

Fig. S1 The rod-like metal ion chain in compound 3.

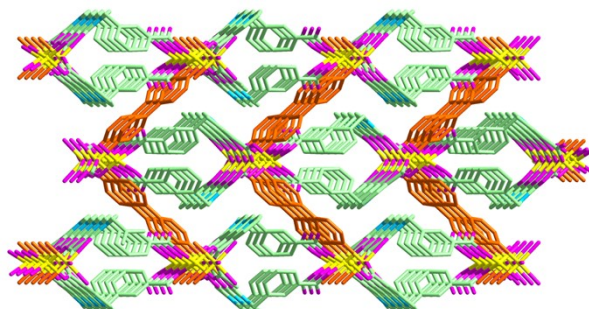
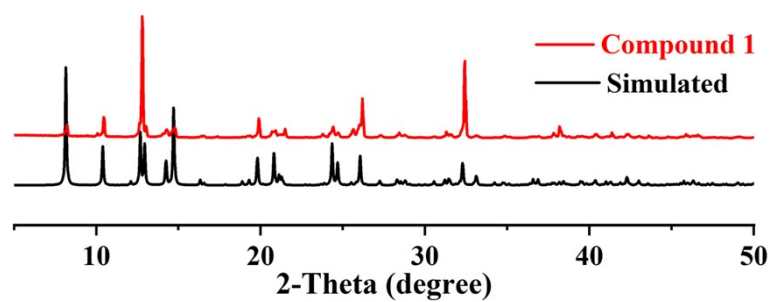
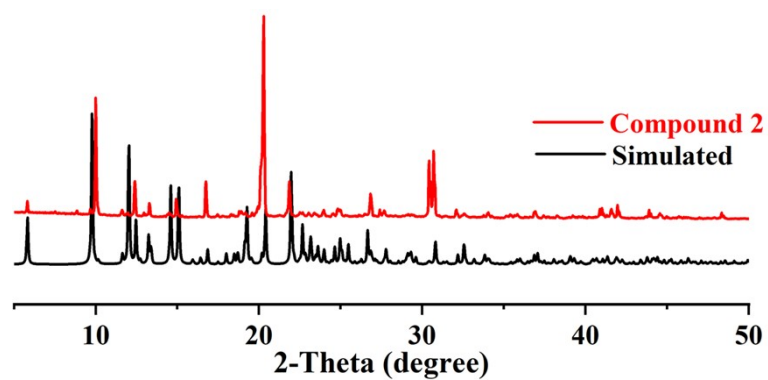


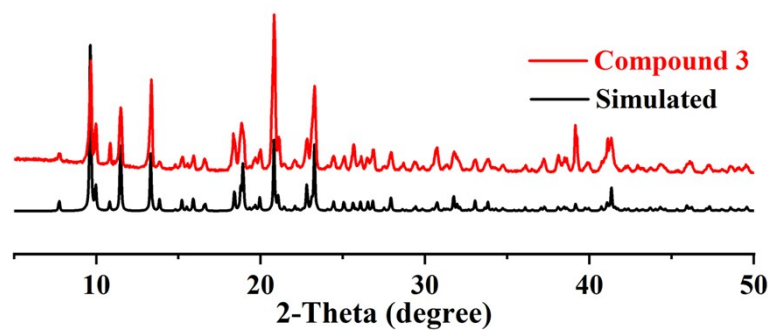
Fig. S2 View of the 3D framework in compound 3.



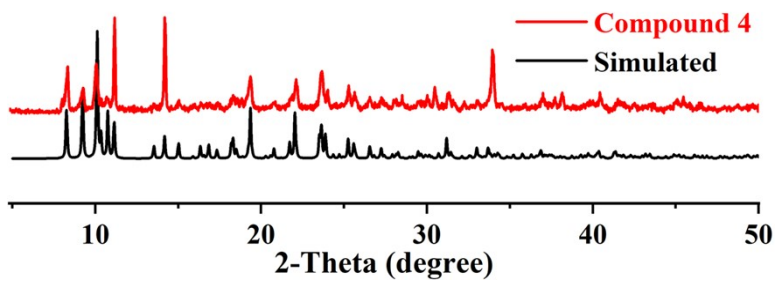
(a)



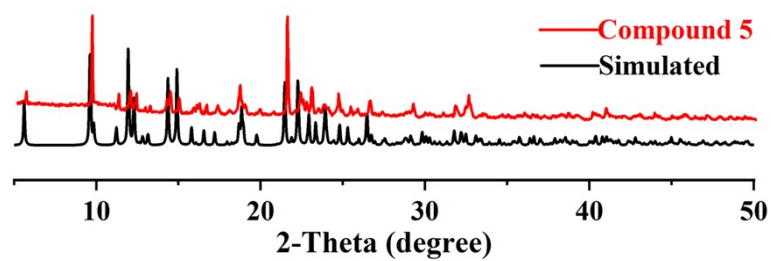
(b)



(c)

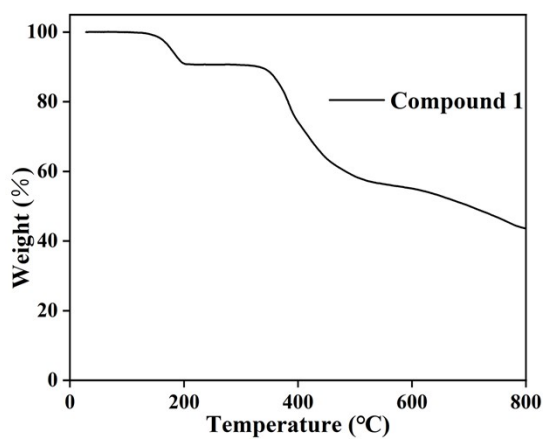


(d)

