

Supporting information

Constructions of a series of lanthanide metal-organic frameworks: structure, luminescence and white light emission

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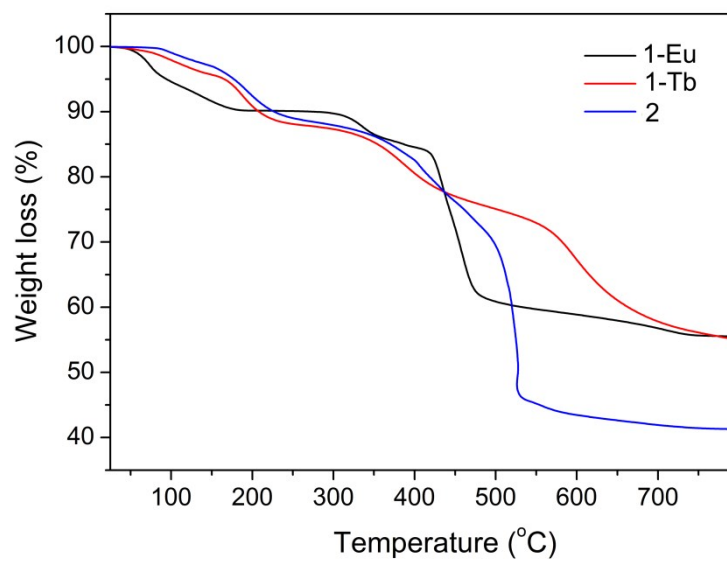


Fig.S1 TG curves of **1-Eu**, **1-Tb** and **2**.

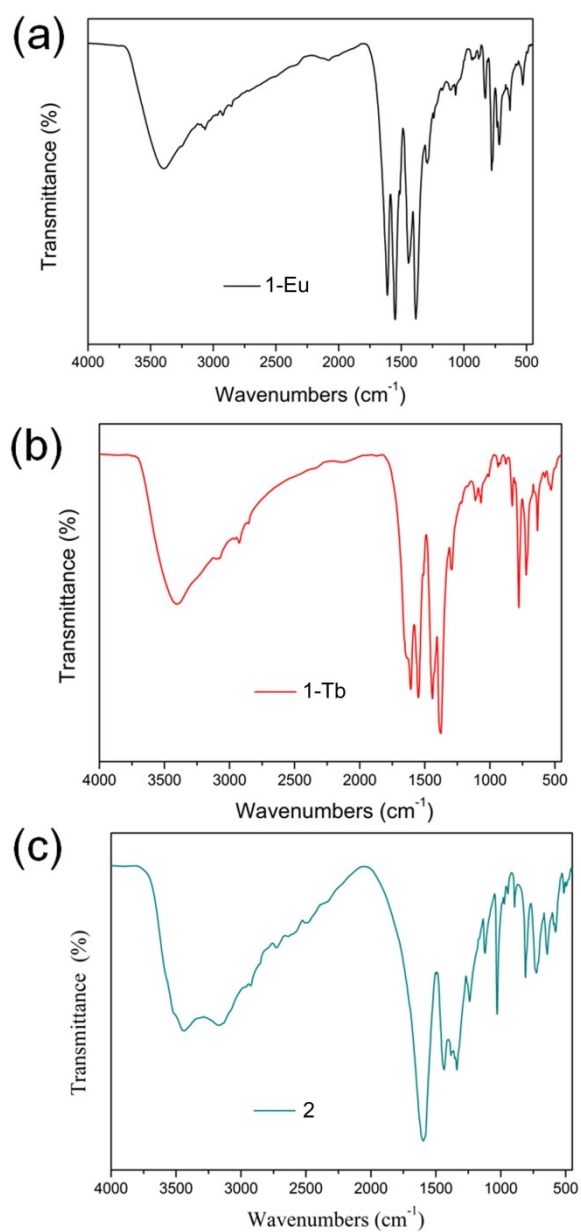


Fig.S2 IR spectra of **1-Eu**, **1-Tb** and **2**..

