

Supporting Information

Lanthanide coordination frameworks constructed from 3,3',4,4'-diphenylsulfonetetracarboxylic and 1,10-phenanthroline: Synthesis, crystal structures and luminescence properties

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Table S1. Selected crystal data and structural refinement parameters.

Compound	1	2	3	4
Empirical formula	C ₁₆ H ₇ SmO ₁₃ S	C ₁₆ H ₁₀ EuO ₁₃ S	C ₁₆ H ₁₁ GdO ₁₃ S	C ₁₆ H ₆ TbO ₁₃ S
Formula weight	589.63	594.26	600.56	597.19
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
<i>a</i> (Å)	5.9443(9)	5.9204(10)	5.9188(7)	5.9118(15)
<i>b</i> (Å)	13.177(2)	13.177(2)	13.1837(16)	13.215(3)
<i>c</i> (Å)	13.687(2)	13.667(2)	13.6877(16)	13.723(4)
α (°)	109.604(2)	109.572(2)	109.804(2)	110.088(4)
β (°)	95.076(2)	94.896(2)	94.954(2)	94.904(4)
γ (°)	93.038(2)	93.260(3)	93.385(2)	93.524(4)
<i>V</i> (Å ³)	1002.1(3)	996.8(3)	996.7(2)	998.5(4)
<i>Z</i>	2	2	2	2
ρ_{calc} (g · cm ⁻³)	1.954	1.980	2.001	1.986
<i>F</i> (000)	570	578	582	574
Reflections collected	4935	4882	4912	4838
<i>S</i> on <i>F</i> ²	1.068	0.0278	1.037	0.391
<i>R</i> _{int}	0.0220	1.029	0.0147	1.158
<i>R</i> ₁ , <i>wR</i> ₂ ^a [<i>I</i> > 2σ(<i>I</i>)]	0.0351, 0.0970	0.0394, 0.1066	0.0263, 0.0721	0.0783, 0.2164
<i>R</i> ₁ , <i>wR</i> ₂ ^a (all data)	0.0376, 0.0988	0.0408, 0.1086	0.0408, 0.1086	0.0824, 0.2201
<i>CCDC</i>	1489387	1489388	1489389	1489390
Compound	5	6	7	8

empirical formula	C ₁₆ H ₇ DyO ₁₃ S	C ₁₆ H ₇ HoO ₁₃ S	C ₁₆ H ₇ ErO ₁₃ S	C ₁₆ H ₇ YbO ₁₃ S
formula weight	601.78	604.21	606.54	612.32
crystal system	Triclinic	Triclinic	Triclinic	Triclinic
space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
<i>a</i> (Å)	5.8841(9)	5.8683(11)	5.8366(12)	5.9317(12)
<i>b</i> (Å)	13.181(2)	13.161(3)	13.138(3)	13.181(3)
<i>c</i> (Å)	13.718(2)	13.719(3)	13.748(3)	13.685(3)
α (°)	110.236(2)	110.324(3)	110.348(3)	109.756(3)
β (°)	94.862(2)	94.741(3)	94.596(3)	95.029(3)
γ (°)	93.699(2)	93.886(3)	94.043(3)	93.180(3)
<i>V</i> (Å ³)	989.7(3)	984.8(3)	979.8(4)	999.0(3)
<i>Z</i>	2	2	2	2
ρ_{calcd} (mg·m ⁻³)	2.019	2.038	2.056	2.036
<i>F</i> (000)	578	580	582	586
Reflections collected	4922	4827	4857	4865
<i>R</i> _(int)	1.039	1.166	1.033	1.047
S on <i>F</i> ²	0.0229	0.0351	0.0303	0.0301
<i>R</i> ₁ , w <i>R</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0327,0.0780	0.0566,0.1137	0.0424, 0.1147	0.047, 0.1222
<i>R</i> ₁ , w <i>R</i> ₂ (all data)	0.0374,0.0811	0.0624,0.1172	0.0467, 0.1192	0.054, 0.1276
CCDC	1489391	1489492	1489393	1489394
Compound	9	10	11	12
empirical formula	C ₂₈ H ₁₉ PrN ₂ O _{12.5} S	C ₂₈ H ₁₉ NdN ₂ O _{12.5} S	C ₂₈ H ₁₉ EuN ₂ O _{12.5} S	C ₂₈ H ₁₉ TbN ₂ O _{12.5} S
formula weight	756.42	759.75	767.47	774.43

crystal system	Triclinic	Triclinic	Triclinic	Triclinic
space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
<i>a</i> (Å)	10.5654(17)	10.5704(13)	10.6041(15)	10.6026(13)
<i>b</i> (Å)	11.668(2)	11.6325(13)	11.5157(17)	11.5116(14)
<i>c</i> (Å)	12.0378(19)	12.0347(14)	12.0048(17)	11.9957(15)
α (°)	109.547(3)	109.448(2)	108.843(2)	108.870(2)
β (°)	105.454(3)	105.460(2)	105.804(2)	105.771(2)
γ (°)	90.547(3)	90.611(2)	90.751(2)	90.769(2)
<i>V</i> (Å ³)	1339.9(4)	1336.8(3)	1326.7(3)	1325.0(3)
<i>Z</i>	2	2	2	2
ρ_{calcd} (mg·m ⁻³)	1.875	1.887	1.921	1.941
<i>F</i> (000)	752	754	760	764
Reflections collected	4661	4659	4619	4626
<i>R</i> _(int)	1.046	1.095	0.0279	0.0212
S on <i>F</i> ²	0.0409	0.0201	1.002	1.017
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> >2σ(<i>I</i>)]	0.0578, 0.1090	0.0353, 0.0743	0.0329, 0.0642	0.0316, 0.0700
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0697, 0.1145	0.0389, 0.0762	0.0329, 0.0674	0.0384, 0.0742
CCDC	1489395	1489396	1489397	1489398

$$^aR_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, wR_2 = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2} \right]^{1/2}$$

Table S2. Selected bond lengths [Å] and angles [°] for compounds **1-12**.

