Assembly of one-, two-, and three-dimensional Ln(III) complexes constructed from a novel asymmetric tricarboxylate acid: synthesis, structure, photoluminescence and tunable white-light emission

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Index

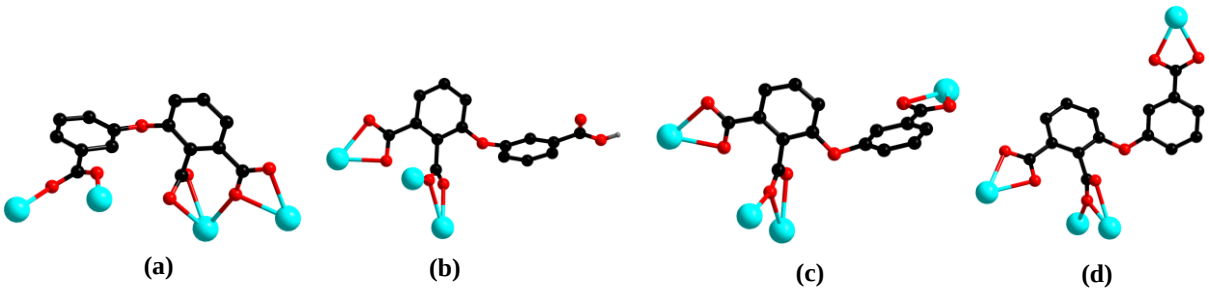

Fig. S1 The coordination modes and configuration H_3dpob ligand.

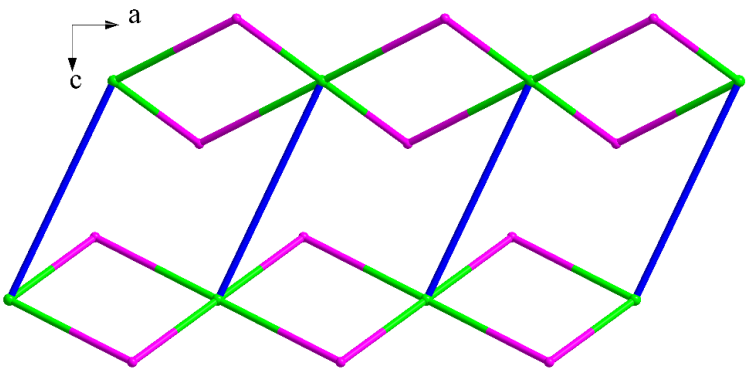

Fig. S2 View of the 2D supramolecular layer net in complex **1** along the *b* axis.

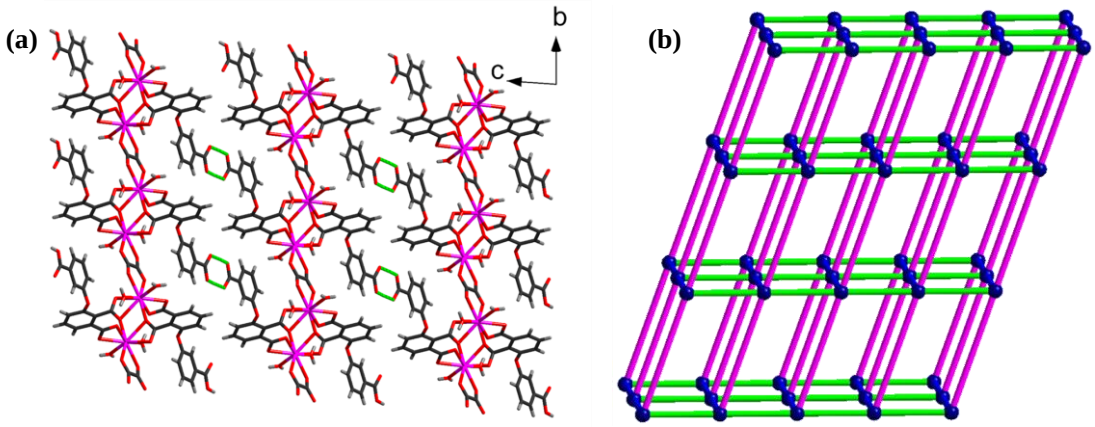

Fig. S3 (a) A 3D supramolecular structure of complex **2** generated through O-H···O hydrogen bonds along the *a* axis (hydrogen bonds are shown by green dots). (b) Topological view the 3D structure of **2** with **pcu** net.

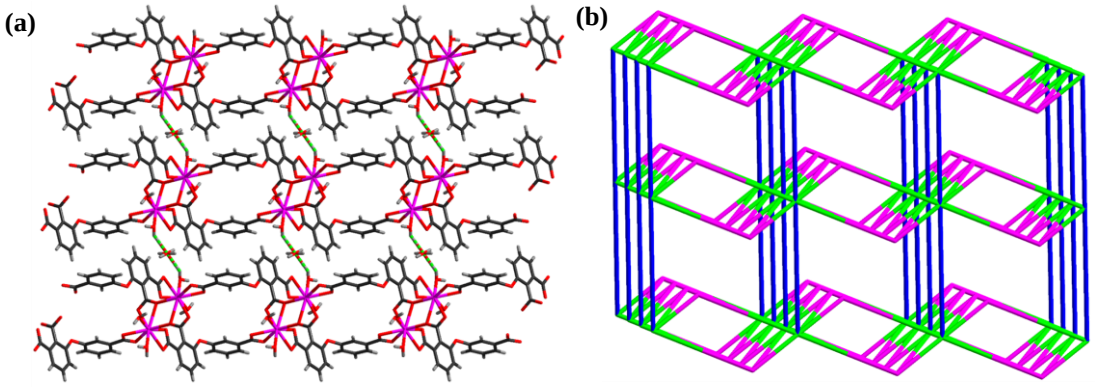

Fig. S4 (a) A 3D supramolecular structure of complex **6** generated through O-H···O hydrogen bonds (hydrogen bonds are shown by green dots). (b) Topological view the 3D structure of **6** with **tfz-d** net.

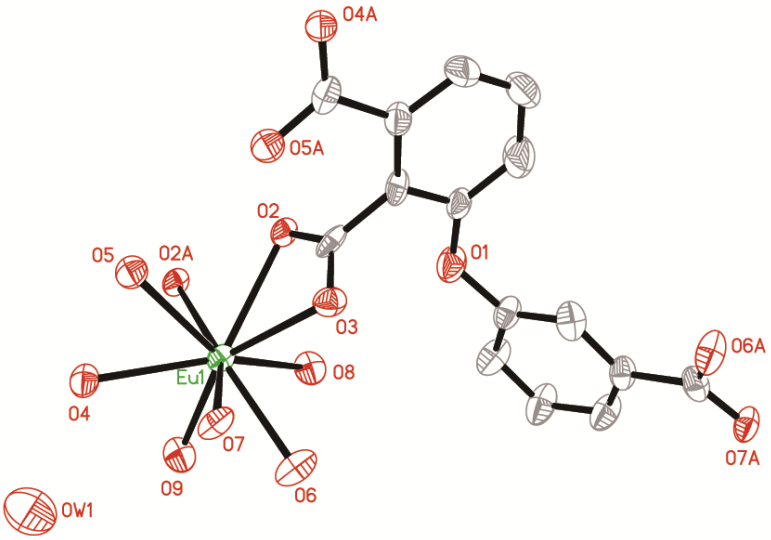

Fig. S5 The metal coordination environment in **7** with labeling scheme and 50% thermal ellipsoids (hydrogen atoms are omitted for clarity).

