

*Electronic Supplementary Information (ESI) for*

# **3D Ln-MOFs as multi-responsive luminescent probe for efficient sensing of Fe<sup>3+</sup>, Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>, and antibiotics in aqueous solution**

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## 1. Experimental section

### X-ray crystallography

Suitable single crystals of the seven compounds were performed on Bruker APEX D8 QUEST diffractometer with a Photon 100 CMOS detector (Mo-K $\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ ). SADABS and SAINT programs were applied for absorption correction and data processing. The structures were solved by direct methods and refined with full-matrix least-squares on  $F^2$  using the SHELXTL-2014 software package.<sup>1</sup> All the non-hydrogen atoms were refined anisotropically. The hydrogen atoms of organic ligands were placed in geometrically calculated positions and refined using the riding model. In compounds **1**, **2**, **3** and **5**, coordinated DMF molecules were disordered and split over two sites. In compound **6**, one coordinated water molecule and O3 atom were disordered and split over two sites. In compound **7**, one coordinated water molecule was disordered and split over two sites. Some C–C bond distances were restrained because of disorder. Details of the crystallographic data are listed in Table S1. Selected bond lengths and angles for compounds **1-7** are provided in Table S2. CCDC numbers: 2071646, 2071647, 2071648, 2071649, 2071650, 2071651, 2071652 for compounds 1-7, respectively.

### Calculations

The calculation of the ligand was performed using the Gaussian 09 program. The structure was completely optimized to the ground state by the DFT method at D-B3LYP/6-31G\* level. Then the singlet and triplet energy of structures were calculated based on TD-SCF method.

## 2. Tables

Table S1. Crystallographic Data collection and Refinement result for compounds **1-7**.

Compound reference	1	2	3	4	5	6	7
chemical formula	C <sub>47</sub> H <sub>55</sub> Ce <sub>2</sub> N <sub>5</sub> O <sub>20</sub>	C <sub>47</sub> H <sub>53</sub> Pr <sub>2</sub> N <sub>5</sub> O <sub>19</sub>	C <sub>47</sub> H <sub>53</sub> Sm <sub>2</sub> N <sub>5</sub> O <sub>19</sub>	C <sub>44</sub> H <sub>46</sub> Eu <sub>2</sub> N <sub>4</sub> O <sub>18</sub>	C <sub>47</sub> H <sub>53</sub> Gd <sub>2</sub> N <sub>5</sub> O <sub>19</sub>	C <sub>32</sub> H <sub>23</sub> Dy <sub>2</sub> O <sub>16.50</sub>	C <sub>32</sub> H <sub>23</sub> Ho <sub>2</sub> O <sub>16.50</sub>
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	trigonal	trigonal
Space group	<i>C2/c</i>	<i>C2/c</i>	<i>C2/c</i>	<i>C2/c</i>	<i>C2/c</i>	<i>R-3</i>	<i>R-3</i>
a/Å	28.6190(12)	28.5809(12)	28.531(2)	28.698(4)	28.4297(13)	19.6983(10)	19.6548(11)
b/Å	14.2049(5)	14.1925(6)	14.3021(9)	14.307(2)	14.2555(6)	19.6983(10)	19.6548(11)
c/Å	14.1485(6)	14.1130(5)	13.7731(9)	13.8772(19)	13.8161(5)	45.340(2)	45.295(3)
α/°	90	90	90	90	90	90	90
β/°	100.1739(14)	99.9937(13)	100.718(2)	99.521(4)	100.144(2)	90	90
γ/°	90	90	90	90	90	120	120
Unit cell volume/Å <sup>3</sup>	5661.4(4)	5637.9(4)	5522.1(6)	5619.2(13)	5511.9(4)	15235.8(17)	15153.5(19)
Temperature/K	150(2)	150(2)	150(2)	293(2)	150(2)	150(2)	150(2)
Z	4	4	4	4	4	9	9
μ(mm <sup>-1</sup> )	1.662	1.780	2.180	2.278	2.459	2.228	2.371
No. of reflections measured	37048	38021	19960	16134	25032	33351	50520
No. of independent reflections	5585	5762	4849	4861	4868	6948	6930
R <sub>int</sub>	0.0378	0.0324	0.0503	0.0654	0.0374	0.0248	0.0397
Final R <sub>I</sub> values (I > 2σ(I))	0.0419	0.0437	0.0428	0.0721	0.0441	0.0371	0.0424
Final wR(F <sup>2</sup> ) values (I > 2σ(I))	0.1000	0.1029	0.1071	0.2097	0.1195	0.1042	0.1246
Final R <sub>1</sub> <sup>a</sup> values (all data)	0.0464	0.0466	0.0566	0.1102	0.0492	0.0436	0.0533
Final wR(F <sup>2</sup> ) <sup>b</sup> values (all data)	0.1019	0.1042	0.1125	0.2330	0.1218	0.1087	0.1305
Goodness of fit on F <sup>2</sup>	1.233	1.169	1.060	1.091	1.087	1.057	1.086

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|. \quad ^b wR_2 = \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]^{1/2}.$$

Table S2. Selected bond lengths (Å) and angles (deg) for compounds 1-7.