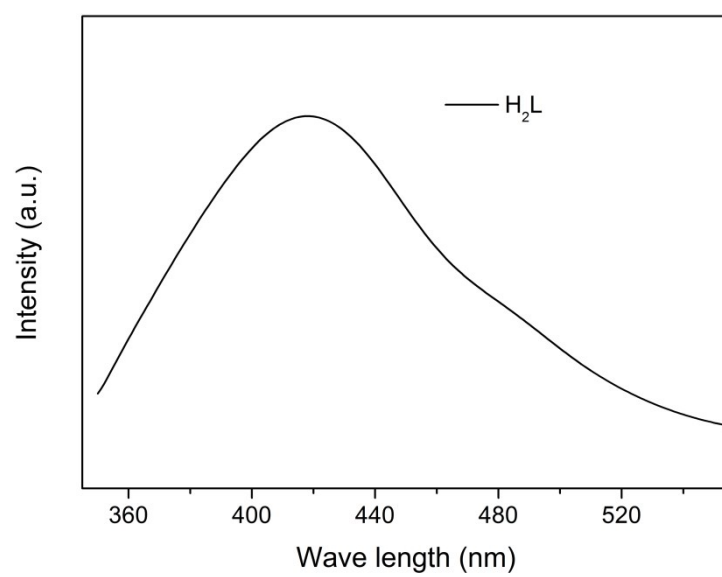


Fig.S3 The emission spectra of H_2L ligand.

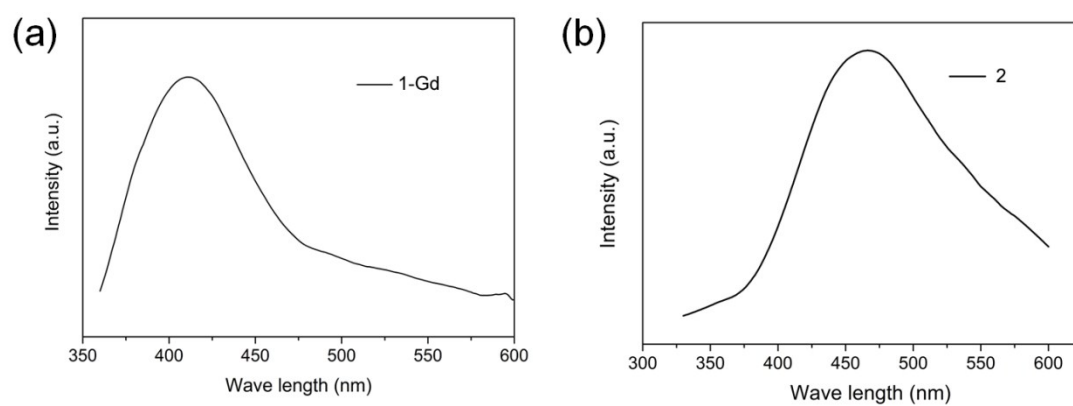


Fig. S4 The emission spectra of **1-Gd** (a) and **2** (b).