Compound 1			
Sm(1)-O(2)#1	2.391(4)	Sm(1)-O(11)	2.414(4)
Sm(1)-O(12)	2.439(4)	Sm(1)-O(3)#2	2.455(4)
Sm(1)-O(4)#2	2.455(4)	Sm(1)-O(6)#3	2.475(4)
Sm(1)-O(1)	2.481(4)	Sm(1)-O(5)#3	2.515(4)
Sm(1)-O(2)	2.687(4)		
O(2)#1-Sm(1)-O(12)	86.43(15)	O(2)#1-Sm(1)-O(3)#2	79.99(15)
O(12)-Sm(1)-O(3)#2	127.49(14)	O(2)#1-Sm(1)-O(4)#2	80.64(15)
O(12)-Sm(1)-O(4)#2	74.60(15)	O(3)#2-Sm(1)-O(4)#2	53.28(13)
O(2)#1-Sm(1)-O(6)#3	154.30(15)	O(12)-Sm(1)-O(6)#3	92.97(16)
O(3)#2-Sm(1)-O(6)#3	80.07(15)	O(4)#2-Sm(1)-O(6)#3	74.46(16)
O(2)#1-Sm(1)-O(1)	114.17(14)	O(12)-Sm(1)-O(1)	148.30(16)
O(3)#2-Sm(1)-O(1)	81.51(14)	O(4)#2-Sm(1)-O(1)	130.19(15)
O(6)#3-Sm(1)-O(1)	78.55(15)	O(2)#1-Sm(1)-O(5)#3	151.78(14)
O(12)-Sm(1)-O(5)#3	80.67(15)	O(3)#2-Sm(1)-O(5)#3	127.52(14)
O(4)#2-Sm(1)-O(5)#3	119.19(15)	O(6)#3-Sm(1)-O(5)#3	52.21(14)
O(1)-Sm(1)-O(5)#3	69.95(14)	O(2)#1-Sm(1)-O(2)	64.29(15)
O(12)-Sm(1)-O(2)	140.94(14)	O(3)#2-Sm(1)-O(2)	74.59(13)
O(4)#2-Sm(1)-O(2)	121.40(14)	O(6)#3-Sm(1)-O(2)	124.73(15)
O(1)-Sm(1)-O(2)	49.91(13)	O(5)#3-Sm(1)-O(2)	112.79(13)
O(1)#1-Sm(1)-O(11)	78.29(16)	O(11)-Sm(1)-O(3)#2	145.05(16)
O(11)-Sm(1)-O(5)#3	74.49(16)	O(11)-Sm(1)-O(12)	77.71(16)
O(11)-Sm(1)-O(6)#3	127.01(16)	O(11)-Sm(1)-O(2)	83.26(17)
Compound 2			
Eu(1)-O(1)#1	2.378(4)	Eu(1)-O(11)	2.398(4)

Eu(1)-O(12)	2.416(4)	Eu(1)-O(3)#2	2.433(4)
Eu(1)-O(4)#2	2.448(4)	Eu(1)-O(6)#3	2.460(4)
Eu(1)-O(2)	2.467(4)	Eu(1)-O(5)#3	2.502(4)
Eu(1)-O(1)	2.682(4)		
O(1)#1-Eu(1)-O(11)	78.29(16)	O(1)#1-Eu(1)-O(12)	86.65(15)
O(11)-Eu(1)-O(12)	77.71(16)	O(1)#1-Eu(1)-O(3)#2	79.64(14)
O(11)-Eu(1)-O(3)#2	145.05(16)	O(12)-Eu(1)-O(3)#2	127.55(14)
O(1)#1-Eu(1)-O(4)#2	80.68(15)	O(11)-Eu(1)-O(4)#2	145.84(17)
O(12)-Eu(1)-O(4)#2	74.46(14)	O(3)#2-Eu(1)-O(4)#2	53.51(13)
O(1)#1-Eu(1)-O(6)#3	154.11(14)	O(11)-Eu(1)-O(6)#3	127.01(16)
O(12)-Eu(1)-O(6)#3	93.33(16)	O(3)#2-Eu(1)-O(6)#3	79.93(14)
O(4)#2-Eu(1)-O(6)#3	74.42(15)	O(1)#1-Eu(1)-O(2)	113.86(13)
O(11)-Eu(1)-O(2)	83.26(17)	O(12)-Eu(1)-O(2)	148.52(15)
O(3)#2-Eu(1)-O(2)	81.30(14)	O(4)#2-Eu(1)-O(2)	130.16(14)
O(6)#3-Eu(1)-O(2)	78.38(15)	O(1)#1-Eu(1)-O(5)#3	151.80(13)
O(11)-Eu(1)-O(5)#3	74.49(16)	O(12)-Eu(1)-O(5)#3	80.51(15)
O(3)#2-Eu(1)-O(5)#3	127.84(14)	O(4)#2-Eu(1)-O(5)#3	119.11(15)
O(6)#3-Eu(1)-O(5)#3	52.54(13)	O(2)-Eu(1)-O(5)#3	70.29(14)
O(1)#1-Eu(1)-O(1)	63.92(14)	O(11)-Eu(1)-O(1)	71.76(15)
O(12)-Eu(1)-O(1)	140.89(14)	O(3)#2-Eu(1)-O(1)	74.29(13)
Compound 3			
Gd(1)-O(1)#1	2.367(3)	Gd(1)-O(11)	2.375(4)
Gd(1)-O(12)	2.403(3)	Gd(1)-O(3)#2	2.430(3)
Gd(1)-O(4)#2	2.437(3)	Gd(1)-O(2)	2.451(3)
Gd(1)-O(5)#3	2.454(3)	Gd(1)-O(6)#3	2.497(3)
Gd(1)-O(1)	2.682(3)		
O(1)#1-Gd(1)-O(11)	77.70(13)	O(1)#1-Gd(1)-O(12)	86.47(13)
O(11)-Gd(1)-O(12)	77.23(13)	O(1)#1-Gd(1)-O(3)#2	79.86(12)

