

Supporting Information

for

Two series of Ln-MOFs by solvent induced self-assembly demonstrating the rapid selectively sensing of Mg²⁺ and Fe³⁺ cations

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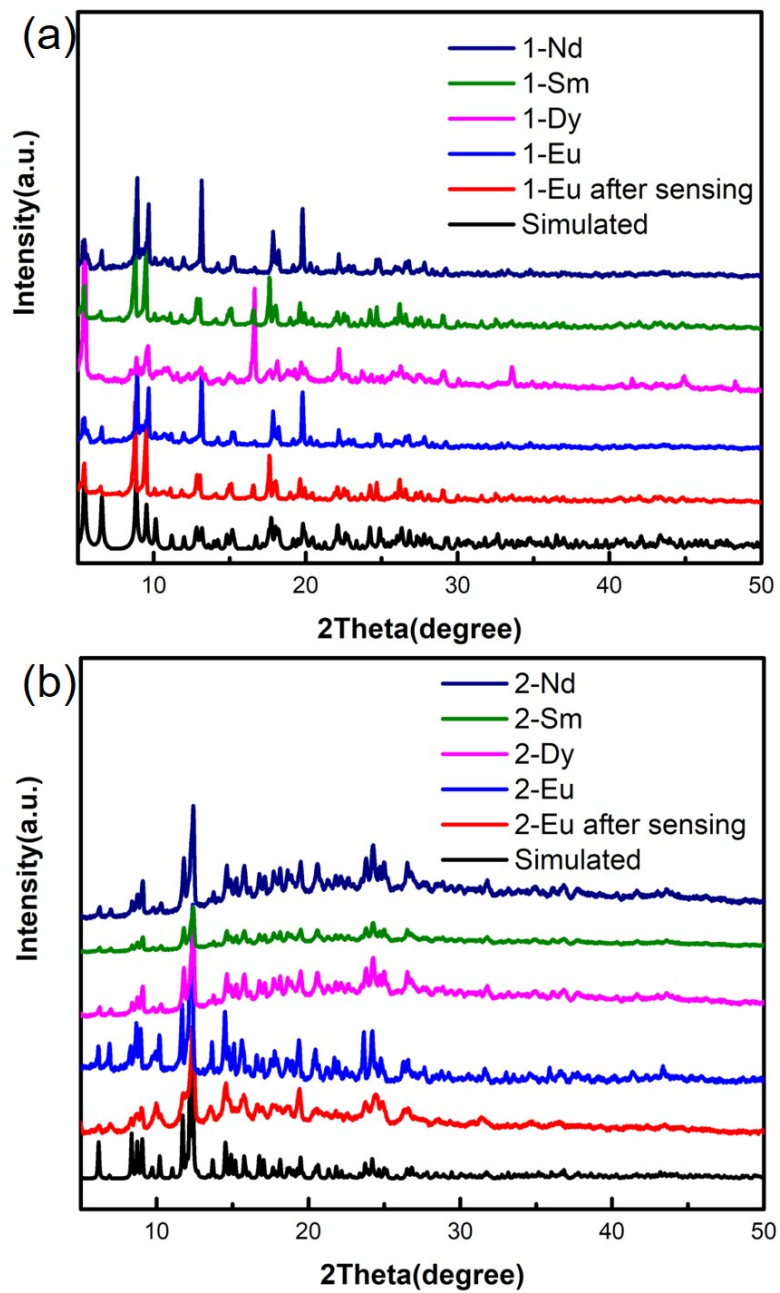


Figure S1 PXR D patterns of the simulated (black), **1-Ln** (a) and **2-Ln** (b).

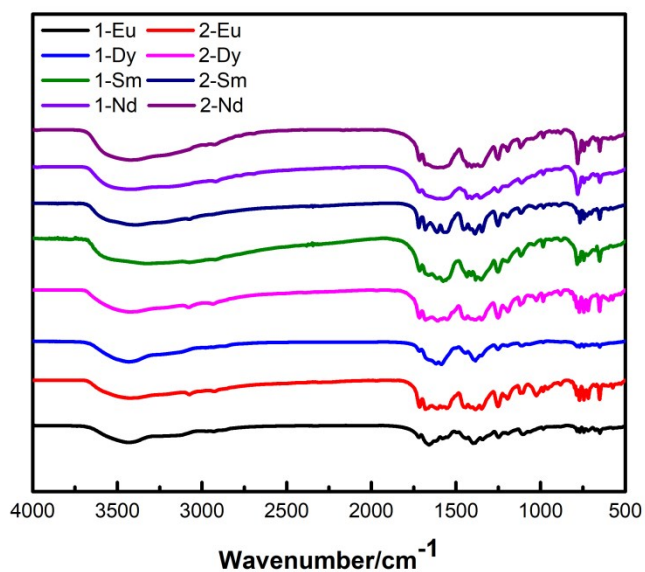


Figure S2 IR spectra of 1-Ln and 2-Ln.