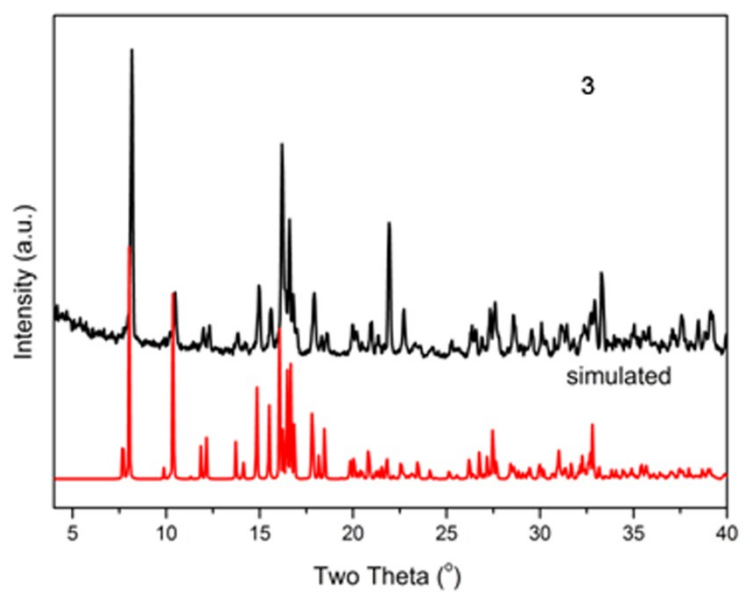


Fig. S5 The experimental PXRD pattern of **3** and simulated PXRD pattern of **1**.

Table S1 Selected bond length [Å] and bond angle [°] for **1-Eu**.

Eu(1)-O(10)	2.3198(14)	Eu(2)-O(19)#2	2.4333(16)
Eu(1)-O(1)	2.3789(15)	Eu(2)-O(16)	2.4414(15)
Eu(1)-O(12)	2.3903(18)	Eu(2)-O(5)	2.4434(15)
Eu(1)-O(17)#1	2.3932(14)	Eu(2)-O(3)#2	2.4815(15)
Eu(1)-O(13)	2.4137(15)	Eu(2)-N(1)	2.4982(17)
Eu(1)-O(15)	2.4346(16)	Eu(2)-O(7)#3	2.5084(15)
Eu(1)-O(11)	2.4495(19)	Eu(2)-N(2)#2	2.5089(17)
Eu(1)-O(14)	2.4827(16)	Eu(2)-O(9)#3	2.5113(15)
O(17)-Eu(1)#6	2.3932(14)	Eu(2)-N(3)#3	2.5560(17)
O(7)-Eu(2)#5	2.5084(15)	N(2)-Eu(2)#4	2.5089(17)
O(9)-Eu(2)#5	2.5113(15)	N(3)-Eu(2)#5	2.5560(17)
O(19)-Eu(2)#4	2.4333(15)	O(3)-Eu(2)#4	2.4815(15)
O(10)-Eu(1)-O(1)	120.79(6)	O(16)-Eu(2)-O(5)	127.70(5)
O(10)-Eu(1)-O(12)	78.20(7)	O(19)#2-Eu(2)-O(3)#2	127.30(5)
O(1)-Eu(1)-O(12)	72.53(6)	O(16)-Eu(2)-O(3)#2	89.34(5)
O(10)-Eu(1)-O(17)#1	132.27(6)	O(5)-Eu(2)-O(3)#2	71.78(5)
O(1)-Eu(1)-O(17)#1	77.11(6)	O(19)#2-Eu(2)-N(1)	135.49(5)
O(12)-Eu(1)-O(17)#1	145.82(7)	O(16)-Eu(2)-N(1)	63.71(5)
O(10)-Eu(1)-O(13)	76.00(6)	O(5)-Eu(2)-N(1)	64.31(5)
O(1)-Eu(1)-O(13)	137.54(5)	O(3)#2-Eu(2)-N(1)	74.55(5)
