Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Ultrahigh luminescence quantum yield lanthanide coordination polymer as multifunctional sensor

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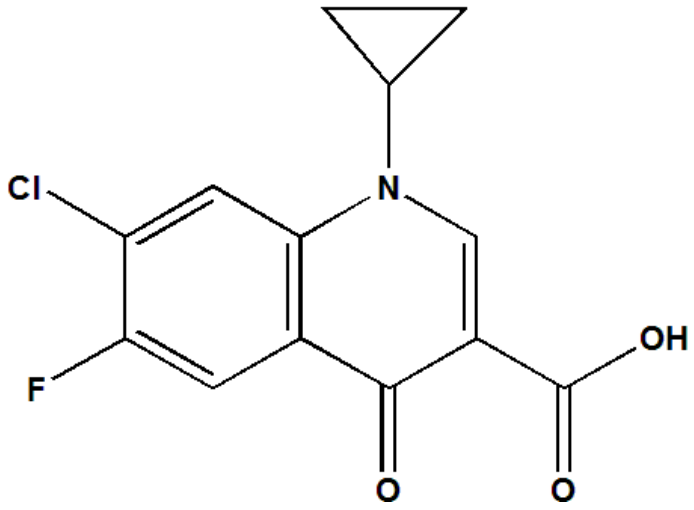

Scheme S1. Structure of the ligand 7-chloro-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid.

Table S1. Crystallographic data and structure refinement parameters for the three series of Ln-CPs**.**

Complex	**1a**	**1b**	**1c**	**1d**	**2a**	**2b**	**2c**	**2d**	**2e**	**2f**
CCDC	1855008	1855010	1855011	1855009	1855015	1855012	1855013	1855014	1855017	1855016
Empirical formula	$EuNaC_{52}Cl_4F_4H_{40}N_4O_{16}$	$GdNaC_{52}Cl_4F_4H_{40}N_4O_{16}$	$TbNaC_{52}Cl_4F_4H_{40}N_4O_{16}$	$HoNaC_{52}Cl_4F_4H_{40}N_4O_{16}$	$EuKC_{52}Cl_4F_4H_{38}N_4O_{15}$	$PrKC_{52}Cl_4F_4H_{38}N_4O_{15}$	$TbKC_{52}Cl_4F_4H_{38}N_4O_{15}$	$DyKC_{52}Cl_4F_4H_{38}N_4O_{15}$	$ErKC_{52}Cl_4F_4H_{38}N_4O_{15}$	$YbKC_{52}Cl_4F_4H_{38}N_4O_{15}$
Formula weight	1369.63	1374.92	1376.60	1382.60	1367.74	1356.67	1374.69	1378.26	1383.02	1388.80
Temperature / K	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
Wavelength / Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P-1
a / Å	10.0557(4)	10.0529(2)	10.0564(2)	10.0685(2)	10.0373(6)	10.0279(3)	10.0496(3)	10.0542(5)	10.0569(5)	10.0457(4)
b / Å	12.7534(5)	12.7458(3)	12.7324(4)	12.7366(3)	12.7525(8)	12.7769(4)	12.7645(4)	12.7549(7)	12.7687(6)	12.7511(5)
c / Å	22.0808(8)	22.0524(5)	22.0394(7)	22.0035(7)	21.8207(14)	22.0478(7)	21.6687(7)	21.7465(12)	21.6123(9)	21.5609(8)
α / °	73.488(3)	73.527(2)	73.580(3)	73.668(2)	74.266(6)	73.703(3)	74.538(3)	74.531(5)	74.868(4)	74.844(3)
β / °	85.530(3)	85.433(2)	85.371(2)	85.270(2)	86.381(3)	86.366(2)	86.700(3)	86.276(4)	86.659(4)	86.508(3)
γ / °	72.201(4)	72.228(2)	72.185(2)	72.024(2)	72.833(6)	72.703(3)	73.095(3)	72.965(5)	72.925(4)	72.910(3)
V / $Å^3$	2584.88(17)	2580.26(10)	2577.03(13)	2575.63(11)	2568.2(3)	2588.14(14)	2562.65(14)	2575.63(11)	2560.9(2)	2548.62(18)
Z	2	2	2	2	2	2	2	2	2	2
Calculated density/$mg{\cdot}m^{-3}$	1.760	1.770	1.774	1.783	1.769	1.741	1.782	1.781	1.794	1.810
F(000)	1372	1374	1376	1380	1352	1360	1372	1374	1378	1382
Data/restraints/ parameters	9006/0/745	8891/0/745	9007/1/751	8802/0/745	17062/0/731	9069/0/751	8985/0/748	9005/0/735	11405/0/730	11307/0/730
Goodness-of-fit on F^2	1.005	1.006	1.006	1.006	1.039	1.057	1.024	1.013	1.083	1.082
Final R indices [a][I > 2sigma(I)]	R1=0.0379, wR2=0.0852	R1=0.0320, wR2=0.0832	R1=0.0397, wR2=0.0955	R1=0.0355 wR2=0.0907	R1=0.0515 wR2=0.1289	R1=0.0382, wR2=0.0795	R1=0.0367, wR2=0.0833	R1=0.0666 wR2=0.1510	R1=0.0607 wR2=0.1415	R1=0.0588, wR2=0.1324

[a] $R = \sum||Fo|-|Fc||/\sum|Fo|$, $wR = [\sum w(|Fo^2|-|Fc^2|)^2/\sum w(|Fo^2|)^2]^{1/2}$

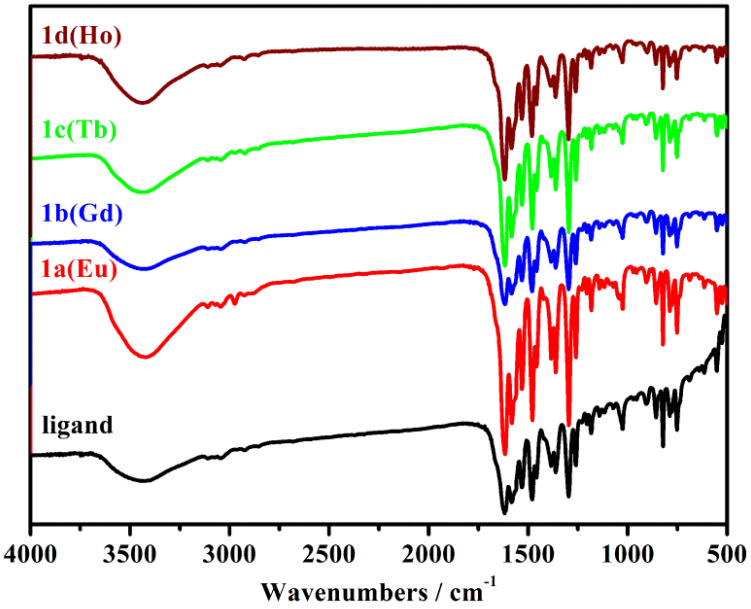

Fig. S1. FT-IR spectra of the ligand, **1a-1d**.