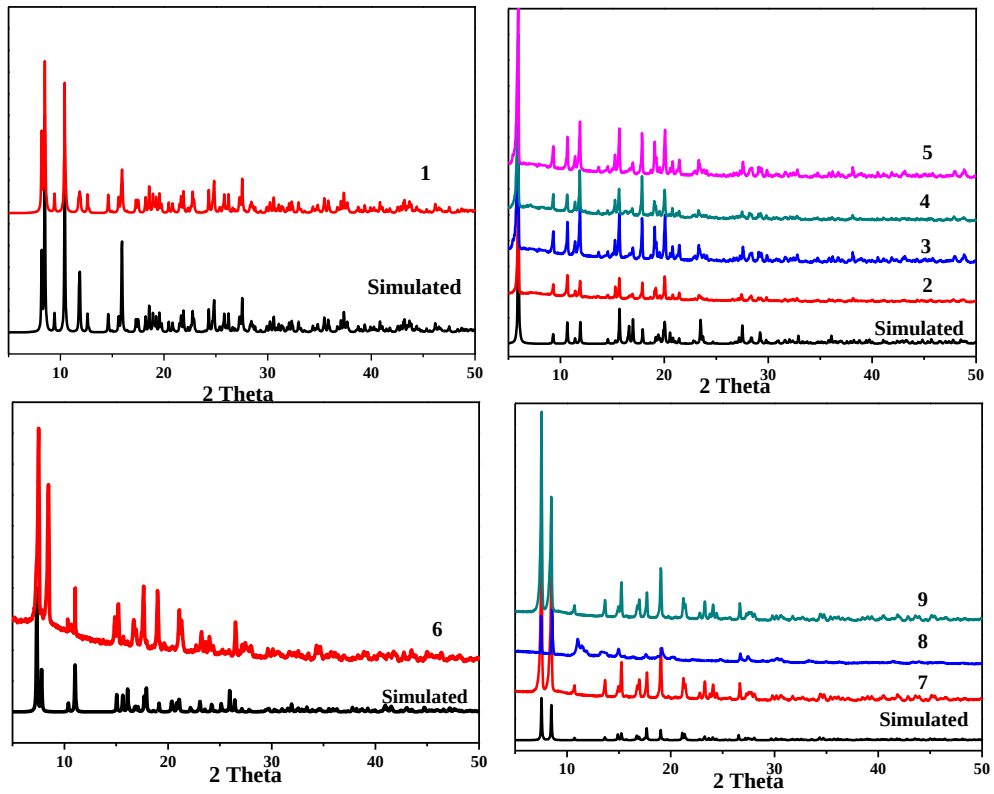

Fig. S6 The PXRD patterns of complexes **1-9** with the relevant simulated patterns.

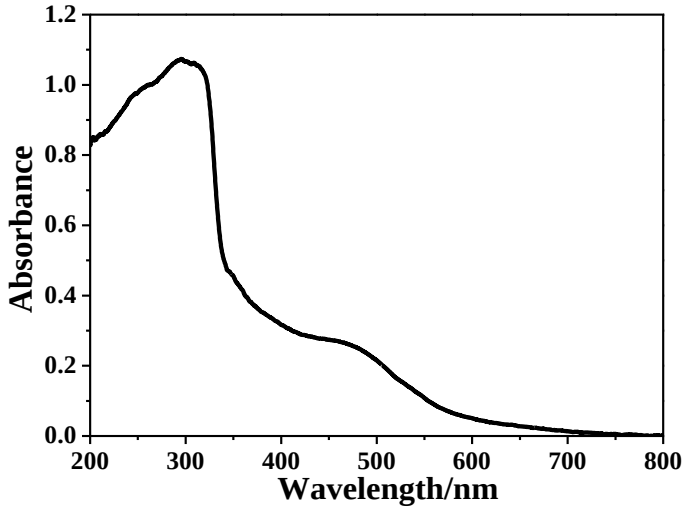

Fig. S7 UV-vis absorption spectrum of H_3dpob ligand in the solid state.

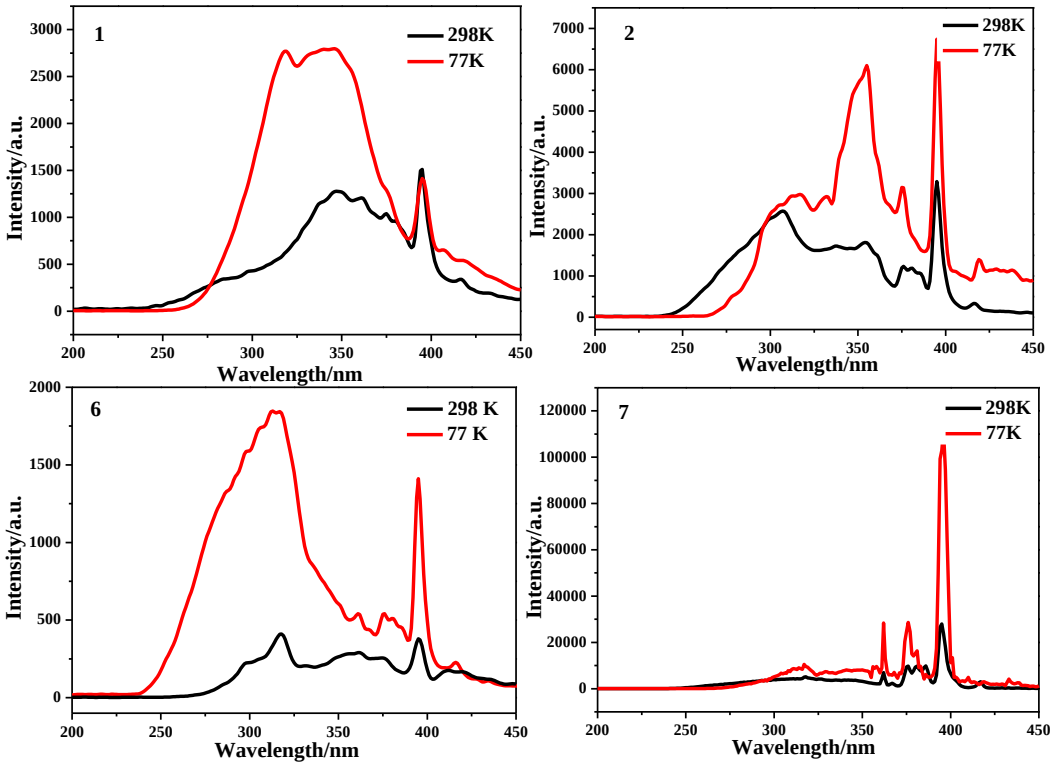

Fig. S8 Excitation spectra of complexes **1**, **2**, **6**, and **7** in the solid state at 298 K and 77 K.

