

**Metal–organic frameworks with 5,5'-(1,4-xylylenediamino)
diisophthalic acid and varied nitrogen-containing ligands for
selectively sensing Fe(III)/Cr(VI) and nitroaromatic**

Cungang Xu^a, Caifeng Bi^a, Zheng Zhu^c, Rong Luo^a, Xia Zhang^a, Dongmei Zhang^a, Chuanbin Fan^a, Liansheng Cui^{b*}, Yuhua Fan^{a*}

- a. Key Laboratory of Marine Chemistry Theory and Technology, Ministry of Education, College of Chemistry and Chemical Engineering, Ocean University of China, Qingdao, Shandong 266100, P.R. China
b. College of Chemistry and Environmental Engineering, Baise University, Baise, Guangxi 533000, China
c. College of Materials Science and Engineering, Hebei University of Engineering, Handan, Hebei, 056038, P.R. China

Table S1. Selected Bond lengths [Å] and angles [°] for complexes **1-4**

Complex 1			
Zn1—O1	1.950 (3)	Zn1—N3	1.995 (3)
Zn1—O3 ⁱ	1.950 (3)	Zn1—N5	2.022 (3)
O3—Zn1 ⁱⁱ	1.950 (3)		
O1—Zn1—O3 ⁱ	107.31 (12)	O3 ⁱ —Zn1—N5	108.00 (14)
O1—Zn1—N3	110.64 (13)	N3—Zn1—N5	105.34 (14)
O1—Zn1—N5	98.96 (13)	O3 ⁱ —Zn1—N3	123.74 (13)
Complex 2			
Zn1—O1	1.947 (4)	Zn1—N4	2.007 (6)
Zn1—O4 ⁱ	1.958 (4)	Zn1—N2	2.013 (5)
O4—Zn1 ⁱⁱ	1.958 (4)		
O1—Zn1—O4 ⁱ	109.95 (17)	O4 ⁱ —Zn1—N4	108.2 (2)
O1—Zn1—N4	118.4 (2)	O4 ⁱ —Zn1—N2	113.37 (19)
O1—Zn1—N2	95.68 (18)	N4—Zn1—N2	110.9 (2)
Complex 3			
Zn1—N2	2.0930 (18)	Zn1—O1 ⁱⁱ	1.9513 (15)
Zn1—O3	2.2418 (16)	N4—Zn1 ⁱ	2.0485 (18)
Zn1—O4	2.0885 (15)	O1—Zn1 ^{iv}	1.9513 (15)
Zn1—N4 ⁱ	2.0485 (18)		
N2—Zn1—O3	154.21 (7)	N4 ⁱ —Zn1—O3	90.07 (7)
N2—Zn1—C2	126.07 (7)	N4 ⁱ —Zn1—O4	127.15 (7)

O3—Zn1—C2	30.10 (6)	O1 ⁱⁱ —Zn1—N2	102.28 (7)
O4—Zn1—N2	96.52 (7)	O1 ⁱⁱ —Zn1—O3	97.22 (7)
O4—Zn1—O3	60.49 (6)	O1 ⁱⁱ —Zn1—O4	110.58 (6)
N4 ⁱ —Zn1—N2	96.18 (7)	O1 ⁱⁱ —Zn1—N4 ⁱ	116.29 (7)

Complex 4

Zn1—O1	1.942 (3)	Zn1—O3 ⁱⁱ	2.349 (3)
Zn1—N4 ⁱ	2.017 (4)	N4—Zn1 ⁱ	2.017 (4)
Zn1—O4 ⁱⁱ	2.063 (3)	O3—Zn1 ⁱⁱⁱ	2.349 (3)
Zn1—N2	2.081 (4)	O4—Zn1 ⁱⁱⁱ	2.063 (3)
O1—Zn1—N4 ⁱ	119.77 (15)	O4 ⁱⁱ —Zn1—N2	97.83 (14)
O1—Zn1—O4 ⁱⁱ	106.91 (13)	O1—Zn1—O3 ⁱⁱ	100.62 (13)
N4 ⁱ —Zn1—O4 ⁱⁱ	125.71 (15)	N4 ⁱ —Zn1—O3 ⁱⁱ	85.24 (13)
O1—Zn1—N2	102.61 (15)	O4 ⁱⁱ —Zn1—O3 ⁱⁱ	59.05 (13)
N4 ⁱ —Zn1—N2	97.53 (16)	N2—Zn1—O3 ⁱⁱ	151.30 (14)

Symmetry codes **1**: (i) $x-1/2, -y+3/2, z-1/2$; (ii) $x+1/2, -y+3/2, z+1/2$; (iii) $-x+3, -y+1, -z+1$; (iv) $-x-1/2, y-1/2, -z+1/2$; (v) $-x-1/2, y+1/2, -z+1/2$.

Symmetry codes **2**: (i) $x-1/2, -y+1/2, z-1/2$; (ii) $x+1/2, -y+1/2, z+1/2$; (iii) $-x+3, -y+1, -z+1$; (iv) $-x, -y, -z+1$; (v) $-x, -y+1, -z$.

Symmetry codes **3**: (i) $-x+1, -y+1, -z$; (ii) $x-1, -y+3/2, z-1/2$; (iii) $-x+3, -y+1, -z+2$; (iv) $x+1, -y+3/2, z+1/2$.

Symmetry codes **4**: (i) $-x+2, -y, -z+2$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $x-1/2, -y+1/2, z+1/2$; (iv) $-x+1, -y+1, -z+1$.

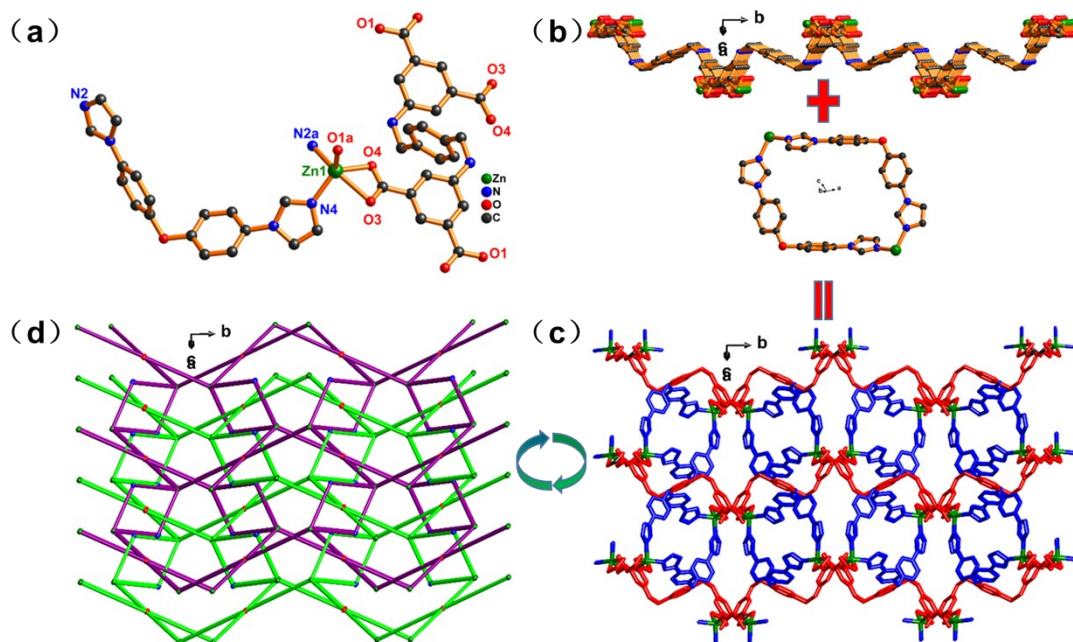


Figure S1. (a) Coordination environment of Zn(II) in complex 4 (all the H atoms are omitted for clarity). Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $x-1/2, -y+1/2, z+1/2$; (iv) $-x+1, -y+1, -z+1$; (b) The 2D "W" type plane of [Zn-L]_n (upper) and a loop of [Zn-bidpe]_n (under); (c) A unit of 3D framework of complex 4 (red spheres: L⁴ ligands; blue spheres: bidpe ligands); and (d) the 3D topology view of 2-fold interpenetrated frameworks of complex 4.