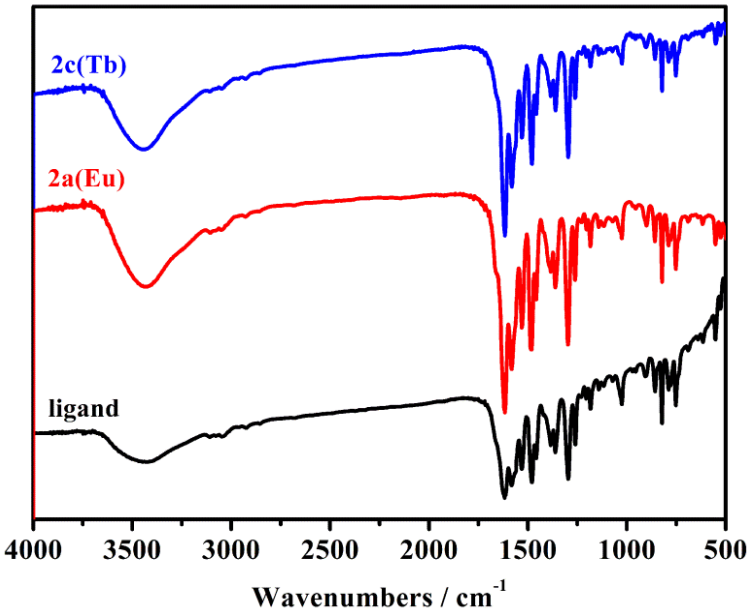

Fig. S2. FT-IR spectra of the ligand, **2a** and **2c**.

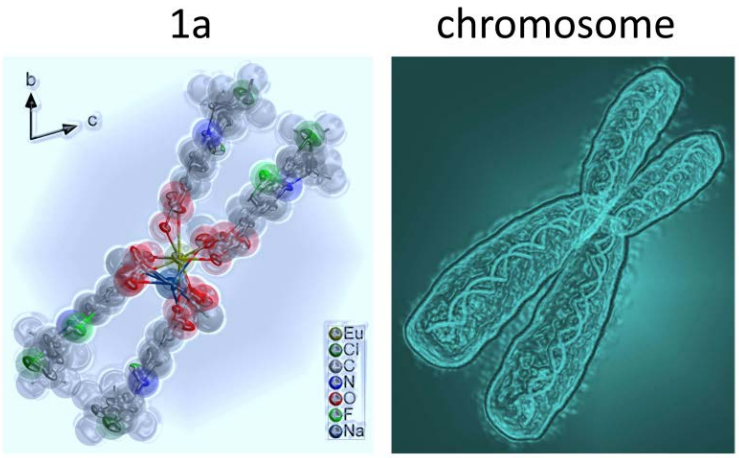

Fig. S3. The structure of **1a** is similar to the chromosome.

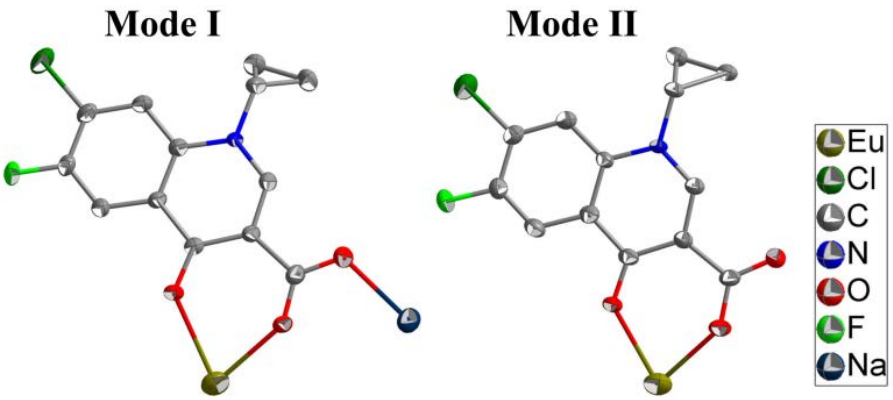

Fig. S4. Ligand coordination modes in **1a**.

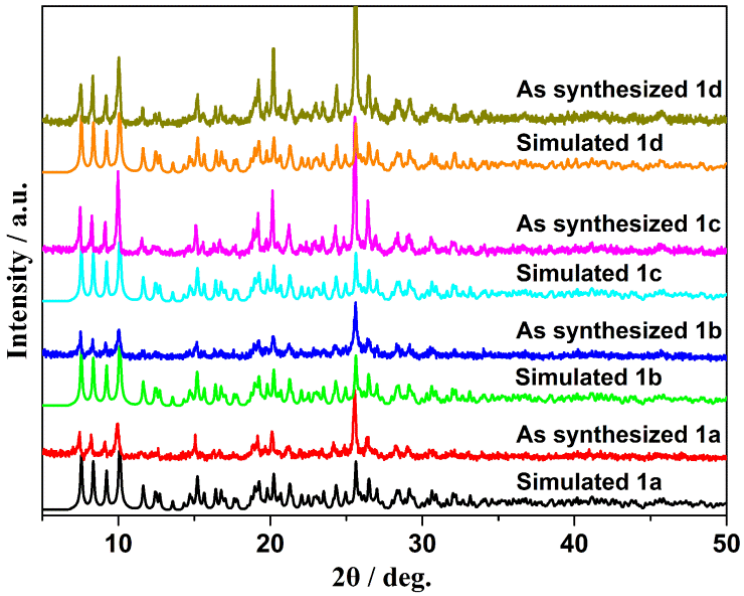

Fig. S5. PXRD peak positions of as synthesized **1a-1d** compete well with their simulated results.

