Three Types of Lanthanide Coordination Polymers from 1D-3D Based on a Tetracarboxylate Ligand: Synthesis, Structural Diversities and Properties

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Supporting Information

Table S1 Selected bond distances (Å) and angles (°) for **3**

Tm(1)-O(2)	2.180(4)	Tm(1)-O(6)#4	2.227(4)
Tm(1)-O(1)#1	2.268(4)	Tm(1)-O(5)#3	2.276(4)
Tm(1)-O(3)#2	2.282(4)	Tm(1)-O(9)	2.287(5)
Tm(1)-O(10)	2.415(4)	O(3)#2-Tm(1)-O(9)	143.51(15)
O(2)-Tm(1)-O(6)#4	171.94(14)	O(2)-Tm(1)-O(10)	94.10(14)
O(2)-Tm(1)-O(1)#1	89.35(15)	O(6)#4-Tm(1)-O(10)	77.87(15)
O(6)#4-Tm(1)-O(1)#1	97.10(15)	O(1)#1-Tm(1)-O(10)	147.73(14)
O(2)-Tm(1)-O(5)#3	89.68(14)	O(5)#3-Tm(1)-O(10)	72.96(14)
O(6)#4-Tm(1)-O(5)#3	88.57(15)	O(3)#2-Tm(1)-O(10)	74.29(14)
O(1)#1-Tm(1)-O(5)#3	139.22(14)	O(10)-Tm(1)-O(9)	141.77(15)
O(2)-Tm(1)-O(3)#2	85.12(15)	O(5)#3-Tm(1)-O(9)	70.01(15)
O(6)#4-Tm(1)-O(3)#2	91.99(15)	O(1)#1-Tm(1)-O(9)	69.46(15)
O(1)#1-Tm(1)-O(3)#2	74.05(14)	O(6)#4-Tm(1)-O(9)	91.9(2)
O(5)#3-Tm(1)-O(3)#2	146.35(14)	O(2)-Tm(1)-O(9)	94.9(2)

Symmetry transformations used to generate equivalent atoms:

#1 1+x, +y, +z; #2 2-x, 1-y, 1-z; #3 1/2+x, 1/2-y, -1/2+z;
#4 3/2+x, 1/2-y, -1/2+z; #5 -1+x, +y, +z #6 -1/2+x, 1/2-y, 1/2+z;
#7 -3/2+x, 1/2-y, 1/2+z

Table S2 Selected bond distances (Å) and angles (°) for **4**

Gd(1)-O(1)	2.305(2)	Gd(1)-O(10)	2.380(3)
Gd(1)-O(11)	2.354(2)	Gd(1)-O(4)#3	2.430(2)
Gd(1)-O(2)#1	2.355(2)	Gd(1)-O(3)#3	2.449(2)
Gd(1)-O(7)#2	2.377(2)	Gd(1)-O(9)	2.513(2)
O(1)-Gd(1)-O(11)	156.63(9)	O(1)-Gd(1)-O(2)#1	96.71(8)
O(11)-Gd(1)-O(2)#1	73.99(9)	O(1)-Gd(1)-O(7)#2	95.70(9)
O(11)-Gd(1)-O(7)#2	79.07(9)	O(2)#1-Gd(1)-O(7)#2	138.40(8)
O(1)-Gd(1)-O(10)	76.58(9)	O(11)-Gd(1)-O(10)	118.35(9)
O(2)#1-Gd(1)-O(10)	70.52(9)	O(7)#2-Gd(1)-O(10)	151.07(8)
O(1)-Gd(1)-O(4)#3	75.65(8)	O(11)-Gd(1)-O(4)#3	123.54(8)
O(2)#1-Gd(1)-O(4)#3	147.28(9)	O(7)#2-Gd(1)-O(4)#3	74.31(8)
O(10)-Gd(1)-O(4)#3	76.77(9)	O(1)-Gd(1)-O(3)#3	127.52(8)
O(11)-Gd(1)-O(3)#3	74.99(8)	O(2)#1-Gd(1)-O(3)#3	117.64(8)
O(7)#2-Gd(1)-O(3)#3	84.14(8)	O(10)-Gd(1)-O(3)#3	79.16(9)
O(4)#3-Gd(1)-O(3)#3	53.71(8)	O(1)-Gd(1)-O(9)	73.30(8)
O(11)-Gd(1)-O(9)	83.45(8)	O(2)#1-Gd(1)-O(9)	73.39(9)
O(7)#2-Gd(1)-O(9)	72.55(8)	O(10)-Gd(1)-O(9)	129.09(8)
O(4)#3-Gd(1)-O(9)	131.31(8)	O(3)#3-Gd(1)-O(9)	150.86(8)