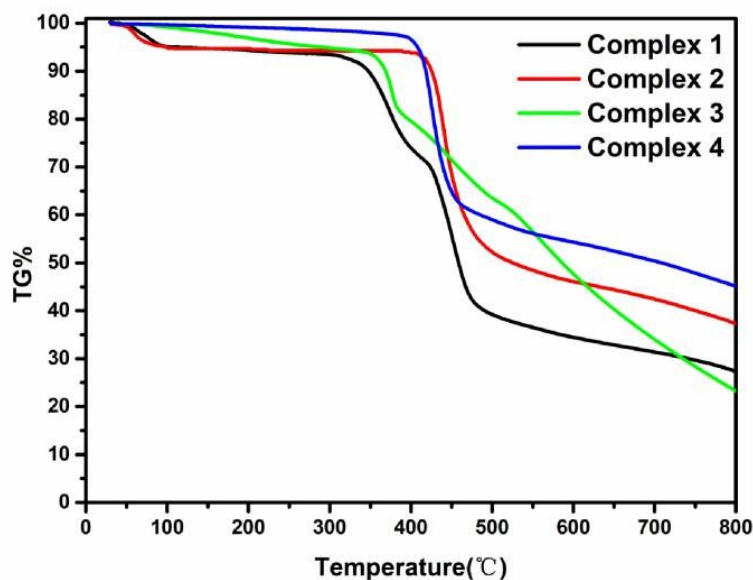


Figure S2. The TG curves for complexes 1-4.

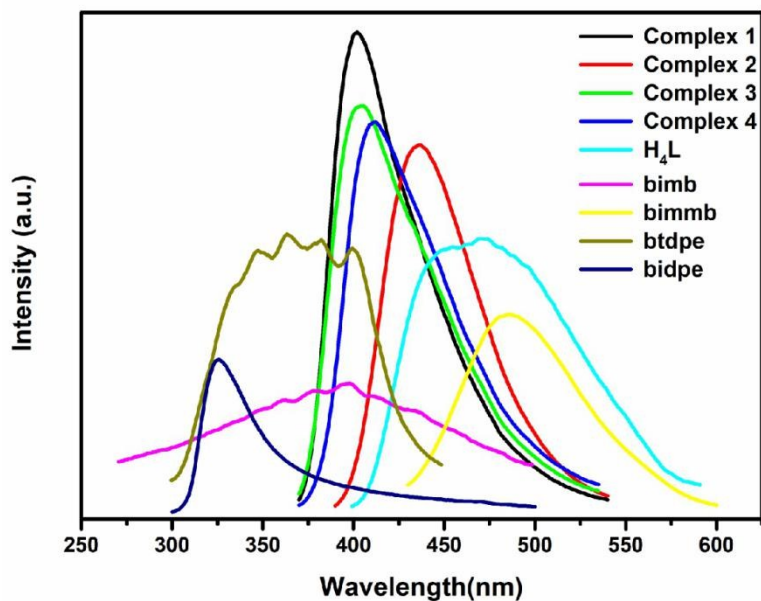


Figure S3. The emission spectra of complexes **1-4** and free organic ligands in solid state at room temperature.

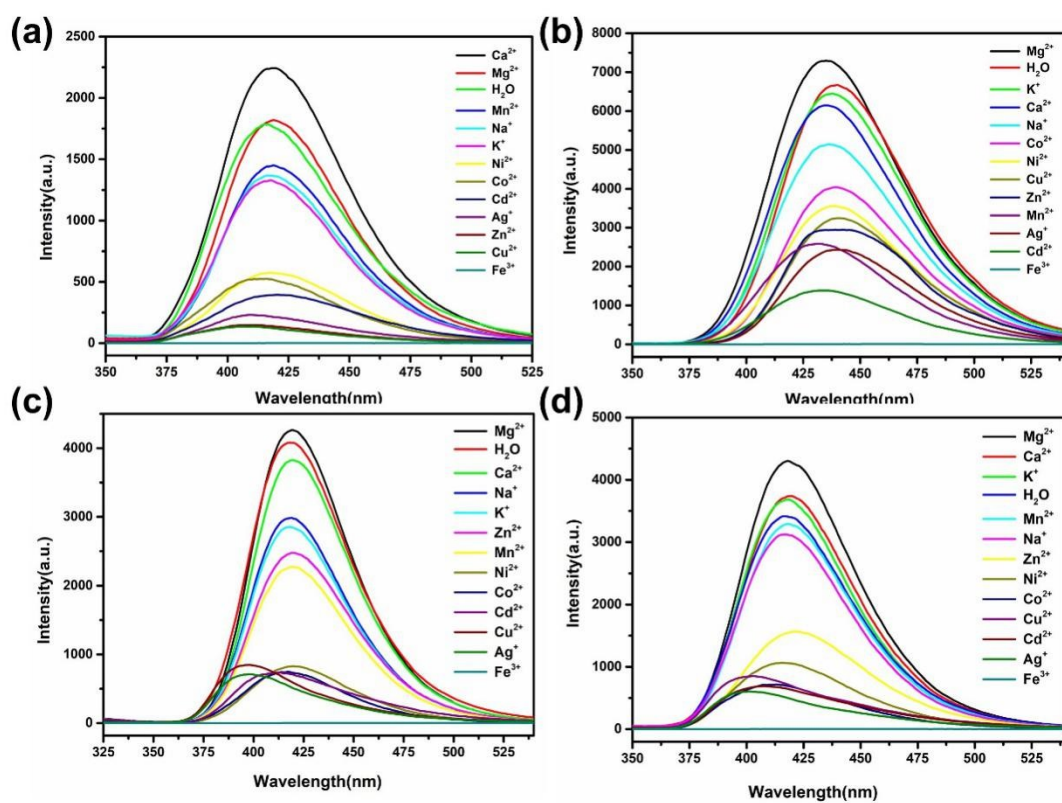


Figure S4. The photoluminescence spectra for **1-4** in aqueous solution with various inorganic cations.