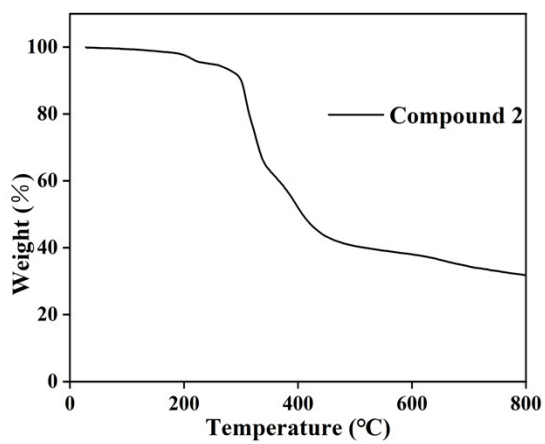


(e)

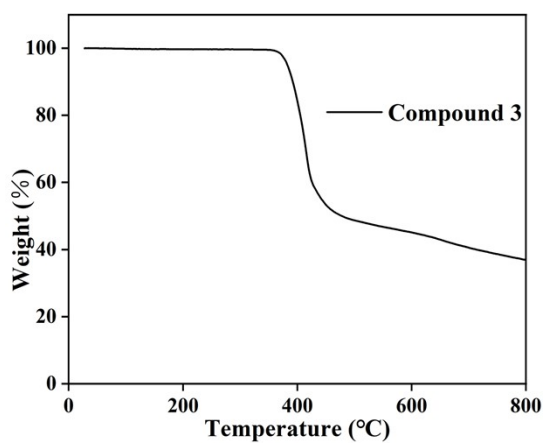
Fig. S3 Simulated PXRD patterns of **1-5** (black) and PXRD patterns of the as-synthesized samples (red).



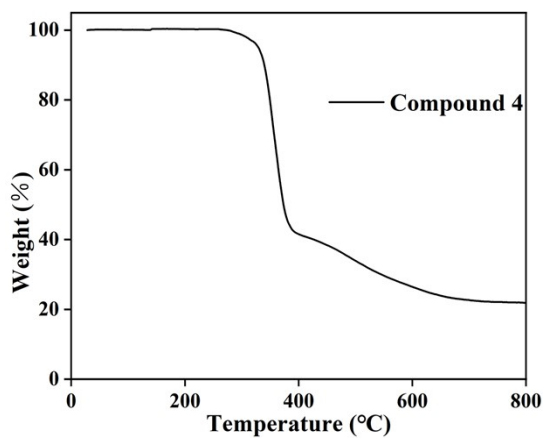
(a)



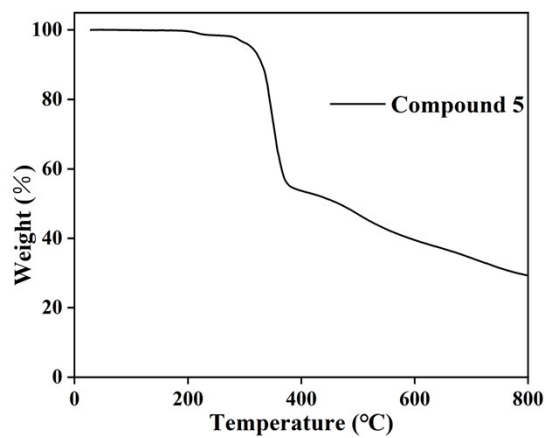
(b)



(c)



(d)



(e)

Fig. S4 TG curves of compounds 1-5.

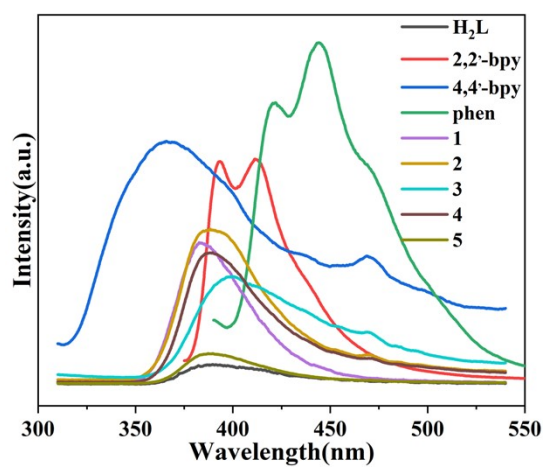
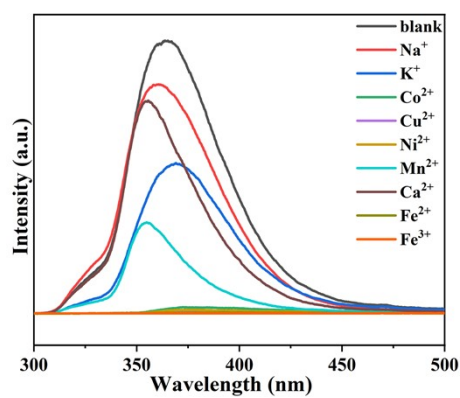
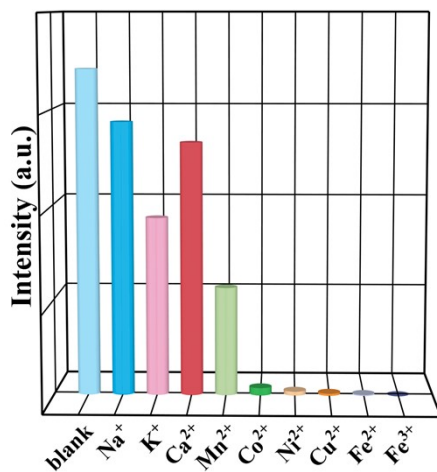


Fig. S5 Solid-state emission spectra at room temperature.