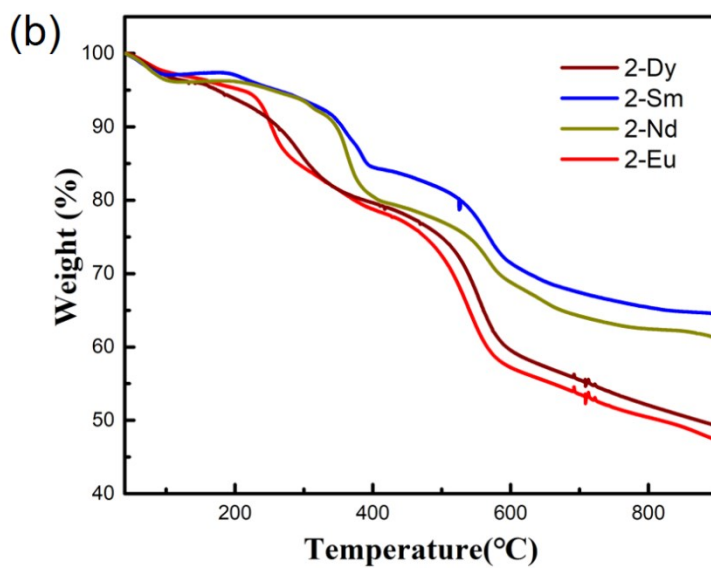
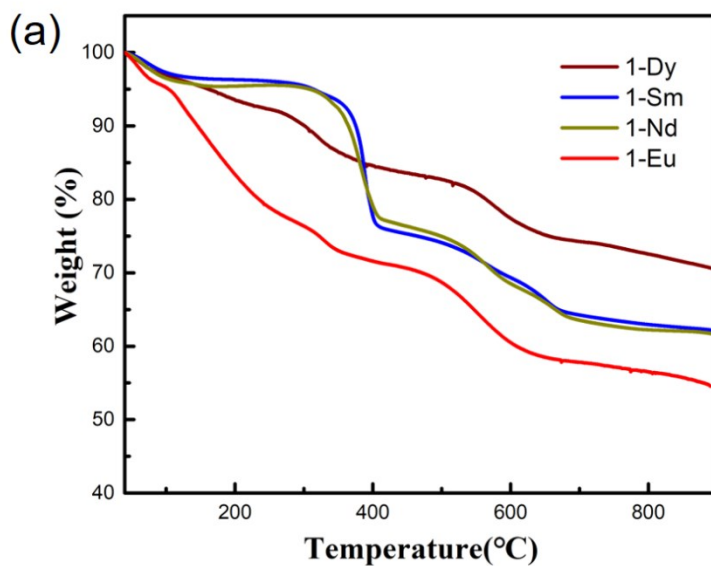


Figure S3 TGA curves of 1-Ln (a) and 2-Ln (b).

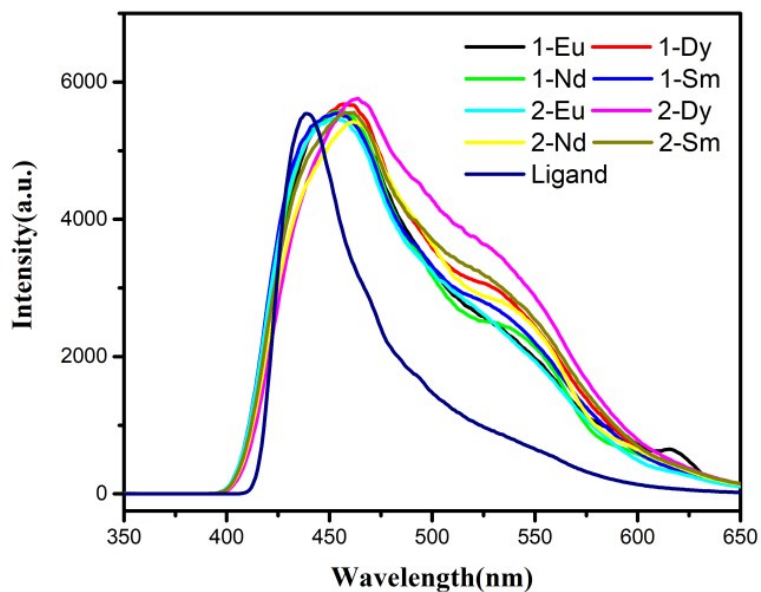


Figure S4 The solid-state fluorescence spectra of ligand, **1-Ln** and **2-Ln**.

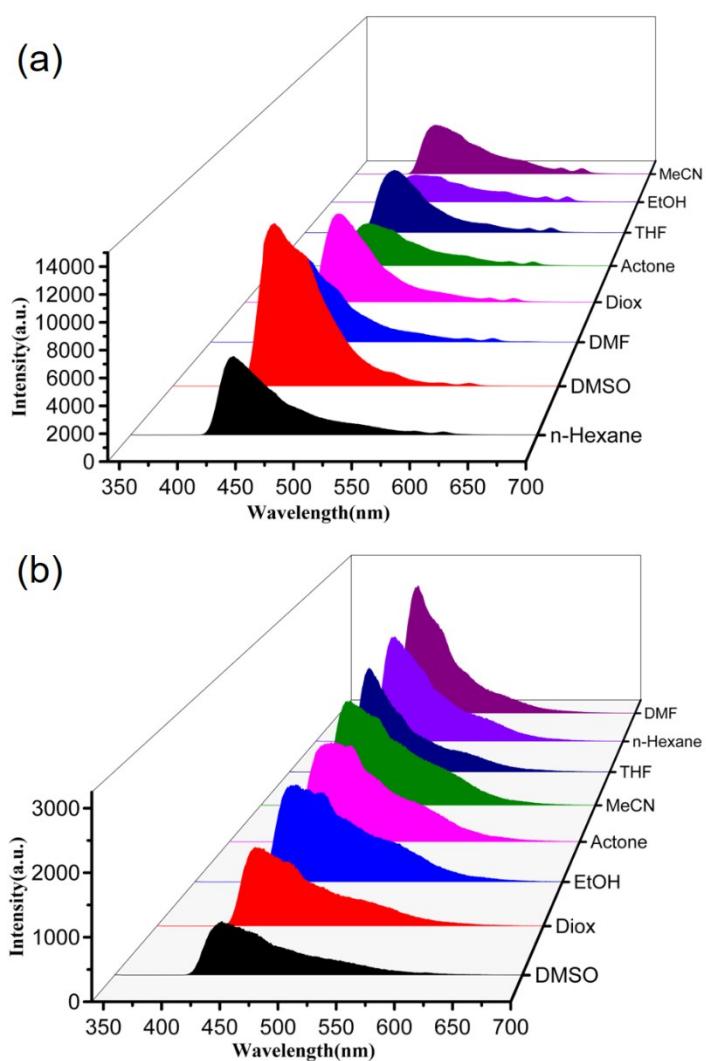


Figure S5 The fluorescence spectra of **1-Eu** (a) and **2-Eu** (b) dispersed in different solvents.