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

Table S3 Selected bond distances (Å) and angles (°) for **5**

Er(1)-O(10)	2.462(5)	Er(1)-O(1)	2.402(5)
Er(1)-O(5)#1	2.326(5)	Er(1)-O(8)#3	2.295(6)
Er(1)-O(2)	2.395(5)	Er(1)-O(9)	2.336(5)
Er(1)-O(7)#2	2.275(5)	Er(1)-O(11)	2.312(5)
O(1)-Er(1)-O(10)	149.43(17)	O(5)#1-Er(1)-O(10)	72.14(18)
O(5)#1-Er(1)-O(1)	84.32(17)	O(5)#1-Er(1)-O(2)	74.89(18)
O(5)#1-Er(1)-O(9)	150.59(19)	O(8)#3-Er(1)-O(10)	73.64(18)
O(8)#3-Er(1)-O(1)	116.39(17)	O(8)#3-Er(1)-O(5)#1	138.34(18)
O(8)#3-Er(1)-O(2)	146.76(18)	O(8)#3-Er(1)-O(9)	71.04(19)
O(8)#3-Er(1)-O(11)	73.33(19)	O(2)-Er(1)-O(10)	131.85(18)
O(2)-Er(1)-O(1)	55.12(17)	O(9)-Er(1)-O(10)	131.15(17)
O(9)-Er(1)-O(1)	78.00(18)	O(9)-Er(1)-O(2)	75.72(19)
O(7)#2-Er(1)-O(10)	74.58(17)	O(7)#2-Er(1)-O(1)	128.52(18)
O(7)#2-Er(1)-O(5)#1	96.28(17)	O(7)#2-Er(1)-O(8)#3	96.85(18)
O(7)#2-Er(1)-O(2)	75.26(18)	O(7)#2-Er(1)-O(9)	77.30(17)
O(7)#2-Er(1)-O(11)	156.48(18)	O(11)-Er(1)-O(10)	82.09(17)
O(11)-Er(1)-O(1)	74.35(18)	O(11)-Er(1)-O(5)#1	79.07(18)
O(11)-Er(1)-O(2)	124.46(18)	O(11)-Er(1)-O(9)	117.57(18)

Symmetry transformations used to generate equivalent atoms:

#1 1−x, 1−y, 1−z; #2 1+x, +y, 1+z; #3 1−x, −y, 1−z; #4 −1+x, +y, −1+z

Table S4 Selected bond distances (Å) and angles (°) for **6**

Tm(1)-O(7)#2	2.261(2)	Tm(1)-O(11)	2.296(2)
Tm(1)-O(8)#3	2.295(2)	Tm(1)-O(9)	2.312(3)
Tm(1)-O(5)#1	2.319(2)	Tm(1)-O(2)	2.373(2)
Tm(1)-O(1)	2.403(2)	Tm(1)-O(10)	2.446(2)
O(7)#2-Tm(1)-O(8)#3	95.76(8)	O(7)#2-Tm(1)-O(11)	155.81(8)
O(8)#3-Tm(1)-O(10)	73.56(9)	O(7)#2-Tm(1)-O(5)#1	96.95(8)
O(8)#3-Tm(1)-O(5)#1	138.79(8)	O(9)-Tm(1)-O(1)	78.94(9)
O(7)#2-Tm(1)-O(9)	76.74(9)	O(8)#3-Tm(1)-O(9)	70.66(9)
O(11)-Tm(1)-O(9)	118.09(9)	O(9)-Tm(1)-O(5)#1	150.54(9)
O(7)#2-Tm(1)-O(2)	75.84(8)	O(8)#3-Tm(1)-O(2)	146.50(8)
O(11)-Tm(1)-O(2)	124.67(8)	O(5)#1-Tm(1)-O(2)	74.71(8)
O(9)-Tm(1)-O(2)	75.85(9)	O(7)#2-Tm(1)-O(1)	129.00(8)
O(8)#3-Tm(1)-O(1)	117.11(8)	O(11)-Tm(1)-O(1)	74.58(8)
O(5)#1-Tm(1)-O(1)	83.42(8)	O(11)-Tm(1)-O(5)#1	78.87(8)
O(2) -Tm(1)-O(1)	54.94(7)	O(7)#2-Tm(1)-O(10)	74.20(8)
O(8)#3-Tm(1)-O(11)	73.74(8)	O(11)-Tm(1)-O(10)	81.88(8)
O(5)#1-Tm(1)-O(10)	72.57(9)	O(10)-Tm(1)-O(9)	130.62(9)
O(2) -Tm(1)-O(10)	131.87(8)	O(1) -Tm(1)-O(10)	149.15(8)