Compound 1							
Ce1 O1 <sup>i</sup>	2.475(4)	Ce1 O4 <sup>ii</sup>	2.705(4)	Ce1 O7 <sup>iv</sup>	2.488(3)	Ce1 O11	2.462(8)
Ce1 O2	2.463(3)	Ce1 O4 <sup>iii</sup>	2.462(4)	Ce1 O8 <sup>i</sup>	2.665(4)	Ce1 O3A	2.421(10)
Ce1 O3	2.461(6)	Ce1 O5 <sup>ii</sup>	2.569(4)	Ce1 O9	2.537(6)		
O1 <sup>i</sup> Ce1 O4 <sup>ii</sup>	128.38(13)	O2 Ce1 O9	143.21(19)	O3A Ce1 O11	80.4(11)	O5 <sup>ii</sup> Ce1 O8 <sup>i</sup>	123.48(12)
O1 <sup>i</sup> Ce1 O5 <sup>ii</sup>	81.91(13)	O3 Ce1 O1 <sup>i</sup>	92.4(3)	O4 <sup>iii</sup> Ce1 O1 <sup>i</sup>	135.69(12)	O7 <sup>iv</sup> Ce1 O4 <sup>ii</sup>	68.46(12)
O1 <sup>i</sup> Ce1 O7 <sup>iv</sup>	140.99(14)	O3 Ce1 O2	133.4(3)	O4 <sup>iii</sup> Ce1 O2	72.97(12)	O7 <sup>iv</sup> Ce1 O5 <sup>ii</sup>	93.37(13)
O1 <sup>i</sup> Ce1 O8 <sup>i</sup>	50.65(12)	O3 Ce1 O4 <sup>iii</sup>	80.7(4)	O4 <sup>iii</sup> Ce1 O4 <sup>ii</sup>	75.69(12)	O7 <sup>iv</sup> Ce1 O8 <sup>i</sup>	142.29(13)
O1 <sup>i</sup> Ce1 O9	71.9(2)	O3 Ce1 O4 <sup>ii</sup>	138.1(3)	O4 <sup>iii</sup> Ce1 O5 <sup>ii</sup>	122.56(12)	O7 <sup>iv</sup> Ce1 O9	69.26(19)
O2 Ce1 O1 <sup>i</sup>	81.23(14)	O3 Ce1 O5 <sup>ii</sup>	151.1(4)	O4 <sup>iii</sup> Ce1 O7 <sup>iv</sup>	78.81(12)	O8 <sup>i</sup> Ce1 O4 <sup>ii</sup>	140.58(12)
O2 Ce1 O4 <sup>ii</sup>	70.68(11)	O3 Ce1 O7 <sup>iv</sup>	73.4(3)	O4 <sup>iii</sup> Ce1 O8 <sup>i</sup>	86.50(12)	O9 Ce1 O4 <sup>ii</sup>	107.1(2)
O2 Ce1 O5 <sup>ii</sup>	73.91(13)	O3 Ce1 O8 <sup>i</sup>	70.1(3)	O4 <sup>iii</sup> Ce1 O9	143.45(19)	O9 Ce1 O5 <sup>ii</sup>	77.7(2)
O2 Ce1 O7 <sup>iv</sup>	134.73(12)	O3 Ce1 O9	73.6(4)	O4 <sup>iii</sup> Ce1 O11	148.6(4)	O9 Ce1 O8 <sup>i</sup>	108.0(2)
O2 Ce1 O8 <sup>i</sup>	70.55(13)	O3A Ce1 O2	135.5(9)	O5 <sup>ii</sup> Ce1 O4 <sup>ii</sup>	49.45(11)	O11 Ce1 O2	134.6(4)
Compound 2							
Pr1 O1	2.457(4)	Pr1 O5 <sup>iii</sup>	2.466(3)	Pr1 O7 <sup>v</sup>	2.442(3)	Pr1 O8	2.447(4)
Pr1 O2	2.652(4)	Pr1 O6 <sup>iv</sup>	2.550(4)	Pr1 O7 <sup>iv</sup>	2.684(3)	Pr1 O9	2.516(5)
Pr1 O4 <sup>ii</sup>	2.444(3)						
O1 Pr1 O2	51.09(12)	O4 <sup>ii</sup> Pr1 O6 <sup>iv</sup>	74.08(13)	O6 <sup>iv</sup> Pr1 O7 <sup>iv</sup>	49.81(11)	O8 Pr1 O1	90.64(16)
O1 Pr1 O5 <sup>iii</sup>	140.62(14)	O4 <sup>ii</sup> Pr1 O7 <sup>iv</sup>	70.74(11)	O7 <sup>v</sup> Pr1 O1	135.87(12)	O8 Pr1 O2	69.69(14)
O1 Pr1 O6 <sup>iv</sup>	81.98(13)	O4 <sup>ii</sup> Pr1 O8	133.82(15)	O7 <sup>v</sup> Pr1 O2	86.06(12)	O8 Pr1 O5 <sup>iii</sup>	74.08(15)
O1 Pr1 O7 <sup>iv</sup>	128.78(13)	O4 <sup>ii</sup> Pr1 O9	141.36(14)	O7 <sup>v</sup> Pr1 O4 <sup>ii</sup>	73.23(12)	O8 Pr1 O6 <sup>iv</sup>	149.87(16)
O1 Pr1 O9	71.48(15)	O5 <sup>iii</sup> Pr1 O2	142.24(13)	O7 <sup>v</sup> Pr1 O5 <sup>iii</sup>	78.80(12)	O8 Pr1 O7 <sup>iv</sup>	139.30(14)
O2 Pr1 O7 <sup>iv</sup>	140.11(12)	O5 <sup>iii</sup> Pr1 O6 <sup>iv</sup>	93.32(14)	O7 <sup>v</sup> Pr1 O6 <sup>iv</sup>	122.83(12)	O8 Pr1 O9	74.65(18)
O4 <sup>ii</sup> Pr1 O1	81.38(14)	O5 <sup>iii</sup> Pr1 O7 <sup>iv</sup>	68.51(12)	O7 <sup>v</sup> Pr1 O7 <sup>iv</sup>	75.50(12)	O9 Pr1 O2	109.61(16)
O4 <sup>ii</sup> Pr1 O2	70.14(13)	O5 <sup>iii</sup> Pr1 O9	69.53(14)	O7 <sup>v</sup> Pr1 O8	82.21(15)	O9 Pr1 O6 <sup>iv</sup>	75.31(16)
O4 <sup>ii</sup> Pr1 O5 <sup>iii</sup>	134.98(12)	O6 <sup>iv</sup> Pr1 O2	123.65(12)	O7 <sup>v</sup> Pr1 O9	144.72(13)	O9 Pr1 O7 <sup>iv</sup>	105.63(16)
Compound 3							
Sm4 O1 <sup>i</sup>	2.432(4)	Sm4 O4 <sup>iv</sup>	2.393(4)	Sm4 O6 <sup>ii</sup>	2.629(4)	Sm4 O8	2.405(5)
Sm4 O2	2.402(4)	Sm4 O4 <sup>iii</sup>	2.678(4)	Sm4 O7 <sup>ii</sup>	2.421(4)	Sm4 O9	2.494(5)
Sm4 O3 <sup>iii</sup>	2.477(4)						
O1 <sup>i</sup> Sm4 O3 <sup>iii</sup>	91.99(15)	O2 Sm4 O9	140.90(15)	O4 <sup>iv</sup> Sm4 O8	82.12(16)	O7 <sup>ii</sup> Sm4 O6 <sup>ii</sup>	51.51(14)
O1 <sup>i</sup> Sm4 O4 <sup>iii</sup>	68.53(13)	O2 Sm4 O6 <sup>ii</sup>	70.42(14)	O4 <sup>iv</sup> Sm4 O4 <sup>iii</sup>	76.01(14)	O8 Sm4 O3 <sup>iii</sup>	148.25(16)
O1 <sup>i</sup> Sm4 O9	69.04(15)	O3 <sup>iii</sup> Sm4 O4 <sup>iii</sup>	50.38(12)	O4 <sup>iv</sup> Sm4 O6 <sup>ii</sup>	84.24(13)	O8 Sm4 O4 <sup>iii</sup>	139.78(16)
O1 <sup>i</sup> Sm4 O6 <sup>ii</sup>	141.58(15)	O3 <sup>iii</sup> Sm4 O9	74.18(17)	O4 <sup>iv</sup> Sm4 O9	144.51(15)	O8 Sm4 O9	74.15(17)
O2 Sm4 O7 <sup>ii</sup>	80.66(15)	O3 <sup>iii</sup> Sm4 O6 <sup>ii</sup>	125.59(13)	O6 <sup>ii</sup> Sm4 O4 <sup>iii</sup>	139.79(14)	O8 Sm4 O6 <sup>ii</sup>	68.78(16)

O2	Sm4	O1 <sup>i</sup>	135.41(13)	O4 <sup>iv</sup>	Sm4	O2	74.02(14)	O7 <sup>ii</sup>	Sm4	O1 <sup>i</sup>	140.81(15)	O8	Sm4	O7 <sup>ii</sup>	89.72(19)
O2	Sm4	O3 <sup>iii</sup>	74.97(15)	O4 <sup>iv</sup>	Sm4	O7 <sup>ii</sup>	134.52(14)	O7 <sup>ii</sup>	Sm4	O3 <sup>iii</sup>	82.79(15)	O8	Sm4	O1 <sup>i</sup>	74.62(17)
O2	Sm4	O8	134.24(16)	O4 <sup>iv</sup>	Sm4	O1 <sup>i</sup>	79.54(14)	O7 <sup>ii</sup>	Sm4	O4 <sup>iii</sup>	129.39(15)	O9	Sm4	O4 <sup>iii</sup>	105.96(15)
O2	Sm4	O4 <sup>iii</sup>	70.60(13)	O4 <sup>iv</sup>	Sm4	O3 <sup>iii</sup>	124.34(14)	O7 <sup>ii</sup>	Sm4	O9	72.19(16)	O9	Sm4	O6 <sup>ii</sup>	110.29(16)