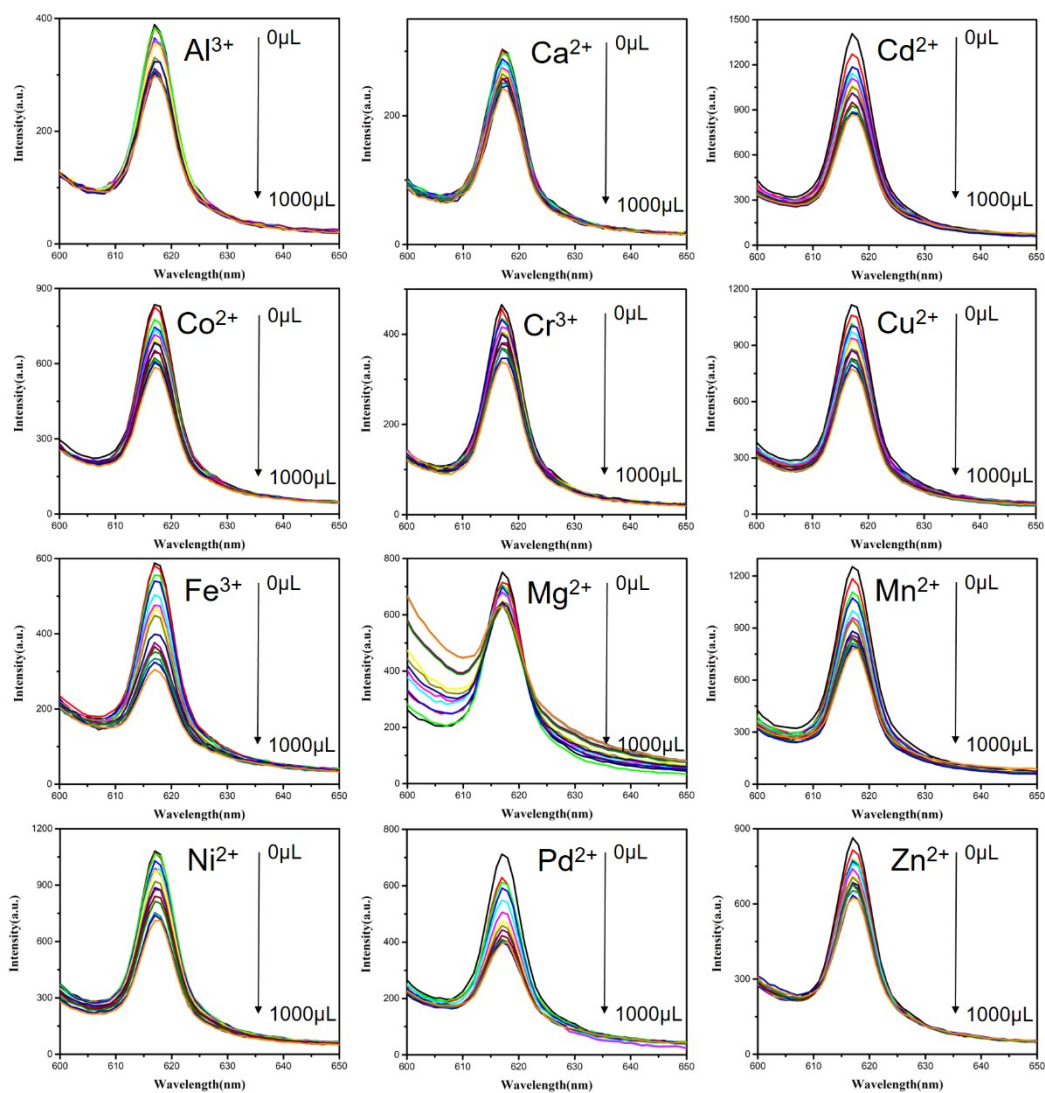


Figure S6 Effect on the emission spectra of **1-Eu** dispersed in EtOH upon incremental addition of a metal ion (Mg^{2+} , Ca^{2+} , Mn^{2+} , Co^{2+} , Ni^{2+} , Cu^{2+} , Zn^{2+} , Cd^{2+} , Pd^{2+} , Al^{3+} , Cr^{3+} or Fe^{3+}) solution (1 mM) in EtOH.