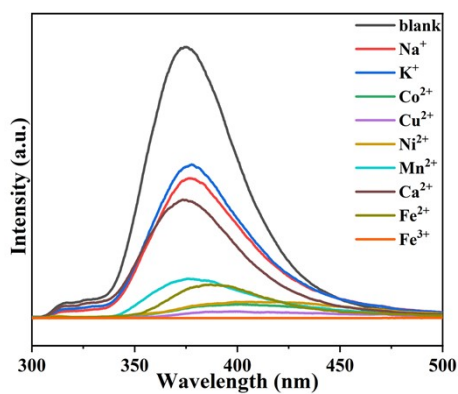


(a)

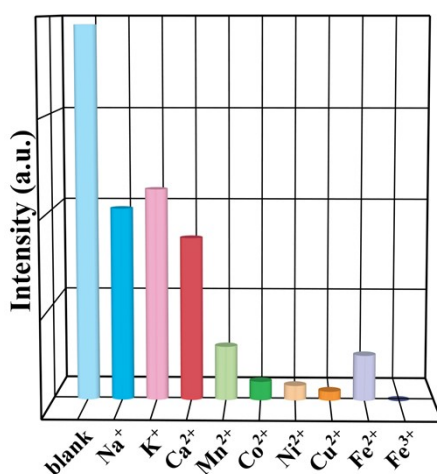


(b)

Fig. S6 Luminescent spectra (a) and intensities (b) for compound **2** treated with 0.01 M different ions.

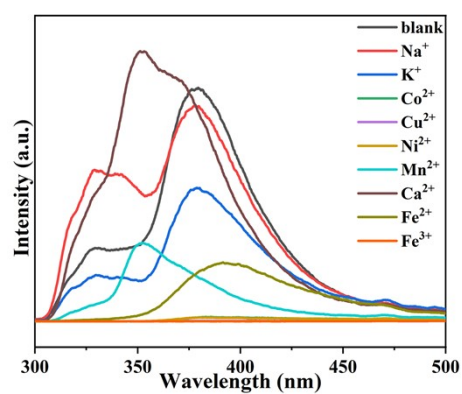


(a)

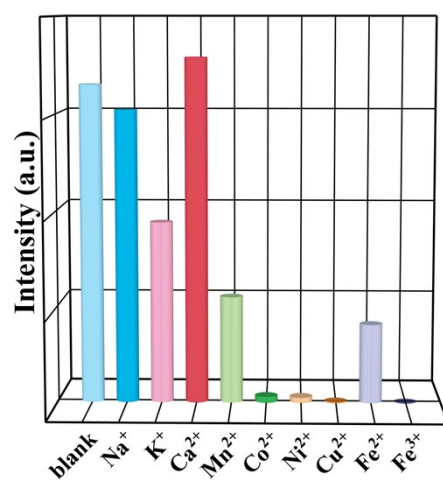


(b)

Fig. S7 Luminescent spectra (a) and intensities (b) for compound **3** treated with 0.01 M different ions.

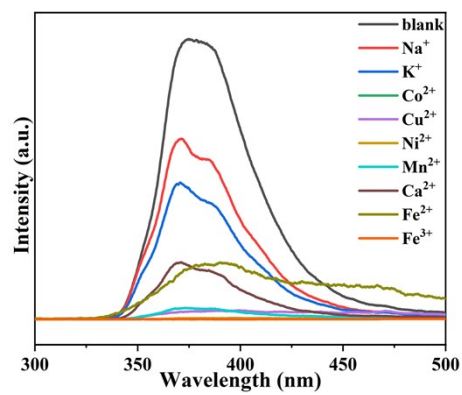


(a)

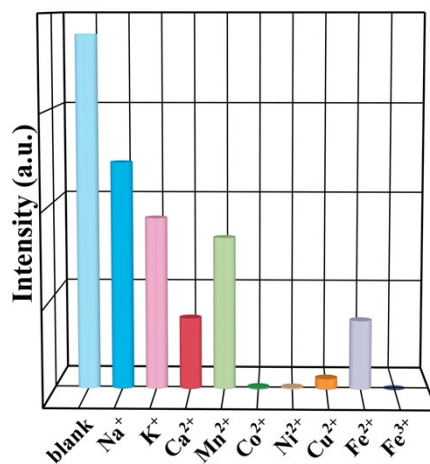


(b)

Fig. S8 Luminescent spectra (a) and intensities (b) for compound **4** treated with 0.01 M different ions.

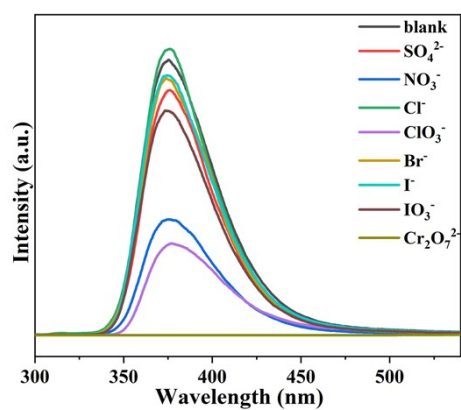


(a)

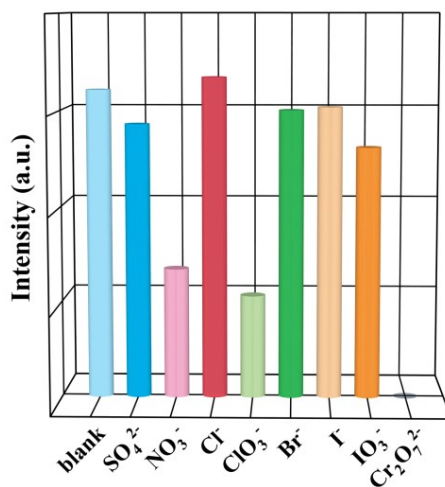


(b)

Fig. S9 Luminescent spectra (a) and intensities (b) for compound **5** treated with 0.01 M different ions.