#### Compound 4

Eu1	O1	2.475(6)	Eu1	O6 <sup>iv</sup>	2.594(6)	Eu2	O2	2.690(8)	Eu2	O6 <sup>iv</sup>	2.610(7)				
Eu1	O2 <sup>i</sup>	2.370(5)	Eu1	O7 <sup>iv</sup>	2.412(7)	Eu2	O2 <sup>i</sup>	2.388(7)	Eu2	O7 <sup>iv</sup>	2.404(8)				
Eu1	O2	2.711(6)	Eu1	O8	2.485(8)	Eu2	O3 <sup>ii</sup>	2.439(7)	Eu2	O8	2.480(9)				
Eu1	O3 <sup>ii</sup>	2.433(5)	Eu1	O9	2.427(9)	Eu2	O4 <sup>iii</sup>	2.396(7)	Eu2	O9	2.458(11)				
Eu1	O4 <sup>iii</sup>	2.410(6)	Eu2	O1	2.442(8)										
O1	Eu1	O2	49.10(19)	O4 <sup>iii</sup>	Eu1	O6 <sup>iv</sup>	71.25(18)	O1	Eu2	O2	49.6(2)	O4 <sup>iii</sup>	Eu2	O2	70.4(2)
O1	Eu1	O6 <sup>iv</sup>	126.8(2)	O4 <sup>iii</sup>	Eu1	O7 <sup>iv</sup>	79.4(2)	O1	Eu2	O6 <sup>iv</sup>	127.6(3)	O4 <sup>iii</sup>	Eu2	O3 <sup>ii</sup>	135.0(3)
O1	Eu1	O8	73.9(3)	O4 <sup>iii</sup>	Eu1	O8	140.0(2)	O1	Eu2	O8	74.6(3)	O4 <sup>iii</sup>	Eu2	O6 <sup>iv</sup>	71.2(2)
O2 <sup>i</sup>	Eu1	O1	123.7(2)	O4 <sup>iii</sup>	Eu1	O9	134.5(2)	O1	Eu2	O9	148.7(3)	O4 <sup>iii</sup>	Eu2	O7 <sup>iv</sup>	79.8(3)
O2 <sup>i</sup>	Eu1	O2	76.21(19)	O6 <sup>iv</sup>	Eu1	O2	140.0(2)	O2 <sup>i</sup>	Eu2	O1	124.4(3)	O4 <sup>iii</sup>	Eu2	O8	141.2(3)
O2 <sup>i</sup>	Eu1	O3 <sup>ii</sup>	80.12(19)	O7 <sup>iv</sup>	Eu1	O1	82.5(2)	O2 <sup>i</sup>	Eu2	O2	76.3(2)	O4 <sup>iii</sup>	Eu2	O9	133.5(3)
O2 <sup>i</sup>	Eu1	O4 <sup>iii</sup>	74.35(19)	O7 <sup>iv</sup>	Eu1	O2	127.1(2)	O2 <sup>i</sup>	Eu2	O3 <sup>ii</sup>	79.6(2)	O6 <sup>iv</sup>	Eu2	O2	140.3(3)
O2 <sup>i</sup>	Eu1	O6 <sup>iv</sup>	84.9(2)	O7 <sup>iv</sup>	Eu1	O3 <sup>ii</sup>	141.5(2)	O2 <sup>i</sup>	Eu2	O4 <sup>iii</sup>	74.3(2)	O7 <sup>iv</sup>	Eu2	O1	83.4(3)
O2 <sup>i</sup>	Eu1	O7 <sup>iv</sup>	134.9(2)	O7 <sup>iv</sup>	Eu1	O6 <sup>iv</sup>	51.8(2)	O2 <sup>i</sup>	Eu2	O6 <sup>iv</sup>	84.2(3)	O7 <sup>iv</sup>	Eu2	O2	128.5(3)
O2 <sup>i</sup>	Eu1	O8	145.2(2)	O7 <sup>iv</sup>	Eu1	O8	71.9(2)	O2 <sup>i</sup>	Eu2	O7 <sup>iv</sup>	134.3(3)	O7 <sup>iv</sup>	Eu2	O3 <sup>ii</sup>	141.6(3)
O2 <sup>i</sup>	Eu1	O9	81.2(2)	O7 <sup>iv</sup>	Eu1	O9	92.3(3)	O2 <sup>i</sup>	Eu2	O8	144.2(3)	O7 <sup>iv</sup>	Eu2	O6 <sup>iv</sup>	51.7(2)
O3 <sup>ii</sup>	Eu1	O1	89.2(2)	O8	Eu1	O2	106.6(2)	O2 <sup>i</sup>	Eu2	O9	80.2(3)	O7 <sup>iv</sup>	Eu2	O8	72.1(3)
O3 <sup>ii</sup>	Eu1	O2	67.89(19)	O8	Eu1	O6 <sup>iv</sup>	108.9(3)	O3 <sup>ii</sup>	Eu2	O1	89.9(3)	O7 <sup>iv</sup>	Eu2	O9	91.7(3)
O3 <sup>ii</sup>	Eu1	O6 <sup>iv</sup>	143.0(2)	O9	Eu1	O1	148.5(3)	O3 <sup>ii</sup>	Eu2	O2	68.2(2)	O8	Eu2	O2	107.4(3)
O3 <sup>ii</sup>	Eu1	O8	69.7(2)	O9	Eu1	O2	139.6(2)	O3 <sup>ii</sup>	Eu2	O6 <sup>iv</sup>	141.6(3)	O8	Eu2	O6 <sup>iv</sup>	108.6(3)
O4 <sup>iii</sup>	Eu1	O1	75.2(2)	O9	Eu1	O3 <sup>ii</sup>	75.6(3)	O3 <sup>ii</sup>	Eu2	O8	69.7(3)	O9	Eu2	O2	139.0(3)
O4 <sup>iii</sup>	Eu1	O2	69.81(19)	O9	Eu1	O6 <sup>iv</sup>	68.8(2)	O3 <sup>ii</sup>	Eu2	O9	74.9(3)	O9	Eu2	O6 <sup>iv</sup>	68.1(3)
O4 <sup>iii</sup>	Eu1	O3 <sup>ii</sup>	134.5(2)	O9	Eu1	O8	75.0(3)	O4 <sup>iii</sup>	Eu2	O1	76.1(3)	O9	Eu2	O8	74.5(3)

#### Compound 5

Gd4	O1	2.605(5)	Gd4	O4 <sup>v</sup>	2.362(4)	Gd4	O5 <sup>iv</sup>	2.454(5)	Gd4	O7 <sup>ii</sup>	2.380(5)				
Gd4	O2	2.387(5)	Gd4	O4 <sup>iv</sup>	2.656(5)	Gd4	O6 <sup>iii</sup>	2.400(4)	Gd4	O8	2.373(5)				
Gd4	O9	2.467(6)													
O1	Gd4	O4 <sup>iv</sup>	138.90(17)	O4 <sup>v</sup>	Gd4	O6 <sup>iii</sup>	79.91(16)	O6 <sup>iii</sup>	Gd4	O4 <sup>iv</sup>	68.04(15)	O8	Gd4	O2	91.5(2)
O2	Gd4	O6 <sup>iii</sup>	140.91(17)	O4 <sup>v</sup>	Gd4	O5 <sup>iv</sup>	124.56(16)	O6 <sup>iii</sup>	Gd4	O9	69.31(17)	O8	Gd4	O7 <sup>ii</sup>	133.41(19)
O2	Gd4	O5 <sup>iv</sup>	81.78(17)	O4 <sup>v</sup>	Gd4	O4 <sup>iv</sup>	75.57(16)	O6 <sup>iii</sup>	Gd4	O1	143.26(17)	O8	Gd4	O6 <sup>iii</sup>	75.60(19)
O2	Gd4	O4 <sup>iv</sup>	128.30(16)	O4 <sup>v</sup>	Gd4	O1	84.58(16)	O7 <sup>ii</sup>	Gd4	O2	79.81(17)	O8	Gd4	O5 <sup>iv</sup>	148.93(19)
O2	Gd4	O1	51.93(16)	O4 <sup>v</sup>	Gd4	O9	144.62(17)	O7 <sup>ii</sup>	Gd4	O6 <sup>iii</sup>	135.21(16)	O8	Gd4	O4 <sup>iv</sup>	139.36(18)
O2	Gd4	O9	71.73(18)	O5 <sup>iv</sup>	Gd4	O4 <sup>iv</sup>	50.75(14)	O7 <sup>ii</sup>	Gd4	O5 <sup>iv</sup>	75.42(16)	O8	Gd4	O1	69.14(19)

O4 <sup>v</sup>	Gd4	O8	80.89(19)	O5 <sup>iv</sup>	Gd4	O1	125.31(16)	O7 <sup>ii</sup>	Gd4	O4 <sup>iv</sup>	70.37(15)	O8	Gd4	O9	75.0(2)
O4 <sup>v</sup>	Gd4	O2	135.13(16)	O5 <sup>iv</sup>	Gd4	O9	74.05(19)	O7 <sup>ii</sup>	Gd4	O1	69.75(17)	O9	Gd4	O4 <sup>iv</sup>	107.05(18)
O4 <sup>v</sup>	Gd4	O7 <sup>ii</sup>	74.35(15)	O6 <sup>iii</sup>	Gd4	O5 <sup>iv</sup>	90.58(17)	O7 <sup>ii</sup>	Gd4	O9	140.59(18)	O9	Gd4	O1	109.8(2)

### Compound 6

Dy1	O0AA	2.447(6)	Dy1	O1	2.300(3)	Dy1	O5 <sup>iii</sup>	2.408(3)	Dy1	O7 <sup>ii</sup>	2.839(3)				
Dy1	O1AA	2.447(6)	Dy1	O2 <sup>iv</sup>	2.318(4)	Dy1	O6 <sup>ii</sup>	2.346(3)	Dy1	O7 <sup>i</sup>	2.276(3)				
Dy1	O2AA	2.215(12)	Dy1	O4 <sup>iii</sup>	2.399(3)										
O1	Dy1	O7 <sup>ii</sup>	66.12(13)	O2 <sup>iv</sup>	Dy1	O0AA	139.3(2)	O6 <sup>ii</sup>	Dy1	O4 <sup>iii</sup>	133.05(14)	O0AA	Dy1	O7 <sup>ii</sup>	112.6(2)
O1	Dy1	O6 <sup>ii</sup>	80.88(16)	O2 <sup>iv</sup>	Dy1	O1AA	141.1(2)	O6 <sup>ii</sup>	Dy1	O0AA	72.5(2)	O0AA	Dy1	O1AA	69.2(3)
O1	Dy1	O5 <sup>iii</sup>	142.59(13)	O4 <sup>iii</sup>	Dy1	O7 <sup>ii</sup>	142.46(15)	O6 <sup>ii</sup>	Dy1	O1AA	137.4(2)	O2AA	Dy1	O1	77.7(3)
O1	Dy1	O2 <sup>iv</sup>	131.09(12)	O4 <sup>iii</sup>	Dy1	O5 <sup>iii</sup>	54.26(13)	O7 <sup>i</sup>	Dy1	O7 <sup>ii</sup>	76.21(11)	O2AA	Dy1	O4 <sup>iii</sup>	73.6(4)
O1	Dy1	O4 <sup>iii</sup>	143.58(17)	O4 <sup>iii</sup>	Dy1	O0AA	100.2(2)	O7 <sup>i</sup>	Dy1	O6 <sup>ii</sup>	125.52(11)	O2AA	Dy1	O7 <sup>ii</sup>	143.0(3)
O1	Dy1	O0AA	75.12(17)	O4 <sup>iii</sup>	Dy1	O1AA	72.7(2)	O7 <sup>i</sup>	Dy1	O5 <sup>iii</sup>	138.75(13)	O2AA	Dy1	O7 <sup>i</sup>	104.2(4)
O1	Dy1	O1AA	71.9(2)	O5 <sup>iii</sup>	Dy1	O7 <sup>ii</sup>	121.88(12)	O7 <sup>i</sup>	Dy1	O2 <sup>iv</sup>	76.83(15)	O2AA	Dy1	O6 <sup>ii</sup>	119.0(4)
O2 <sup>iv</sup>	Dy1	O7 <sup>ii</sup>	67.69(13)	O5 <sup>iii</sup>	Dy1	O0AA	68.23(18)	O7 <sup>i</sup>	Dy1	O1	77.50(14)	O2AA	Dy1	O5 <sup>iii</sup>	82.7(4)
O2 <sup>iv</sup>	Dy1	O6 <sup>ii</sup>	81.26(16)	O5 <sup>iii</sup>	Dy1	O1AA	100.9(2)	O7 <sup>i</sup>	Dy1	O4 <sup>iii</sup>	88.13(13)	O2AA	Dy1	O2 <sup>iv</sup>	149.2(3)
O2 <sup>iv</sup>	Dy1	O5 <sup>iii</sup>	77.66(13)	O6 <sup>ii</sup>	Dy1	O7 <sup>ii</sup>	49.32(10)	O7 <sup>i</sup>	Dy1	O0AA	143.8(2)	O2AA	Dy1	O0AA	46.9(4)
O2 <sup>iv</sup>	Dy1	O4 <sup>iii</sup>	75.65(16)	O6 <sup>ii</sup>	Dy1	O5 <sup>iii</sup>	81.29(12)	O7 <sup>i</sup>	Dy1	O1AA	80.1(2)				