O(12)-Eu(1)-O(13)	73.98(6)	O(19)#2-Eu(2)-O(7)#3	80.77(6)
O(17)#1-Eu(1)-O(13)	122.59(5)	O(16)-Eu(2)-O(7)#3	148.43(5)
O(10)-Eu(1)-O(15)	150.42(6)	O(5)-Eu(2)-O(7)#3	80.28(5)
O(1)-Eu(1)-O(15)	78.07(6)	O(3)#2-Eu(2)-O(7)#3	86.41(5)
O(12)-Eu(1)-O(15)	87.62(7)	N(1)-Eu(2)-O(7)#3	143.43(6)
O(17)#1-Eu(1)-O(15)	70.87(6)	O(19)#2-Eu(2)-N(2)#2	64.38(5)
O(13)-Eu(1)-O(15)	75.17(5)	O(16)-Eu(2)-N(2)#2	74.73(5)
O(10)-Eu(1)-O(11)	70.91(7)	O(5)-Eu(2)-N(2)#2	129.29(5)
O(1)-Eu(1)-O(11)	72.45(7)	O(3)#2-Eu(2)-N(2)#2	62.93(5)
O(12)-Eu(1)-O(11)	109.75(8)	N(1)-Eu(2)-N(2)#2	119.75(5)
O(17)#1-Eu(1)-O(11)	74.73(6)	O(7)#3-Eu(2)-N(2)#2	75.51(5)
O(13)-Eu(1)-O(11)	144.82(6)	O(19)#2-Eu(2)-O(9)#3	84.60(5)
O(15)-Eu(1)-O(11)	138.65(6)	O(16)-Eu(2)-O(9)#3	75.10(5)
O(10)-Eu(1)-O(14)	73.39(6)	O(5)-Eu(2)-O(9)#3	89.48(6)
O(1)-Eu(1)-O(14)	143.68(6)	O(3)#2-Eu(2)-O(9)#3	140.78(5)
O(12)-Eu(1)-O(14)	142.70(6)	N(1)-Eu(2)-O(9)#3	66.26(6)
O(17)#1-Eu(1)-O(14)	70.56(6)	O(7)#3-Eu(2)-O(9)#3	124.95(5)
O(13)-Eu(1)-O(14)	76.05(6)	N(2)#2-Eu(2)-O(9)#3	140.59(6)
O(15)-Eu(1)-O(14)	105.64(6)	O(19)#2-Eu(2)-N(3)#3	71.49(5)
O(11)-Eu(1)-O(14)	83.28(7)	O(16)-Eu(2)-N(3)#3	128.94(5)
O(19)#2-Eu(2)-O(16)	77.10(6)	O(5)-Eu(2)-N(3)#3	81.36(6)
O(19)#2-Eu(2)-O(5)	151.92(5)	O(3)#2-Eu(2)-N(3)#3	141.70(5)