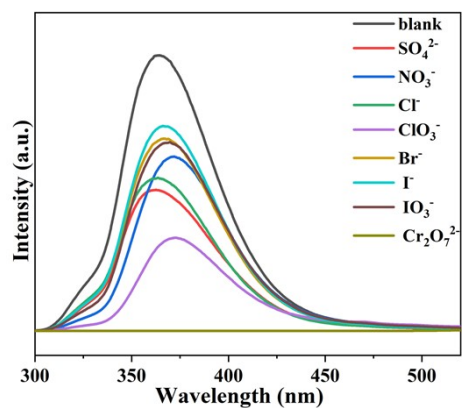
(a)



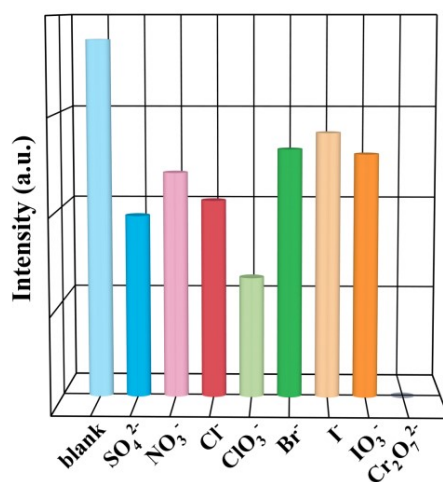
(b)

Fig. S10 Luminescent spectra (a) and intensities (b) for compound **1** treated with 0.01 M different ions.

M different ions.

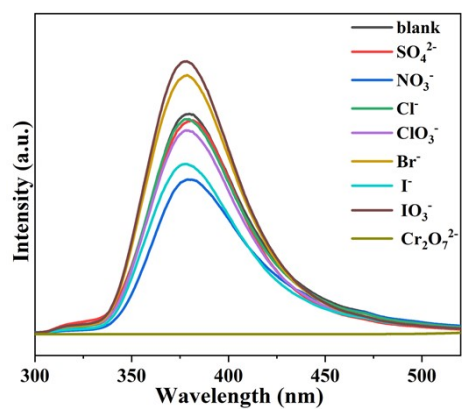


(a)

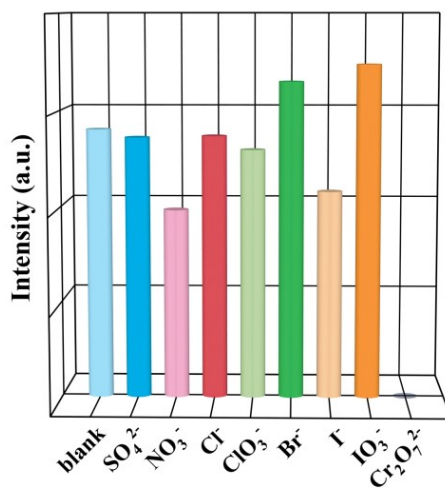


(b)

Fig. S11 Luminescent spectra (a) and intensities (b) for compound **2** treated with 0.01 M different ions.

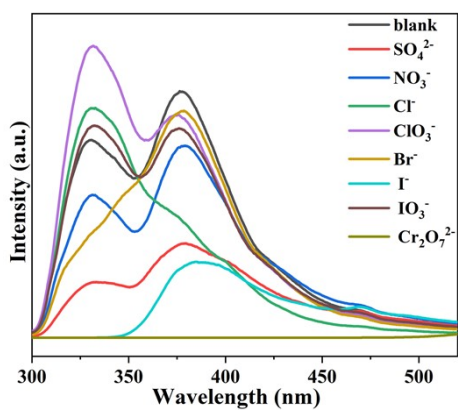


(a)

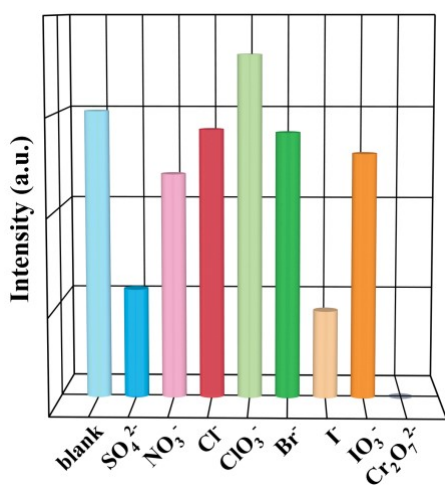


(b)

Fig. S12 Luminescent spectra (a) and intensities (b) for compound **3** treated with 0.01 M different ions.