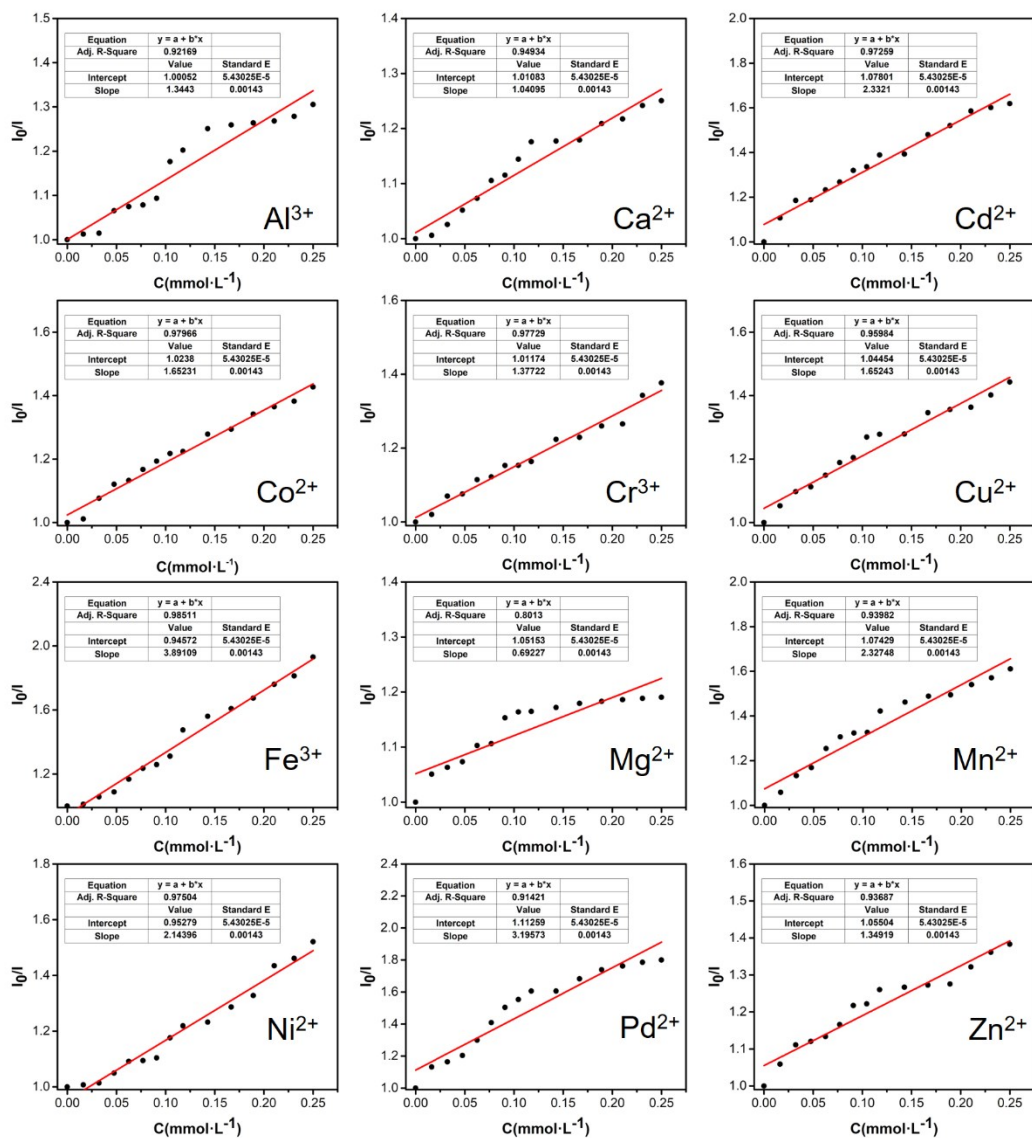


Figure S7 The Stern-Volmer plots of I_0/I versus the ion concentration of 1-Eu.

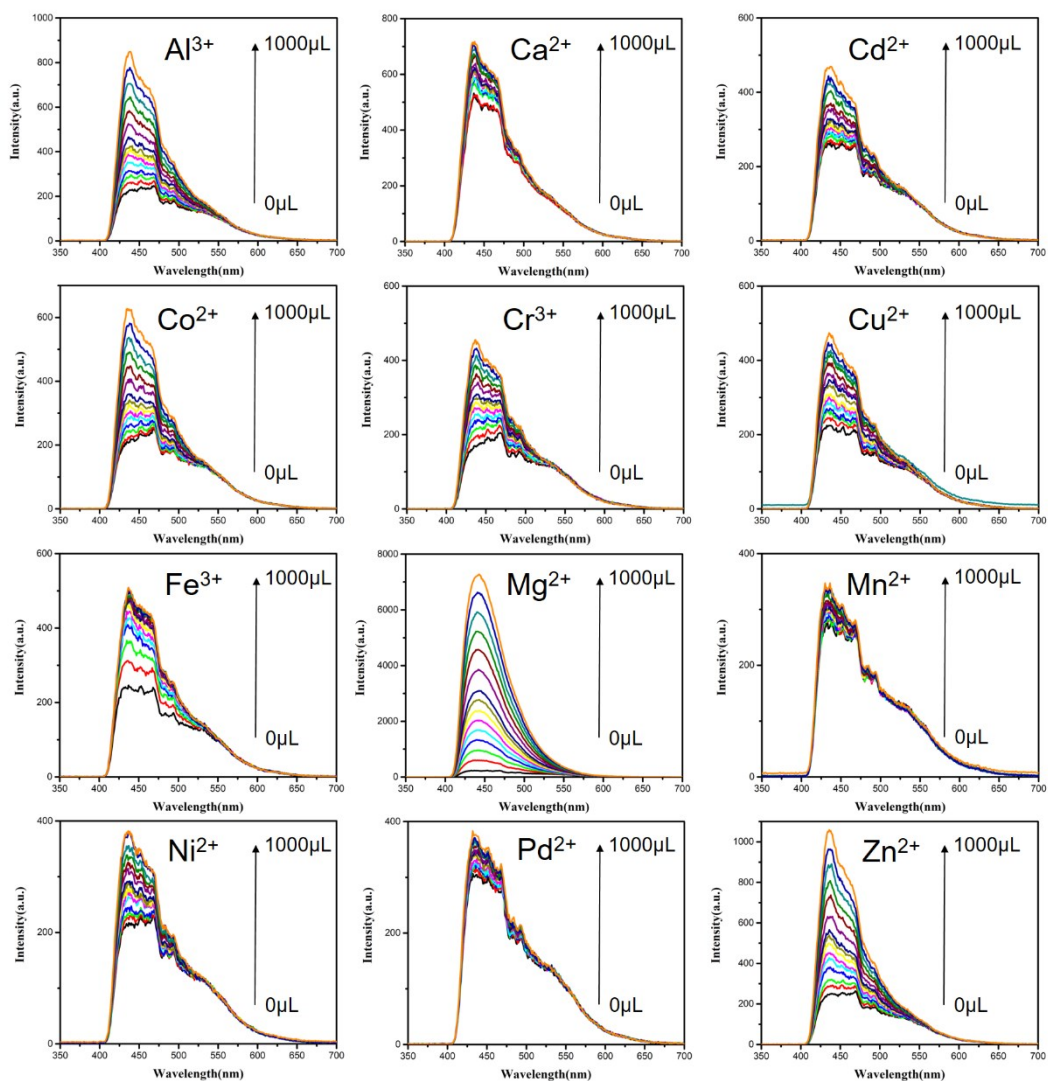


Figure S8 Effect on the emission spectra of **2-Eu** dispersed in EtOH upon incremental addition of a metal ion (Mg²⁺, Ca²⁺, Mn²⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, Pd²⁺, Al³⁺, Cr³⁺ or Fe³⁺) solution (1mM) in EtOH.