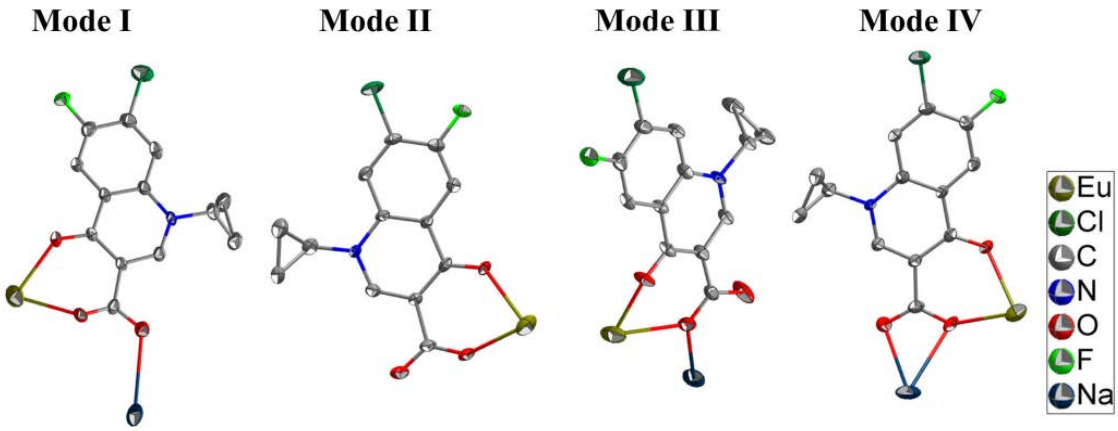

Fig. S6. Ligand coordination modes in **2a**.

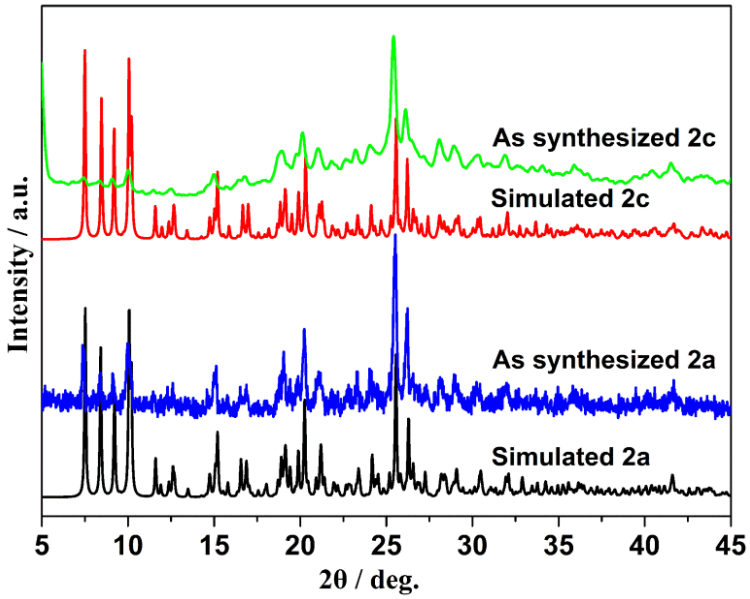

Fig. S7. PXRD peak positions comparison of as synthesized **2a**, **2c** and their simulated results.

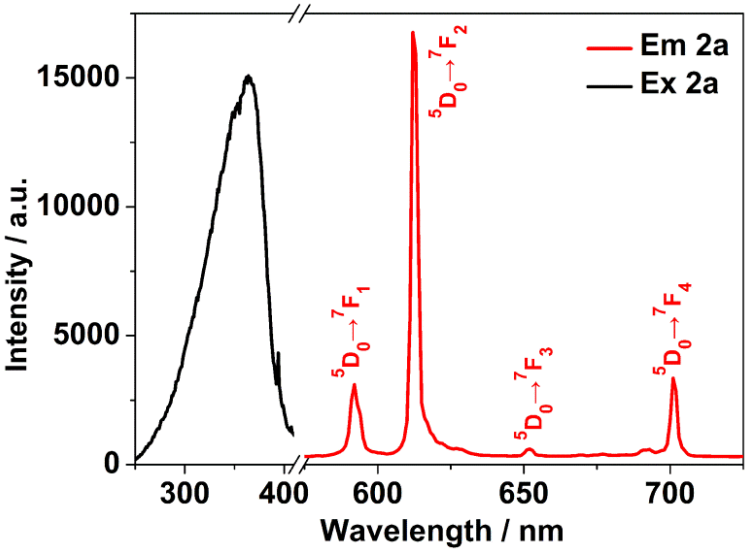

Fig. S8. Excitation and emission spectra of solid sample **2a**.

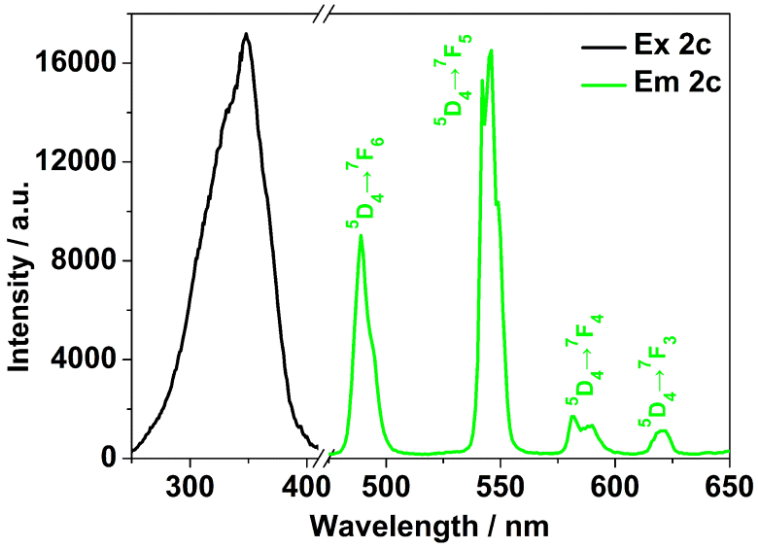

Fig. S9. Excitation and emission spectra of solid sample **2c**.