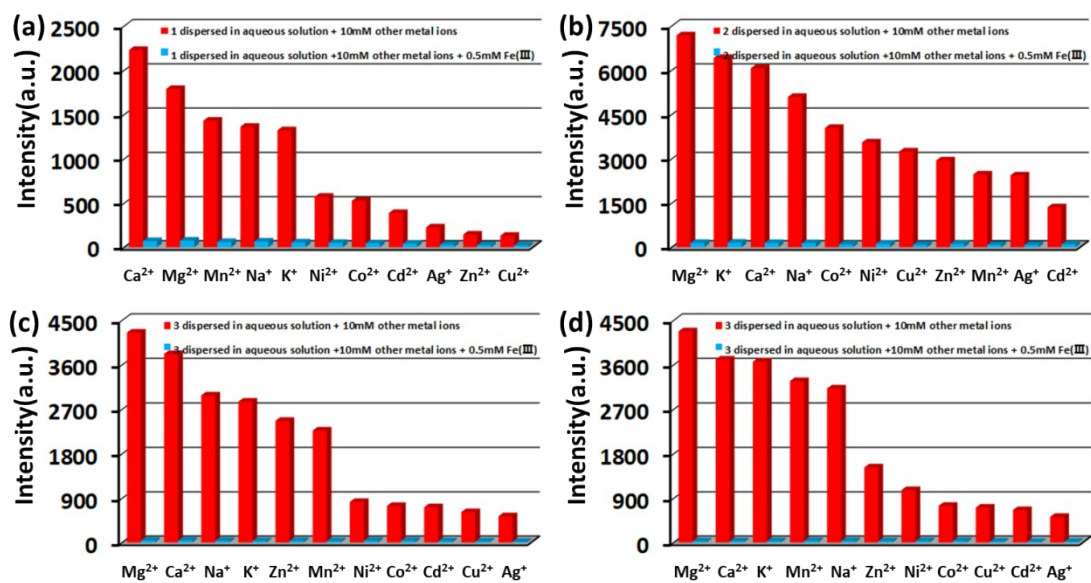


Figure S5. Fluorescence intensity of **1-4** in aqueous solution with the introduction of diverse other metal ions (red) and introduction of Fe(III) (blue).

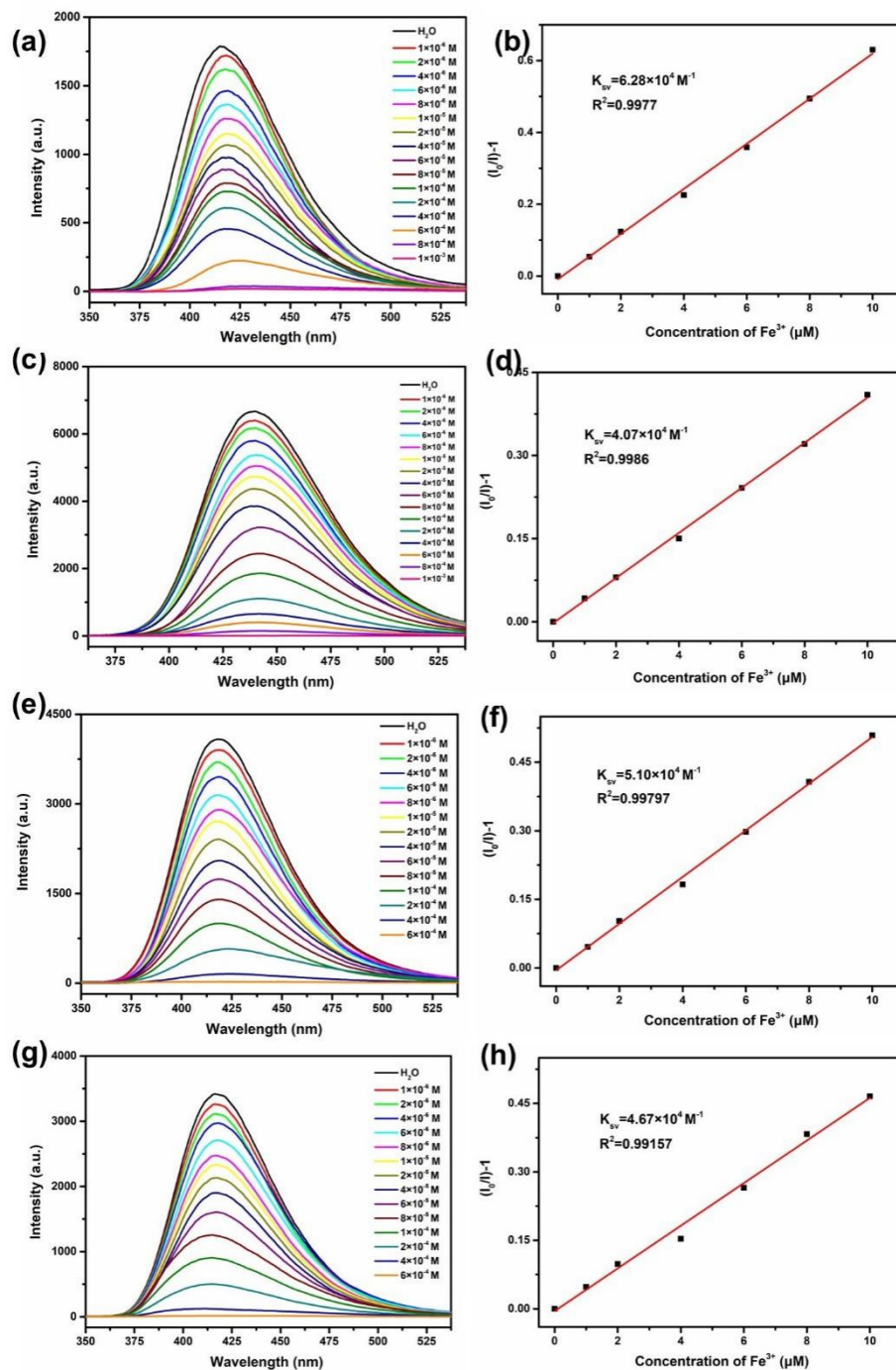


Figure S6. Emission spectra and linear relationships for 1-4 aqueous solutions of different Fe^{3+} concentrations.