O(16)-Eu(2)-O(5)	127.70(5)	N(1)-Eu(2)-N(3)#3	117.65(6)
O(19)#2-Eu(2)-O(3)#2	127.30(5)	O(7)#3-Eu(2)-N(3)#3	62.06(5)
O(16)-Eu(2)-O(3)#2	89.34(5)	N(2)#2-Eu(2)-N(3)#3	122.30(6)
O(5)-Eu(2)-O(3)#2	71.78(5)	O(9)#3-Eu(2)-N(3)#3	62.96(5)
O(19)#2-Eu(2)-N(1)	135.49(5)	O(7)#3-Eu(2)-N(2)#2	75.51(5)
O(16)-Eu(2)-N(1)	63.71(5)	O(19)#2-Eu(2)-O(9)#3	84.60(5)
O(5)-Eu(2)-N(1)	64.31(5)	O(16)-Eu(2)-O(9)#3	75.10(5)
O(3)#2-Eu(2)-N(1)	74.55(5)	O(5)-Eu(2)-O(9)#3	89.48(6)
O(19)#2-Eu(2)-O(7)#3	80.77(6)	O(3)#2-Eu(2)-O(9)#3	140.78(5)
O(16)-Eu(2)-O(7)#3	148.43(5)	N(1)-Eu(2)-O(9)#3	66.26(6)
O(5)-Eu(2)-O(7)#3	80.28(5)	O(7)#3-Eu(2)-O(9)#3	124.95(5)
O(3)#2-Eu(2)-O(7)#3	86.41(5)	N(2)#2-Eu(2)-O(9)#3	140.59(6)
N(1)-Eu(2)-O(7)#3	143.43(6)	O(19)#2-Eu(2)-N(3)#3	71.49(5)
O(19)#2-Eu(2)-N(2)#2	64.38(5)	O(16)-Eu(2)-N(3)#3	128.94(5)
O(16)-Eu(2)-N(2)#2	74.73(5)	O(5)-Eu(2)-N(3)#3	81.36(6)
O(5)-Eu(2)-N(2)#2	129.29(5)	O(3)#2-Eu(2)-N(3)#3	141.70(5)
O(3)#2-Eu(2)-N(2)#2	62.93(5)	N(1)-Eu(2)-N(3)#3	117.65(6)
N(1)-Eu(2)-N(2)#2	119.75(5)	O(7)#3-Eu(2)-N(3)#3	62.06(5)
O(9)#3-Eu(2)-N(3)#3	62.96(5)	N(2)#2-Eu(2)-N(3)#3	122.30(6)