O(11)-Gd(1)-O(3)#2	145.10(12)	O(12)-Gd(1)-O(3)#2	127.63(12)
O(1)#1-Gd(1)-O(4)#2	80.75(12)	O(11)-Gd(1)-O(4)#2	145.03(14)
O(12)-Gd(1)-O(4)#2	74.24(12)	O(3)#2-Gd(1)-O(4)#2	53.80(11)
O(1)#1-Gd(1)-O(2)	114.04(11)	O(11)-Gd(1)-O(2)	83.80(14)
O(12)-Gd(1)-O(2)	148.39(12)	O(3)#2-Gd(1)-O(2)	81.35(11)
O(4)#2-Gd(1)-O(2)	130.46(12)	O(1)#1-Gd(1)-O(5)#3	154.27(12)
O(11)-Gd(1)-O(5)#3	127.34(13)	O(12)-Gd(1)-O(5)#3	93.25(13)
O(3)#2-Gd(1)-O(5)#3	80.02(12)	O(4)#2-Gd(1)-O(5)#3	74.45(13)
O(2)-Gd(1)-O(5)#3	78.41(12)	O(1)#1-Gd(1)-O(6)#3	151.43(11)
O(11)-Gd(1)-O(6)#3	74.73(13)	O(12)-Gd(1)-O(6)#3	80.33(13)
O(3)#2-Gd(1)-O(6)#3	128.02(11)	O(4)#2-Gd(1)-O(6)#3	119.05(12)
O(2)-Gd(1)-O(6)#3	70.34(11)	O(5)#3-Gd(1)-O(6)#3	52.62(11)
O(1)#1-Gd(1)-O(1)	63.97(12)	O(11)-Gd(1)-O(1)	71.98(12)
O(12)-Gd(1)-O(1)	140.83(11)	O(3)#2-Gd(1)-O(1)	74.25(10)
O(4)#2-Gd(1)-O(1)	121.49(11)	O(2)-Gd(1)-O(1)	50.10(10)
O(5)#3-Gd(1)-O(1)	124.66(12)	O(6)#3-Gd(1)-O(1)	113.22(11)
Compound 4			
Tb(1)-O(2)#1	2.341(10)	Tb(1)-O(11)	2.385(10)
Tb(1)-O(12)	2.404(11)	Tb(1)-O(3)#2	2.425(10)
Tb(1)-O(6)#3	2.434(11)	Tb(1)-O(1)	2.439(10)
Tb(1)-O(4)#2	2.441(10)	Tb(1)-O(5)#3	2.475(11)
Tb(1)-O(2)	2.717(10)		
O(2)#1-Tb(1)-O(11)	77.4(4)	O(2)#1-Tb(1)-O(12)	86.2(4)
O(11)-Tb(1)-O(12)	76.7(4)	O(2)#1-Tb(1)-O(3)#2	79.5(4)
O(11)-Tb(1)-O(3)#2	145.0(4)	O(12)-Tb(1)-O(3)#2	127.5(3)
O(2)#1-Tb(1)-O(6)#3	154.1(4)	O(11)-Tb(1)-O(6)#3	127.7(4)
O(12)-Tb(1)-O(6)#3	93.5(4)	O(3)#2-Tb(1)-O(6)#3	80.3(4)
O(2)#1-Tb(1)-O(1)	113.8(3)	O(11)-Tb(1)-O(1)	84.4(4)
O(12)-Tb(1)-O(1)	148.9(4)	O(3)#2-Tb(1)-O(1)	81.3(3)