### Compound 7

Ho1	O1	2.263(4)	Ho1	O3 <sup>i</sup>	2.336(4)	Ho1	O6 <sup>ii</sup>	2.384(4)	Ho1	O9	2.451(7)				
Ho1	O1 <sup>i</sup>	2.837(4)	Ho1	O4 <sup>iii</sup>	2.294(4)	Ho1	O8	2.416(6)	Ho1	O10	2.333(9)				
Ho1	O2 <sup>ii</sup>	2.396(4)	Ho1	O5 <sup>iv</sup>	2.298(4)										
O1	Ho1	O1 <sup>i</sup>	76.30(13)	O2 <sup>ii</sup>	Ho1	O9	68.0(2)	O4 <sup>iii</sup>	Ho1	O8	72.4(2)	O6 <sup>ii</sup>	Ho1	O1 <sup>i</sup>	142.70(17)
O1	Ho1	O2 <sup>ii</sup>	139.33(15)	O3 <sup>i</sup>	Ho1	O1 <sup>i</sup>	49.33(11)	O4 <sup>iii</sup>	Ho1	O9	75.1(2)	O6 <sup>ii</sup>	Ho1	O2 <sup>ii</sup>	54.52(15)
O1	Ho1	O3 <sup>i</sup>	125.63(13)	O3 <sup>i</sup>	Ho1	O2 <sup>ii</sup>	81.20(14)	O4 <sup>iii</sup>	Ho1	O10	76.9(4)	O6 <sup>ii</sup>	Ho1	O8	72.0(2)
O1	Ho1	O4 <sup>iii</sup>	77.26(16)	O3 <sup>i</sup>	Ho1	O6 <sup>ii</sup>	133.32(15)	O5 <sup>iv</sup>	Ho1	O1 <sup>i</sup>	67.35(14)	O6 <sup>ii</sup>	Ho1	O9	99.7(2)
O1	Ho1	O5 <sup>iv</sup>	77.29(17)	O3 <sup>i</sup>	Ho1	O8	138.2(3)	O5 <sup>iv</sup>	Ho1	O2 <sup>ii</sup>	77.97(14)	O8	Ho1	O1 <sup>i</sup>	135.2(2)
O1	Ho1	O6 <sup>ii</sup>	88.37(15)	O3 <sup>i</sup>	Ho1	O9	72.8(3)	O5 <sup>iv</sup>	Ho1	O3 <sup>i</sup>	81.18(17)	O8	Ho1	O9	69.8(4)
O1	Ho1	O8	78.9(3)	O4 <sup>iii</sup>	Ho1	O1 <sup>i</sup>	66.14(15)	O5 <sup>iv</sup>	Ho1	O6 <sup>ii</sup>	76.25(18)	O9	Ho1	O1 <sup>i</sup>	113.0(2)
O1	Ho1	O9	143.1(3)	O4 <sup>iii</sup>	Ho1	O2 <sup>ii</sup>	142.21(15)	O5 <sup>iv</sup>	Ho1	O8	140.5(3)	O10	Ho1	O1 <sup>i</sup>	142.0(4)
O1	Ho1	O10	104.4(6)	O4 <sup>iii</sup>	Ho1	O3 <sup>i</sup>	80.59(18)	O5 <sup>iv</sup>	Ho1	O9	139.6(2)	O10	Ho1	O6 <sup>ii</sup>	74.5(4)
O2 <sup>ii</sup>	Ho1	O1 <sup>i</sup>	121.79(14)	O4 <sup>iii</sup>	Ho1	O5 <sup>iv</sup>	130.86(14)	O5 <sup>iv</sup>	Ho1	O10	150.6(4)	O10	Ho1	O9	45.6(6)
O2 <sup>ii</sup>	Ho1	O8	101.2(3)	O4 <sup>iii</sup>	Ho1	O6 <sup>ii</sup>	143.44(19)								

Symmetry codes for **1**: (i) 1-x, y, 0.5-z; (ii) 0.5-x, -0.5+y, 0.5-z; (iii) x, 1-y, 0.5+z; (iv) 0.5-x, 0.5-y, 1-z; (v) x, 1-y, -0.5+z; (vi) 0.5-x, 0.5+y, 0.5-z. For **2**: (i) 0.5-x, 0.5-y, 1-z; (ii) 1-x, y, 0.5-z; (iii) -0.5+x, 0.5-y, 0.5+z; (iv) -0.5+x, 0.5+y, z; (v) 1-x, -y, 1-z; (vi) 0.5+x, 0.5-y, -0.5+z; (vii) 0.5+x, -0.5+y, z. For **3**: (i) 0.5-x, 0.5-y, 1-z; (ii) 1-x, y, 0.5-z; (iii) 0.5-x, -0.5+y, 0.5-z; (iv) x, 1-y, 0.5+z; (v) 0.5-x, 0.5+y, 0.5-z; (vi) x, 1-y, -0.5+z. For **4**: (i) 0.5-x, -0.5-y, 1-z; (ii) x, -y, -0.5+z; (iii) 0.5-x, -0.5+y, 1.5-z; (iv) -0.5+x, -0.5+y, z; (v) x, -y, 0.5+z; (vi) 0.5-x, 0.5+y, 1.5-z; (vii) 0.5+x, 0.5+y, z. For **5**: (i) 1.5-x, 1.5-y, 1-z; (ii) 1-x, y, 1.5-z; (iii) 0.5+x, 1.5-y,

-0.5+z; (iv)  $0.5+x, 0.5+y, z$ ; (v)  $1-x, 1-y, 1-z$ ; (vi)  $-0.5+x, 1.5-y, 0.5+z$ ; (vii)  $-0.5+x, -0.5+y, z$ . For 6: (i)  $0.33333+y, 0.66667-x+y, 1.66667-z$ ; (ii)  $1-y, 1+x-y, z$ ; (iii)  $0.66667-x+y, 1.33333-x, 0.33333+z$ ; (iv)  $1.33333-x, 1.66667-y, 1.66667-z$ ; (v)  $0.33333+x-y, -0.33333+x, 1.66667-z$ ; (vi)  $-x+y, 1-x, z$ ; (vii)  $1.33333-y, 0.66667+x-y, -0.33333+z$ . For 7: (i)  $0.33333-x, 0.66667-y, 0.66667-z$ ; (ii)  $x-y, x, 1-z$ ; (iii)  $0.33333+y, 0.66667-x+y, 0.66667-z$ ; (iv)  $-y, x-y, z$ ; (v)  $y, -x+y, 1-z$ ; (vi)  $0.33333+x-y, -0.33333+x, 0.66667-z$ ; (vii)  $-x+y, -x, z$ .



Table S3. Comparison of various MOFs sensors for the detection of Fe<sup>3+</sup> and Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> ions.