Symmetry transformations used to generate equivalent atoms:

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

Table S2 Selected bond length [Å] and bond angle [°] for **1-Tb**.

O(8)-Tb(1)#1	2.327(3)	O(10)-Tb(1)	2.290(3)
N(1)-Tb(3)#2	2.440(4)	O(11)-Tb(1)	2.343(3)
N(2)-Tb(3)	2.456(4)	O(12)-Tb(1)	2.444(4)
N(3)-Tb(3)#3	2.512(4)	O(14)-Tb(3)#3	2.459(3)
O(1)-Tb(1)	2.366(3)	O(15)-Tb(1)	2.394(4)
O(2)-Tb(1)	2.337(3)	O(18)-Tb(3)#3	2.491(3)
O(3)-Tb(3)	2.433(3)	Tb(1)-O(8)#4	2.352(3)
O(4)-Tb(3)	2.390(3)	Tb(3)-O(7)#5	2.410(3)
O(5)-Tb(3)#2	2.394(3)	Tb(3)-O(5)#5	2.417(3)
O(6)-Tb(1)	2.391(3)	Tb(3)-N(1)#5	2.439(4)
O(7)-Tb(3)#2	2.386(3)	Tb(3)-O(14)#6	2.469(3)
Tb(3)-N(3)#6	2.496(4)	Tb(3)-O(18)#6	2.472(3)
O(10)-Tb(1)-O(2)	78.62(14)	O(4)-Tb(3)-O(5)#5	76.55(12)
O(10)-Tb(1)-O(11)	131.93(12)	O(7)#5-Tb(3)-O(5)#5	129.18(11)
O(2)-Tb(1)-O(11)	145.51(13)	O(4)-Tb(3)-O(3)	128.07(10)
O(10)-Tb(1)-O(8)#4	122.00(13)	O(7)#5-Tb(3)-O(3)	71.73(11)
O(2)-Tb(1)-O(8)#4	72.07(12)	O(5)#5-Tb(3)-O(3)	90.14(11)
O(11)-Tb(1)-O(8)#4	76.75(12)	O(4)-Tb(3)-N(1)#5	135.09(12)
O(10)-Tb(1)-O(1)	75.36(12)	O(7)#5-Tb(3)-N(1)#5	65.37(11)
O(2)-Tb(1)-O(1)	74.59(13)	O(5)#5-Tb(3)-N(1)#5	64.11(12)
O(11)-Tb(1)-O(1)	123.01(11)	O(3)-Tb(3)-N(1)#5	74.78(12)
O(8)#4-Tb(1)-O(1)	137.31(11)	O(4)-Tb(3)-N(2)	64.68(11)
O(10)-Tb(1)-O(6)	150.40(12)	O(7)#5-Tb(3)-N(2)	129.33(11)
O(2)-Tb(1)-O(6)	88.34(14)	O(5)#5-Tb(3)-N(2)	74.54(12)
O(11)-Tb(1)-O(6)	70.65(12)	O(3)-Tb(3)-N(2)	63.39(11)
O(8)#4-Tb(1)-O(6)	77.53(12)	N(1)#5-Tb(3)-N(2)	119.94(12)
O(1)-Tb(1)-O(6)	75.59(12)	O(4)-Tb(3)-O(14)#6	81.42(12)
O(10)-Tb(1)-O(15)	70.90(13)	O(7)#5-Tb(3)-O(14)#6	79.06(11)
O(2)-Tb(1)-O(15)	108.48(15)	O(5)#5-Tb(3)-O(14)#6	148.17(11)
O(11)-Tb(1)-O(15)	75.07(12)	O(3)-Tb(3)-O(14)#6	85.59(11)
O(8)#4-Tb(1)-O(15)	72.73(13)	N(1)#5-Tb(3)-O(14)#6	143.16(12)
O(1)-Tb(1)-O(15)	144.52(12)	N(2)-Tb(3)-O(14)#6	75.38(12)
O(6)-Tb(1)-O(15)	138.70(12)	O(4)-Tb(3)-O(18)#6	84.11(12)
O(10)-Tb(1)-O(12)	72.97(13)	O(7)#5-Tb(3)-O(18)#6	90.01(11)
O(2)-Tb(1)-O(12)	142.82(13)	O(5)#5-Tb(3)-O(18)#6	74.43(11)
O(11)-Tb(1)-O(12)	70.85(12)	O(3)-Tb(3)-O(18)#6	140.50(12)
O(8)#4-Tb(1)-O(12)	144.22(12)	N(1)#5-Tb(3)-O(18)#6	65.75(12)
O(1)-Tb(1)-O(12)	75.38(12)	N(2)-Tb(3)-O(18)#6	140.09(12)
O(6)-Tb(1)-O(12)	104.86(14)	O(14)#6-Tb(3)-O(18)#6	125.95(10)
O(15)-Tb(1)-O(12)	84.45(14)	O(4)-Tb(3)-N(3)#6	71.86(12)
O(4)-Tb(3)-O(7)#5	150.83(11)	O(7)#5-Tb(3)-N(3)#6	79.91(12)