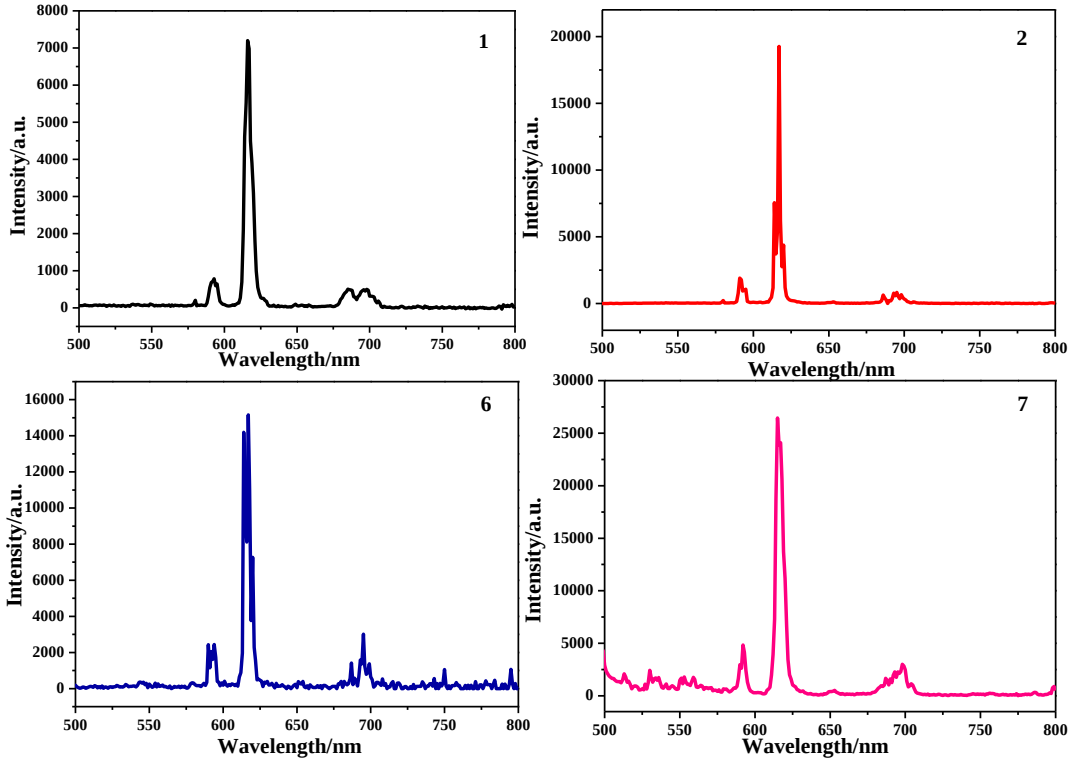

Fig. S9 Solid-state emission spectra of complexes **1**, **2**, **6**, and **7** at 77 K.

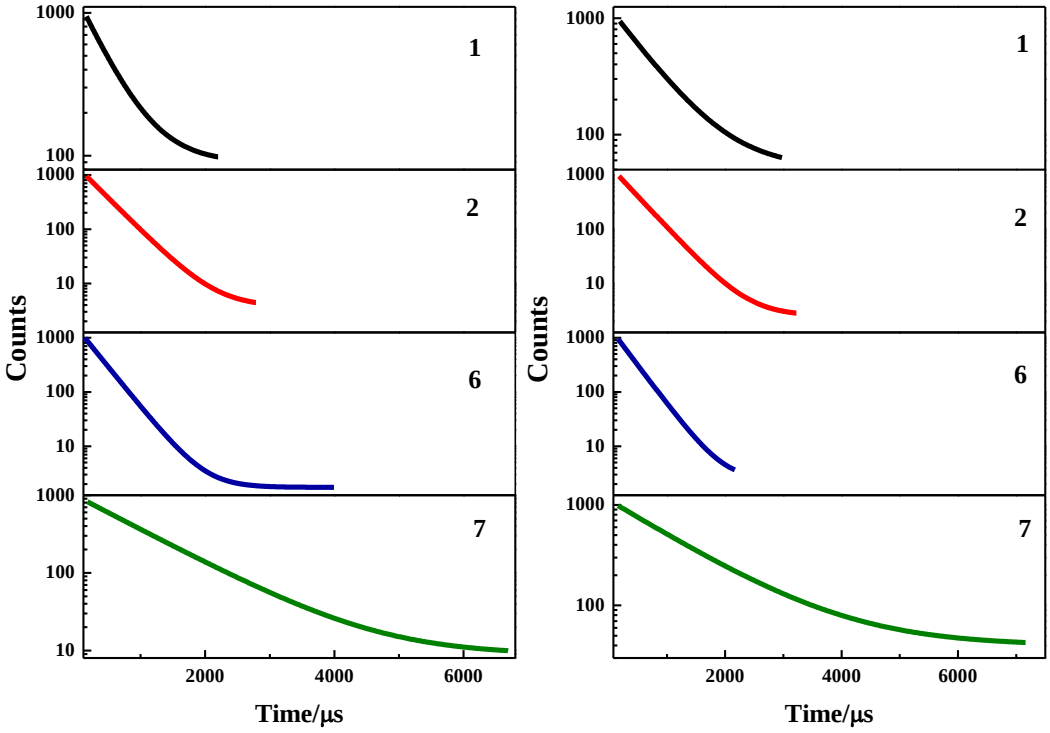

Fig. S10 Luminescence decay curves of complexes **1**, **2**, **6**, and **7** in the solid state at 298 K (left) and 77 K (right).