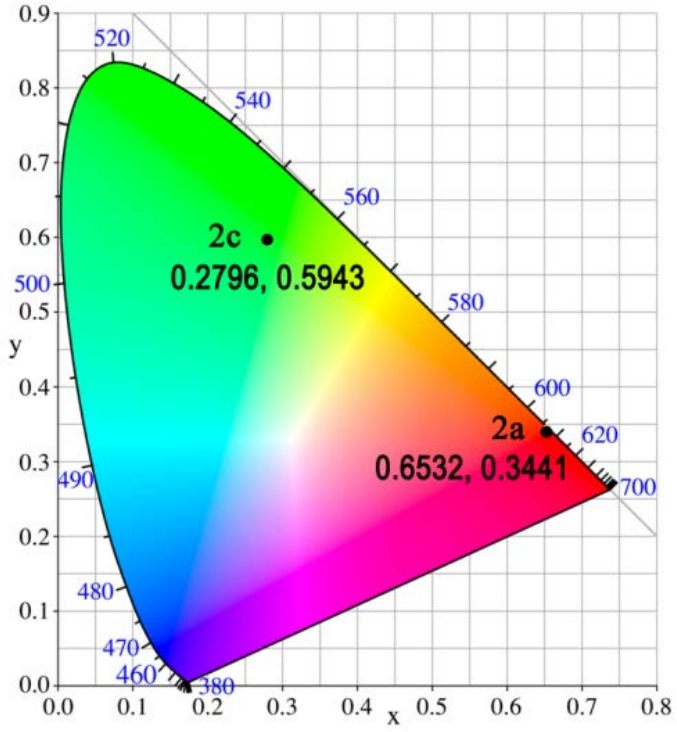

Fig. S10. CIE coordinate diagram of **2a** and **2c**.

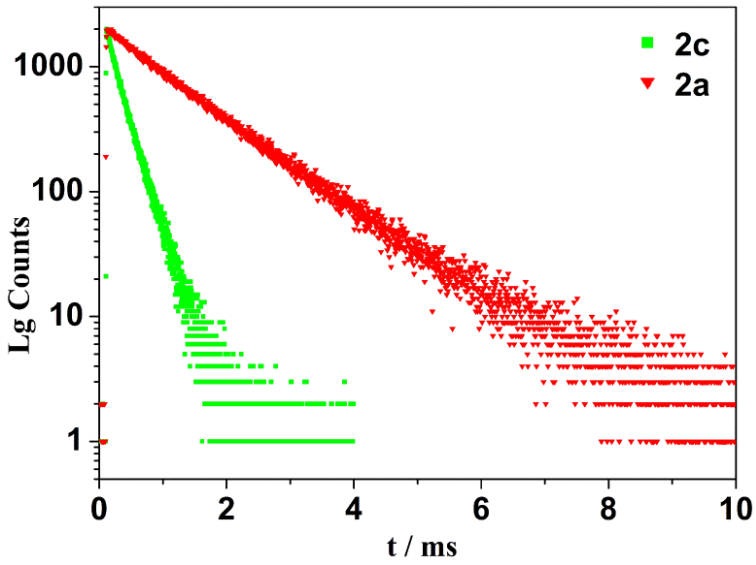

Fig. S11. Luminescence decay of **2a** and **2c**, R(t) = 0.691 + 490.123exp$^{(-t/0.755)}$ + 1400.028exp$^{(-t/1.262)}$ and R(t) = 0.521 + 1794.646exp$^{(-t/0.238)}$ are utilized for fitting the luminescence decay curve of **2a** and **2c**. The best parameters of χ^2 are 1.148 and 1.109, lifetimes are 0.94 and 0.238 for **2a** and **2c**, respectively.

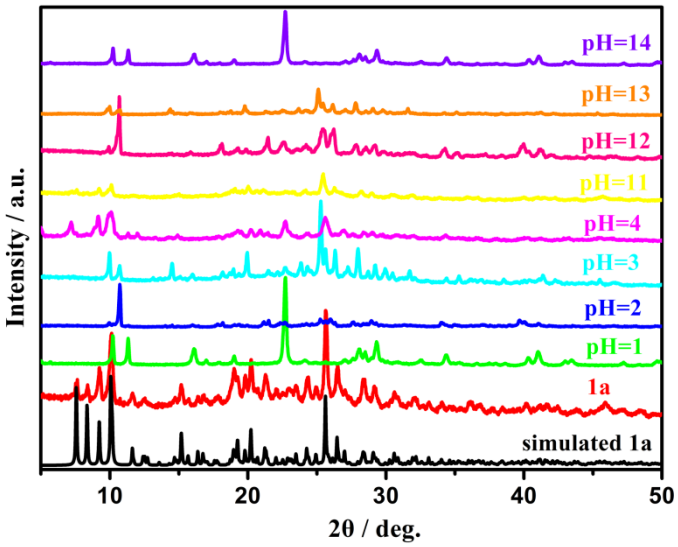

Fig. S12. PXRD of **1a** soaked in solution with various pH.

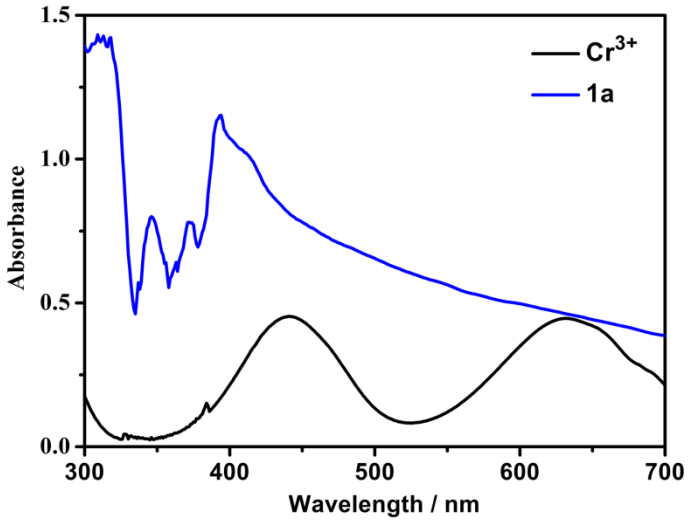

Fig. S13. UV-vis of Cr^{3+} and **1a** sloutions.