Symmetry transformations used to generate equivalent atoms:

#1 2-x, -y, 2-z; #2 -1+x, +y, -1+z; #3 2-x, 1-y, 2-z; #4 1+x, +y, 1+z

Table S5 Selected bond distances (Å) and angles (°) for **7**

Gd(1)-O(5)#3	2.286(7)	Gd(1)-O(9)	2.425(9)
Gd(1)-O(5)#2	2.286(7)	Gd(1)-O(2)#1	2.480(7)
Gd(1)-O(1)#1	2.419(12)	Gd(1)-O(2)	2.480(7)
Gd(1)-O(1)	2.419(12)	O(1)#1-Gd(1)-O(9)	125.7(4)
O(5)#3-Gd(1)-O(5)#2	89.8(4)	O(1)-Gd(1)-O(9)	125.7(4)
O(5)#2-Gd(1)-O(1)#1	156.1(4)	O(5)#2-Gd(1)-O(2)#1	151.8(3)
O(5)#3-Gd(1)-O(1)#1	95.6(5)	O(5)#3-Gd(1)-O(2)#1	79.9(3)
O(5)#2-Gd(1)-O(1)	95.6(5)	O(1)#1-Gd(1)-O(2)#1	52.0(3)
O(5)#3-Gd(1)-O(1)	156.1(4)	O(1)-Gd(1)-O(2)#1	104.5(5)
O(1)#1-Gd(1)-O(1)	70.7(8)	O(9)-Gd(1)-O(2)	74.0(2)
O(5)#2-Gd(1)-O(9)	78.2(3)	O(5)#2-Gd(1)-O(2)	79.9(3)
O(5)#3-Gd(1)-O(9)	78.2(3)	O(5)#3-Gd(1)-O(2)	151.8(3)
O(1)#1-Gd(1)-O(2)	104.5(5)	O(2)#1-Gd(1)-O(2)	96.9(3)

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

Table S6 Selected bond distances (Å) and angles (°) for **8**

Dy(1)-O(1)	2.258(5)	Dy(1)-O(1)#1	2.258(5)
Dy(1)-O(5)#3	2.400(9)	Dy(1)-O(5)#2	2.400(9)
Dy(1)-O(9)	2.412(7)	Dy(1)-O(6)#3	2.452(5)
Dy(1)-O(6)#2	2.452(5)	O(1)-Dy(1)-O(1)#1	90.4(3)
O(1)#1-Dy(1)-O(5)#2	155.3(3)	O(1) -Dy(1)-O(5)#2	94.1(4)
O(1)#1-Dy(1)-O(5)#3	94.1(4)	O(1) -Dy(1)-O(5)#3	155.3(3)
O(5)#2-Dy(1)-O(5)#3	72.3(6)	O(1)-Dy(1)-O(9)	78.1(2)
O(1)#1-Dy(1)-O(9)	78.1(2)	O(5)#2-Dy(1)-O(9)	126.6(3)
O(5)#3-Dy(1)-O(9)	126.6(3)	O(1)#1-Dy(1)-O(6)#3	79.62(19)
O(1) -Dy(1)-O(6)#3	151.7(2)	O(5)#2-Dy(1)-O(6)#3	106.0(4)
O(5)#2-Dy(1)-O(6)#2	52.8(3)	O(9)-Dy(1)-O(6)#2	73.91(17)
O(1)#1-Dy(1)-O(6)#2	151.7(2)	O(1)-Dy(1)-O(6)#2	79.62(19)
O(5)#3-Dy(1)-O(6)#2	106.0(4)	O(6)#2-Dy(1)-O(6)#3	96.7(3)
O(9)-Dy(1)-O(6)#3	73.91(17)		