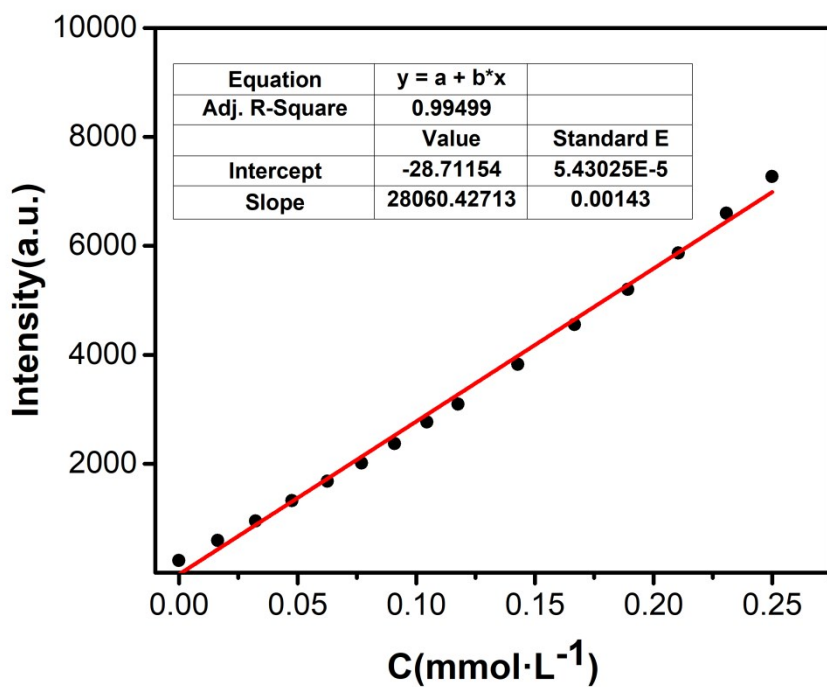


Figure S9 Correlation between the luminescence intensity of 2-Eu and the concentration of Mg^{2+} .

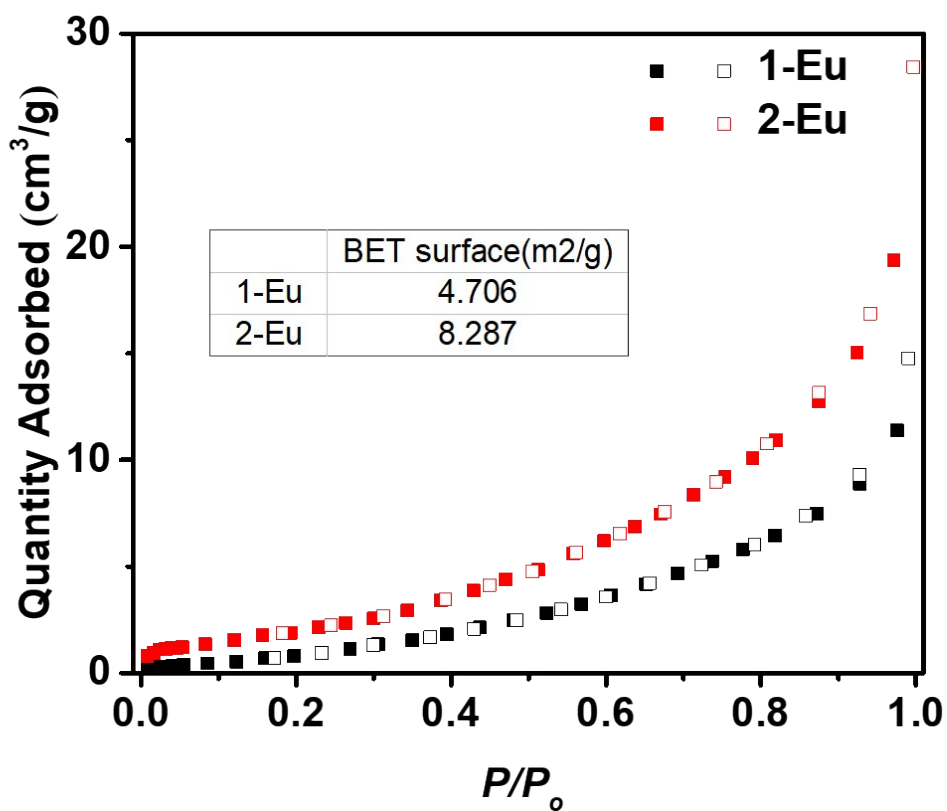


Figure S10 N_2 sorption isotherms of 1-Eu and 2-Eu at 77 K (insert, BET surface).

Table S1. Selected bond lengths (Å) for **1-Eu**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Eu1	O1	2.375(3)	Eu1	O7	2.356(3)
Eu1	O2 ¹	2.392(3)	Eu1	O8 ²	2.567(3)
Eu1	O3	2.536(4)	Eu1	O8 ³	2.464(3)
Eu1	O4	2.492(4)	Eu1	O9 ²	2.468(3)
Eu1	O6	2.423(4)			

Table S2. Selected bond angles (°) for **1-Eu**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Eu1	O2 ¹	135.32(11)	O6	Eu1	O8 ³	81.95(13)
O1	Eu1	O3	73.82(13)	O6	Eu1	O8 ²	137.20(12)
O1	Eu1	O4	124.00(14)	O6	Eu1	O9 ³	71.93(14)
O1	Eu1	O6	142.65(13)	O7	Eu1	O1	85.24(13)
O1	Eu1	O8 ²	70.31(11)	O7	Eu1	O2 ¹	139.33(14)
O1	Eu1	O8 ³	80.81(10)	O7	Eu1	O3	68.56(14)
O1	Eu1	O9 ³	71.34(12)	O7	Eu1	O4	77.73(16)
O2 ¹	Eu1	O3	113.66(13)	O7	Eu1	O6	77.99(15)
O2 ¹	Eu1	O4	75.60(14)	O7	Eu1	O8 ³	124.93(12)
O2 ¹	Eu1	O6	69.55(13)	O7	Eu1	O8 ²	143.41(13)
O2 ¹	Eu1	O8 ³	74.61(11)	O7	Eu1	O9 ³	73.15(12)
O2 ¹	Eu1	O8 ²	68.65(11)	O8 ²	Eu1	O3	78.48(12)
O2 ¹	Eu1	O9 ³	116.84(11)	O8 ²	Eu1	O4	93.49(15)
O3	Eu1	O8 ³	150.31(12)	O8 ²	Eu1	O8 ³	78.63(10)
O4	Eu1	O3	50.25(15)	O8 ²	Eu1	O9 ³	120.69(11)
O4	Eu1	O8 ³	150.04(13)	O9 ³	Eu1	O3	129.50(12)
O6	Eu1	O3	127.73(15)	O9 ³	Eu1	O4	145.75(15)
O6	Eu1	O4	84.81(17)	O9 ³	Eu1	O8 ³	51.87(9)