Table S2. Selected bond lengths and bond angles of **1a**.

Eu(2)-O(4)	2.332(3)	Eu(2)-O(9)	2.388(3)
Eu(2)-O(10)	2.345(3)	Eu(2)-O(3)	2.402(3)
Eu(2)-O(7)	2.365(3)	Eu(2)-O(6)	2.464(2)
Eu(2)-O(1)	2.379(3)	Eu(2)-O(12)	2.506(3)
O(4)-Eu(2)-O(10)	108.37(11)	O(1)-Eu(2)-O(6)	73.90(9)
O(4)-Eu(2)-O(7)	83.40(10)	O(9)-Eu(2)-O(6)	142.48(8)
O(10)-Eu(2)-O(7)	137.92(9)	O(3)-Eu(2)-O(6)	75.94(9)
O(4)-Eu(2)-O(1)	137.27(9)	O(4)-Eu(2)-O(12)	75.92(9)
O(10)-Eu(2)-O(1)	85.41(10)	O(10)-Eu(2)-O(12)	69.85(9)
O(7)-Eu(2)-O(1)	113.57(10)	O(7)-Eu(2)-O(12)	74.59(9)
O(4)-Eu(2)-O(9)	145.43(9)	O(1)-Eu(2)-O(12)	144.92(9)
O(10)-Eu(2)-O(9)	77.63(10)	O(9)-Eu(2)-O(12)	74.57(9)
O(7)-Eu(2)-O(9)	71.76(9)	O(3)-Eu(2)-O(12)	140.42(9)
O(1)-Eu(2)-O(9)	76.13(9)	O(6)-Eu(2)-O(12)	121.90(9)
O(4)-Eu(2)-O(3)	79.06(11)	O(9)-Eu(2)-O(3)	114.17(11)
O(10)-Eu(2)-O(3)	148.35(9)	O(4)-Eu(2)-O(6)	70.13(9)
O(7)-Eu(2)-O(3)	72.47(9)	O(10)-Eu(2)-O(6)	77.96(9)
O(1)-Eu(2)-O(3)	70.41(9)	O(7)-Eu(2)-O(6)	141.95(8)

Table S3. Selected bond lengths and bond angles of **1b**.

Gd(1)-O(10)	2.321(2)	Gd(1)-O(3)	2.378(2)
Gd(1)-O(4)	2.337(2)	Gd(1)-O(9)	2.388(2)
Gd(1)-O(1)	2.352(2)	Gd(1)-O(12)	2.453(2)
Gd(1)-O(7)	2.368(2)	Gd(1)-O(6)	2.487(2)
O(10)-Gd(1)-O(4)	108.31(9)	O(1)-Gd(1)-O(12)	141.99(7)
O(10)-Gd(1)-O(1)	83.11(9)	O(7)-Gd(1)-O(12)	74.02(8)
O(4)-Gd(1)-O(1)	138.04(8)	O(3)-Gd(1)-O(12)	142.33(8)
O(10)-Gd(1)-O(7)	137.76(8)	O(9)-Gd(1)-O(12)	75.95(8)
O(4)-Gd(1)-O(7)	85.13(9)	O(10)-Gd(1)-O(6)	75.60(8)
O(1)-Gd(1)-O(7)	113.78(9)	O(4)-Gd(1)-O(6)	70.06(8)
O(10)-Gd(1)-O(3)	145.26(8)	O(1)-Gd(1)-O(6)	74.42(8)
O(4)-Gd(1)-O(3)	77.65(8)	O(7)-Gd(1)-O(6)	144.75(8)
O(1)-Gd(1)-O(3)	71.96(8)	O(3)-Gd(1)-O(6)	74.65(8)
O(7)-Gd(1)-O(3)	75.87(8)	O(12)-Gd(1)-O(6)	121.85(8)
O(3)-Gd(1)-O(9)	114.39(9)	O(10)-Gd(1)-O(9)	79.03(9)
O(10)-Gd(1)-O(12)	70.39(8)	O(4)-Gd(1)-O(9)	148.25(8)
O(4)-Gd(1)-O(12)	77.73(8)	O(1)-Gd(1)-O(9)	72.54(8)
O(9)-Gd(1)-O(6)	140.23(8)		

Table S4. Selected bond lengths and bond angles of **1c**.

Tb(1)-O(20)	2.302(13)	Tb(1)-O(22)	2.368(12)
Tb(1)-O(11)	2.313(13)	Tb(1)-O(23)	2.377(13)
Tb(1)-O(13)	2.332(12)	Tb(1)-O(21)	2.442(11)
Tb(1)-O(18)	2.352(12)	Tb(1)-O(12)	2.476(12)
O(20)-Tb(1)-O(11)	108.1(5)	O(22)-Tb(1)-O(21)	74.1(4)
O(20)-Tb(1)-O(13)	83.1(5)	O(23)-Tb(1)-O(21)	142.0(4)
O(11)-Tb(1)-O(13)	138.7(4)	O20)-Tb(1)-O(12)	75.8(4)
O(20)-Tb(1)-O(18)	137.9(4)	O(11)-Tb(1)-O(12)	75.3(4)
O(11)-Tb(1)-O(18)	85.1(5)	O(13)-Tb(1)-O(12)	70.6(4)
O(13)-Tb(1)-O(18)	113.5(5)	O(18)-Tb(1)-O(12)	74.5(4)

O(20)-Tb(1)-O(22)	145.3(4)	O(22)-Tb(1)-O(12)	145.0(5)
O(11)-Tb(1)-O(22)	77.8(5)	O(23)-Tb(1)-O(12)	74.8(4)
O(13)-Tb(1)-O(22)	72.3(4)	O(21)-Tb(1)-O(12)	139.8(4)
O(18)-Tb(1)-O(22)	75.7(4)	O(18)-Tb(1)-O(21)	131.5(12)
O(20)-Tb(1)-O(23)	78.7(5)	O(22)-Tb(1)-O(23)	114.9(5)
O(11)-Tb(1)-O(23)	147.9(4)	O(20)-Tb(1)-O(21)	70.5(4)
O(13)-Tb(1)-O(23)	72.3(4)	O(11)-Tb(1)-O(21)	77.3(4)
O(18)-Tb(1)-O(23)	71.1(5)	O(13)-Tb(1)-O(21)	141.9(4)

Table S5. Selected bond lengths and bond angles of **1d**.