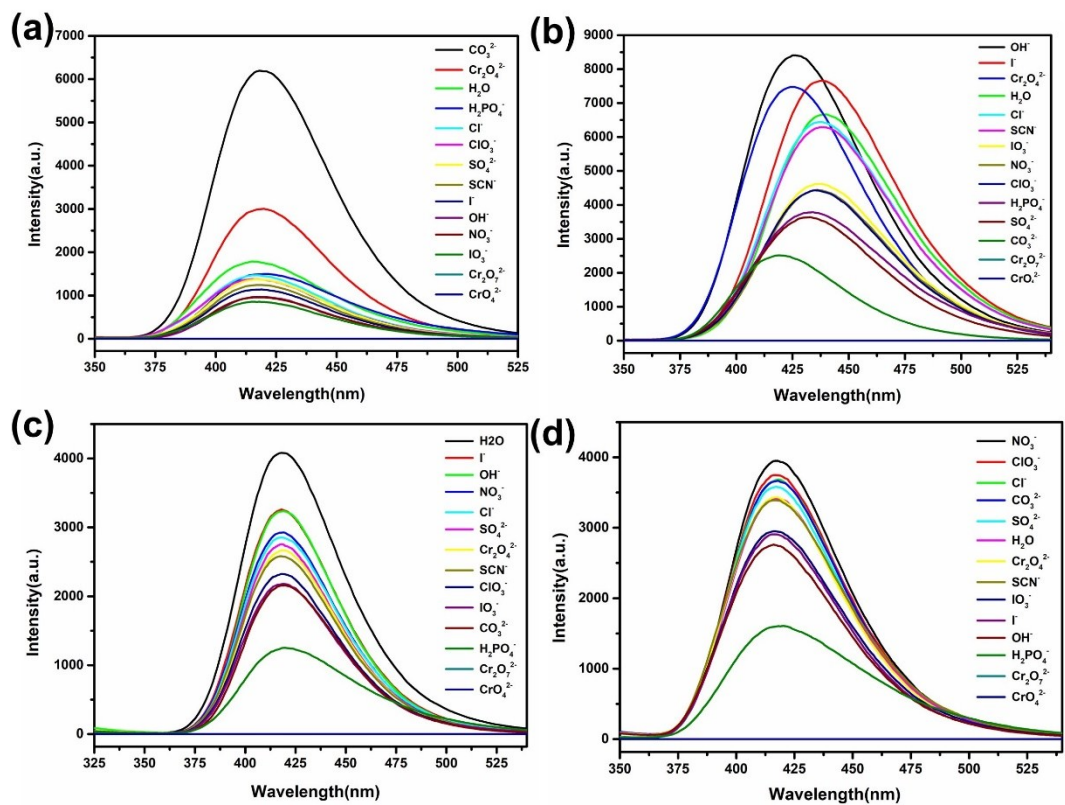


Figure S7. The photoluminescence spectra for 1-4 in aqueous solution with various inorganic anions.

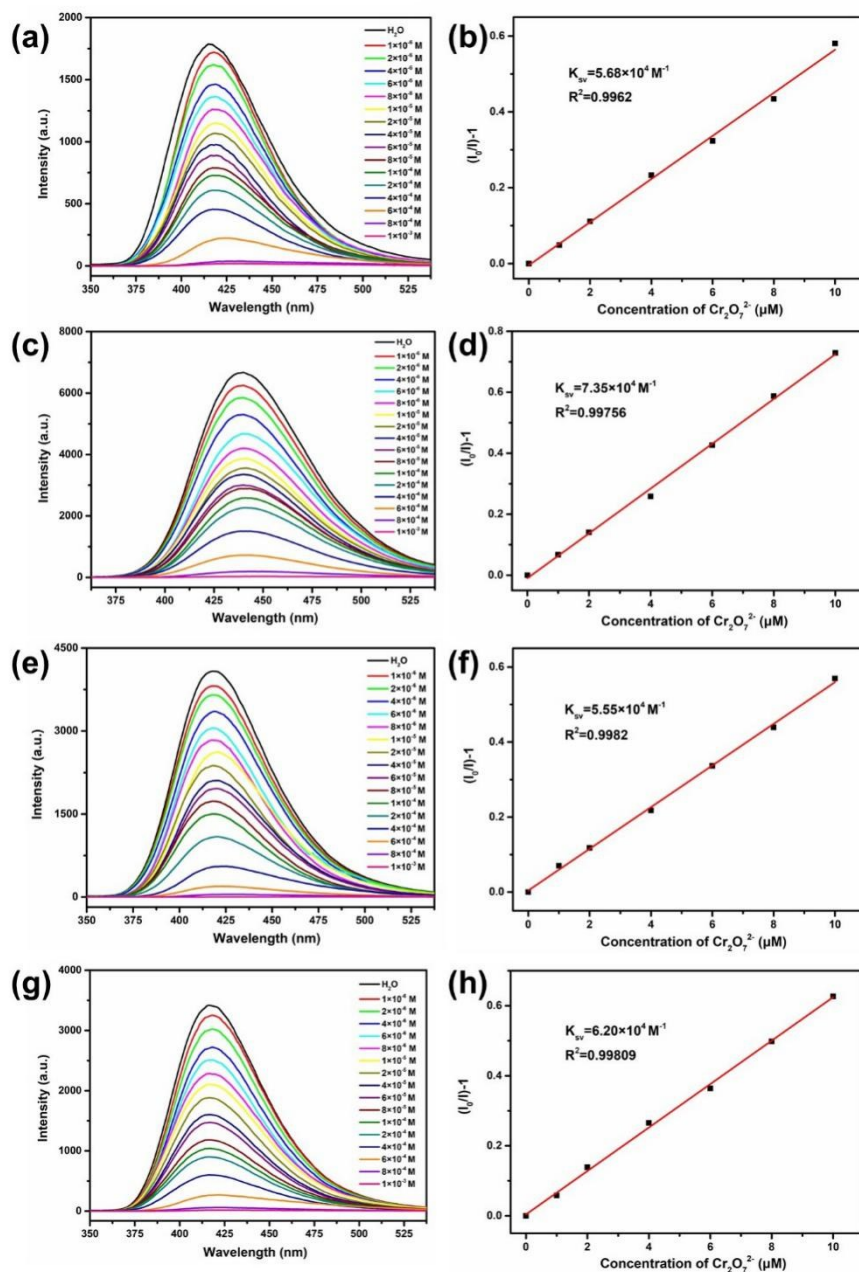


Figure S8. Emission spectra and linear relationships for 1-4 aqueous solutions of different $\text{Cr}_2\text{O}_7^{2-}$ concentrations.