O(6)#3-Tb(1)-O(1)	78.6(4)	O(2)#1-Tb(1)-O(4)#2	80.5(4)
O(11)-Tb(1)-O(4)#2	144.2(4)	O(12)-Tb(1)-O(4)#2	73.9(4)
O(3)#2-Tb(1)-O(4)#2	54.0(3)	O(6)#3-Tb(1)-O(4)#2	74.6(4)
O(1)-Tb(1)-O(4)#2	130.7(3)	O(2)#1-Tb(1)-O(5)#3	151.1(4)
O(11)-Tb(1)-O(5)#3	74.6(4)	O(12)-Tb(1)-O(5)#3	80.7(4)
O(3)#2-Tb(1)-O(5)#3	128.6(3)	O(6)#3-Tb(1)-O(5)#3	53.1(3)
O(1)-Tb(1)-O(5)#3	70.5(4)	O(4)#2-Tb(1)-O(5)#3	119.5(4)
O(2)#1-Tb(1)-O(2)	64.0(4)	O(11)-Tb(1)-O(2)	72.1(4)
O(12)-Tb(1)-O(2)	140.6(4)	O(3)#2-Tb(1)-O(2)	74.2(3)
O(6)#3-Tb(1)-O(2)	124.7(4)	O(1)-Tb(1)-O(2)	49.8(3)
O(4)#2-Tb(1)-O(2)	121.7(3)	O(5)#3-Tb(1)-O(2)	112.8(4)
Compound 5			
Dy(1)-O(2)#1	2.328(4)	Dy(1)-O(12)	2.362(4)
Dy(1)-O(11)	2.372(4)	Dy(1)-O(3)#2	2.399(4)
Dy(1)-O(4)#2	2.409(4)	Dy(1)-O(1)	2.419(4)
Dy(1)-O(6)#3	2.421(4)	Dy(1)-O(5)#3	2.463(4)
Dy(1)-O(2)	2.723(4)		
O(2)#1-Dy(1)-O(12)	77.13(14)	O(2)#1-Dy(1)-O(11)	86.40(15)
O(12)-Dy(1)-O(11)	77.19(15)	O(2)#1-Dy(1)-O(3)#2	79.69(14)
O(12)-Dy(1)-O(3)#2	144.34(14)	O(11)-Dy(1)-O(3)#2	127.94(14)
O(2)#1-Dy(1)-O(4)#2	80.65(15)	O(12)-Dy(1)-O(4)#2	144.67(15)
O(11)-Dy(1)-O(4)#2	74.31(14)	O(3)#2-Dy(1)-O(4)#2	54.08(13)
O(2)#1-Dy(1)-O(1)	113.68(13)	O(12)-Dy(1)-O(1)	83.83(15)
O(11)-Dy(1)-O(1)	148.55(15)	O(3)#2-Dy(1)-O(1)	81.12(13)
O(4)#2-Dy(1)-O(1)	130.61(14)	O(2)#1-Dy(1)-O(6)#3	154.23(14)
O(12)-Dy(1)-O(6)#3	127.98(14)	O(11)-Dy(1)-O(6)#3	93.46(16)
O(3)#2-Dy(1)-O(6)#3	80.17(14)	O(4)#2-Dy(1)-O(6)#3	74.55(15)
O(1)-Dy(1)-O(6)#3	78.69(15)	O(2)#1-Dy(1)-O(5)#3	150.89(14)
O(12)-Dy(1)-O(5)#3	74.77(14)	O(11)-Dy(1)-O(5)#3	80.16(15)

O(3)#2-Dy(1)-O(5)#3	128.67(13)	O(4)#2-Dy(1)-O(5)#3	119.53(14)
O(1)-Dy(1)-O(5)#3	70.70(14)	O(6)#3-Dy(1)-O(5)#3	53.23(13)
O(2)#1-Dy(1)-O(2)	63.96(15)	O(12)-Dy(1)-O(2)	71.87(14)
O(11)-Dy(1)-O(2)	140.84(13)	O(3)#2-Dy(1)-O(2)	73.72(12)
O(4)#2-Dy(1)-O(2)	121.27(13)	O(1)-Dy(1)-O(2)	49.74(12)
O(6)#3-Dy(1)-O(2)	124.48(14)	O(5)#3-Dy(1)-O(2)	113.16(13)
Compound 6			
Ho(1)-O(2)#1	2.325(8)	Ho(1)-O(11)	2.347(8)
Ho(1)-O(12)	2.362(7)	Ho(1)-O(1)	2.385(7)
Ho(1)-O(4)#2	2.388(8)	Ho(1)-O(3)#2	2.391(8)
Ho(1)-O(5)#3	2.414(8)	Ho(1)-O(6)#3	2.443(8)
Ho(1)-O(2)	2.736(8)		
O(2)#1-Ho(1)-O(11)	77.3(3)	O(2)#1-Ho(1)-O(12)	86.7(3)
O(11)-Ho(1)-O(12)	77.4(3)	O(2)#1-Ho(1)-O(1)	113.5(3)
O(11)-Ho(1)-O(1)	83.5(3)	O(12)-Ho(1)-O(1)	148.4(3)
O(2)#1-Ho(1)-O(4)#2	80.5(3)	O(11)-Ho(1)-O(4)#2	144.5(3)
O(12)-Ho(1)-O(4)#2	73.9(3)	O(1)-Ho(1)-O(4)#2	131.1(3)
O(2)#1-Ho(1)-O(3)#2	79.3(3)	O(11)-Ho(1)-O(3)#2	143.7(3)
O(12)-Ho(1)-O(3)#2	128.3(2)	O(1)-Ho(1)-O(3)#2	80.9(3)
O(4)#2-Ho(1)-O(3)#2	54.8(2)	O(2)#1-Ho(1)-O(5)#3	153.9(3)
O(11)-Ho(1)-O(5)#3	128.3(3)	O(12)-Ho(1)-O(5)#3	93.6(3)
O(1)-Ho(1)-O(5)#3	78.7(3)	O(4)#2-Ho(1)-O(5)#3	74.6(3)
O(3)#2-Ho(1)-O(5)#3	80.1(3)	O(2)#1-Ho(1)-O(6)#3	150.9(3)
O(11)-Ho(1)-O(6)#3	74.6(3)	O(12)-Ho(1)-O(6)#3	80.1(3)
O(1)-Ho(1)-O(6)#3	70.6(2)	O(4)#2-Ho(1)-O(6)#3	119.7(3)
O(3)#2-Ho(1)-O(6)#3	128.9(3)	O(5)#3-Ho(1)-O(6)#3	53.7(3)
O(2)#1-Ho(1)-O(2)	64.1(3)	O(11)-Ho(1)-O(2)	71.4(2)
O(12)-Ho(1)-O(2)	140.9(3)	O(1)-Ho(1)-O(2)	49.5(2)
O(4)#2-Ho(1)-O(2)	121.9(2)	O(3)#2-Ho(1)-O(2)	73.6(2)