	Analyte	CPS-based fluorescent Materials	Quenching constant (K <sub>SV</sub> × 10 <sup>4</sup> M <sup>-1</sup> )	Detection Limits (DL)	Ref
1	Fe <sup>3+</sup>	{[Tb(CmdcpBr)(H <sub>2</sub> O) <sub>3</sub> ] <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ·5H <sub>2</sub> O} <sub>n</sub>	0.5532	1.5 mM	2
2		{[Eu(L)(HCOO)]·H <sub>2</sub> O} <sub>n</sub>	0.7461	1 μM	3
3		[Eu <sub>2</sub> (2,3'-oba) <sub>3</sub> (phen) <sub>2</sub> ] <sub>n</sub>	1.37	7.93 μM	4
4		[Tb(HMDIA)(H <sub>2</sub> O) <sub>3</sub> ]·H <sub>2</sub> O	1.73		5
5		[Eu(L <sub>1</sub> )(H <sub>2</sub> O)]·1.5H <sub>2</sub> O	6.607	0.87 μM	6
		[[Tb(μ <sub>6</sub> -H <sub>2</sub> cpboda)(μ <sub>2</sub> -OH <sub>2</sub> ) <sub>2</sub> ]·H <sub>2</sub> O] <sub>n</sub>	6.50	0.84 μM	7
6		[Tb(TATAB)(H <sub>2</sub> O)]·2H <sub>2</sub> O	12.5	0.0221 μM	8
7		Eu-MOF	13.4	3.69 μM	This work
8		[H <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> [Zn <sub>2</sub> L(HPO <sub>3</sub> ) <sub>2</sub> ]	39.6	0.116 μM	9
9		{[Zn <sub>3</sub> (HL) <sub>2</sub> H <sub>2</sub> O]·4H <sub>2</sub> O} <sub>n</sub>	50		10
10	CTGU-1 (Tb)	188.3	0.001 μM	11	
1	Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup>	[Cd <sub>2</sub> (L <sub>1</sub> )(1,4-NDC) <sub>2</sub> ] <sub>n</sub>	5.86	0.031 ppm	12
2		[Zr <sub>6</sub> O <sub>4</sub> (OH) <sub>8</sub> (H <sub>2</sub> O) <sub>4</sub> (TCPP) <sub>4</sub> ] □9DMF□3.5H <sub>2</sub> O	5.91		13
3		{[Zn(H <sub>2</sub> BCA)(m-bib)]·H <sub>2</sub> O} <sub>n</sub>	5.3	0.07 μM	14
		{[Zn <sub>2</sub> (tpeb) <sub>2</sub> (2,3-ndc) <sub>2</sub> ]·H <sub>2</sub> O} <sub>n</sub>	7.09	2.623 ppb	15
4		[Zn(NH <sub>2</sub> -bdc)(4,4'-bpy)]	7.62	1.30 μM	16
5		[Ln(Hbptc)(H <sub>2</sub> O) <sub>4</sub> ]·H <sub>2</sub> O	10.4	2.36 μM	17
6	Eu-MOF	11.3	4.01 μM	This work	

Table S4. Comparison of various MOFs sensors for the detection of NZF and NFT.

	Analyte	CPs-based fluorescent Materials	Quenching constant ( $K_{SV} \times 10^4 \text{ M}^{-1}$ )	Detection Limits (DL)	Ref
1	NZF	$[\text{Zn}(\text{L})_2] \cdot \text{CH}_2\text{Cl}_2 \cdot \text{CH}_3\text{OH}$	1.62		18
2		$\{\text{Tb}(\text{TATMA})(\text{H}_2\text{O}) \cdot 2\text{H}_2\text{O}\}_n$	3.00		19
3		Eu-MOF	4.38		This work
4		$[\text{Cd}(\text{tpc})_{0.5}(\text{o-bimb})]_n$	4.4		20
5		$\{[\text{Cd}_3(\text{TDCPB}) \cdot 2\text{DMAc}] \cdot \text{DMAc} \cdot 4\text{H}_2\text{O}\}_n$	7.46		21
6		$[\text{Zn}_2(\text{azdc})_2(\text{dpta})] \cdot (\text{DMF})_4$	13	0.63 ppm	22
7		$[\text{Cd}(\text{H}_2\text{tpc})_{0.5}(\text{mbimb})(\text{Cl})]_n$	21		20
1	NFT	$[\text{Zn}(\text{L})_2] \cdot \text{CH}_2\text{Cl}_2 \cdot \text{CH}_3\text{OH}$	1.58		18
		$\{\text{Tb}(\text{TATMA})(\text{H}_2\text{O}) \cdot 2\text{H}_2\text{O}\}_n$	3.35		19
		$[\text{Cd}(\text{tpc})_{0.5}(\text{o-bimb})]_n$	3.4		20
2		$[\text{TbL} \cdot 2\text{H}_2\text{O}]_n$	5.26		23
3		Eu-MOF	5.29		This work
		$[\text{Zn}_2(\text{azdc})_2(\text{dpta})] \cdot (\text{DMF})_4$	7.14		22
6		$\{[\text{Cd}_3(\text{TDCPB}) \cdot 2\text{DMAc}] \cdot \text{DMAc} \cdot 4\text{H}_2\text{O}\}_n$	10.5		21
7	$[\text{Cd}(\text{H}_2\text{tpc})_{0.5}(\text{mbimb})(\text{Cl})]_n$	26		20	

### 3. Figures

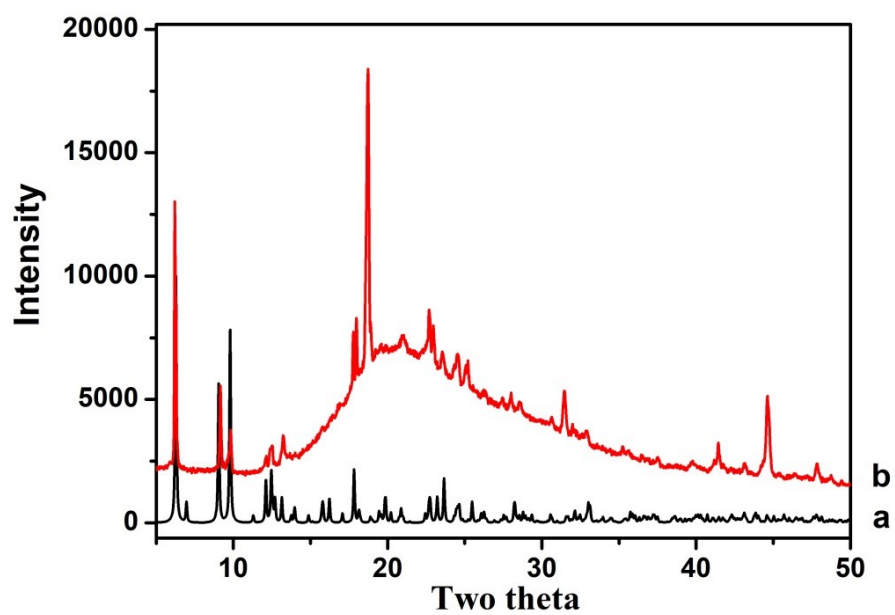


Figure S1. PXRD pattern of compound Ce(1).

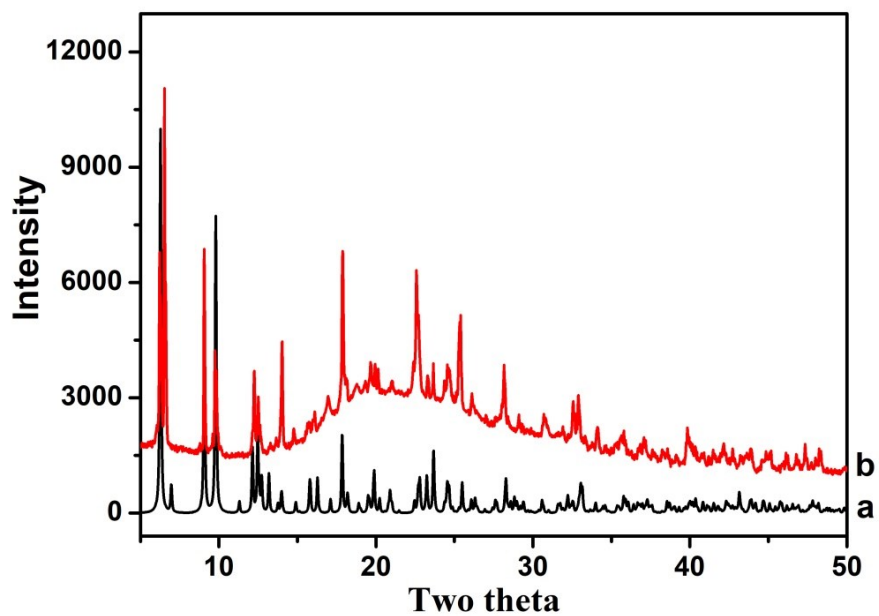


Figure S2. PXRD pattern of compound Pr(2).

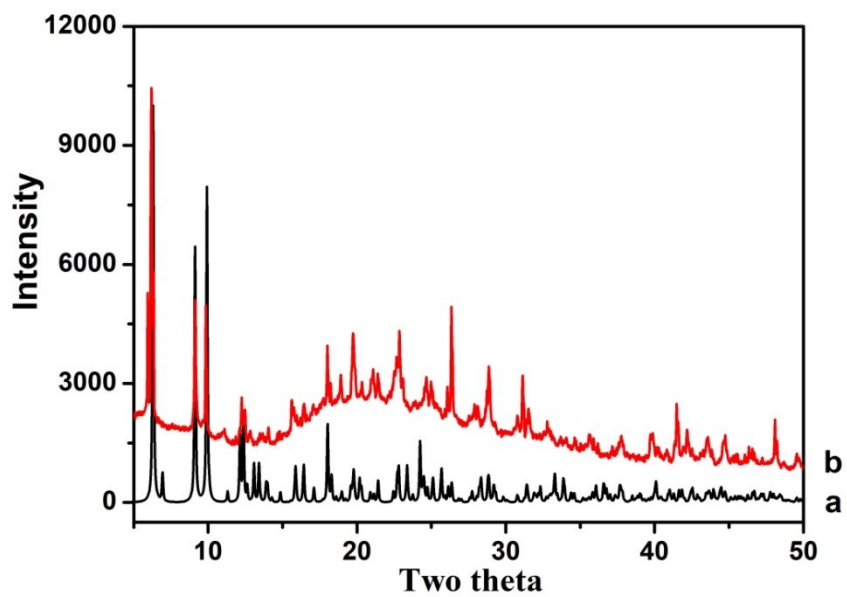


Figure S3. PXRD pattern of compound Sm(3).