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

Table S7 Selected bond distances (Å) and angles (°) for **9**

Er(1)-O(1)#1	2.234(6)	Er(1)-O(1)	2.234(6)
Er(1)-O(5)#2	2.370(10)	Er(1)-O(5)#3	2.370(10)
Er(1)-O(9)	2.385(8)	Er(1)-O(6)#3	2.421(6)
Er(1)-O(6)#2	2.421(6)	O(1)#1-Er(1)-O(1)	90.8(3)
O(1)#1-Er(1)-O(5)#3	155.0(3)	O(1)-Er(1)-O(5)#3	94.6(4)
O(1)#1-Er(1)-O(5)#2	94.6(4)	O(1)-Er(1)-O(5)#2	155.0(3)
O(5)#3-Er(1)-O(5)#2	70.9(7)	O(1)#1-Er(1)-O(9)	78.3(2)
O(1)-Er(1)-O(9)	78.3(2)	O(5)#3-Er(1)-O(9)	126.7(3)
O(5)#2-Er(1)-O(9)	126.7(3)	O(1)#1-Er(1)-O(6)#3	151.9(2)
O(1)-Er(1)-O(6)#3	79.6 (2)	O(5)#3-Er(1)-O(6)#3	53.0(3)
O(5)#2-Er(1)-O(6)#3	105.2(5)	O(9)-Er(1)-O(6)#3	73.92(19)
O(1)#1-Er(1)-O(6)#2	79.6 (2)	O(1)-Er(1)-O(6)#2	151.9(2)
O(5)#3-Er(1)-O(6)#2	105.2(5)	O(5)#2-Er(1)-O(6)#2	53.0(3)
O(9)-Er(1)-O(6)#2	73.92(19)	O(6)#3-Er(1)-O(6)#2	96.5(3)

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

Table S8 Selected bond distances (Å) and angles (°) for **10**

Tm(1)-O(5)#2	2.228(6)	Tm(1)-O(5)#3	2.228(6)
Tm(1)-O(1)	2.355(11)	Tm(1)-O(1)#1	2.355(11)
Tm(1)-O(9)	2.364(8)	Tm(1)-O(2)	2.424(6)
Tm(1)-O(2)#1	2.424(6)	O(5)#2-Tm(1)-O(5)#3	90.4(3)
O(5)#2-Tm(1)-O(1)	154.9(3)	O(5)#3-Tm(1)-O(1)	94.9(5)
O(5)#2-Tm(1)-O(1)#1	94.9(5)	O(5)#3-Tm(1)-O(1)#1	154.9(3)
O(1)-Tm(1)-O(1)#1	70.6(7)	O(5)#3-Tm(1)-O(9)	78.4(2)
O(5)#2-Tm(1)-O(9)	78.4(2)	O(1)-Tm(1)-O(9)	126.7(3)
O(1)#1-Tm(1)-O(9)	126.7(3)	O(5)#2-Tm(1)-O(2)	152.0(2)
O(5)#3-Tm(1)-O(2)	80.0(2)	O(1)-Tm(1)-O(2)	52.9(3)
O(2)#1-Tm(1)-O(1)	105.0(5)	O(9)-Tm(1)-O(2)	74.0(2)
O(5)#2-Tm(1)-O(2)#1	80.0(2)	O(5)#2-Tm(1)-O(2)	152.0(2)
O(2)-Tm(1)-O(1)#1	105.0(5)	O(1)#1-Tm(1)-O(2)#1	52.9(3)
O(9)-Tm(1)-O(2)#1	74.0(2)	O(2)-Tm(1)-O(2)#1	96.3(3)

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

Table S9 Comparision of Ln–O bond lengths in **3– 10**.