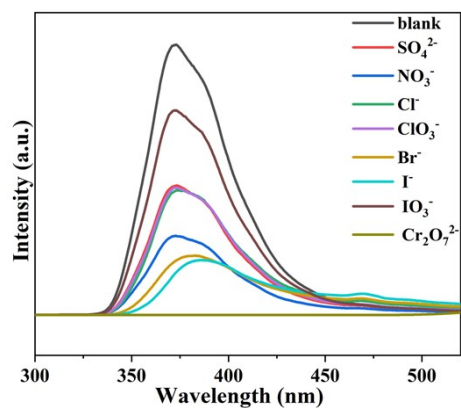
(a)



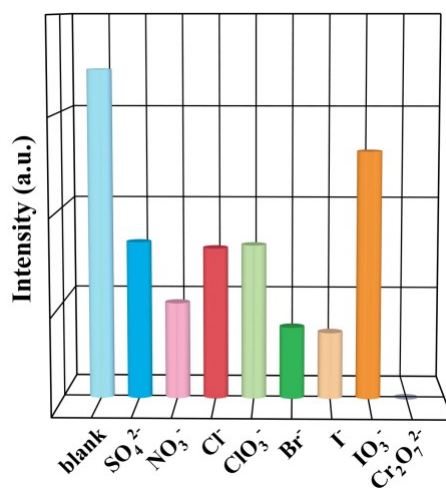
(b)

Fig. S13 Luminescent spectra (a) and intensities (b) for compound **4** treated with 0.01

M different ions.

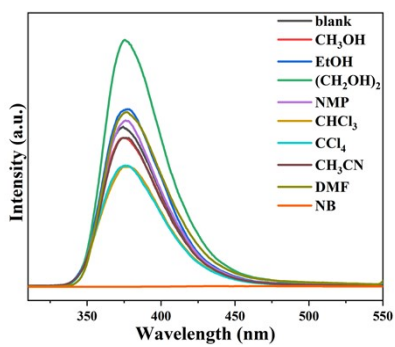


(a)



(b)

Fig. S14 Luminescent spectra (a) and intensities (b) for compound **5** treated with 0.01 M different ions.



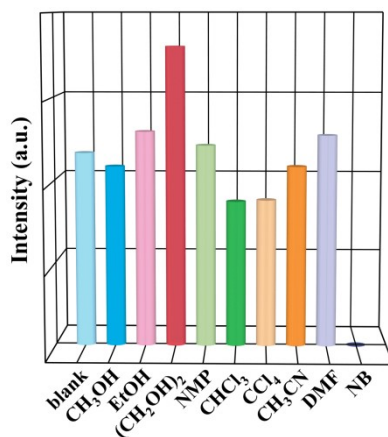
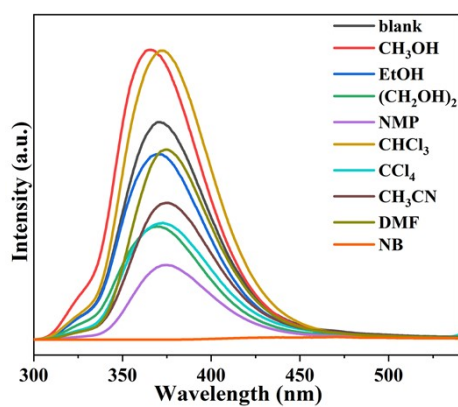
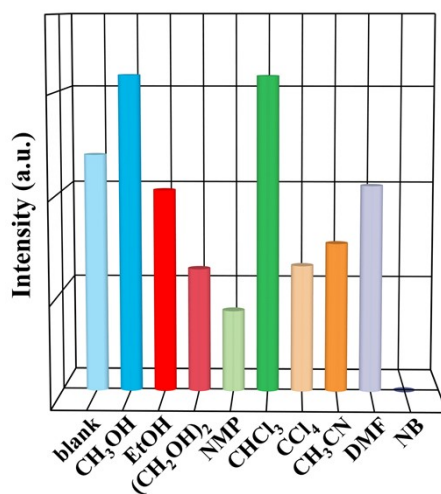


Fig. S15 Luminescent spectra (a) and intensities (b) for compound **1** treated with different organic solvents.

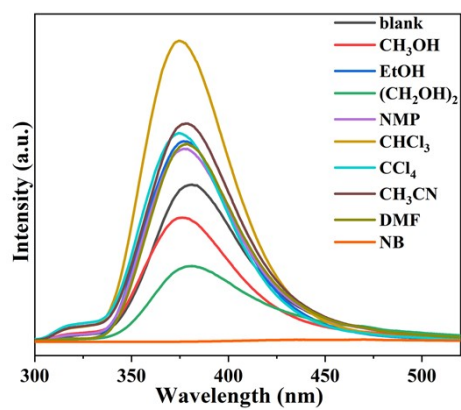


(a)

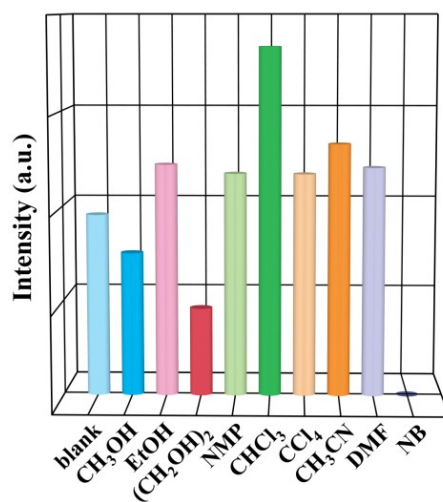


(b)

Fig. S16 Luminescent spectra (a) and intensities (b) for compound **2** treated with different organic solvents.