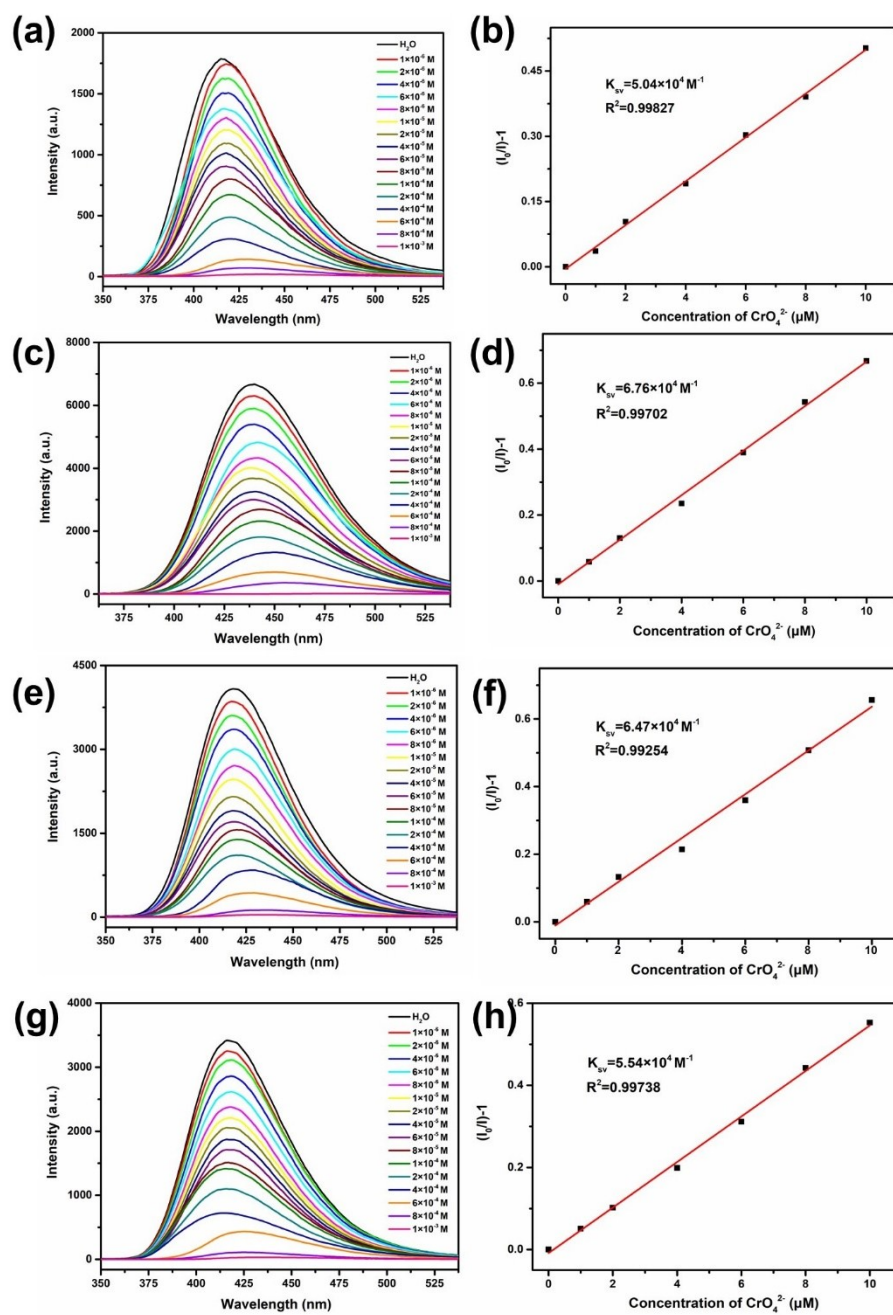


Figure S9. Emission spectra and linear relationships for 1-4 aqueous solutions of different CrO_4^{2-} concentrations.

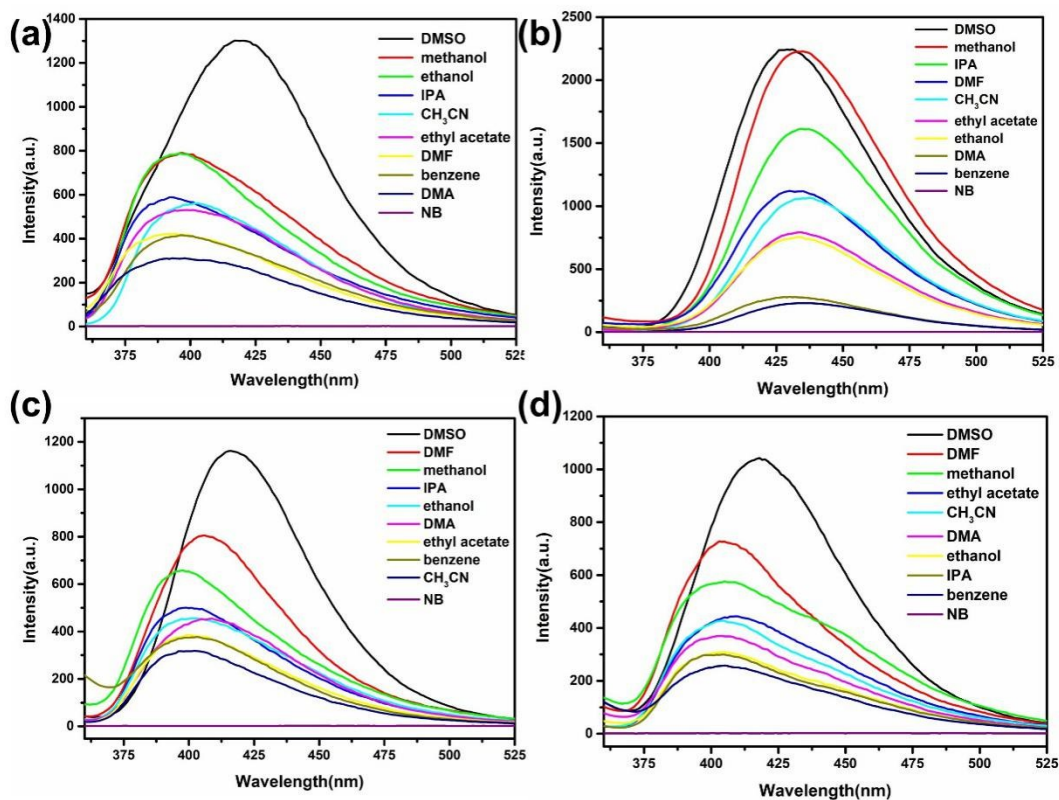


Figure S10. Emission spectra of 1-4 in diverse organic solvents.

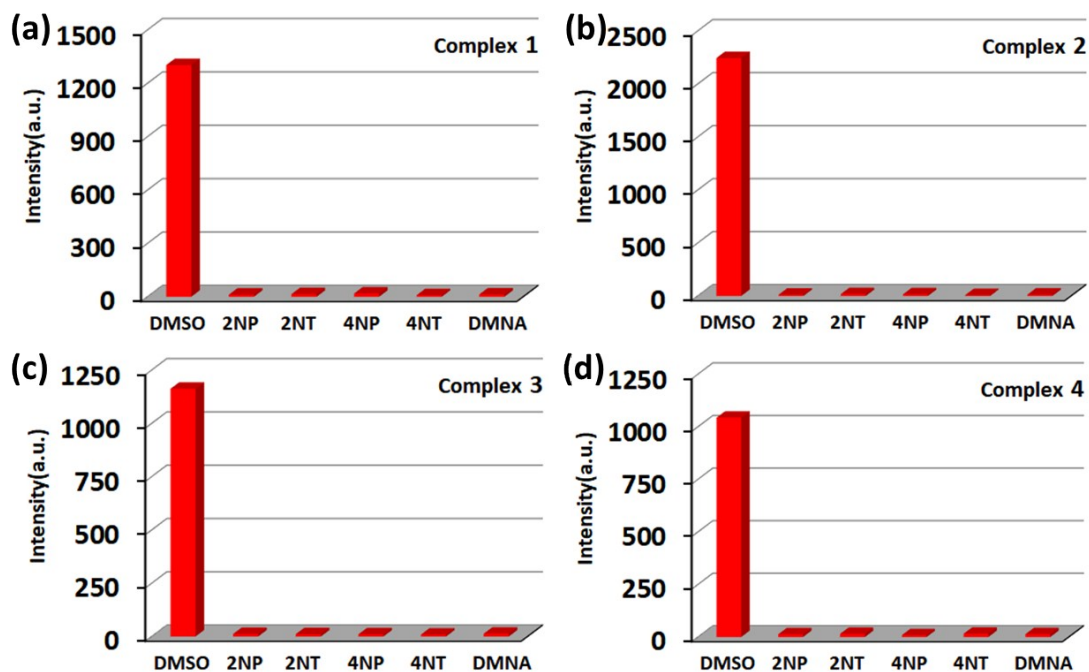


Figure S11. The photoluminescence intensities of 1-4 for nitroaromatic compounds in DMSO.

