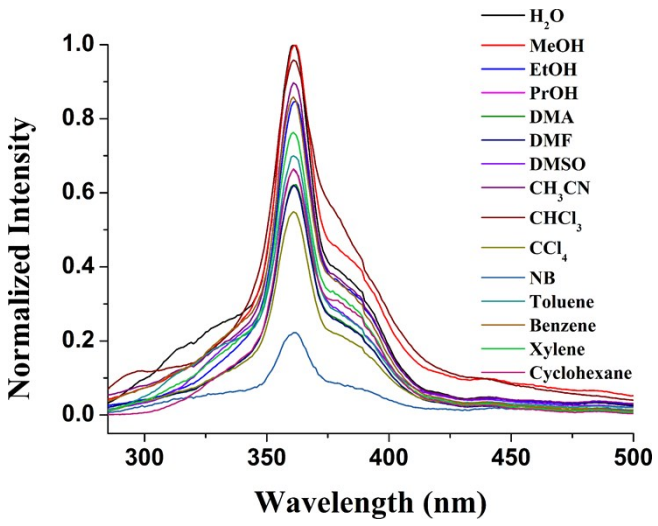

Fig. S20 Normalized luminescent intensities of compound **1** dispersed in different organic solvents.

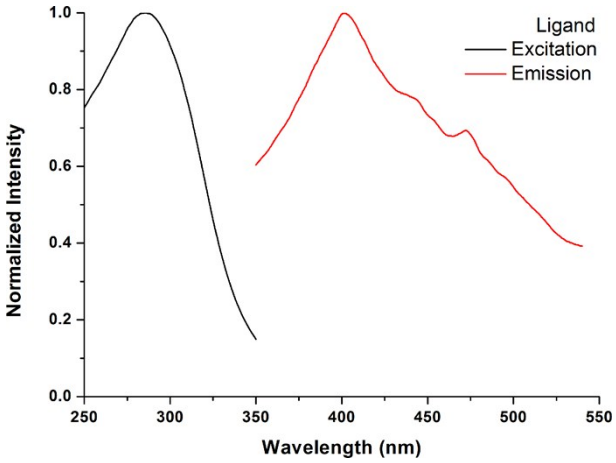

Fig. S21 Solid state excitation and emission spectra of free ligand. (λ_{ex} = 280 nm, λ_{em} = 402 nm)