Compounds	The range of Ln–O bond lengths / Å	Average Ln–O bond lengths / Å
3 (Tm^{III})	2.180(4)-2.415(4)	2.276
4 (Gd^{III})	2.305(2)-2.513(2)	2.395
5 (Er^{III})	2.275(5)-2.462(5)	2.350
6 (Tm^{III})	2.261(2)-2.446(2)	2.338
7 (Gd^{III})	2.286(7)- 2.480(7)	2.399
8 (Dy^{III})	2.258(5)-2.452(5)	2.376
9 (Er^{III})	2.234(6)-2.421(6)	2.348
10 (Tm^{III})	2.228(6)-2.424(6)	2.340

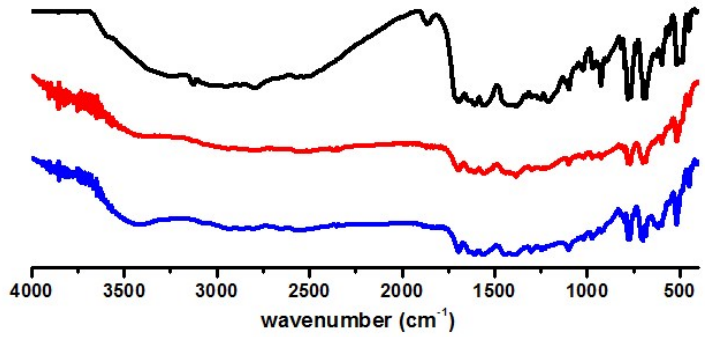

Fig. S1 IR spectra of **1-3**. Black: **1** Red: **2** Blue: **3**

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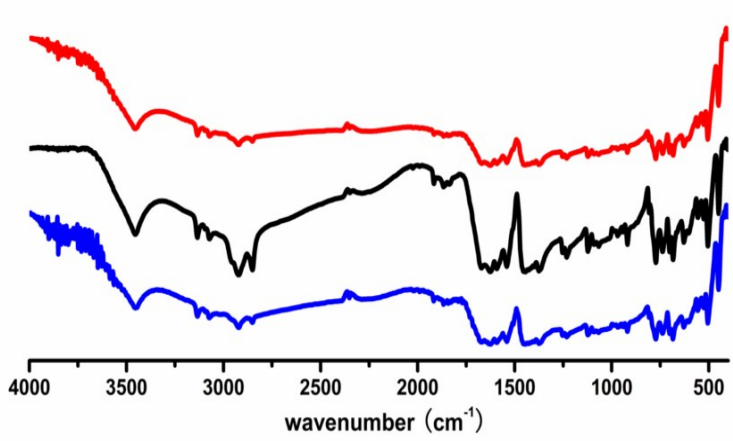

Fig. S2 IR spectra of **4-6**. Red: **4** Black: **5** Blue: **6**.

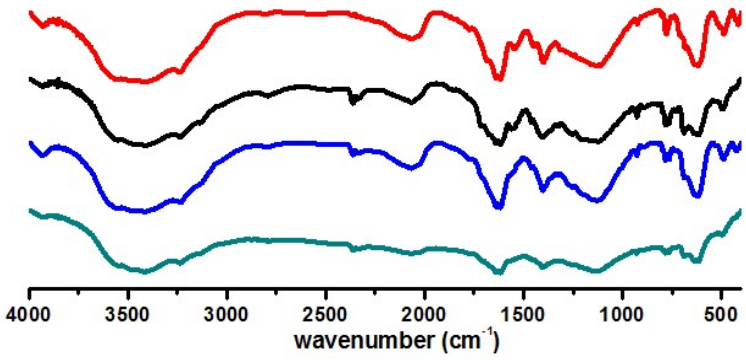

Fig. S3 IR spectra of **7-10**. Red: **7** Black: **8** Blue: **9** Green **10**.