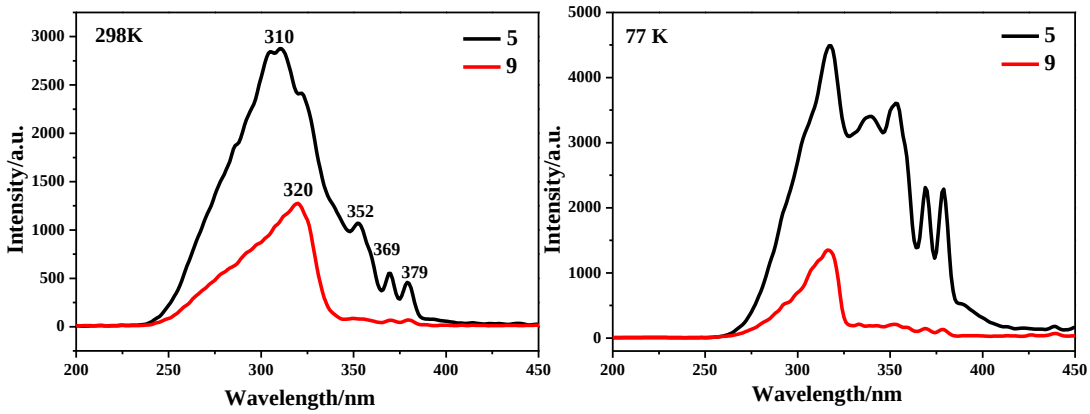

Fig. S11 Excitation spectra of complexes **5** and **9** in the solid state at 298 K and 77 K.

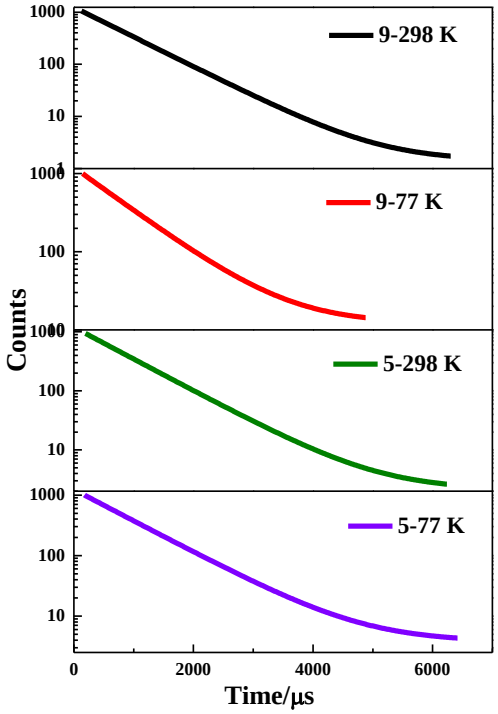

Fig. S12 Luminescence decay curves of complexes **5** and **9** in the solid state at 298 K and 77 K.

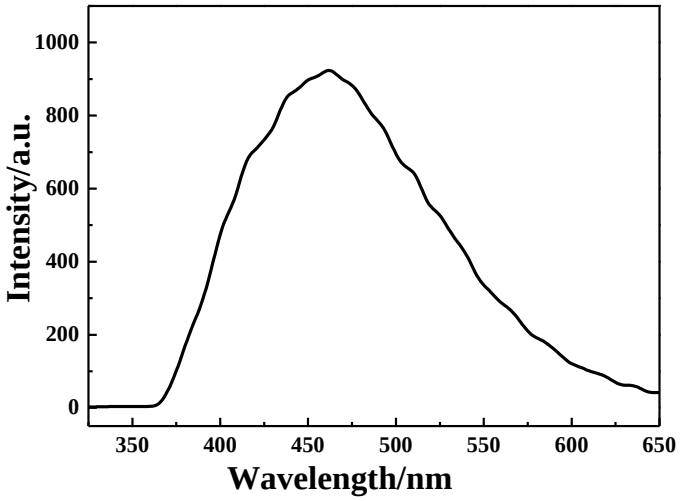

Fig. S13 Emission spectrum of complex **8** in the solid state at 298 K.

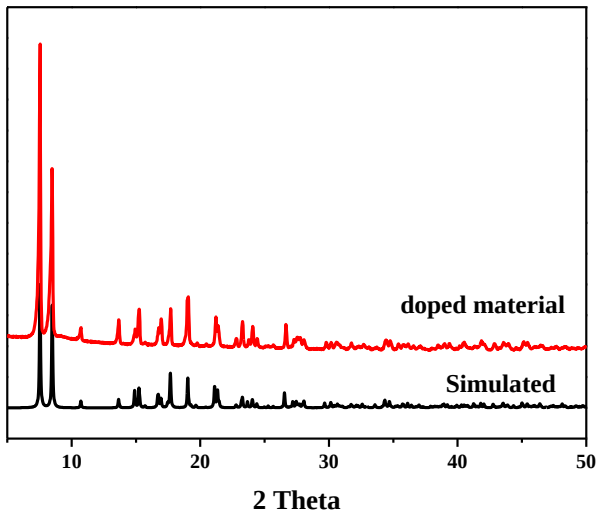

Fig. S14 The PXRD patterns of doped material $\{[Gd_{0.92}Eu_{0.04}Tb_{0.04}(dpob)(H_2O)_2]\cdot 0.5H_2O\}_n$ with the relevant simulated pattern.

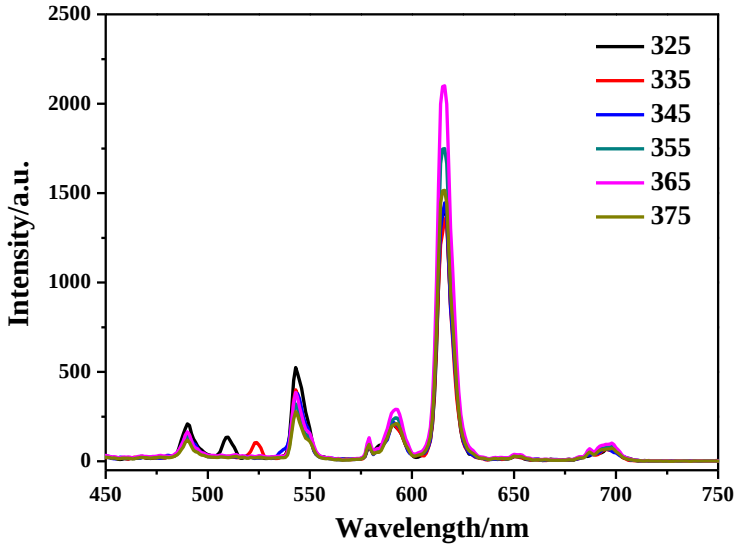

Fig. S15 Solid-state emission spectra of mixed lanthanide complex $\{[Gd_{0.92}Eu_{0.04}Tb_{0.04}(dpob)(H_2O)_2]\cdot 0.5H_2O\}_n$ excited at different wavelength.

Table S1 Selected bond lengths in complexes **1**-**9**.