O(5)#3-Ho(1)-O(2)	124.2(3)	O(6)#3-Ho(1)-O(2)	112.7(2)
Compound 7			
Er(1)-O(1)	2.274(5)	Er(1)-O(11)	2.330(6)
Er(1)-O(12)	2.340(5)	Er(1)-O(2)#1	2.371(5)
Er(1)-O(5)#2	2.385(6)	Er(1)-O(3)#3	2.387(5)
Er(1)-O(4)#3	2.391(6)	Er(1)-O(6)#2	2.449(5)
Er(1)-O(1)#1	2.820(6)		
O(1)-Er(1)-O(11)	77.0(2)	O(1)-Er(1)-O(12)	86.2(2)
O(11)-Er(1)-O(12)	77.7(2)	O(1)-Er(1)-O(2)#1	112.96(19)
O(11)-Er(1)-O(2)#1	83.0(2)	O(12)-Er(1)-O(2)#1	148.9(2)
O(1)-Er(1)-O(5)#2	153.9(2)	O(11)-Er(1)-O(5)#2	128.71(19)
O(12)-Er(1)-O(5)#2	94.1(2)	O(2)#1-Er(1)-O(5)#2	79.2(2)
O(1)-Er(1)-O(3)#3	78.94(19)	O(11)-Er(1)-O(3)#3	142.52(19)
O(12)-Er(1)-O(3)#3	128.69(19)	O(2)#1-Er(1)-O(3)#3	80.54(19)
O(5)#2-Er(1)-O(3)#3	80.54(18)	O(1)-Er(1)-O(4)#3	80.0(2)
O(11)-Er(1)-O(4)#3	144.8(2)	O(12)-Er(1)-O(4)#3	74.42(19)
O(2)#1-Er(1)-O(4)#3	131.0(2)	O(5)#2-Er(1)-O(4)#3	74.9(2)
O(3)#3-Er(1)-O(4)#3	54.80(18)	O(1)-Er(1)-O(6)#2	151.07(19)
O(11)-Er(1)-O(6)#2	75.27(18)	O(12)-Er(1)-O(6)#2	80.18(19)
O(2)#1-Er(1)-O(6)#2	71.42(18)	O(5)#2-Er(1)-O(6)#2	53.49(17)
O(3)#3-Er(1)-O(6)#2	129.16(17)	O(4)#3-Er(1)-O(6)#2	119.83(18)
Er(1)-O(1)	2.274(5)	Er(1)-O(11)	2.330(6)
Er(1)-O(12)	2.340(5)	Er(1)-O(2)#1	2.371(5)
Er(1)-O(5)#2	2.385(6)	Er(1)-O(3)#3	2.387(5)
Er(1)-O(4)#3	2.391(6)	Er(1)-O(6)#2	2.449(5)
Compound 8			
Yb(1)-O(2)#1	2.388(6)	Yb(1)-O(11)	2.406(7)
Yb(1)-O(12)	2.424(7)	Yb(1)-O(3)#2	2.441(6)
Yb(1)-O(4)#2	2.448(6)	Yb(1)-O(1)	2.463(6)