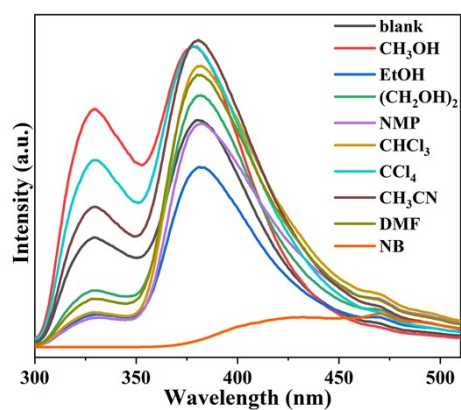


(a)

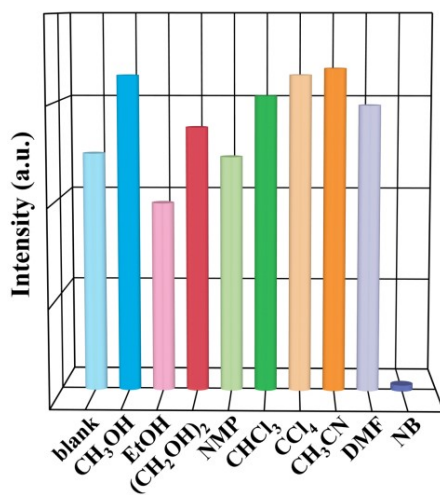


(b)

Fig. S17 Luminescent spectra (a) and intensities (b) for compound **3** treated with different organic solvents.

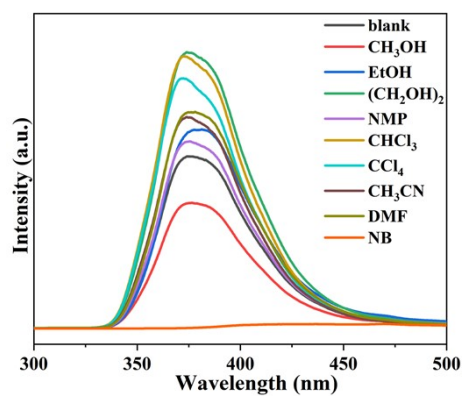


(a)

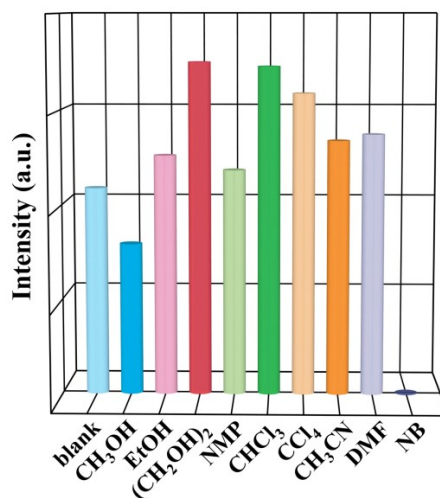


(b)

Fig. S18 Luminescent spectra (a) and intensities (b) for compound **4** treated with different organic solvents.



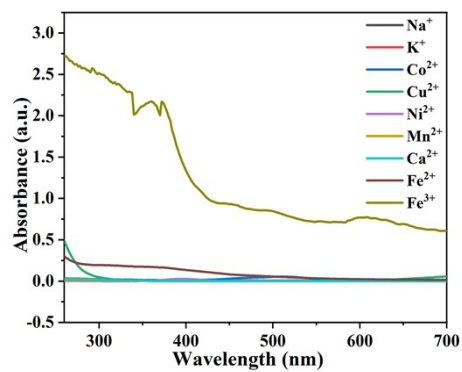
(a)



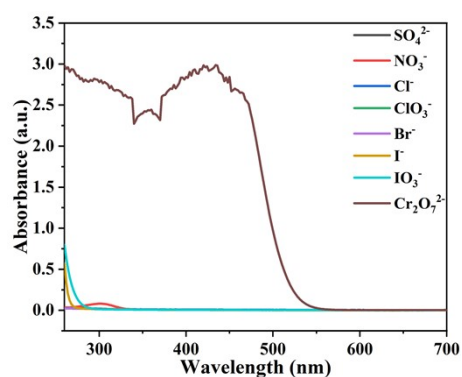
(b)

Fig. S19 Luminescent spectra (a) and intensities (b) for compound **5** treated with

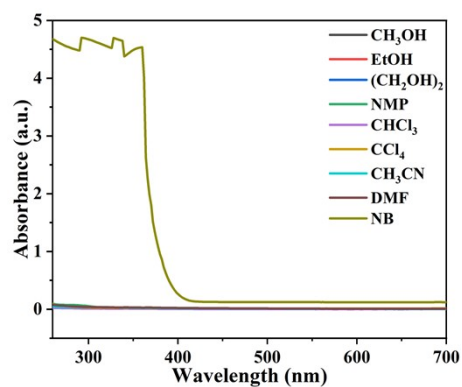
different organic solvents.



(a)



(b)



(c)

Fig. S20 The UV-Vis absorption spectra of cations, anions, and organic small molecules.

Table S1 Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(3)	2.0091(12)	Zn(1)-O(1W)	2.0531(13)
Zn(1)-O(5) ^{#1}	2.0837(12)	Zn(1)-O(1)	2.0924(11)
Zn(1)-O(2W)	2.1676(12)	Zn(1)-O(1) ^{#2}	2.1835(11)
O(3)-Zn(1)-O(1W)	98.93(5)	O(3)-Zn(1)-O(5) ^{#1}	93.57(5)
O(1W)-Zn(1)-O(5) ^{#1}	95.86(5)	O(3)-Zn(1)-O(1)	86.06(5)
O(1W)-Zn(1)-O(1)	174.81(5)	O(5) ^{#1} -Zn(1)-O(1)	85.21(5)
O(3)-Zn(1)-O(2W)	93.11(5)	O(1W)-Zn(1)-O(2W)	92.48(5)
O(5) ^{#1} -Zn(1)-O(2W)	168.38(5)	O(1)-Zn(1)-O(2W)	85.77(4)
O(3)-Zn(1)-O(1) ^{#2}	166.30(5)	O(1W)-Zn(1)-O(1) ^{#2}	94.27(5)
O(5) ^{#1} -Zn(1)-O(1) ^{#2}	88.70(5)	O(1)-Zn(1)-O(1) ^{#2}	80.66(4)
O(2W)-Zn(1)-O(1) ^{#2}	82.61(4)	C(1)-O(1)-Zn(1)	129.23(10)
C(1)-O(1)-Zn(1) ^{#2}	125.80(10)	Zn(1)-O(1)-Zn(1) ^{#2}	99.34(4)
C(3)-O(3)-Zn(1)	125.24(11)	C(14)-O(5)-Zn(1) ^{#1}	126.27(11)