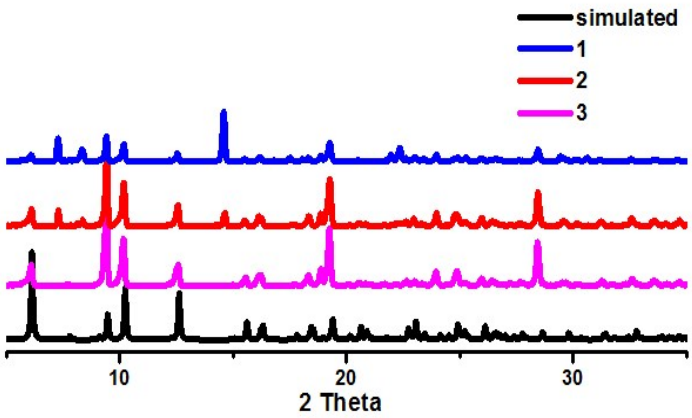

Fig. S4 Experimental and calculated powder X-ray diffraction (PXRD) patterns for **1-3**.

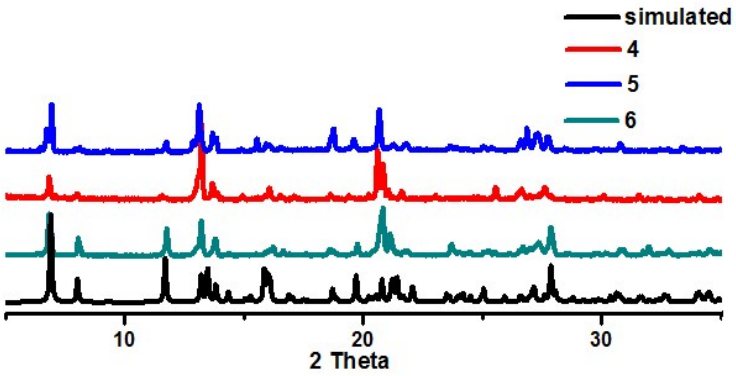

Fig. S5 Experimental and calculated powder X-ray diffraction (PXRD) patterns for **4-6**.

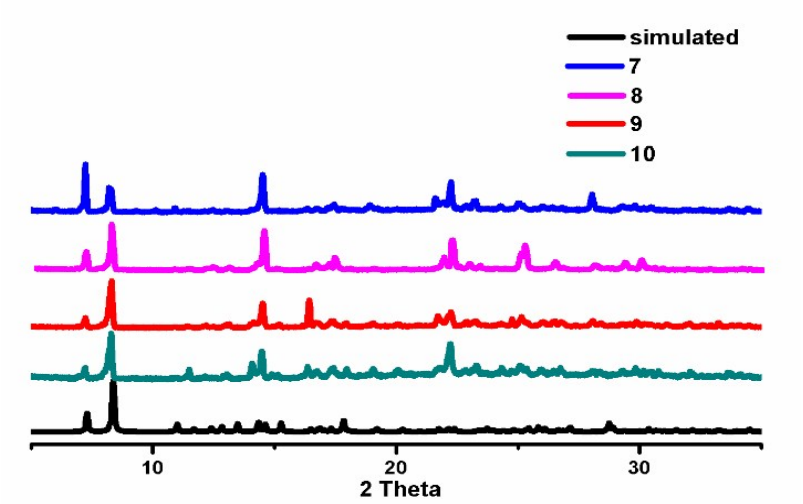

Fig. S6 Experimental and calculated powder X-ray diffraction (PXRD) patterns for **7-10**.

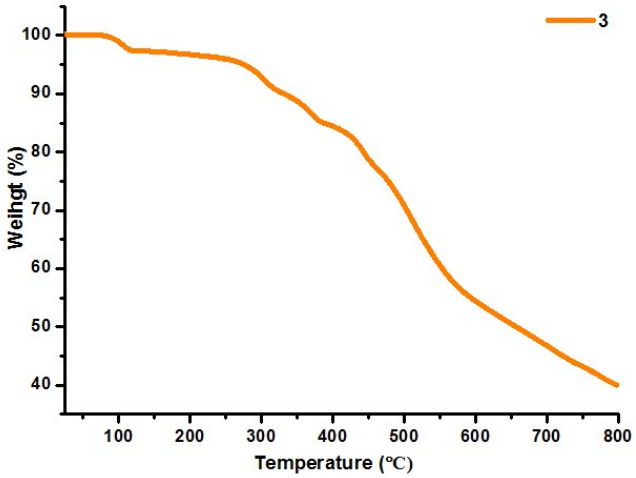

Fig. S7 TGA curves for complex **3**.