Ho(2)-O(1)	2.297(3)	Ho(2)-O(6)	2.340(3)
Ho(2)-O(4)	2.314(3)	Ho(2)-O(9)	2.354(3)
Ho(2)-O(7)	2.325(3)		
O(10)-Ho(2)-O(1)	107.83(11)	O(10)-Ho(2)-O(6)	144.96(9)
O(10)-Ho(2)-O(4)	83.01(10)	O(1)-Ho(2)-O(6)	77.71(10)
O(1)-Ho(2)-O(4)	19.26(9)	O(4)-Ho(2)-O(6)	72.64(9)
O(10)-Ho(2)-O(7)	138.85(9)	O(7)-Ho(2)-O(6)	75.27(9)
O(1)-Ho(2)-O(7)	84.57(10)	O(10)-Ho(2)-O(9)	78.88(11)
O(4)-Ho(2)-O(7)	113.34(11)	O(1)-Ho(2)-O(9)	147.73(9)
O(1)-Ho(2)-O(12)	76.85(9)	O(4)-Ho(2)-O(9)	72.02(9)
O(4)-Ho(2)-O(12)	141.85(9)	O(7)-Ho(2)-O(9)	71.77(10)
O(7)-Ho(2)-O(12)	74.17(10)	O(6)-Ho(2)-O(9)	115.36(11)
O(6)-Ho(2)-O(12)	141.64(9)	O(10)-Ho(2)-O(12)	71.07(9)

Table S6. Selected bond lengths and bond angles of **2a**.

Eu(1)-O(8)	2.316(4)	Eu(1)-O(3)	2.508(4)
Eu(1)-O(2)	2.346(4)	K(1)-O(1W)	2.515(8)
Eu(1)-O(5)	2.377(4)	K(1)-O(2W)	2.711(7)
Eu(1)-O(12)	2.376(4)	K(1)-O(1)	2.771(6)

Eu(1)-O(6)	2.382(4)	K(1)-O(4)	2.948(6)
Eu(1)-O(11)	2.406(4)	K(1)-O(2)	2.965(5)
Eu(1)-O(9)	2.477(4)	O(4)-K(1)	2.948(6)
O(8)-Eu(1)-O(2)	108.58(16)	O(6)-Eu(1)-O(3)	74.47(13)
O(8)-Eu(1)-O(5)	81.80(14)	O(11)-Eu(1)-O(3)	144.00(13)
O(2)-Eu(1)-O(5)	137.53(13)	O(9)-Eu(1)-O(3)	121.98(13)
O(8)-Eu(1)-O(12)	81.83(15)	O(1W)-K(1)-O(2W)	80.05(19)
O(2)-Eu(1)-O(12)	148.36(14)	O(1W)-K(1)-O(1)	120.6(2)
O(5)-Eu(1)-O(12)	72.37(13)	O(2W)-K(1)-O(1)	78.81(17)
O(8)-Eu(1)-O(6)	144.21(13)	O(1W)-K(1)-O(4)	118.7(2)
O(2)-Eu(1)-O(6)	78.51(14)	O(2W)-K(1)-O(4)	80.75(16)
O(5)-Eu(1)-O(6)	71.43(13)	O(1)-K(1)-O(4)	111.53(18)
O(12)-Eu(1)O(6)	110.89(15)	O(1W)-K(1)-O(2)	96.5(2)
O(8)-Eu(1)-O(11)	137.86(13)	O(2W)-K(1)-O(2)	111.42(18)
O(2)-Eu(1)-O(11)	83.25(14)	O(1)-K(1)-O(2)	44.69(13)
O(5)-Eu(1)-O(11)	117.04(14)	O(4)-K(1)-O(2)	144.59(16)
O(12)-Eu(1)-O(11)	70.42(14)	O(6)-Eu(1)-O(9)	144.28(12)
O(6)-Eu(1)-O(11)	76.93(13)	O(11)-Eu(1)-O(9)	73.33(13)
O(8)-Eu(1)-O(9)	69.91(13)	O(8)-Eu(1)-O(3)	75.42(13)
O(2)-Eu(1)-O(9)	78.77(13)	O(2)-Eu(1)-O(3)	70.06(13)
O(5)-Eu(1)-O(9)	140.82(12)	O(5)-Eu(1)-O(3)	73.40(13)
O(12)-Eu(1)-O(9)	77.12(14)	O(12)-Eu(1)-O(3)	141.05(12)

Table S7. Selected bond lengths and bond angles of **2b**.

Pr(1)-O(7)	2.383(3)	Pr(1)-O(3)	2.442(2)
Pr(1)-O(4)	2.396(2)	Pr(1)-O(10)	2.449(2)
Pr(1)-O(1)	2.425(2)	Pr(1)-O(9)	2.516(2)
Pr(1)-O(11)	2.429(2)	Pr(1)-O(6)	2.566(2)