1		**2**		**3**	
Eu(1)-O(6)#1	2.335(11)	Eu(1)-O(10)	2.391(4)	Sm(1)-O(3)	2.390(4)
Eu(1)-O(4)#2	2.383(12)	Eu(1)-O(2)#3	2.398(4)	Sm(1)-O(11)	2.408(4)
Eu(1)-O(7)	2.396(12)	Eu(1)-O(11)	2.408(4)	Sm(1)-O(10)	2.420(4)
Eu(1)-O(3)#2	2.472(10)	Eu(1)-O(9)#2	2.420(4)	Sm(1)-O(8)	2.435(4)
Eu(1)-O(5)#3	2.503(10)	Eu(1)-O(8)	2.439(4)	Sm(1)-O(9)	2.439(3)
Eu(1)-O(2)#2	2.516(13)	Eu(1)-O(5)	2.442(4)	Sm(1)-O(5)	2.453(4)
Eu(1)-O(4)#3	2.529(12)	Eu(1)-O(4)	2.473(4)	Sm(1)-O(4)	2.476(4)
Eu(1)-N(2)	2.559(14)	Eu(1)-O(3)#1	2.487(3)	Sm(1)-O(2)	2.495(4)
Eu(1)-N(1)	2.576(15)	Eu(1)-O(2)#1	2.580(4)	Sm(1)-O(3)#1	2.588(4)
4		**5**		**6**	
Gd(1)-O(3)	2.383(4)	Tb(1)-O(11)	2.379(4)	Eu(1)-O(9)	2.397(10)
Gd(1)-O(10)	2.384(4)	Tb(1)-O(10)	2.381(5)	Eu(1)-O(8)	2.418(9)
Gd(1)-O(11)	2.404(5)	Tb(1)-O(3)#1	2.380(4)	Eu(1)-O(5)#1	2.428(8)
Gd(1)-O(9)	2.416(4)	Tb(1)-O(9)	2.416(4)	Eu(1)-O(6)#2	2.437(9)
Gd(1)-O(8)	2.423(4)	Tb(1)-O(8)	2.426(4)	Eu(1)-O(7)#2	2.464(10)
Gd(1)-O(4)	2.439(4)	Tb(1)-O(4)	2.436(4)	Eu(1)-O(4)#3	2.476(10)
Gd(1)-O(2)	2.459(5)	Tb(1)-O(2)	2.446(4)	Eu(1)-O(3)	2.480(10)
Gd(1)-O(5)	2.468(4)	Tb(1)-O(5)	2.462(5)	Eu(1)-O(2)	2.498(9)
Gd(1)-O(3)#1	2.598(4)	Tb(1)-O(3)	2.620(4)	Eu(1)-O(5)#3	2.604(10)
7		**8**		**9**	
Eu(1)-O(2)#1	2.406(5)	Gd(1)-O(2)#1	2.380(12)	Tb(1)-O(8)	2.375(5)
Eu(1)-O(8)	2.413(6)	Gd(1)-O(8)	2.413(13)	Tb(1)-O(4)#1	2.376(5)
Eu(1)-O(9)	2.430(6)	Gd(1)-O(9)	2.424(14)	Tb(1)-O(9)	2.412(6)
Eu(1)-O(6)	2.436(6)	Gd(1)-O(7)	2.429(14)	Tb(1)-O(3)	2.415(6)
Eu(1)-O(4)	2.450(6)	Gd(1)-O(4)	2.454(14)	Tb(1)-O(7)	2.436(5)
Eu(1)-O(5)	2.464(6)	Gd(1)-O(5)	2.465(12)	Tb(1)-O(6)	2.437(6)
Eu(1)-O(3)	2.481(6)	Gd(1)-O(6)	2.498(13)	Tb(1)-O(5)	2.452(5)
Eu(1)-O(7)	2.504(6)	Gd(1)-O(3)	2.513(14)	Tb(1)-O(2)	2.473(6)
Eu(1)-O(2)	2.548(6)	Gd(1)-O(2)	2.551(13)	Tb(1)-O(4)	2.538(6)

Symmetry transformations used to generate equivalent atoms: #1 –x. –y, –z; #2 –x+1, –y, –z; #3 x–1, y, z (for **1**). #1 –x+1, –y+1, –z+1; #2 –x+1. –y+2, –z+1; #3 x+1, y, z (for **2**). #1 –x, –y+1, –z (for **3**). #1 –x+2, –y+1,–z+1 (for **4**). #1 –x+2, –y+1, –z (for **5**). #1 x, y, z+1, #2 x+1, y, z+1; #3 –x+1, –y, –z+1 (for **6**). #1 –x+1, –y+1, –z (for **7**). #1 –x+1, –y, –z (for **8**). #1 –x, –y+1, –z (for **9**).

Table S2 Selected bond angles in complexes **1-9**.