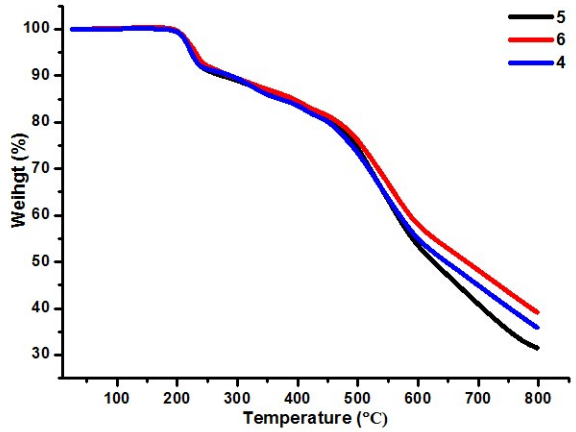

Fig. S8 TGA curves for complexes **4-6**.

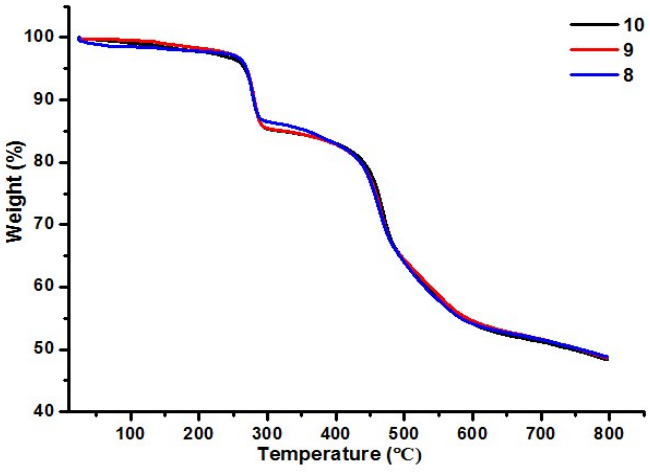

Fig. S9 TGA curves for complexes **8-10**.

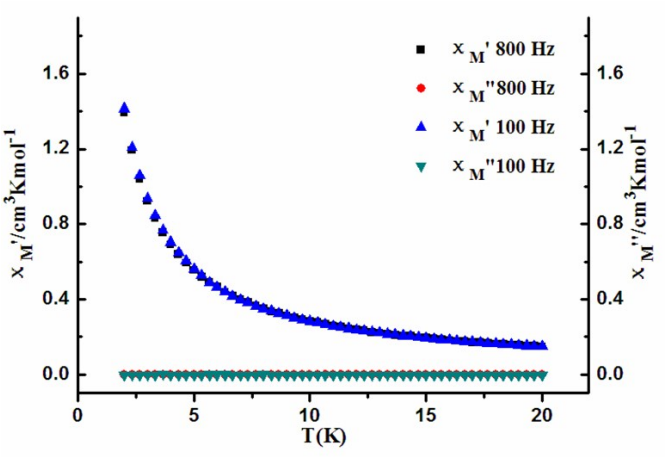

Fig. S10 The temperature dependence of the alternating-current (ac) magnetic susceptibilities for **8** were collected at zero direct-current (dc) fields.

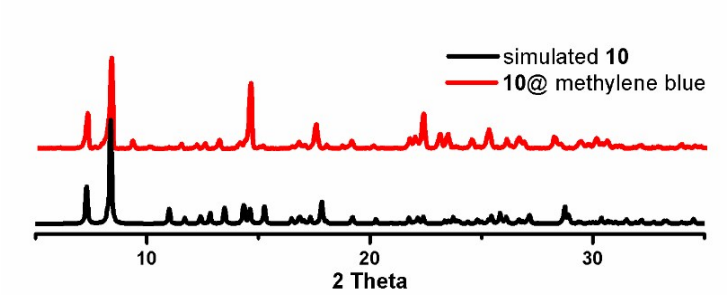

Fig. S11 PXRD data for **10**@ methylene blue.