Yb(1)-O(6)#3	2.465(7)	Yb(1)-O(5)#3	2.494(6)
Yb(1)-O(2)	2.669(6)		
O(2)#1-Yb(1)-O(11)	78.0(2)	O(2)#1-Yb(1)-O(12)	86.9(2)
O(11)-Yb(1)-O(12)	77.0(2)	O(2)#1-Yb(1)-O(3)#2	79.7(2)
O(11)-Yb(1)-O(3)#2	145.5(2)	O(12)-Yb(1)-O(3)#2	127.6(2)
O(2)#1-Yb(1)-O(4)#2	80.8(2)	O(11)-Yb(1)-O(4)#2	145.3(3)
O(12)-Yb(1)-O(4)#2	74.8(2)	O(3)#2-Yb(1)-O(4)#2	53.2(2)
O(2)#1-Yb(1)-O(1)	113.8(2)	O(11)-Yb(1)-O(1)	83.4(3)
O(12)-Yb(1)-O(1)	147.9(2)	O(3)#2-Yb(1)-O(1)	81.9(2)
O(4)#2-Yb(1)-O(1)	130.6(2)	O(2)#1-Yb(1)-O(6)#3	154.1(2)
O(11)-Yb(1)-O(6)#3	127.3(2)	O(12)-Yb(1)-O(6)#3	93.1(3)
O(3)#2-Yb(1)-O(6)#3	79.8(2)	O(4)#2-Yb(1)-O(6)#3	74.3(2)
O(1)-Yb(1)-O(6)#3	78.7(2)	O(2)#1-Yb(1)-O(5)#3	151.8(2)
O(11)-Yb(1)-O(5)#3	74.7(2)	O(12)-Yb(1)-O(5)#3	80.4(2)
O(3)#2-Yb(1)-O(5)#3	127.7(2)	O(4)#2-Yb(1)-O(5)#3	119.2(2)
O(1)-Yb(1)-O(5)#3	69.9(2)	O(6)#3-Yb(1)-O(5)#3	52.6(2)
O(2)#1-Yb(1)-O(2)	64.0(2)	O(11)-Yb(1)-O(2)	71.9(2)
O(12)-Yb(1)-O(2)	140.8(2)	O(3)#2-Yb(1)-O(2)	74.7(2)
O(4)#2-Yb(1)-O(2)	121.6(2)	O(1)-Yb(1)-O(2)	49.8(2)
O(6)#3-Yb(1)-O(2)	124.6(2)	O(5)#3-Yb(1)-O(2)	112.7(2)
Compound 9			
Pr(1)-O(8)#1	2.367(6)	Pr(1)-O(7)#2	2.404(5)
Pr(1)-O(2)	2.502(5)	Pr(1)-O(3)#3	2.529(5)
Pr(1)-O(1)	2.536(5)	Pr(1)-O(11)	2.586(6)
Pr(1)-O(4)#3	2.639(5)	Pr(1)-N(2)	2.669(6)
Pr(1)-N(1)	2.694(6)		
O(8)#1-Pr(1)-O(7)#2	84.54(18)	O(8)#1-Pr(1)-O(2)	136.55(18)
O(7)#2-Pr(1)-O(2)	96.06(17)	O(8)#1-Pr(1)-O(3)#3	126.45(18)

O(7)#2-Pr(1)-O(3)#3	141.07(17)	O(2)-Pr(1)-O(3)#3	77.40(16)
O(8)#1-Pr(1)-O(1)	87.6(2)	O(7)#2-Pr(1)-O(1)	74.07(18)
O(2)-Pr(1)-O(1)	51.70(17)	O(3)#3-Pr(1)-O(1)	123.89(18)
O(8)#1-Pr(1)-O(11)	80.76(19)	O(7)#2-Pr(1)-O(11)	140.87(18)
O(2)-Pr(1)-O(11)	71.66(18)	O(3)#3-Pr(1)-O(11)	73.98(18)
O(1)-Pr(1)-O(11)	69.29(19)	O(8)#1-Pr(1)-O(4)#3	76.71(18)
O(7)#2-Pr(1)-O(4)#3	141.64(17)	O(2)-Pr(1)-O(4)#3	120.53(16)
O(3)#3-Pr(1)-O(4)#3	50.30(16)	O(1)-Pr(1)-O(4)#3	136.85(18)
O(11)-Pr(1)-O(4)#3	68.64(18)	O(8)#1-Pr(1)-N(2)	143.28(19)
O(7)#2-Pr(1)-N(2)	72.22(18)	O(2)-Pr(1)-N(2)	75.35(18)
O(3)#3-Pr(1)-N(2)	68.98(18)	O(1)-Pr(1)-N(2)	111.7(2)
O(11)-Pr(1)-N(2)	134.6(2)	O(4)#3-Pr(1)-N(2)	104.30(18)
O(8)#1-Pr(1)-N(1)	85.2(2)	O(7)#2-Pr(1)-N(1)	72.50(18)
O(2)-Pr(1)-N(1)	136.53(18)	O(3)#3-Pr(1)-N(1)	86.03(19)
O(1)-Pr(1)-N(1)	146.29(19)	O(11)-Pr(1)-N(1)	141.04(19)
O(4)#3-Pr(1)-N(1)	72.82(18)	N(2)-Pr(1)-N(1)	61.2(2)
Compound 10			
Nd(1)-O(8)#1	2.356(3)	Nd(1)-O(7)#2	2.393(3)
Nd(1)-O(2)	2.485(3)	Nd(1)-O(3)#3	2.514(3)
Nd(1)-O(1)	2.530(3)	Nd(1)-O(11)	2.572(3)
Nd(1)-O(4)#3	2.628(3)	Nd(1)-N(2)	2.661(4)
Nd(1)-N(1)	2.668(4)		
O(8)#1-Nd(1)-O(7)#2	84.67(12)	O(8)#1-Nd(1)-O(2)	136.96(12)
O(7)#2-Nd(1)-O(2)	96.46(11)	O(8)#1-Nd(1)-O(3)#3	126.17(12)
O(7)#2-Nd(1)-O(3)#3	141.19(11)	O(2)-Nd(1)-O(3)#3	76.96(10)
O(8)#1-Nd(1)-O(1)	87.62(13)	O(7)#2-Nd(1)-O(1)	74.29(11)
O(2)-Nd(1)-O(1)	52.18(11)	O(3)#3-Nd(1)-O(1)	123.80(10)
O(8)#1-Nd(1)-O(11)	80.31(11)	O(7)#2-Nd(1)-O(11)	140.54(12)
O(2)-Nd(1)-O(11)	71.77(11)	O(3)#3-Nd(1)-O(11)	74.30(11)