Table S3. Selected bond lengths (Å) for **1-Nd**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Nd1	O1	2.418(5)	Nd1	O7	2.380(5)
Nd1	O2 ¹	2.442(5)	Nd1	O8 ²	2.619(5)
Nd1	O3	2.571(6)	Nd1	O8 ³	2.517(5)
Nd1	O4	2.545(7)	Nd1	O9 ²	2.525(5)
Nd1	O6	2.448(6)			

Table S4. Selected bond angles (°) for **1-Nd**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Nd1	O2 ¹	134.44(17)	O6	Nd1	O8 ²	81.7(2)
O1	Nd1	O3	74.5(2)	O6	Nd1	O8 ³	135.99(19)
O1	Nd1	O4	123.7(2)	O6	Nd1	O9 ²	72.2(2)
O1	Nd1	O6	142.8(2)	O7	Nd1	O1	86.7(2)
O1	Nd1	O8 ²	78.89(16)	O7	Nd1	O2 ¹	138.8(2)
O1	Nd1	O8 ³	70.24(18)	O7	Nd1	O3	68.9(2)
O1	Nd1	O9 ²	70.90(19)	O7	Nd1	O4	76.5(3)
O2 ¹	Nd1	O3	113.4(2)	O7	Nd1	O6	78.3(2)
O2 ¹	Nd1	O4	76.6(2)	O7	Nd1	O8 ³	144.1(2)
O2 ¹	Nd1	O6	69.1(2)	O7	Nd1	O8 ²	123.88(19)
O2 ¹	Nd1	O8 ²	76.22(18)	O7	Nd1	O9 ²	73.57(19)
O2 ¹	Nd1	O8 ³	68.03(18)	O8 ³	Nd1	O3	78.47(18)
O2 ¹	Nd1	O9 ²	117.05(18)	O8 ³	Nd1	O4	93.5(2)
O3	Nd1	O8 ²	149.76(18)	O8 ³	Nd1	O8 ²	79.26(17)
O4	Nd1	O3	49.2(2)	O8 ³	Nd1	O9 ²	120.61(18)
O4	Nd1	O8 ²	152.7(2)	O9 ²	Nd1	O3	129.59(18)
O6	Nd1	O3	128.5(2)	O9 ²	Nd1	O4	145.7(2)
O6	Nd1	O4	85.8(3)	O9 ²	Nd1	O8 ²	50.40(15)

Table S5. Selected bond lengths (Å) for **2-Eu**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Eu1	O3	2.519(9)	Eu2	O2	2.332(11)
Eu1	O4	2.450(10)	Eu2	O11	3.008(14)
Eu1	O12 ¹	2.338(7)	Eu2	O14 ⁴	2.424(7)
Eu1	O13 ²	2.277(7)	Eu2	O16 ⁵	2.322(8)
Eu1	O15 ³	2.414(7)	Eu2	O18 ⁴	2.449(9)
Eu1	O17 ³	2.455(7)	Eu2	O19	2.538(12)
Eu1	O22	2.327(13)	Eu2	O20	2.446(13)
Eu1	O23	2.413(8)	Eu2	O21	2.256(14)
Eu2	O1	2.35(3)	Eu2	O1A	2.28(2)

Table S6. Selected bond angles (°) for **2-Eu**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Eu1	O3	51.9(3)	O2	Eu2	O11	43.6(4)
O4	Eu1	O17 ¹	85.2(4)	O2	Eu2	O14 ⁴	75.2(3)
O12 ²	Eu1	O3	76.0(3)	O2	Eu2	O18 ⁴	126.3(3)
O12 ²	Eu1	O4	123.2(3)	O2	Eu2	O19	73.5(4)
O12 ²	Eu1	O15 ¹	77.0(3)	O2	Eu2	O20	84.3(4)
O12 ²	Eu1	O17 ¹	118.5(3)	O14 ⁴	Eu2	O11	65.9(3)
O12 ²	Eu1	O23	155.1(3)	O14 ⁴	Eu2	O18 ⁴	52.7(3)
O13 ³	Eu1	O3	76.1(3)	O14 ⁴	Eu2	O19	128.3(4)
O13 ³	Eu1	O4	99.3(4)	O14 ⁴	Eu2	O20	71.8(4)
O13 ³	Eu1	O12 ²	86.7(3)	O16 ⁵	Eu2	O1	84.4(7)
O13 ³	Eu1	O15 ¹	160.4(3)	O16 ⁵	Eu2	O2	87.6(4)
O13 ³	Eu1	O17 ¹	146.5(3)	O16 ⁵	Eu2	O11	82.6(4)
O13 ³	Eu1	O22	85.1(5)	O16 ⁵	Eu2	O14 ⁴	147.5(4)
O13 ³	Eu1	O23	77.0(3)	O16 ⁵	Eu2	O18 ⁴	143.6(4)
O15 ¹	Eu1	O3	89.3(3)	O16 ⁵	Eu2	O19	69.6(4)
O15 ¹	Eu1	O4	81.1(4)	O16 ⁵	Eu2	O20	134.5(5)
O15 ¹	Eu1	O17 ¹	53.0(2)	O18 ⁴	Eu2	O11	111.7(4)
O17 ¹	Eu1	O3	128.5(3)	O18 ⁴	Eu2	O19	127.6(4)
O22	Eu1	O3	148.6(4)	O19	Eu2	O11	112.0(4)
O22	Eu1	O4	158.3(4)	O20	Eu2	O11	118.5(4)
O22	Eu1	O12 ²	78.0(4)	O20	Eu2	O18 ⁴	69.4(5)
O22	Eu1	O15 ¹	101.8(5)	O20	Eu2	O19	65.1(4)
O22	Eu1	O17 ¹	79.8(4)	O21	Eu2	O1	105.2(8)
O22	Eu1	O23	81.8(4)	O21	Eu2	O2	107.5(6)
O23	Eu1	O3	117.1(3)	O21	Eu2	O11	64.2(5)
O23	Eu1	O4	78.6(4)	O21	Eu2	O14 ⁴	83.1(5)
O23	Eu1	O15 ¹	121.9(3)	O21	Eu2	O16 ⁵	76.0(6)
O23	Eu1	O17 ¹	71.4(3)	O21	Eu2	O18 ⁴	80.6(6)
O1	Eu2	O11	164.9(7)	O21	Eu2	O19	145.6(6)
O1	Eu2	O14 ⁴	125.4(7)	O21	Eu2	O20	148.7(6)
O1	Eu2	O18 ⁴	75.2(7)	O1A	Eu2	O2	158.1(6)
O1	Eu2	O19	70.1(7)	O1A	Eu2	O11	148.8(6)
O1	Eu2	O20	76.3(7)	O1A	Eu2	O19	85.4(6)
O2	Eu2	O1	143.3(7)	O1A	Eu2	O20	92.1(7)