O(7)-Pr(1)-O(4)	109.58(10)	O(11)-Pr(1)-O(6)	142.41(8)
O(7)-Pr(1)-O(1)	83.02(9)	O(3)-Pr(1)-O(6)	73.82(8)
O(4)-Pr(1)-O(1)	135.49(8)	O(10)-Pr(1)-O(6)	143.87(8)
O(7)-Pr(1)-O(11)	81.58(10)	O(9)-Pr(1)-O(6)	121.93(8)
O(4)-Pr(1)-O(11)	148.89(8)	O(7)-Pr(1)-O(9)	68.62(8)
O(1)-Pr(1)-O(11)	73.26(8)	O(4)-Pr(1)-O(9)	80.26(8)
O(7)-Pr(1)-O(3)	145.14(8)	O(1)-Pr(1)-O(9)	141.47(8)
O(4)-Pr(1)-O(3)	77.55(9)	O(11)-Pr(1)-O(9)	77.12(9)
O(1)-Pr(1)-O(3)	70.29(8)	O(3)-Pr(1)-O(9)	144.84(8)
O(11)-Pr(1)-O(3)	110.31(10)	O(10)-Pr(1)-O(9)	73.21(8)
O(7)-Pr(1)-O(10)	135.95(8)	O(7)-Pr(1)-O(6)	77.43(8)
O(4)-Pr(1)-O(10)	84.19(9)	O(4)-Pr(1)-O(6)	68.44(8)
O(1)-Pr(1)-O(10)	116.76(9)	O(1)-Pr(1)-O(6)	73.50(8)
O(11)-Pr(1)-O(10)	69.03(9)	O(3)-Pr(1)-O(10)	77.69(8)

Table S8. Selected bond lengths and bond angles of **2c**.

Tb(2)-O(4)	2.292(3)	Tb(2)-O(9)	2.367(3)
Tb(2)-O(10)	2.312(3)	Tb(2)-O(1)	2.388(3)
Tb(2)-O(3)	2.332(3)	Tb(2)-O(6)	2.451(3)
Tb(2)-O(7)	2.361(3)	Tb(2)-O(12)	2.480(3)
O(4)-Tb(2)-(10)	108.25(12)	O(7)-Tb(2)-O(6)	140.29(9)
O(4)-Tb(2)-O(3)	82.69(11)	O(9)-Tb(2)-O(6)	144.00(9)
O(10)-Tb(2)-O(3)	148.01(10)	O(1)-Tb(2)-O(6)	73.47(9)
O(4)-Tb(2)-O(7)	81.08(10)	O(4)-Tb(2)-O(12)	74.35(9)
O(10)-Tb(2)-O(7)	138.27(9)	O(10)-Tb(2)-O(12)	70.96(10)
O(3)-Tb(2)-O(7)	72.03(9)	O(3)-Tb(2)-O(12)	140.53(10)
O(4)-Tb(2)-O(9)	143.63(9)	O(7)-Tb(2)-O(12)	73.00(10)
O(10)-Tb(2)-O(9)	78.50(10)	O(9)-Tb(2)-O(12)	74.53(9)
O(3)-Tb(2)-O(9)	110.84(11)	O(1)-Tb(2)-O(12)	143.06(9)
O(7)-Tb(2)-O(9)	72.18(9)	O(6)-Tb(2)-O(12)	122.45(9)
O(4)-Tb(2)-O(1)	139.61(9)	O(9)-Tb(2)-O(1)	76.08(9)
O(10)-Tb(2)-O(1)	81.69(10)	O(4)-Tb(2)-O(6)	70.63(9)

O(3)-Tb(2)-O(1)	71.73(10)	O(10)-Tb(2)-O(6)	78.52(9)
O(7)-Tb(2)-O(1)	117.93(10)	O(3)-Tb(2)-O(6)	77.11(10)

Table S9. Selected bond lengths and bond angles of **2d**.

Dy(2)-O(7)	2.284(6)	Dy(2)-O(4)	2.348(5)
Dy(2)-O(2)	2.303(5)	Dy(2)-O(10)	2.370(6)
Dy(2)-O(12)	2.318(5)	Dy(2)-O(9)	2.438(5)
Dy(2)-O(6)	2.346(5)	Dy(2)-O(3)	2.461(5)
O(7)-Dy(2)-O(2)	107.3(2)	O(6)-Dy(2)-O(9)	143.47(18)
O(7)-Dy(2)-O(12)	82.4(2)	O(4)-Dy(2)-O(9)	140.45(18)
O(2)-Dy(2)-O(12)	147.84(19)	O(10)-Dy(2)-O(9)	73.84(18)
O(7)-Dy(2)-O(6)	143.99(18)	O(7)-Dy(2)-O(3)	74.05(19)
O(2)-Dy(2)-O(6)	78.7(2)	O(2)-Dy(2)-O(3)	71.09(19)
O(12)-Dy(2)-O(6)	111.7(2)	O(12)-Dy(2)-O(3)	140.29(19)
O(7)-Dy(2)-O(4)	81.6(2)	O(6)-Dy(2)-O(3)	74.77(19)
O(2)-Dy(2)-O(4)	138.71(18)	O(4)-Dy(2)-O(3)	73.17(19)
O(12)-Dy(2)-O(4)	72.09(19)	O(10)-Dy(2)-O(3)	143.39(18)
O(6)-Dy(2)-O(4)	72.51(19)	O(9)-Dy(2)-O(3)	122.37(18)
O(7)-Dy(2)-O(10)	139.80(18)	O(4)-Dy(2)-O(10)	117.0(2)
O(2)-Dy(2)-O(10)	82.5(2)	O(7)-Dy(2)-O(9)	70.59(18)
O(12)-Dy(2)-O(10)	71.67(19)	O(2)-Dy(2)-O(9)	77.92(18)
O(6)-Dy(2)-O(10)	75.58(18)	O(12)-Dy(2)-O(9)	76.7(2)

Table S10. Selected bond lengths and bond angles of **2e.**

Er(1)-O(8)	2.262(4)	Er(1)-K(1)	4.332(3)
Er(1)-O(2)	2.277(5)	K(1)-O(1W)	2.618(8)
Er(1)-O(12)	2.298(4)	K(1)-O(2W)	2.805(8)
Er(1)-O(6)	2.324(4)	K(1)-O(1)	2.812(6)
Er(1)-O(5)	2.331(5)	K(1)-O(4)	2.922(6)
Er(1)-O(11)	2.348(4)	K(1)-O(2)	2.965(5)
Er(1)-O(9)	2.428(4)	K(1)-O(11)	3.051(6)
Er(1)-O(3)	2.446(4)	K(1)-O(10)	3.399(6)