1		**2**		**3**	
O(6)#1-Eu(1)-O(4)#2	73.4(4)	O(10)-Eu(1)-O(2)#3	74.88(13)	O(3)-Sm(1)-O(11)	75.22(13)
O(6)#1-Eu(1)-O(7)	136.3(4)	O(10)-Eu(1)-O(11)	76.81(14)	O(3)-Sm(1)-O(10)	82.51(14)
O(4)#2-Eu(1)-O(7)	78.0(4)	O(2)#3-Eu(1)-O(11)	83.19(14)	O(11)-Sm(1)-O(10)	76.69(13)
O(6)#1-Eu(1)-O(3)#2	122.0(4)	O(10)-Eu(1)-O(9)#2	66.95(14)	O(3)-Sm(1)-O(8)	139.88(12)
O(4)#2-Eu(1)-O(3)#2	72.5(4)	O(2)#3-Eu(1)-O(9)#2	139.61(13)	O(11)-Sm(1)-O(8)	66.88(13)
O(7)-Eu(1)-O(3)#2	78.2(4)	O(11)-Eu(1)-O(9)#2	75.92(14)	O(10)-Sm(1)-O(8)	76.61(14)
O(6)#1-Eu(1)-O(5)#3	85.5(4)	O(10)-Eu(1)-O(8)	133.43(13)	O(3)-Sm(1)-O(9)	151.17(13)
O(4)#2-Eu(1)-O(5)#3	125.2(4)	O(2)#3-Eu(1)-O(8)	151.24(12)	O(11)-Sm(1)-O(9)	133.20(13)
O(7)-Eu(1)-O(5)#3	84.6(4)	O(11)-Eu(1)-O(8)	97.34(15)	O(10)-Sm(1)-O(9)	98.12(13)
O(3)#2-Eu(1)-O(5)#3	152.0(4)	O(9)#2-Eu(1)-O(8)	66.83(13)	O(8)-Sm(1)-O(9)	66.70(12)
O(6)#1-Eu(1)-O(2)#2	73.2(4)	O(10)-Eu(1)-O(5)	144.81(13)	O(3)-Sm(1)-O(5)	79.44(12)
O(4)#2-Eu(1)-O(2)#2	71.0(4)	O(2)#3-Eu(1)-O(5)	79.72(12)	O(11)-Sm(1)-O(5)	144.79(13)
O(7)-Eu(1)-O(2)#2	126.7(4)	O(11)-Eu(1)-O(5)	124.01(13)	O(10)-Sm(1)-O(5)	123.79(13)
O(3)#2-Eu(1)-O(2)#2	51.9(4)	O(9)#2-Eu(1)-O(5)	140.43(13)	O(8)-Sm(1)-O(5)	140.44(12)
O(5)#3-Eu(1)-O(2)#2	148.6(4)	O(8)-Eu(1)-O(5)	76.24(12)	O(9)-Sm(1)-O(5)	76.37(12)
O(6)#1-Eu(1)-O(4)#3	69.9(4)	O(10)-Eu(1)-O(4)	141.75(14)	O(3)-Sm(1)-O(4)	80.77(12)
O(4)#2-Eu(1)-O(4)#3	72.8(4)	O(2)#3-Eu(1)-O(4)	80.52(13)	O(11)-Sm(1)-O(4)	142.17(13)
O(7)-Eu(1)-O(4)#3	70.3(4)	O(11)-Eu(1)-O(4)	71.52(13)	O(10)-Sm(1)-O(4)	71.50(13)
O(3)#2-Eu(1)-O(4)#3	136.9(4)	O(9)#2-Eu(1)-O(4)	123.06(13)	O(8)-Sm(1)-O(4)	122.76(12)
O(5)#3-Eu(1)-O(4)#3	52.4(4)	O(8)-Eu(1)-O(4)	72.54(13)	O(9)-Sm(1)-O(4)	72.30(13)
O(2)#2-Eu(1)-O(4)#3	134.0(4)	O(5)-Eu(1)-O(4)	53.27(12)	O(5)-Sm(1)-O(4)	53.29(12)
O(6)#1-Eu(1)-N(2)	78.4(4)	O(10)-Eu(1)-O(3)#1	85.91(14)	O(3)-Sm(1)-O(2)	116.96(12)
O(4)#2-Eu(1)-N(2)	139.0(4)	O(2)#3-Eu(1)-O(3)#1	116.85(12)	O(11)-Sm(1)-O(2)	85.59(13)
O(7)-Eu(1)-N(2)	140.9(4)	O(11)-Eu(1)-O(3)#1	149.24(13)	O(10)-Sm(1)-O(2)	149.49(14)
O(3)#2-Eu(1)-N(2)	99.1(4)	O(9)#2-Eu(1)-O(3)#1	73.93(13)	O(8)-Sm(1)-O(2)	73.62(13)
O(5)#3-Eu(1)-N(2)	80.7(4)	O(8)-Eu(1)-O(3)#1	76.27(12)	O(9)-Sm(1)-O(2)	76.14(12)
O(2)#2-Eu(1)-N(2)	72.7(5)	O(5)-Eu(1)-O(3)#1	84.24(12)	O(5)-Sm(1)-O(2)	84.53(12)
O(4)#3-Eu(1)-N(2)	123.8(4)	O(4)-Eu(1)-O(3)#1	131.75(12)	O(4)-Sm(1)-O(2)	131.76(12)
O(6)#1-Eu(1)-N(1)	140.2(5)	O(10)-Eu(1)-O(2)#1	71.57(13)	O(3)-Sm(1)-O(3)#1	65.84(14)
O(4)#2-Eu(1)-N(1)	144.7(5)	O(2)#3-Eu(1)-O(2)#1	65.79(13)	O(11)-Sm(1)-O(3)#1	71.37(12)
O(7)-Eu(1)-N(1)	78.1(5)	O(11)-Eu(1)-O(2)#1	140.17(14)	O(10)-Sm(1)-O(3)#1	139.46(12)
O(3)#2-Eu(1)-N(1)	77.4(4)	O(9)#2-Eu(1)-O(2)#1	111.72(12)	O(8)-Sm(1)-O(3)#1	111.53(12)
O(5)#3-Eu(1)-N(1)	77.6(4)	O(8)-Eu(1)-O(2)#1	121.96(12)	O(9)-Sm(1)-O(3)#1	121.91(12)
O(2)#2-Eu(1)-N(1)	104.1(5)	O(5)-Eu(1)-O(2)#1	76.00(11)	O(5)-Sm(1)-O(3)#1	76.16(12)
O(4)#3-Eu(1)-N(1)	121.8(4)	O(4)-Eu(1)-O(2)#1	123.32(12)	O(4)-Sm(1)-O(3)#1	123.73(12)
N(2)-Eu(1)-N(1)	63.5(5)	O(3)#1-Eu(1)-O(2)#1	51.07(12)	O(2)-Sm(1)-O(3)#1	51.13(11)
4		**5**		**6**	
O(3)-Gd(1)-O(10)	75.23(15)	O(11)-Tb(1)-O(10)	77.48(17)	O(9)-Eu(1)-O(8)	75.3(4)
O(3)-Gd(1)-O(11)	83.54(18)	O(11)-Tb(1)-O(3)#1	74.78(15)	O(9)-Eu(1)-O(5)#1	79.3(3)
O(10)-Gd(1)-O(11)	77.12(17)	O(10)-Tb(1)-O(3)#1	83.23(18)	O(8)-Eu(1)-O(5)#1	81.7(3)
O(3)-Gd(1)-O(9)	150.63(15)	O(11)-Tb(1)-O(9)	134.19(15)	O(9)-Eu(1)-O(6)#2	147.9(4)
O(10)-Gd(1)-O(9)	133.61(15)	O(10)-Tb(1)-O(9)	96.52(18)	O(8)-Eu(1)-O(6)#2	125.4(3)