O(1)-Nd(1)-O(11)	68.84(12)	O(8)#1-Nd(1)-O(4)#3	75.97(12)
O(7)#2-Nd(1)-O(4)#3	141.51(11)	O(2)-Nd(1)-O(4)#3	120.39(10)
O(3)#3-Nd(1)-O(4)#3	50.74(10)	O(1)-Nd(1)-O(4)#3	136.26(11)
O(11)-Nd(1)-O(4)#3	68.56(11)	O(8)#1-Nd(1)-N(2)	143.21(12)
O(7)#2-Nd(1)-N(2)	72.13(11)	O(2)-Nd(1)-N(2)	75.26(11)
O(3)#3-Nd(1)-N(2)	69.20(11)	O(1)-Nd(1)-N(2)	111.95(12)
O(11)-Nd(1)-N(2)	135.12(12)	O(4)#3-Nd(1)-N(2)	104.90(11)
O(8)#1-Nd(1)-N(1)	84.71(12)	O(7)#2-Nd(1)-N(1)	72.73(12)
O(2)-Nd(1)-N(1)	136.82(11)	O(3)#3-Nd(1)-N(1)	86.09(12)
O(1)-Nd(1)-N(1)	146.67(12)	O(11)-Nd(1)-N(1)	140.70(12)
O(4)#3-Nd(1)-N(1)	72.62(12)	N(2)-Nd(1)-N(1)	61.59(12)
Compound 11			
Eu(1)-O(1)	2.320(3)	Eu(1)-O(2)#1	2.348(3)
Eu(1)-O(7)#2	2.425(3)	Eu(1)-O(6)#3	2.475(3)
Eu(1)-O(8)#2	2.506(3)	Eu(1)-O(11)	2.527(3)
Eu(1)-O(5)#3	2.597(3)	Eu(1)-N(1)	2.615(4)
Eu(1)-N(2)	2.626(4)		
O(1)-Eu(1)-O(2)#1	84.46(11)	O(1)-Eu(1)-O(7)#2	135.94(11)
O(2)#1-Eu(1)-O(7)#2	96.30(11)	O(1)-Eu(1)-O(6)#3	126.17(11)
O(2)#1-Eu(1)-O(6)#3	141.85(10)	O(7)#2-Eu(1)-O(6)#3	77.37(10)
O(1)-Eu(1)-O(8)#2	85.94(11)	O(2)#1-Eu(1)-O(8)#2	73.72(11)
O(7)#2-Eu(1)-O(8)#2	52.86(10)	O(6)#3-Eu(1)-O(8)#2	124.61(10)
O(1)-Eu(1)-O(11)	79.26(11)	O(2)#1-Eu(1)-O(11)	139.92(11)
O(7)#2-Eu(1)-O(11)	72.16(11)	O(6)#3-Eu(1)-O(11)	74.50(11)
O(8)#2-Eu(1)-O(11)	68.83(12)	O(1)-Eu(1)-O(5)#3	75.65(10)
O(2)#1-Eu(1)-O(5)#3	141.19(11)	O(7)#2-Eu(1)-O(5)#3	121.17(10)
O(6)#3-Eu(1)-O(5)#3	51.20(9)	O(8)#2-Eu(1)-O(5)#3	135.90(11)
O(11)-Eu(1)-O(5)#3	68.54(11)	O(1)-Eu(1)-N(1)	84.83(11)
O(2)#1-Eu(1)-N(1)	73.84(11)	O(7)#2-Eu(1)-N(1)	137.82(11)

O(6)#3-Eu(1)-N(1)	85.81(11)	O(8)#2-Eu(1)-N(1)	146.95(11)
O(11)-Eu(1)-N(1)	139.48(12)	O(5)#3-Eu(1)-N(1)	71.49(11)
O(1)-Eu(1)-N(2)	144.13(11)	O(2)#1-Eu(1)-N(2)	73.00(11)
O(7)#2-Eu(1)-N(2)	75.34(11)	O(6)#3-Eu(1)-N(2)	68.99(11)
O(8)#2-Eu(1)-N(2)	112.88(11)	O(11)-Eu(1)-N(2)	135.25(11)
Compound 12			
Tb(1)-O(5)#1	2.315(3)	Tb(1)-O(6)#2	2.346(3)
Tb(1)-O(3)#3	2.437(3)	Tb(1)-O(1)	2.474(3)
Tb(1)-O(4)#3	2.499(3)	Tb(1)-O(11)	2.535(4)
Tb(1)-O(2)	2.597(3)	Tb(1)-N(2)	2.615(4)
Tb(1)-N(1)	2.626(4)		
O(5)#1-Tb(1)-O(6)#2	84.14(12)	O(5)#1-Tb(1)-O(3)#3	135.90(11)
O(6)#2-Tb(1)-O(3)#3	96.49(12)	O(5)#1-Tb(1)-O(1)	126.36(11)
O(6)#2-Tb(1)-O(1)	141.79(11)	O(3)#3-Tb(1)-O(1)	77.46(11)
O(5)#1-Tb(1)-O(4)#3	85.88(12)	O(6)#2-Tb(1)-O(4)#3	73.85(12)
O(3)#3-Tb(1)-O(4)#3	52.82(10)	O(1)-Tb(1)-O(4)#3	124.70(11)
O(5)#1-Tb(1)-O(11)	79.39(11)	O(6)#2-Tb(1)-O(11)	139.81(12)
O(3)#3-Tb(1)-O(11)	72.03(11)	O(1)-Tb(1)-O(11)	74.75(11)
O(4)#3-Tb(1)-O(11)	68.64(12)	O(5)#1-Tb(1)-O(2)	75.84(11)
O(6)#2-Tb(1)-O(2)	141.14(11)	O(3)#3-Tb(1)-O(2)	121.07(10)
O(1)-Tb(1)-O(2)	51.15(10)	O(4)#3-Tb(1)-O(2)	135.79(12)
O(11)-Tb(1)-O(2)	68.60(11)	O(5)#1-Tb(1)-N(2)	84.92(12)
O(6)#2-Tb(1)-N(2)	73.62(12)	O(3)#3-Tb(1)-N(2)	137.72(11)
O(1)-Tb(1)-N(2)	85.70(12)	O(4)#3-Tb(1)-N(2)	146.90(12)
O(11)-Tb(1)-N(2)	139.79(12)	O(2)-Tb(1)-N(2)	71.74(12)
O(5)#1-Tb(1)-N(1)	144.12(12)	O(6)#2-Tb(1)-N(1)	73.09(12)
O(3)#3-Tb(1)-N(1)	75.28(11)	O(1)-Tb(1)-N(1)	68.86(11)
O(4)#3-Tb(1)-N(1)	112.82(12)	O(11)-Tb(1)-N(1)	135.21(11)
O(2)-Tb(1)-N(1)	105.08(12)	N(2)-Tb(1)-N(1)	62.46(12)