O(4)-K(1)	2.922(6)		
O(8)-Er(1)-O(2)	106.97(18)	O(2W)-K(1)-O(4)	78.43(18)
O(8)-Er(1)-O(12)	82.33(17)	O(1)-K(1)-O(4)	110.37(19)
O(2)-Er(1)-O(12)	147.81(15)	O(1W)-K(1)-O(2)	100.0(2)
O(8)-Er(1)-O(6)	143.62(15)	O(2W)-K(1)-O(2)	110.16(18)
O(2)-Er(1)-O(6)	78.81(16)	O(1)-K(1)-O(2)	44.93(14)
O(12)-Er(1)-O(6)	112.25(17)	O(4)-K(1)-O(2)	145.07(15)
O(8)-Er(1)-O(5)	81.09(17)	O(1W)-K(1)-O(11)	80.31(19)
O(2)-Er(1)-O(5)	139.36(14)	O(2W)-K(1)-O(11)	78(18)
O(12)-Er(1)-O(5)	71.69(15)	O(1)-K(1)-O(11)	103.58(16)
O(6)-Er(1)-O(5)	73.13(15)	O(4)-K(1)-O(11)	122.62(17)
O(8)-Er(1)-O(11)	140.69(14)	O(2)-K(1)-O(11)	60.66(13)
O(2)-Er(1)-O(11)	82.13(16)	O(1W)-K(1)-O(10)	56.4(2)
O(12)-Er(1)-O(11)	72.50(15)	O(2W)-K(1)-O(10)	131.58(18)
O(6)-Er(1)-O(11)	75.16(14)	O(1)-K(1)-O(10)	142.03(17)
O(5)-Er(1)-O(11)	117.15(16)	O(4)-K(1)-O(10)	101.34(17)
O(8)-Er(1)-O(9)	71.24(15)	O(2)-K(1)-O(10)	97.21(14)
O(2)-Er(1)-O(9)	77.44(15)	O(11)-K(1)-O(10)	39.61(12)
O(12)-Er(1)-O(9)	76.71(16)	O(5)-Er(1)-O(3)	73.24(15)
O(6)-Er(1)-O(9)	143.02(15)	O(11)-Er(1)-O(3)	143.13(14)
O(5)-Er(1)-O(9)	140.25(14)	O(9)-Er(1)-O(3)	122.48(15)
O(11)-Er(1)-O(9)	73.85(14)	O(1W)-K(1)-O(2W)	79.5(2)
O(8)-Er(1)-O(3)	73.38(15)	O(1W)-K(1)-O(1)	122.3(3)
O(2)-Er(1)-O(3)	71.43(15)	O(2W)-K(1)-O(1)	76.47(18)
O(12)-Er(1)-O(3)	139.80(15)	O(1W)-K(1)-O(4)	115.0(2)
O(6)-Er(1)-O(3)	74.85(15)		

Table S11. Selected bond lengths and bond angles of **2f**.

Yb(1)-(8)	2.238(4)	K(1)-O(1W)	2.580(9)
Yb(1)-O(2)	2.262(4)	K(1)-O(1)	2.792(6)
Yb(1)-O(12)	2.282(4)	K(1)-O(2W)	2.793(7)

Yb(1)-O(5)	2.304(4)	K(1)-O(4)	2.932(6)
Yb(1)-O(6)	2.314(4)	K(1)-O(2)	2.945(6)
Yb(1)-O(11)	2.325(4)	K(1)-O(11)	3.059(6)
Yb(1)-O(9)	2.411(4)	K(1)-O(10)	3.398(6)
Yb(1)-O(3)	2.427(4)	O(4)-K(1)	2.932(6)
Yb(1)-K(1)	4.324(3)		
O(8)-Yb(1)-O(2)	106.85(17)	O(1)-K(1)-O(4)	111.4(2)
O(8)-Yb(1)-O(12)	82.00(17)	O(2W)-K(1)-O(4)	77.77(18)
O(2)-Yb(1)-O(1)	147.61(15)	O(1W)-K(1)-O(2)	99.9(2)
O(8)-Yb(1)-O(5)	80.88(16)	O(1)-K(1)-O(2)	44.92(14)
O(2)-Yb(1)-O(5)	140.00(14)	O(2W)-K(1)-O(2)	110.98(18)
O(12)-Yb(1)-O(5)	71.39(15)	O(40-K(1)-O(2)	145.75(17)
O(8)-Yb(1)-O(6)	143.55(15)	O(1W)-K(1)-O(11)	80.43(19)
O(2)-Yb(1)-O(6)	78.85(16)	O(1)-K(1)-O(11)	103.05(15)
O(12)-Yb(1)-O(6)	112.81(16)	O(2W)-K(1)-O(11)	156.39(19)
O(5)-Yb(1)-O(6)	73.58(15)	O(4)-K(1)-O(11)	122.63(18)
O(8)-Yb(1)-O(11)	141.14(15)	O(2)-K(1)-O(11)	60.05(13)
O(2)-Yb(1)-O(11)	81.89(16)	O(1W)-K(1)-O(10)	56.3(2)
O(12)-Yb(1)-O(11)	73.05(15)	O(1)-K(1)-O(10)	141.30(17)
O(5)-Yb(1)-O(11)	117.01(16)	O(2W)-K(1)-O(10)	131.94(18)
O(2)-Yb(1)-O(9)	76.90(14)	O(11)-K(1)-O(10)	39.49(12)
O(12)-Yb(1)-O(9)	76.61(15)	O(6)-Yb(1)-O(3)	75.01(15)
O(5)-Yb(1)-O(9)	140.26(14)	O(11)-Yb(1)-O(3)	143.27(14)
O(6)-Yb(1)-O(9)	142.45(14)	O(9)-Yb(1)-O(3)	122.77(14)
O(11)-Yb(1)-O(9)	73.73(15)	O(1W)-K(1)-O(1)	122.1(3)
O(8)-Yb(1)-O(3)	72.92(14)	O(1W)-K(1)-O(2W)	79.9(2)
O(2)-Yb(1)-O(3)	72.14(15)	O(1)-K(1)-O(2W)	76.79(17)
O(12)-Yb(1)-O(3)	139.10(15)	O(1W)-K(1)-O(4)	114.3(2)
O(5)-Yb(1)-O(3)	73.09(15)		