Symmetry transformations used to generate equivalent atoms: ^{#1} -x+1,-y+2,-z+1; ^{#2} -x+1,-y+2,-z+2.

Table S2 Selected bond distances (Å) and angles (°) for **2**.

Zn(1)-O(5)	2.0592(13)	Zn(1)-O(2) ^{#1}	2.0992(13)
Zn(1)-O(3) ^{#1}	2.1002(12)	Zn(1)-N(2)	2.1469(14)
Zn(1)-O(1W)	2.1480(12)	Zn(1)-N(3)	2.1528(14)
O(5)-Zn(1)-O(2) ^{#1}	85.12(5)	O(5)-Zn(1)-O(3) ^{#1}	104.74(6)
O(2) ^{#1} -Zn(1)-O(3) ^{#1}	83.35(5)	O(5)-Zn(1)-N(2)	167.50(6)
O(2) ^{#1} -Zn(1)-N(2)	96.58(5)	O(3) ^{#1} -Zn(1)-N(2)	87.76(5)
O(5)-Zn(1)-O(1W)	85.98(5)	O(2) ^{#1} -Zn(1)-O(1W)	164.39(5)
O(3) ^{#1} -Zn(1)-O(1W)	86.56(5)	N(2)-Zn(1)-O(1W)	94.89(5)
O(5)-Zn(1)-N(3)	91.71(6)	O(2) ^{#1} -Zn(1)-N(3)	89.99(5)
O(3) ^{#1} -Zn(1)-N(3)	161.59(5)	N(2)-Zn(1)-N(3)	75.93(5)
O(1W)-Zn(1)-N(3)	103.07(5)	C(15)-N(2)-Zn(1)	124.95(12)
C(19)-N(2)-Zn(1)	116.09(11)	C(24)-N(3)-Zn(1)	125.46(12)

C(20)-N(3)-Zn(1)	116.07(11)	C(1)-O(2)-Zn(1) ^{#2}	125.13(11)
C(6)-O(3)-Zn(1) ^{#2}	125.89(11)	C(14)-O(5)-Zn(1)	136.29(12)

Symmetry transformations used to generate equivalent atoms: ^{#1} x,y+1,z; ^{#2} x,y-1,z.

Table S3 Hydrogen bonds for **2** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)
C7-H7A···O1	0.97	2.61	3.543	162.7
C15-H15···O3	0.93	2.47	3.016(2)	117.6
O1W- H1A···O4	0.890(9)	1.874(11)	2.7402(17)	164(2)

Symmetry transformations used to generate equivalent atoms: ^{#1} x,y+1,z; ^{#2} x,y-1,z.

Table S4 Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(1)	2.0713(12)	Zn(1)-O(1) ^{#1}	2.0713(12)
Zn(1)-O(3) ^{#1}	2.1075(12)	Zn(1)-O(3)	2.1076(12)
Zn(1)-N(2)	2.1715(14)	Zn(1)-N(2) ^{#1}	2.1715(14)
Zn(2)-O(5) ^{#1}	1.9413(13)	Zn(2)-O(5)	1.9413(13)
Zn(2)-O(2) ^{#2}	1.9667(13)	Zn(2)-O(2) ^{#3}	1.9667(13)
O(1)-Zn(1)-O(1) ^{#1}	173.56(7)	O(1)-Zn(1)-O(3) ^{#1}	89.71(5)
O(1) ^{#1} -Zn(1)-O(3) ^{#1}	85.90(5)	O(1)-Zn(1)-O(3)	85.90(5)
O(1) ^{#1} -Zn(1)-O(3)	89.71(5)	O(3) ^{#1} -Zn(1)-O(3)	93.94(8)
O(1)-Zn(1)-N(2)	91.63(5)	O(1) ^{#1} -Zn(1)-N(2)	93.08(5)
O(3) ^{#1} -Zn(1)-N(2)	175.83(5)	O(3)-Zn(1)-N(2)	90.09(5)
O(1)-Zn(1)-N(2) ^{#1}	93.08(5)	O(1) ^{#1} -Zn(1)-N(2) ^{#1}	91.63(5)
O(3) ^{#1} -Zn(1)-N(2) ^{#1}	90.10(5)	O(3)-Zn(1)-N(2) ^{#1}	175.83(5)
N(2)-Zn(1)-N(2) ^{#1}	85.89(7)	O(5) ^{#1} -Zn(2)-O(5)	98.24(8)
O(5) ^{#1} -Zn(2)-O(2) ^{#2}	116.70(6)	O(5)-Zn(2)-O(2) ^{#2}	115.68(6)
O(5) ^{#1} -Zn(2)-O(2) ^{#3}	115.68(6)	O(5)-Zn(2)-O(2) ^{#3}	116.70(6)
O(2) ^{#2} -Zn(2)-O(2) ^{#3}	95.19(9)	C(15)-N(2)-Zn(1)	121.82(12)

C(19)-N(2)-Zn(1)	120.69(12)	C(1)-O(1)-Zn(1)	129.11(11)
C(1)-O(2)-Zn(2) ^{#5}	121.84(12)	C(3)-O(3)-Zn(1)	128.40(12)
C(14)-O(5)-Zn(2)	113.42(12)		

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

Table S5 Selected bond distances (Å) and angles (°) for **4**.