N(2)-Tb(3)-N(3)#6	122.58(13)	O(5)#5-Tb(3)-N(3)#6	129.10(11)
O(14)#6-Tb(3)-N(3)#6	62.34(11)	O(3)-Tb(3)-N(3)#6	140.72(11)
O(18)#6-Tb(3)-N(3)#6	63.65(11)	N(1)#5-Tb(3)-N(3)#6	117.21(13)

Symmetry transformations used to generate equivalent atoms:

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

Table S3 Selected bond length [Å] and bond angle [°] for **2**.

Gd(1)-O(12)	2.403(4)	Gd(2)-O(11)	2.295(3)
Gd(1)-O(2)	2.414(4)	Gd(2)-O(14)	2.358(3)
Gd(1)-O(10)	2.421(4)	Gd(2)-O(15)	2.362(4)
Gd(1)-O(5)	2.435(3)	Gd(2)-O(9)	2.409(4)
Gd(1)-O(7)	2.439(3)	Gd(2)-O(8)	2.408(4)
Gd(1)-O(3)	2.448(3)	Gd(2)-O(6)	2.428(4)
Gd(1)-O(1)	2.452(3)	Gd(2)-O(16)	2.451(4)
Gd(1)-N(1)	2.499(4)	Gd(2)-O(13)	2.458(4)
Gd(1)-O(4)	2.555(3)		
O(12)-Gd(1)-O(2)	135.90(12)	O(7)-Gd(1)-O(4)	70.12(12)
O(12)-Gd(1)-O(10)	87.49(14)	O(3)-Gd(1)-O(4)	128.79(12)
O(2)-Gd(1)-O(10)	78.60(14)	O(1)-Gd(1)-O(4)	133.56(11)
O(12)-Gd(1)-O(5)	77.46(13)	N(1)-Gd(1)-O(4)	114.86(12)
O(2)-Gd(1)-O(5)	137.98(13)	O(11)-Gd(2)-O(14)	143.67(14)
O(10)-Gd(1)-O(5)	137.04(12)	O(11)-Gd(2)-O(15)	84.48(14)
O(12)-Gd(1)-O(7)	77.91(13)	O(14)-Gd(2)-O(15)	74.67(13)
O(2)-Gd(1)-O(7)	87.02(13)	O(11)-Gd(2)-O(9)	106.80(13)
O(10)-Gd(1)-O(7)	140.86(13)	O(14)-Gd(2)-O(9)	80.69(13)
O(5)-Gd(1)-O(7)	74.98(12)	O(15)-Gd(2)-O(9)	150.14(13)
O(12)-Gd(1)-O(3)	74.73(12)	O(11)-Gd(2)-O(8)	143.94(14)
O(2)-Gd(1)-O(3)	135.70(13)	O(14)-Gd(2)-O(8)	72.05(14)
O(10)-Gd(1)-O(3)	70.92(12)	O(15)-Gd(2)-O(8)	109.11(15)
O(5)-Gd(1)-O(3)	66.35(11)	O(9)-Gd(2)-O(8)	78.24(13)
O(7)-Gd(1)-O(3)	136.36(12)	O(11)-Gd(2)-O(6)	84.96(13)
O(12)-Gd(1)-O(1)	146.15(12)	O(14)-Gd(2)-O(6)	117.09(13)
O(2)-Gd(1)-O(1)	73.24(12)	O(15)-Gd(2)-O(6)	75.75(14)
O(10)-Gd(1)-O(1)	82.14(13)	O(9)-Gd(2)-O(6)	131.68(12)
O(5)-Gd(1)-O(1)	88.47(12)	O(8)-Gd(2)-O(6)	67.41(12)
O(7)-Gd(1)-O(1)	128.20(11)	O(11)-Gd(2)-O(16)	75.21(13)
O(3)-Gd(1)-O(1)	71.42(12)	O(14)-Gd(2)-O(16)	137.03(13)
O(12)-Gd(1)-N(1)	134.65(13)	O(15)-Gd(2)-O(16)	142.94(13)
O(2)-Gd(1)-N(1)	68.51(13)	O(9)-Gd(2)-O(16)	66.68(12)
O(10)-Gd(1)-N(1)	137.78(13)	O(8)-Gd(2)-O(16)	74.45(14)
O(5)-Gd(1)-N(1)	69.47(12)	O(6)-Gd(2)-O(16)	71.92(12)
O(7)-Gd(1)-N(1)	64.36(12)	O(11)-Gd(2)-O(13)	71.87(14)
O(3)-Gd(1)-N(1)	116.33(12)	O(14)-Gd(2)-O(13)	75.29(14)
O(1)-Gd(1)-N(1)	63.86(12)	O(15)-Gd(2)-O(13)	79.63(15)
O(12)-Gd(1)-O(4)	70.88(12)	O(9)-Gd(2)-O(13)	78.00(14)
O(2)-Gd(1)-O(4)	65.02(12)	O(8)-Gd(2)-O(13)	142.10(13)
O(10)-Gd(1)-O(4)	70.80(12)	O(6)-Gd(2)-O(13)	147.57(13)
O(5)-Gd(1)-O(4)	136.67(12)	O(16)-Gd(2)-O(13)	121.06(14)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1,y,z$	#2 $x-1,y,z$	#3 $-x+1,-y,-z+2$
#4 $x-1,y-1,z$	#5 $-x+2,-y+1,-z+1$	#6 $x+1,y+1,z$