Table S7. Selected bond lengths (Å) for **2-Dy**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O3	2.471(6)	Dy2	O18 ⁴	2.475(7)
Dy1	O4	2.407(7)	Dy2	O19	2.451(8)
Dy1	O12 ¹	2.277(5)	Dy2	O20	2.28(3)
Dy1	O13 ²	2.254(6)	Dy2	O21	2.31(2)
Dy1	O15 ³	2.395(6)	Dy2	O20A	2.38(3)
Dy1	O17 ³	2.433(6)	Dy2A	O14 ⁴	2.459(12)
Dy1	O22	2.290(9)	Dy2A	O16 ⁵	2.149(11)
Dy1	O23	2.411(7)	Dy2A	O18 ⁴	2.444(12)
Dy2	O1	2.283(7)	Dy2A	O19	2.83(2)
Dy2	O2	2.314(7)	Dy2A	O1A	2.21(5)
Dy2	O14 ⁴	2.436(5)	Dy2A	O11A	2.19(5)
Dy2	O16 ⁵	2.314(6)	Dy2A	O21A	1.91(3)

Table S8. Selected bond angles (°) for **2-Dy**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Dy1	O3	52.67(19)	O2	Dy2	O19	77.8(3)
O4	Dy1	O17 ¹	86.2(3)	O2	Dy2	O21	84.7(6)
O4	Dy1	O23	74.7(3)	O2	Dy2	O20A	85.8(6)
O12 ²	Dy1	O3	76.0(2)	O14 ⁴	Dy2	O18 ⁴	52.14(19)
O12 ²	Dy1	O4	124.7(2)	O14 ⁴	Dy2	O19	133.6(3)
O12 ²	Dy1	O15 ¹	77.1(2)	O16 ⁵	Dy2	O14 ⁴	141.5(3)
O12 ²	Dy1	O17 ¹	117.1(2)	O16 ⁵	Dy2	O18 ⁴	137.6(3)
O12 ²	Dy1	O22	79.5(3)	O16 ⁵	Dy2	O19	70.1(3)
O12 ²	Dy1	O23	157.3(2)	O16 ⁵	Dy2	O21	67.0(7)
O13 ³	Dy1	O3	78.1(2)	O16 ⁵	Dy2	O20A	139.9(7)
O13 ³	Dy1	O4	99.4(3)	O19	Dy2	O18 ⁴	136.6(3)
O13 ³	Dy1	O12 ²	87.5(2)	O20	Dy2	O2	99.0(5)
O13 ³	Dy1	O15 ¹	160.4(2)	O20	Dy2	O14 ⁴	79.2(6)
O13 ³	Dy1	O17 ¹	145.7(2)	O20	Dy2	O16 ⁵	137.4(7)
O13 ³	Dy1	O22	83.0(3)	O20	Dy2	O18 ⁴	70.6(7)
O13 ³	Dy1	O23	76.8(2)	O20	Dy2	O19	69.9(7)
O15 ¹	Dy1	O3	86.3(2)	O20	Dy2	O21	155.2(9)
O15 ¹	Dy1	O4	80.0(3)	O20	Dy2	O20A	13.5(8)
O15 ¹	Dy1	O17 ¹	53.87(19)	O21	Dy2	O14 ⁴	78.3(6)
O15 ¹	Dy1	O23	121.3(2)	O21	Dy2	O18 ⁴	87.4(7)
O17 ¹	Dy1	O3	128.7(2)	O21	Dy2	O19	134.4(7)
O22	Dy1	O3	149.6(2)	O21	Dy2	O20A	150.5(8)