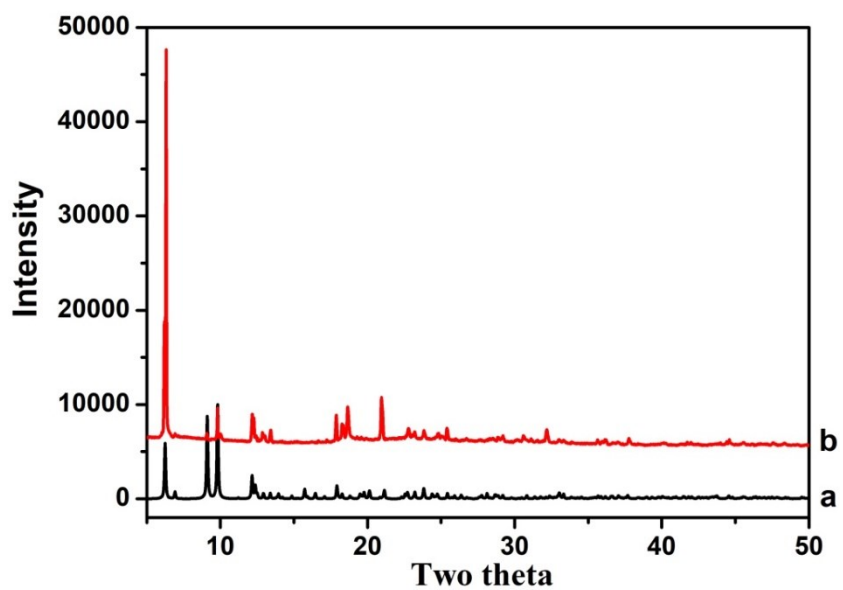


Figure S4. PXRD pattern of compound Eu(4).

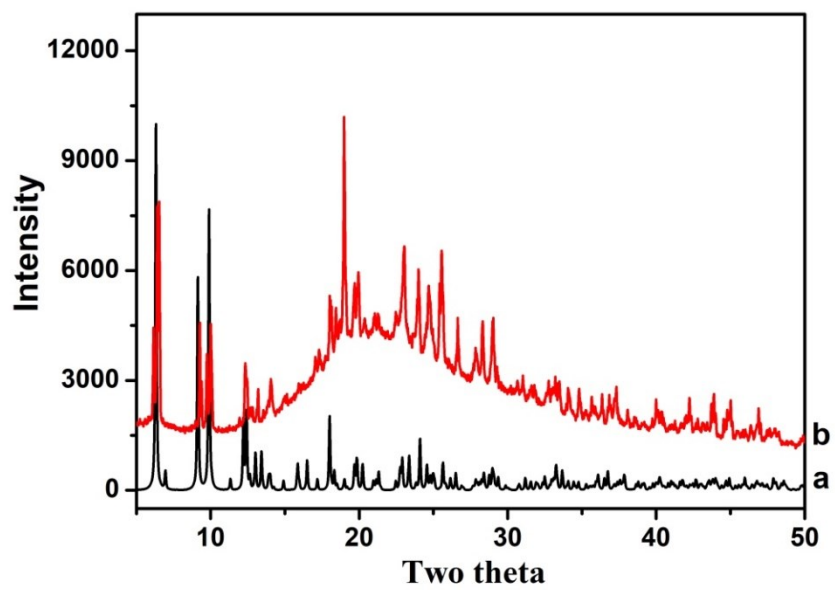


Figure S5. PXRD pattern of compound Gd(5).

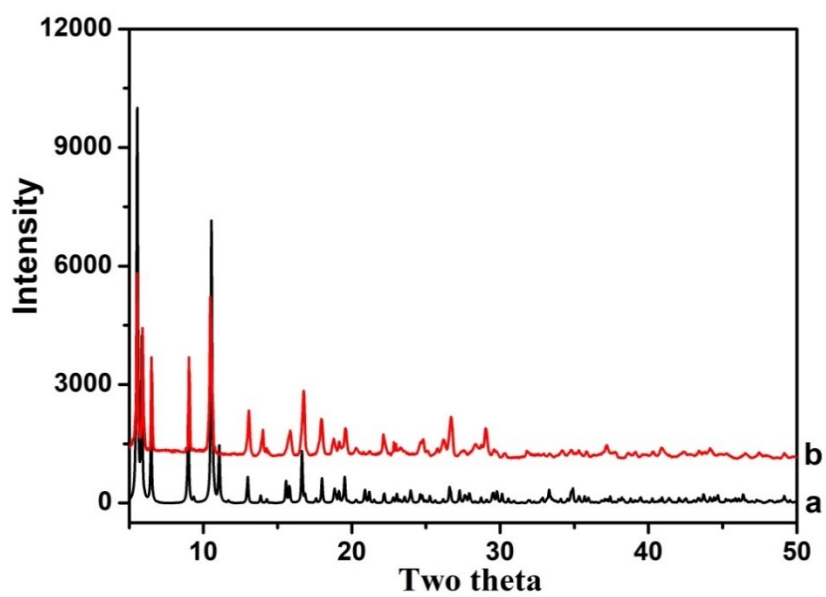


Figure S6. PXRD pattern of compound Dy(6).

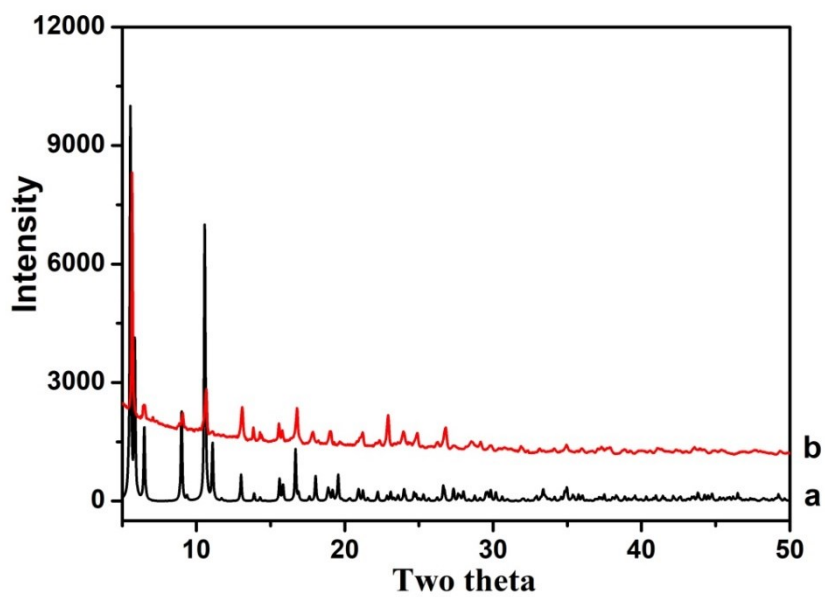


Figure S7. PXRD pattern of compound Ho(7).

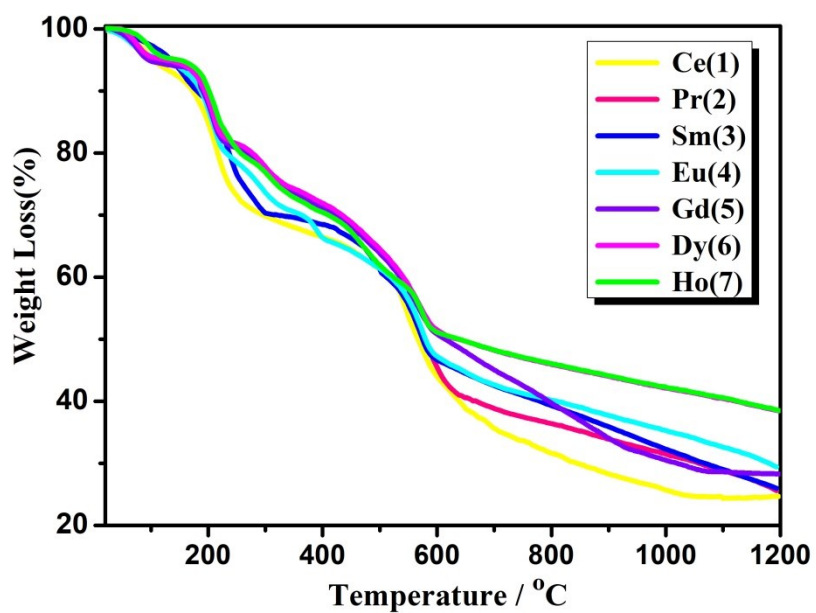


Figure S8. TGA curves for compounds 1-7.