O(11)-Gd(1)-O(9)	96.59(18)	O(3)#1-Tb(1)-O(9)	150.47(14)	O(5)#1-Eu(1)-O(6)#2	80.1(3)
O(3)-Gd(1)-O(8)	139.89(15)	O(11)-Tb(1)-O(8)	67.25(14)	O(9)-Eu(1)-O(7)#2	145.1(4)
O(10)-Gd(1)-O(8)	66.89(14)	O(10)-Tb(1)-O(8)	75.77(17)	O(8)-Eu(1)-O(7)#2	73.1(3)
O(11)-Gd(1)-O(8)	75.84(18)	O(3)#1-Tb(1)-O(8)	139.61(13)	O(5)#1-Eu(1)-O(7)#2	81.7(3)
O(9)-Gd(1)-O(8)	67.02(14)	O(9)-Tb(1)-O(8)	67.27(13)	O(6)#2-Eu(1)-O(7)#2	53.5(3)
O(3)-Gd(1)-O(4)	79.57(15)	O(11)-Tb(1)-O(4)	144.16(14)	O(9)-Eu(1)-O(4)#3	84.3(4)
O(10)-Gd(1)-O(4)	144.79(15)	O(10)-Tb(1)-O(4)	124.15(15)	O(8)-Eu(1)-O(4)#3	149.5(3)
O(11)-Gd(1)-O(4)	124.08(16)	O(3)#1-Tb(1)-O(4)	79.71(15)	O(5)#1-Eu(1)-O(4)#3	116.8(3)
O(9)-Gd(1)-O(4)	76.13(14)	O(9)-Tb(1)-O(4)	76.09(14)	O(6)#2-Eu(1)-O(4)#3	83.3(3)
O(8)-Gd(1)-O(4)	140.30(15)	O(8)-Tb(1)-O(4)	140.45(13)	O(7)#2-Eu(1)-O(4)#3	130.6(3)
O(3)-Gd(1)-O(2)	116.68(14)	O(11)-Tb(1)-O(2)	86.19(16)	O(9)-Eu(1)-O(3)	76.0(3)
O(10)-Gd(1)-O(2)	85.96(16)	O(10)-Tb(1)-O(2)	149.65(16)	O(8)-Eu(1)-O(3)	78.5(4)
O(11)-Gd(1)-O(2)	149.48(17)	O(3)#1-Tb(1)-O(2)	117.13(13)	O(5)#1-Eu(1)-O(3)	151.5(3)
O(9)-Gd(1)-O(2)	76.90(15)	O(9)-Tb(1)-O(2)	76.73(14)	O(6)#2-Eu(1)-O(3)	128.2(3)
O(8)-Gd(1)-O(2)	74.19(16)	O(8)-Tb(1)-O(2)	74.35(15)	O(7)#2-Eu(1)-O(3)	111.4(4)
O(4)-Gd(1)-O(2)	83.80(15)	O(4)-Tb(1)-O(2)	83.46(14)	O(4)#3-Eu(1)-O(3)	74.7(4)
O(3)-Gd(1)-O(5)	79.95(14)	O(11)-Tb(1)-O(5)	140.97(15)	O(9)-Eu(1)-O(2)	127.8(3)
O(10)-Gd(1)-O(5)	141.51(17)	O(10)-Tb(1)-O(5)	70.73(15)	O(8)-Eu(1)-O(2)	98.6(4)
O(11)-Gd(1)-O(5)	71.20(16)	O(3)#1-Tb(1)-O(5)	79.44(14)	O(5)#1-Eu(1)-O(2)	152.3(3)
O(9)-Gd(1)-O(5)	72.44(15)	O(9)-Tb(1)-O(5)	72.73(14)	O(6)#2-Eu(1)-O(2)	77.3(3)
O(8)-Gd(1)-O(5)	123.28(15)	O(8)-Tb(1)-O(5)	123.39(15)	O(7)#2-Eu(1)-O(2)	72.1(3)
O(4)-Gd(1)-O(5)	53.54(15)	O(4)-Tb(1)-O(5)	54.03(13)	O(4)#3-Eu(1)-O(2)	76.2(3)
O(2)-Gd(1)-O(5)	131.88(15)	O(2)-Tb(1)-O(5)	132.09(14)	O(3)-Eu(1)-O(2)	52.3(3)
O(3)-Gd(1)-O(3)#1	65.68(17)	O(11)-Tb(1)-O(3)	71.33(14)	O(9)-Eu(1)-O(5)#3	72.3(3)
O(10)-Gd(1)-O(3)#1	71.51(15)	O(10)-Tb(1)-O(3)	140.59(16)	O(8)-Eu(1)-O(5)#3	137.7(3)
O(11)-Gd(1)-O(3)#1	140.39(16)	O(3)#1-Tb(1)-O(3)	65.94(15)	O(5)#1-Eu(1)-O(5)#3	66.2(3)
O(9)-Gd(1)-O(3)#1	122.54(15)	O(9)-Tb(1)-O(3)	122.48(13)	O(6)#2-Eu(1)-O(5)#3	76.9(3)
O(8)-Gd(1)-O(3)#1	111.79(15)	O(8)-Tb(1)-O(3)	112.03(15)	O(7)#2-Eu(1)-O(5)#3	125.0(3)
O(4)-Gd(1)-O(3)#1	75.90(14)	O(4)-Tb(1)-O(3)	75.47(13)	O(4)#3-Eu(1)-O(5)#3	50.6(3)
O(2)-Gd(1)-O(3)#1	51.02(13)	O(2)-Tb(1)-O(3)	51.21(12)	O(3)-Eu(1)-O(5)#3	118.1(3)
O(5)-Gd(1)-O(3)#1	123.16(14)	O(5)-Tb(1)-O(3)	122.97(14)	O(2)-Eu(1)-O(5)#3	122.7(3)
7		**8**		**9**	
O(2)#1-Eu(1)-O(8)	76.8(2)	O(2)#1-Gd(1)-O(8)	77.8(4)	O(8)-Tb(1)-O(4)#1	76.5(2)
O(2)#1-Eu(1)-O(9)	83.7(2)	O(2)#1-Gd(1)-O(9)	83.2(5)	O(8)-Tb(1)-O(9)	75.0(2)
O(8)-Eu(1)-O(9)	74.3(2)	O(8)-Gd(1)-O(9)	74.9(5)	O(4)#1-Tb(1)-O(9)	83.91(19)
O(2)#1-Eu(1)-O(6)	152.0(2)	O(2)#1-Gd(1)-O(7)	152.2(4)	O(8)-Tb(1)-O(3)	78.35(19)
O(8)-Eu(1)-O(6)	78.3(2)	O(8)-Gd(1)-O(7)	77.9(5)	O(4)#1-Tb(1)-O(3)	151.69(16)
O(9)-Eu(1)-O(6)	77.4(2)	O(9)-Gd(1)-O(7)	77.6(5)	O(9)-Tb(1)-O(3)	77.17(19)
O(2)#1-Eu(1)-O(4)	83.3(2)	O(2)#1-Gd(1)-O(4)	82.7(4)	O(8)-Tb(1)-O(7)	146.85(18)
O(8)-Eu(1)-O(4)	142.2(2)	O(8)-Gd(1)-O(4)	143.1(4)	O(4)#1-Tb(1)-O(7)	78.2(2)
O(9)-Eu(1)-O(4)	71.8(2)	O(9)-Gd(1)-O(4)	71.9(5)	O(9)-Tb(1)-O(7)	123.09(18)
O(6)-Eu(1)-O(4)	109.5(2)	O(7)-Gd(1)-O(4)	109.6(5)	O(3)-Tb(1)-O(7)	129.87(19)
O(2)#1-Eu(1)-O(5)	78.1(2)	O(2)#1-Gd(1)-O(5)	77.2(4)	O(8)-Tb(1)-O(6)	141.86(18)
O(8)-Eu(1)-O(5)	147.3(2)	O(8)-Gd(1)-O(5)	146.7(5)	O(4)#1-Tb(1)-O(6)	83.1(2)