Cd(1)-O(1)	2.1984(16)	Cd(1)-O(3) ^{#1}	2.3175(15)
Cd(1)-O(3) ^{#2}	2.3254(15)	Cd(1)-O(5) ^{#1}	2.3473(15)
Cd(1)-N(3)	2.3520(18)	Cd(1)-N(2)	2.3635(18)
O(1)-Cd(1)-O(3) ^{#1}	114.17(6)	O(1)-Cd(1)-O(3) ^{#2}	93.98(7)
O(3) ^{#1} -Cd(1)-O(3) ^{#2}	69.52(6)	O(1)-Cd(1)-O(5) ^{#1}	99.21(7)
O(3) ^{#1} -Cd(1)-O(5) ^{#1}	74.65(5)	O(3) ^{#2} -Cd(1)-O(5) ^{#1}	144.14(5)
O(1)-Cd(1)-N(3)	156.02(7)	O(3) ^{#1} -Cd(1)-N(3)	89.76(6)
O(3) ^{#2} -Cd(1)-N(3)	96.08(6)	O(5) ^{#1} -Cd(1)-N(3)	85.12(6)
O(1)-Cd(1)-N(2)	86.60(6)	O(3) ^{#1} -Cd(1)-N(2)	154.78(6)
O(3) ^{#2} -Cd(1)-N(2)	125.64(6)	O(5) ^{#1} -Cd(1)-N(2)	88.51(6)
N(3)-Cd(1)-N(2)	69.86(6)	C(15)-N(2)-Cd(1)	123.57(16)
C(19)-N(2)-Cd(1)	117.67(14)	C(24)-N(3)-Cd(1)	122.77(15)
C(20)-N(3)-Cd(1)	118.29(14)	C(1)-O(1)-Cd(1)	131.07(15)
C(14)-O(3)-Cd(1) ^{#3}	139.00(14)	C(14)-O(3)-Cd(1) ^{#2}	108.41(13)
Cd(1) ^{#3} -O(3)-Cd(1) ^{#2}	110.48(6)	C(13)-O(5)-Cd(1) ^{#3}	133.59(14)

Symmetry transformations used to generate equivalent atoms: ^{#1} x-1,y,z; ^{#2} -x+1,-y+1,-z+1; ^{#3} x+1,y,z.

Table S6 Hydrogen bonds for **4** (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
C8-H8B...O2	0.970	2.399	3.298	153.82
C9-H9...O2	0.930	2.423	3.281	153.35

C15-H15 \cdots O1	0.930	2.565	3.164	122.54
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Symmetry transformations used to generate equivalent atoms: ^{#1} x-1,y,z; ^{#2} -x+1,-y+1,-z+1; ^{#3} x+1,y,z.

Table S7 Selected bond distances (Å) and angles (°) for **5**.

Cd(1)-O(1)	2.2210(13)	Cd(1)-O(5) ^{#1}	2.2748(12)
Cd(1)-O(3)	2.2818(12)	Cd(1)-O(1W)	2.3096(13)
Cd(1)-N(3)	2.3579(14)	Cd(1)-N(2)	2.3582(14)
O(1)-Cd(1)-O(5) ^{#1}	83.56(5)	O(1)-Cd(1)-O(3)	78.21(5)
O(5) ^{#1} -Cd(1)-O(3)	122.21(5)	O(1)-Cd(1)-O(1W)	146.06(5)
O(5) ^{#1} -Cd(1)-O(1W)	81.03(5)	O(3)-Cd(1)-O(1W)	84.78(5)
O(1)-Cd(1)-N(3)	96.43(5)	O(5) ^{#1} -Cd(1)-N(3)	82.43(5)
O(3)-Cd(1)-N(3)	153.34(5)	O(1W)-Cd(1)-N(3)	111.17(5)
O(1)-Cd(1)-N(2)	107.83(5)	O(5) ^{#1} -Cd(1)-N(2)	151.56(5)
O(3)-Cd(1)-N(2)	86.02(5)	O(1W)-Cd(1)-N(2)	99.94(5)
N(3)-Cd(1)-N(2)	70.64(5)	C(15)-N(2)-Cd(1)	125.18(12)
C(19)-N(2)-Cd(1)	116.12(11)	C(26)-N(3)-Cd(1)	125.08(12)
C(23)-N(3)-Cd(1)	116.51(11)	C(1)-O(1)-Cd(1)	137.32(11)
C(6)-O(3)-Cd(1)	130.04(11)	C(14)-O(5)-Cd(1) ^{#2}	124.80(11)
Cd(1)-O(1W)-H(1A)	121.3(15)	Cd(1)-O(1W)-H(1B)	100.6(16)

Symmetry transformations used to generate equivalent atoms: ^{#1} x,-y+1,z+1/2; ^{#2} x,-y+1,z-1/2.

Table S8 Hydrogen bonds for **5** (Å and °).

D-H \cdots A	d(D-H)	d(H \cdots A)	d(D \cdots A)	\angle (DHA)
C5-H5 \cdots O4	0.92	2.65	3.269(2)	124.9
C7-H7B \cdots O2	0.97	2.49	3.428(2)	165.4

Symmetry transformations used to generate equivalent atoms: ^{#1} x,-y+1,z+1/2; ^{#2} x,-y+1,z-1/2.