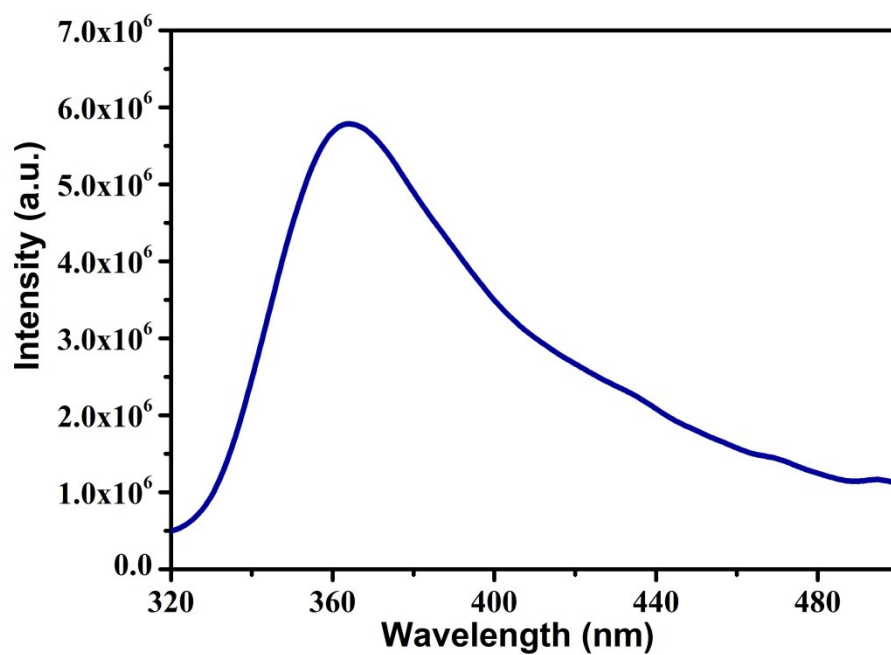


Figure S9. The solid state photoluminescence spectra for H<sub>3</sub>L ligand.

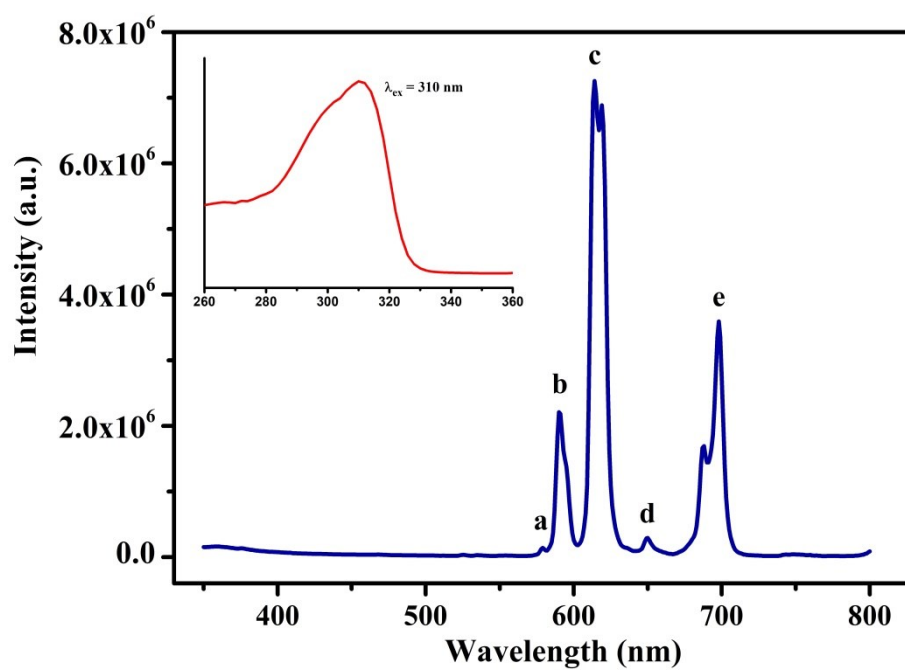


Figure S10. The photoluminescence spectra for Eu(4) (Inset: the excitation spectra of (4)).

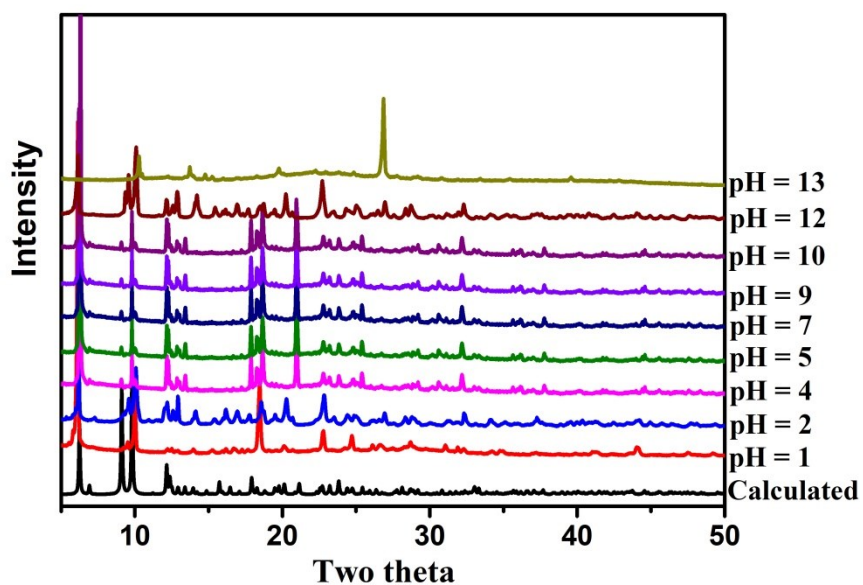


Figure S11. PXRD pattern of Eu(4) soaked into aqueous solutions with different pH values.

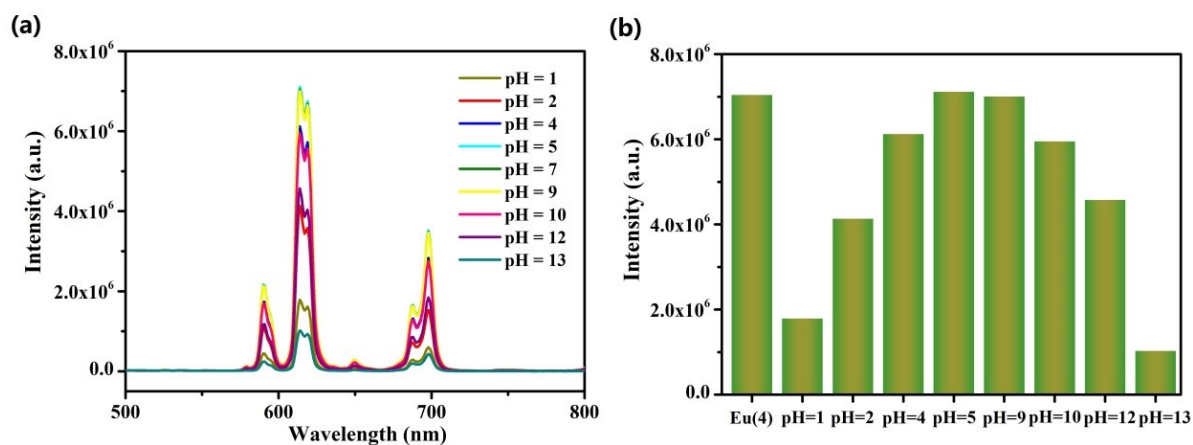


Figure S12 (a) pH-dependent emission spectra of Eu(4) in the aqueous solution with pH ranging from 1.00 to 13.00; (b) Histogram showed fluorescence emission of Eu(4) at 614 nm at different pH values.