O(9)-Eu(1)-O(5)	123.1(2)	O(9)-Gd(1)-O(5)	123.1(4)	O(9)-Tb(1)-O(6)	71.07(19)
O(6)-Eu(1)-O(5)	129.7(2)	O(7)-Gd(1)-O(5)	130.3(4)	O(3)-Tb(1)-O(6)	109.8(2)
O(4)-Eu(1)-O(5)	53.0(2)	O(4)-Gd(1)-O(5)	53.0(4)	O(7)-Tb(1)-O(6)	53.49(17)
O(2)#1-Eu(1)-O(3)	115.1(2)	O(2)#1-Gd(1)-O(6)	152.8(4)	O(8)-Tb(1)-O(5)	84.89(19)
O(8)-Eu(1)-O(3)	84.3(2)	O(8)-Gd(1)-O(6)	129.4(4)	O(4)#1-Tb(1)-O(5)	115.53(18)
O(9)-Eu(1)-O(3)	147.6(2)	O(9)-Gd(1)-O(6)	103.4(5)	O(9)-Tb(1)-O(5)	148.07(19)
O(6)-Eu(1)-O(3)	74.6(2)	O(7)-Gd(1)-O(6)	53.3(4)	O(3)-Tb(1)-O(5)	74.6(2)
O(4)-Eu(1)-O(3)	133.5(2)	O(4)-Gd(1)-O(6)	74.6(4)	O(7)-Tb(1)-O(5)	86.97(19)
O(5)-Eu(1)-O(3)	87.7(2)	O(5)-Gd(1)-O(6)	77.2(4)	O(6)-Tb(1)-O(5)	133.19(18)
O(2)#1-Eu(1)-O(7)	153.5(2)	O(2)#1-Gd(1)-O(3)	115.3(4)	O(8)-Tb(1)-O(2)	130.2(2)
O(8)-Eu(1)-O(7)	129.7(2)	O(8)-Gd(1)-O(3)	83.8(4)	O(4)#1-Tb(1)-O(2)	153.30(17)
O(9)-Eu(1)-O(7)	102.3(2)	O(9)-Gd(1)-O(3)	148.2(4)	O(9)-Tb(1)-O(2)	101.6(2)
O(6)-Eu(1)-O(7)	52.8(2)	O(7)-Gd(1)-O(3)	75.1(5)	O(3)-Tb(1)-O(2)	53.22(17)
O(4)-Eu(1)-O(7)	74.4(2)	O(4)-Gd(1)-O(3)	133.1(4)	O(7)-Tb(1)-O(2)	76.9(2)
O(5)-Eu(1)-O(7)	77.1(2)	O(5)-Gd(1)-O(3)	87.4(4)	O(6)-Tb(1)-O(2)	74.4(2)
O(3)-Eu(1)-O(7)	73.0(2)	O(6)-Gd(1)-O(3)	72.5(4)	O(5)-Tb(1)-O(2)	72.83(19)
O(2)#1-Eu(1)-O(2)	63.6(2)	O(2)#1-Gd(1)-O(2)	63.9(5)	O(8)-Tb(1)-O(4)	71.70(17)
O(8)-Eu(1)-O(2)	72.00(19)	O(8)-Gd(1)-O(2)	71.5(4)	O(4)#1-Tb(1)-O(4)	63.54(19)
O(9)-Eu(1)-O(2)	137.2(2)	O(9)-Gd(1)-O(2)	136.8(4)	O(9)-Tb(1)-O(4)	137.63(17)
O(6)-Eu(1)-O(2)	119.7(2)	O(7)-Gd(1)-O(2)	119.7(5)	O(3)-Tb(1)-O(4)	119.66(18)
O(4)-Eu(1)-O(2)	126.1(2)	O(4)-Gd(1)-O(2)	126.1(4)	O(7)-Tb(1)-O(4)	78.00(16)
O(5)-Eu(1)-O(2)	78.2(2)	O(5)-Gd(1)-O(2)	77.9(4)	O(6)-Tb(1)-O(4)	126.13(18)
O(3)-Eu(1)-O(2)	51.54(19)	O(6)-Gd(1)-O(2)	118.8(4)	O(5)-Tb(1)-O(4)	52.01(17)
O(7)-Eu(1)-O(2)	119.39(19)	O(3)-Gd(1)-O(2)	51.4(4)	O(2)-Tb(1)-O(4)	119.82(17)

Symmetry transformations used to generate equivalent atoms: #1 –x. –y, –z; #2 –x+1, –y, –z; #3 x–1, y, z (for **1**). #1 –x+1, –y+1, –z+1; #2 –x+1. –y+2, –z+1; #3 x+1, y, z (for **2**). #1 –x, –y+1, –z (for **3**). #1 –x+2, –y+1,–z+1 (for **4**). #1 –x+2, –y+1, –z (for **5**). #1 x, y, z+1, #2 x+1, y, z+1; #3 –x+1, –y, –z+1 (for **6**). #1 –x+1, –y+1, –z (for **7**). #1 –x+1, –y, –z (for **8**). #1 –x, –y+1, –z (for **9**).

Table S3 The geometrical parameters of hydrogen bond and π···π stacking interactions of Ln(III) complexes.

	D–H···A	D–H/Å	H···A/Å	D···A/Å	D–H···A/°
1	OW1–HW1B···O3	0.850	2.274	2.975	139.91
	π···π		3.463		
2	O7–H7A···O6	0.930	1.696	2.625	176.13
3	O6–H6···O7 [-x+1, -y+2, -z+1]	0.840	1.789	2.618	168.66
	O10–H10A···O9 [x-1, y, z]	0.850	2.009	2.773	149.18
	O10–H10A···O8 [-x, -y, -z]	0.850	2.608	3.381	151.75
	O11–H11B···O2 [x-1, y, z]	0.850	2.413	2.855	113.03
	O11–H11B···O9 [x-1, y, z]	0.850	2.447	3.220	151.44
4	O7–H7···O6 [-x-1, -y, -z]	0.820	1.820	2.628	168.17
	O10–H10A···O9 [x+1, y, z]	0.850	2.387	3.233	173.18
	O11–H11B···O8 [-x+2, -y+2, -z+1]	0.850	2.540	3.342	157.60
5	O6–H6···O7 [-x+3, -y+2, -z+1]	0.820	1.831	2.641	169.44
	O10–H10C···O8 [-x+2, -y+2, -z]	0.850	2.560	3.359	157.06
	O11–H11A···O9 [x+1, y, z]	0.850	2.401	3.246	173.05
	O11–H11A···O2 [x+1, y, z]	0.850	2.489	2.895	110.21
6	OW1-HW1C···O7 [-x, -y+1, -z+1]	0.850	2.415	2.970	123.50
	O8–H8B···OW1	0.850	2.082	2.799	141.70
	O8–H8C···O2 [x-1, y, z]	0.850	2.136	2.736	127.37
	O9–H9A···O6 [-x, -y, -z+1]	0.850	2.158	2.951	155.09
	O9–H9A···O4 [-x, -y, -z+1]	0.850	2.499	2.906	110.38
	O9–H9B···O2 [x-1, y, z]	0.850	2.524	3.268	146.70