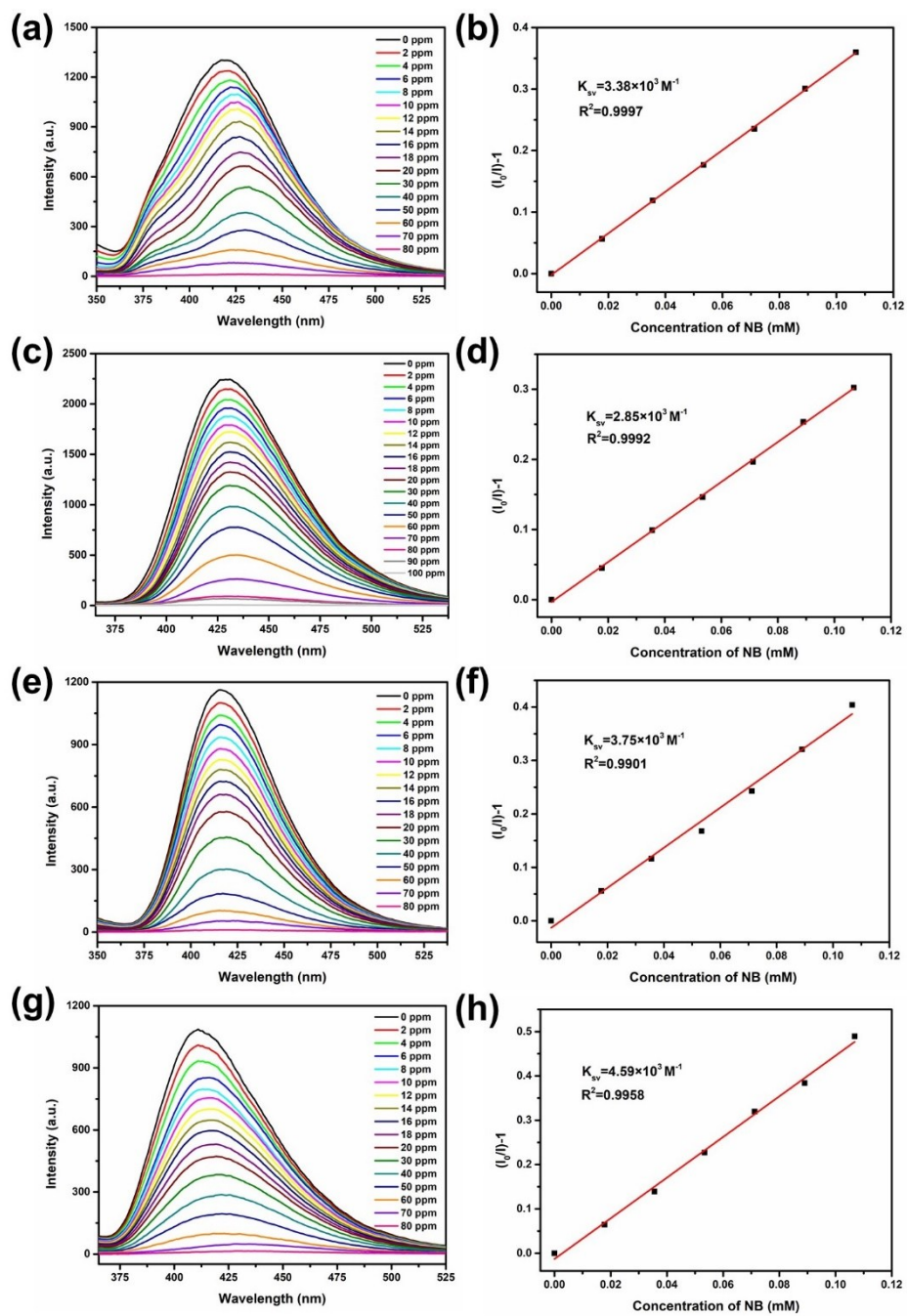


Figure S12. Emission spectra and linear relationships for 1-4 in DMSO with different concentrations of NB.