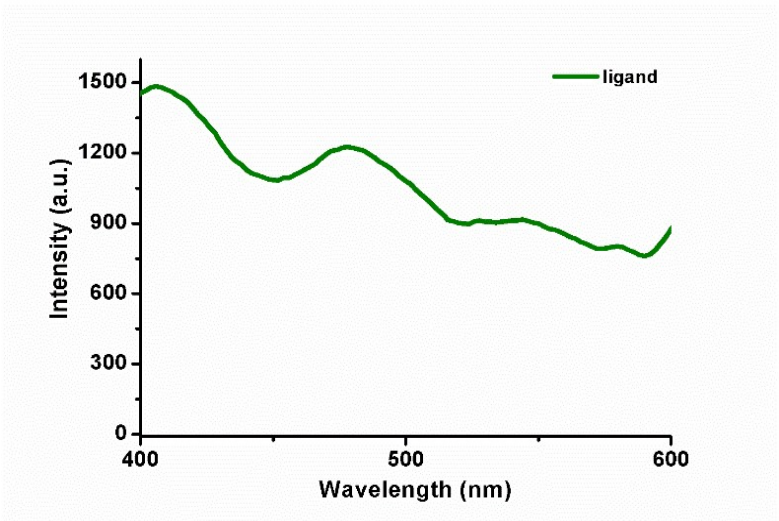

Fig. S12 Solid-state emission spectra of the ligand at room temperature.

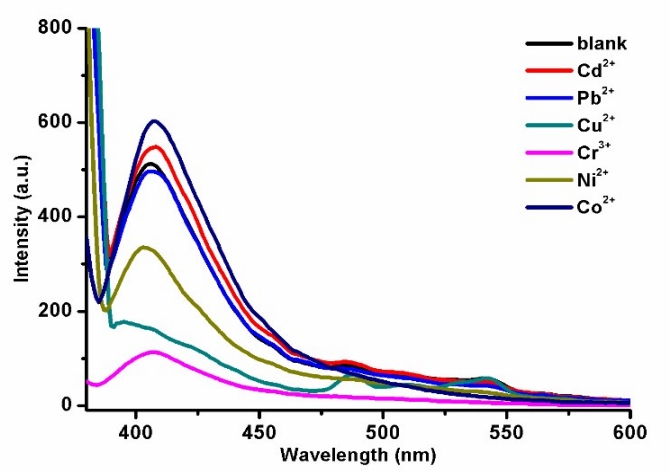

Fig. S13 The emission spectra of ligand in 10^{-2} M DMA solutions of $M(NO_3)_x$ (M= Cd^{2+}, Pb^{2+}, Co^{2+}, Cu^{2+}, Ni^{2+}, Cr^{3+}).

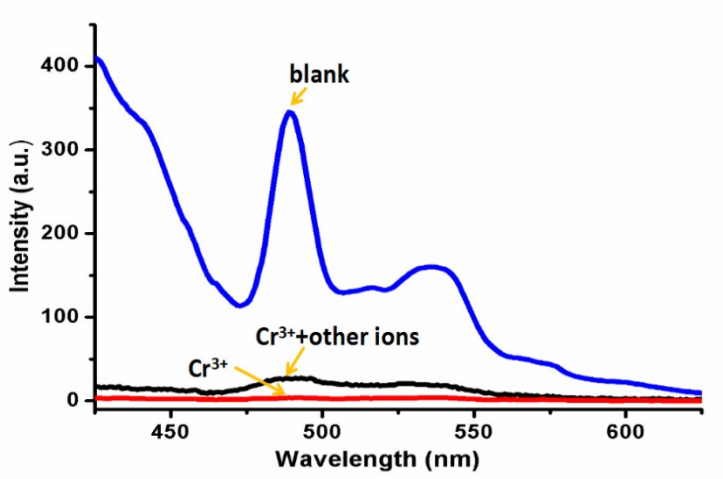

Fig. S14 Competitive tests for the fluorescence responses of **8** to various metal ions.