Table S4 Hydrogen bonds for **1**-Eu [Å] and [°]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(14)-H(29)...O(9)	0.802(18)	2.30(3)	2.979(2)	143(4)
O(14)-H(27)...O(21)#7	0.82	1.97	2.662(4)	141.6
O(6)-H(6)...O(7)#8	0.82	1.83	2.581(2)	150.7
O(4)-H(4)...O(20)#9	0.82	1.91	2.703(3)	163.0
O(2)-H(2)...O(8)#10	0.82	1.79	2.593(2)	166.0
O(21)-H(22)...O(18)#11	0.839(19)	2.47(3)	3.256(5)	157(5)
O(21)-H(21)...O(8)#9	0.85(2)	2.10(2)	2.943(4)	177(7)
O(12)-H(28)...O(14)#3	0.79(4)	2.08(4)	2.858(3)	170(4)
O(12)-H(18)...O(3)	0.84(4)	1.91(4)	2.703(2)	156(3)
O(20)-H(16)...O(6)#12	0.78(4)	2.04(4)	2.820(2)	179(4)
O(20)-H(15)...O(19)#13	0.78(4)	2.00(4)	2.774(2)	175(4)
O(15)-H(26)...O(18)#14	0.80(4)	2.01(4)	2.805(2)	172(4)
O(15)-H(25)...O(16)	0.82(3)	1.92(4)	2.722(2)	163(3)
O(11)-H(3)...O(5)#1	0.70(4)	2.13(4)	2.772(2)	154(4)
O(11)-H(24)...O(20)#2	0.77(3)	2.15(4)	2.906(3)	165(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3,y-1/2,-z+3/2 #2 x+1,y,z #3 -x+2,y+1/2,-z+3/2
 #4 x-1,y,z #5 -x+2,y-1/2,-z+3/2 #6 -x+3,y+1/2,-z+3/2
 #7 -x+1,y-1/2,-z+3/2 #8 x,-y+1/2,z-1/2 #9 -x+1,-y+1,-z+2
 #10 -x+2,-y+1,-z+2 #11 x,-y+3/2,z+1/2 #12 x,-y+1/2,z+1/2
 #13 -x,y-1/2,-z+3/2 #14 -x+1,-y+1,-z+1

Table S5 Hydrogen bonds for **1**-Tb [$\text{\AA}$] and [$^\circ$]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(20)-H(10)...O(17)#2	0.85(2)	2.57(7)	3.127(8)	124(7)
O(20)-H(10)...O(16)#7	0.85(2)	2.45(4)	3.219(9)	151(7)
O(12)-H(7)...O(18)	0.84(2)	2.24(5)	2.973(5)	147(8)
O(20)-H(9)...O(21)#8	0.85(2)	2.12(5)	2.938(9)	163(14)
O(12)-H(8)...O(20)	0.84(2)	1.81(2)	2.632(8)	169(6)
O(2)-H(3)...O(12)#5	0.85(2)	2.00(2)	2.842(5)	171(5)
O(19)-H(11)...O(13)	0.83(2)	1.99(2)	2.816(5)	170(7)
O(15)-H(1)...O(7)	0.84(2)	2.03(5)	2.751(5)	143(6)
O(6)-H(6)...O(16)#7	0.85(2)	1.96(2)	2.799(5)	173(6)
O(15)-H(2)...O(19)#9	0.83(2)	2.09(3)	2.885(5)	160(6)
O(6)-H(5)...O(5)#4	0.86(2)	1.88(3)	2.714(5)	166(6)
O(19)-H(12)...O(4)#10	0.84(2)	1.92(3)	2.739(5)	164(7)
O(17)-H(17A)...O(19)#6	0.82	1.88	2.673(6)	163.3
O(13)-H(13A)...O(14)#8	0.82	1.80	2.550(4)	150.9
O(9)-H(15)...O(21)#11	0.82	1.76	2.563(5)	164.7

Symmetry transformations used to generate equivalent atoms:

#1 $-x-1, y+1/2, -z+1/2$ #2 $-x, y+1/2, -z+1/2$ #3 $-x+1, y+1/2, -z+1/2$
 #4 $-x-1, y-1/2, -z+1/2$ #5 $-x, y-1/2, -z+1/2$ #6 $-x+1, y-1/2, -z+1/2$
 #7 $-x+1, -y, -z+1$ #8 $x, -y+1/2, z+1/2$ #9 $x-1, -y+1/2, z-1/2$
 #10 $-x+2, -y, -z+1$ #11 $x-1, -y+1/2, z+1/2$