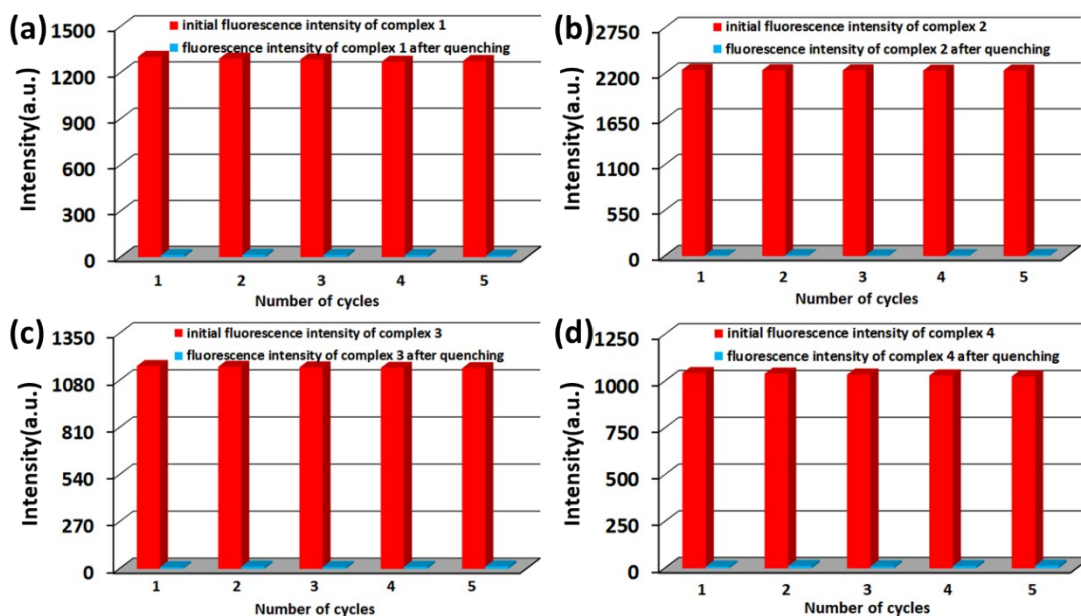
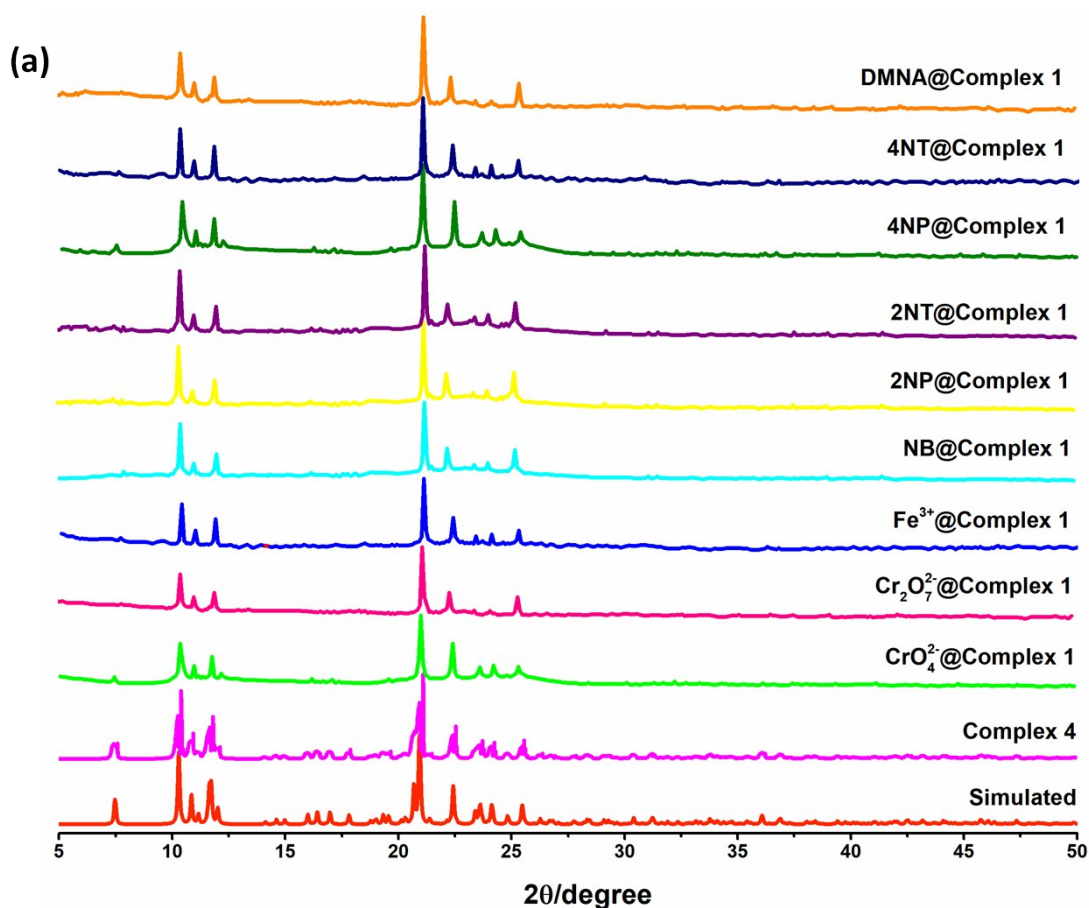
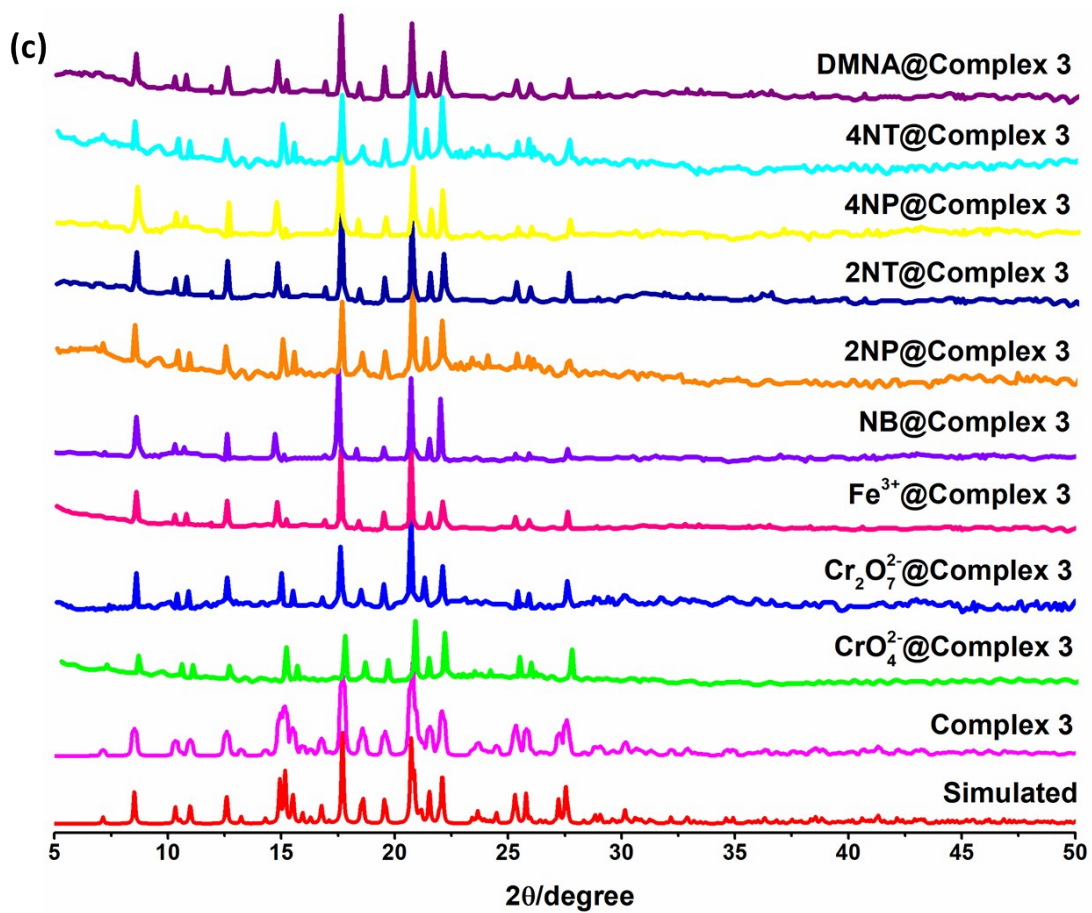
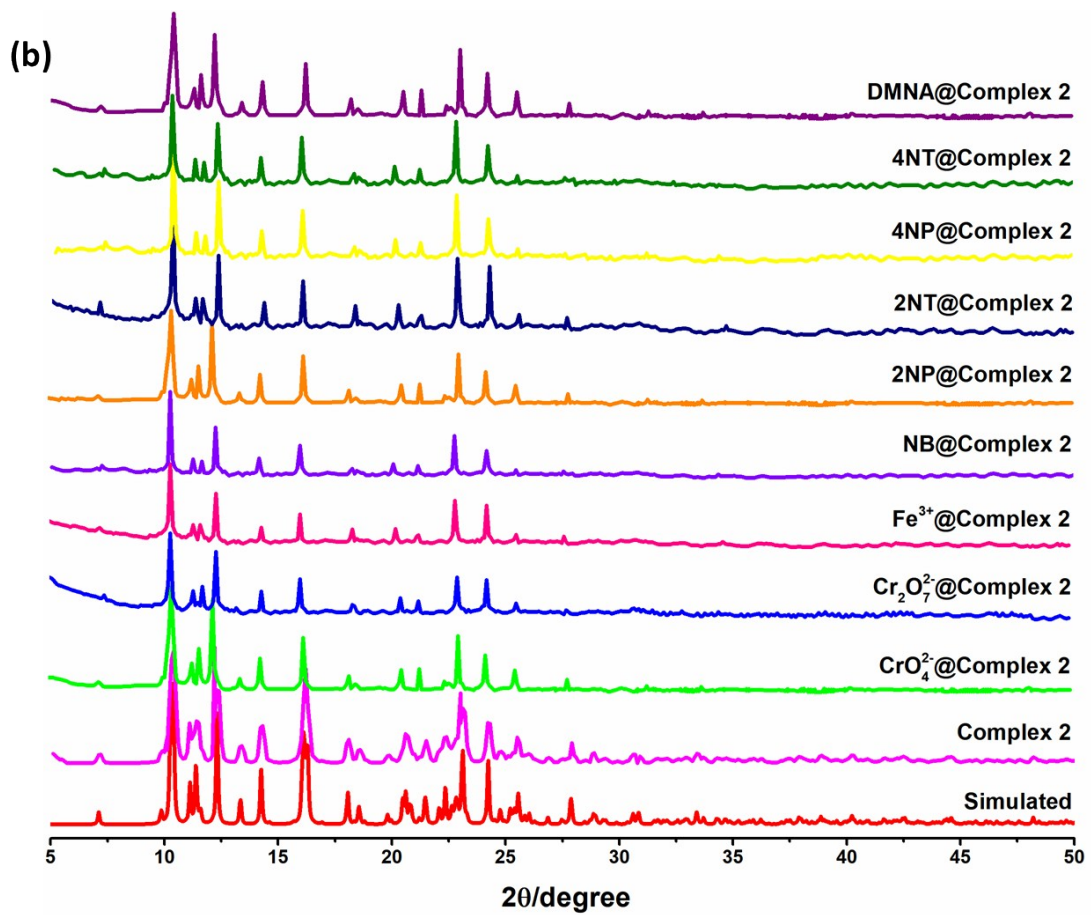