O22	Dy1	O4	155.6(3)	O20A	Dy2	O14 ⁴	72.3(6)
O22	Dy1	O15 ¹	105.7(3)	O20A	Dy2	O18 ⁴	75.9(7)
O22	Dy1	O17 ¹	78.9(3)	O20A	Dy2	O19	69.9(7)
O22	Dy1	O23	82.3(3)	O14 ⁴	Dy2A	O19	116.1(7)
O23	Dy1	O3	115.7(3)	O16 ⁵	Dy2A	O14 ⁴	153.3(7)
O23	Dy1	O17 ¹	72.1(2)	O16 ⁵	Dy2A	O18 ⁴	152.8(5)
O1	Dy2	O2	155.2(3)	O16 ⁵	Dy2A	O19	65.1(6)
O1	Dy2	O14 ⁴	126.7(2)	O16 ⁵	Dy2A	O1A	80.4(13)
O1	Dy2	O16 ⁵	83.0(3)	O16 ⁵	Dy2A	O11A	81.2(16)
O1	Dy2	O18 ⁴	75.4(3)	O18 ⁴	Dy2A	O14 ⁴	52.2(3)
O1	Dy2	O19	77.5(3)	O18 ⁴	Dy2A	O19	120.3(9)
O1	Dy2	O20	74.6(6)	O1A	Dy2A	O19	82.6(12)
O1	Dy2	O21	111.4(6)	O11A	Dy2A	O19	75.5(13)
O1	Dy2	O20A	87.9(6)	O11A	Dy2A	O1A	155.8(19)
O2	Dy2	O14 ⁴	73.7(2)	O21A	Dy2A	O19	150.9(8)
O2	Dy2	O16 ⁵	86.5(3)	O21A	Dy2A	O1A	86.3(12)
O2	Dy2	O18 ⁴	125.8(3)	O21A	Dy2A	O11A	108.1(16)

Table S9. Selected bond lengths (Å) for **2-Sm**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sm1	O3	2.492(6)	Sm2	O2	2.372(6)
Sm1	O4	2.485(7)	Sm2	O11	2.938(12)
Sm1	O12 ¹	2.338(5)	Sm2	O14 ⁴	2.459(5)
Sm1	O13 ²	2.305(5)	Sm2	O16 ⁵	2.366(6)
Sm1	O15 ³	2.443(5)	Sm2	O18 ⁴	2.540(6)
Sm1	O17 ³	2.457(5)	Sm2	O19	2.519(7)
Sm1	O22	2.351(8)	Sm2	O20	2.419(8)
Sm1	O23	2.446(7)	Sm2	O21	2.475(11)
Sm2	O1	2.333(11)	Sm2	O1A	2.374(14)

Table S10. Selected bond angles (°) for **2-Sm**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Sm1	O3	51.80(18)	O1	Sm2	O21	83.0(4)
O12 ¹	Sm1	O3	76.34(19)	O2	Sm2	O11	45.8(3)
O12 ¹	Sm1	O4	124.7(2)	O2	Sm2	O14 ⁴	74.7(2)
O12 ¹	Sm1	O15 ²	78.53(19)	O2	Sm2	O18 ⁴	124.9(2)
O12 ¹	Sm1	O17 ²	118.7(2)	O2	Sm2	O19	72.0(2)
O12 ¹	Sm1	O22	79.2(2)	O2	Sm2	O20	85.4(3)
O12 ¹	Sm1	O23	156.2(2)	O2	Sm2	O21	116.0(4)

O13 ³	Sm1	O3	77.7(2)	O2	Sm2	O1A	141.6(4)
O13 ³	Sm1	O4	98.3(2)	O14 ⁴	Sm2	O11	67.8(2)
O13 ³	Sm1	O12 ¹	86.66(19)	O14 ⁴	Sm2	O18 ⁴	51.69(17)
O13 ³	Sm1	O15 ²	160.36(19)	O14 ⁴	Sm2	O19	131.0(2)
O13 ³	Sm1	O17 ²	146.80(19)	O14 ⁴	Sm2	O21	82.9(3)
O13 ³	Sm1	O22	84.2(3)	O16 ⁵	Sm2	O2	92.2(2)
O13 ³	Sm1	O23	76.6(2)	O16 ⁵	Sm2	O11	79.1(2)
O15 ²	Sm1	O3	86.3(2)	O16 ⁵	Sm2	O14 ⁴	144.1(3)
O15 ²	Sm1	O4	80.1(3)	O16 ⁵	Sm2	O18 ⁴	138.0(2)
O15 ²	Sm1	O17 ²	52.82(18)	O16 ⁵	Sm2	O19	72.0(3)
O15 ²	Sm1	O23	121.1(2)	O16 ⁵	Sm2	O20	139.8(3)
O17 ²	Sm1	O3	126.6(2)	O16 ⁵	Sm2	O21	73.0(4)
O17 ²	Sm1	O4	84.9(2)	O16 ⁵	Sm2	O1A	86.3(4)
O22	Sm1	O3	150.2(2)	O18 ⁴	Sm2	O11	111.4(2)
O22	Sm1	O4	156.0(2)	O19	Sm2	O11	109.1(2)
O22	Sm1	O15 ²	105.3(3)	O19	Sm2	O18 ⁴	133.2(2)
O22	Sm1	O17 ²	80.4(3)	O20	Sm2	O11	123.3(3)
O22	Sm1	O23	82.4(3)	O20	Sm2	O14 ⁴	73.4(3)
O23	Sm1	O3	115.4(3)	O20	Sm2	O18 ⁴	69.6(3)
O23	Sm1	O4	75.1(3)	O20	Sm2	O19	69.1(3)
O23	Sm1	O17 ²	72.3(2)	O20	Sm2	O21	142.7(4)
O1	Sm2	O2	155.9(4)	O21	Sm2	O11	70.2(3)
O1	Sm2	O11	149.2(4)	O21	Sm2	O18 ⁴	73.1(3)
O1	Sm2	O14 ⁴	124.8(3)	O21	Sm2	O19	144.4(3)
O1	Sm2	O16 ⁵	78.8(4)	O1A	Sm2	O11	164.3(4)
O1	Sm2	O18 ⁴	73.1(3)	O1A	Sm2	O19	71.0(4)
O1	Sm2	O19	83.9(4)	O1A	Sm2	O20	72.0(4)
O1	Sm2	O20	87.3(4)	O1A	Sm2	O21	100.2(5)

Table S11. ICP analysis results of **1-Eu** and **2-Eu**.

Name	Weight/mg	Volume/mL	Ion	Concentration/mg L ⁻¹	Weight Percentage/wt.%
1-Eu	17.6	100	Fe ³⁺	0.041	0.023
1-Eu	16.3	100	Zn ²⁺	-0.021	-
2-Eu	17.2	100	Mg ²⁺	0.186	0.108
2-Eu	15.9	100	Zn ²⁺	-0.030	-