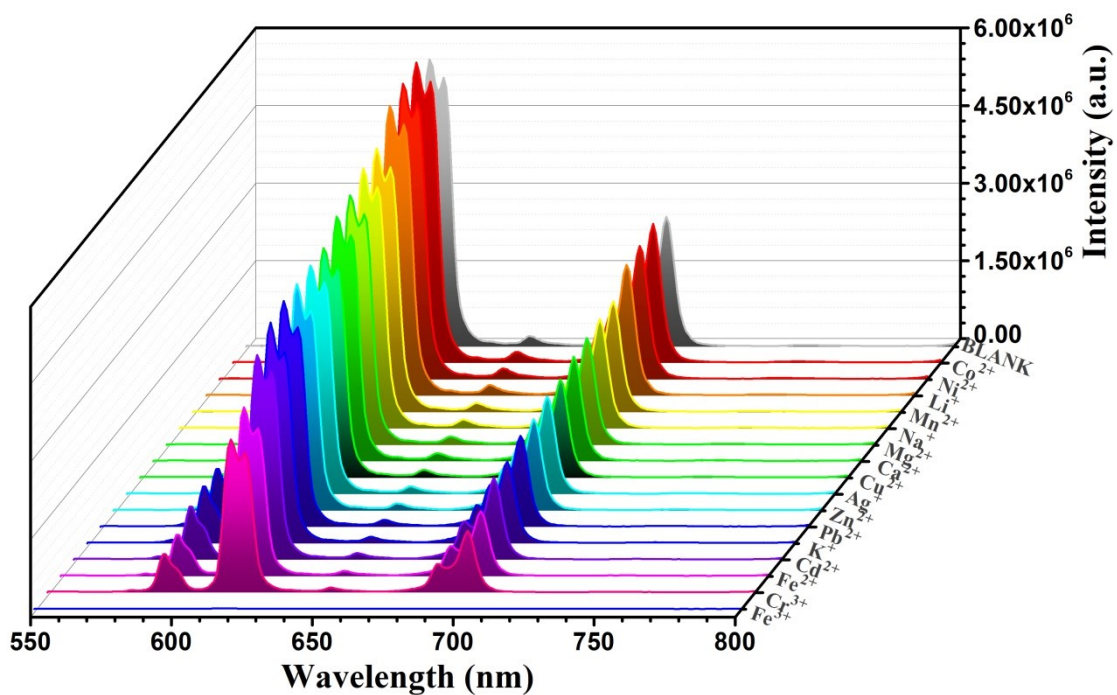


Figure S13. The emission spectra of Eu(4) dispersed in 0.01 M metal ion aqueous solutions.

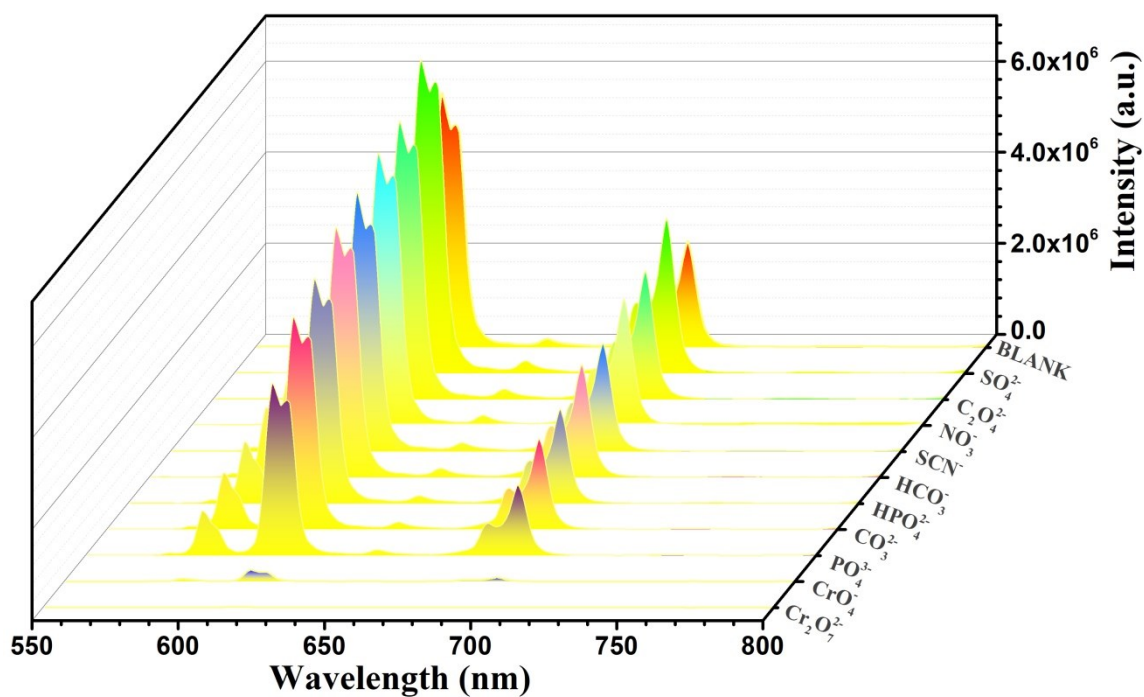


Figure S14. The emission spectra of Eu(4) dispersed in 0.01 M anion aqueous solutions.

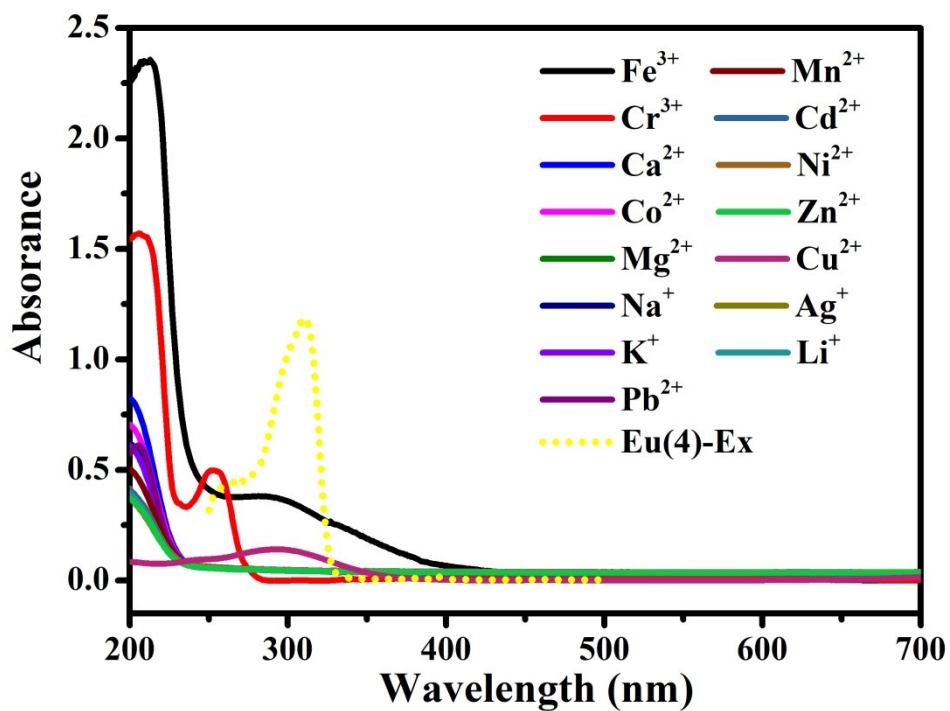


Figure S15. UV-vis spectra of different metal ions in aqueous solutions, and the excitation spectra of Eu(4).

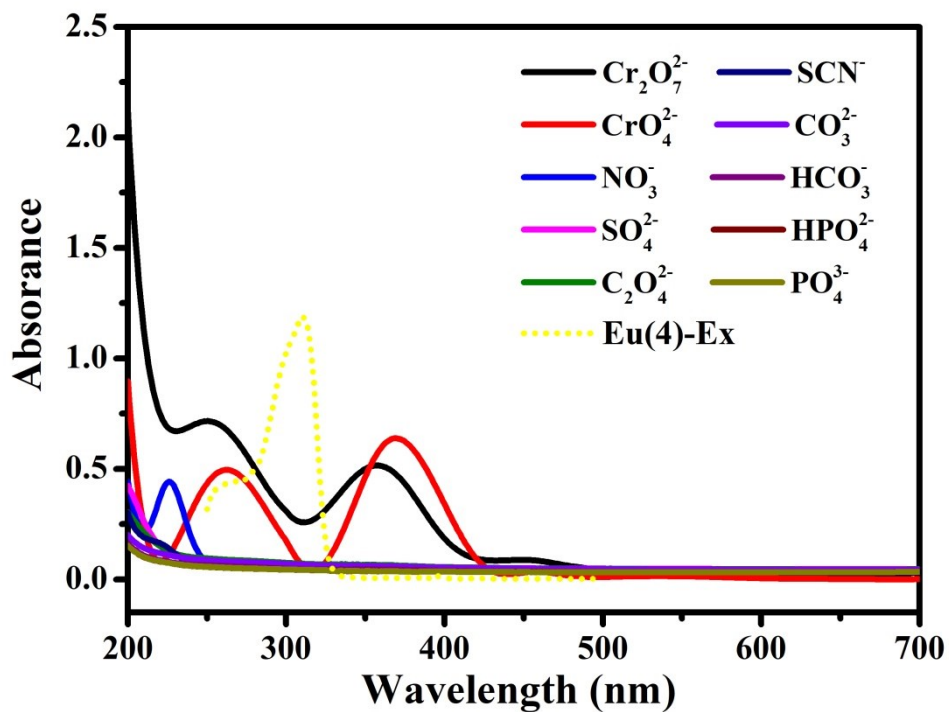


Figure S16. UV-vis spectra of different anions in aqueous solutions, and the excitation spectra of Eu(4).



Reference:

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2. K.-Y. Wu, L. Qin, C. Fan, S.-L. Cai, T.-T. Zhang, W.-H. Chen, X.-Y. Tang and J.-X. Chen, *Dalton Trans.*, 2019, **48**, 8911.
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