Figure S13. Fluorescence quenching and repeatability test of 1-4 for NB.





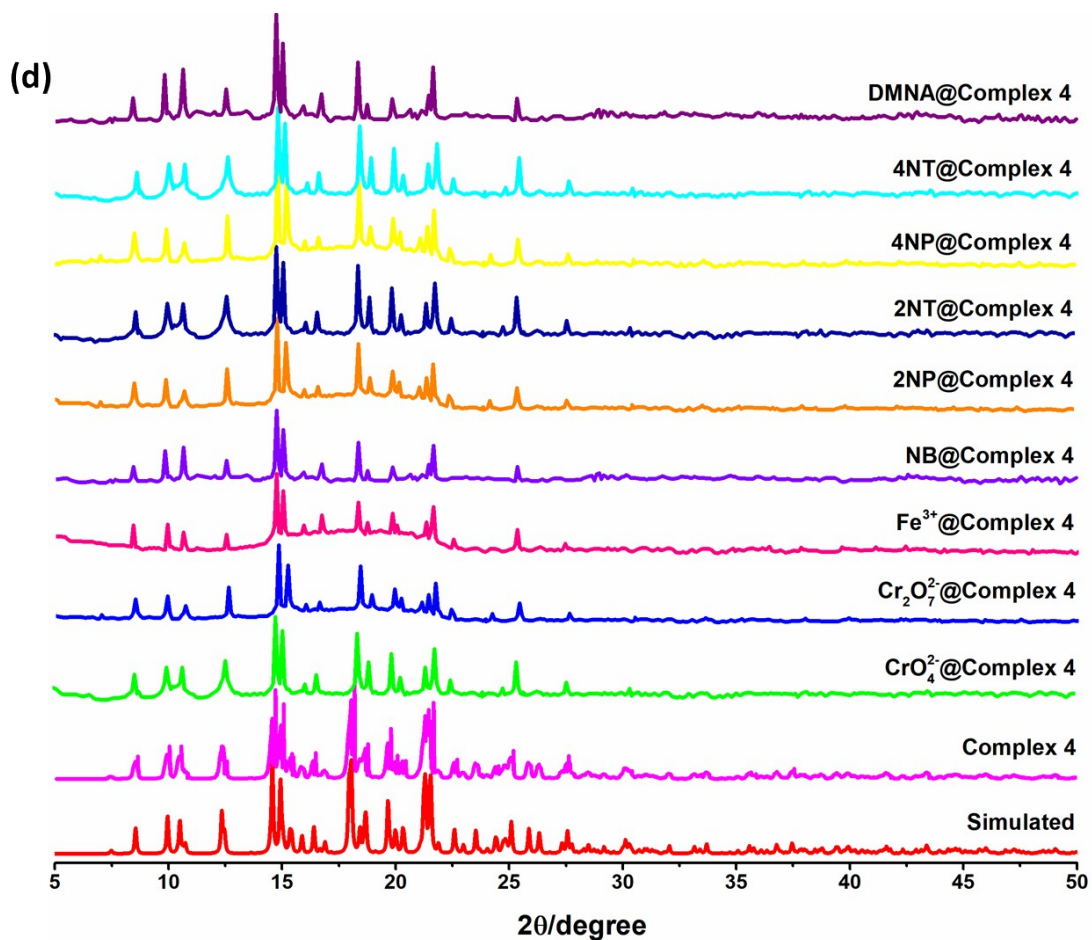


Figure S14. The PXRD patterns of complexes 1-4 before and after the quenching test.

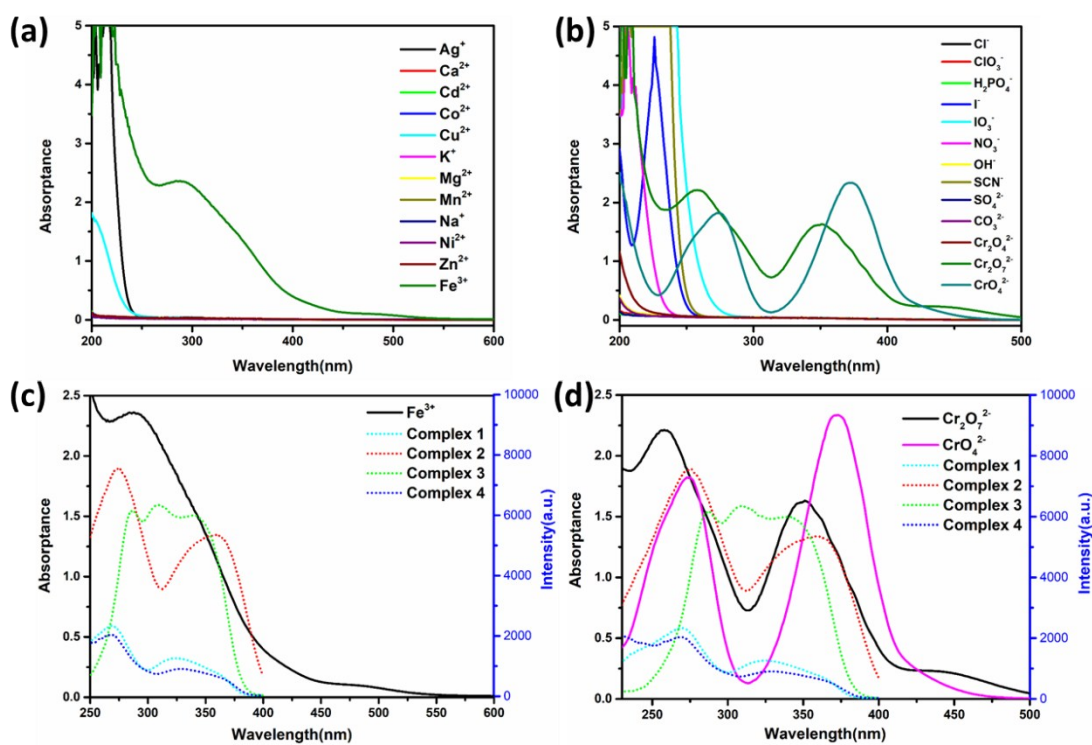


Figure S15. Liquid UV-Vis spectra of various anions and excitation spectra of complexes **1-4** in aqueous solution.