Symmetry transformations used to generate equivalent atoms: For **1** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **2** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **3** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **4** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **5** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **6** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **7** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **8** #1 1-x,1-y,-z; #2 2-x,1-y,-z; #3 2-x,1-y,1-z. For **9** #1 1-x,-y,1-z; 1-x,-y,1-z; x,-1+y,-1+z. For **10** #1 1-x,-y,1-z; 1-x,-y,1-z; x,-1+y,-1+z. For **11** #1 1-x,-y,1-z; 1-x,-y,1-z; x,-1+y,-1+z. For **12** #1 1-x,-y,1-z; 1-x,-y,1-z; x,-1+y,-1+z.

Figure S1. The PXRD patterns for compounds 1-12.

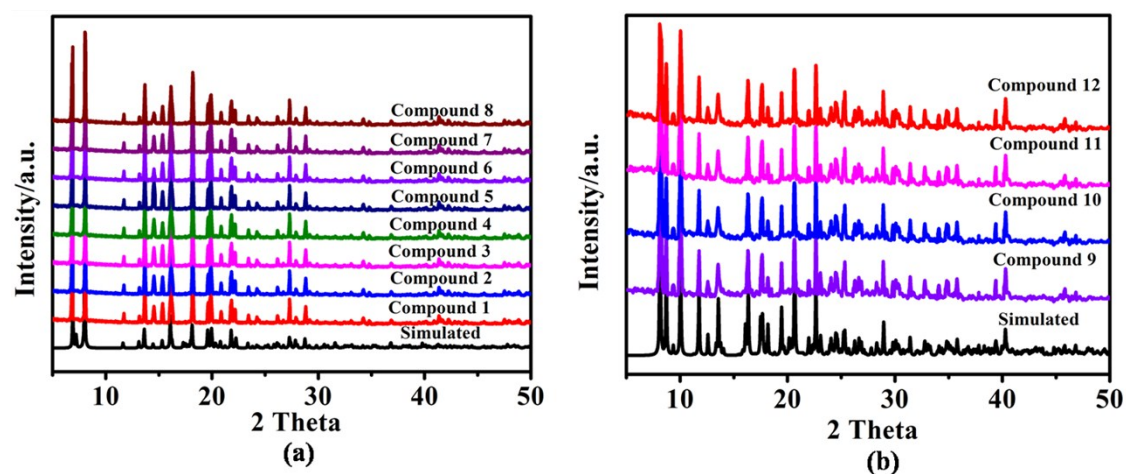


Figure S2. The TGA curves of compounds 1-12.

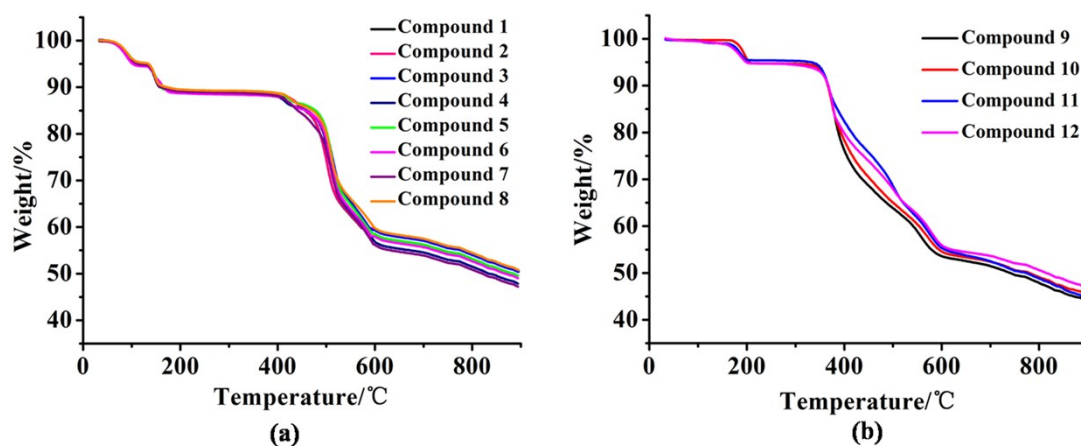


Figure S3. Excitation spectra of compounds **2**, **4**, **11** and **12**.

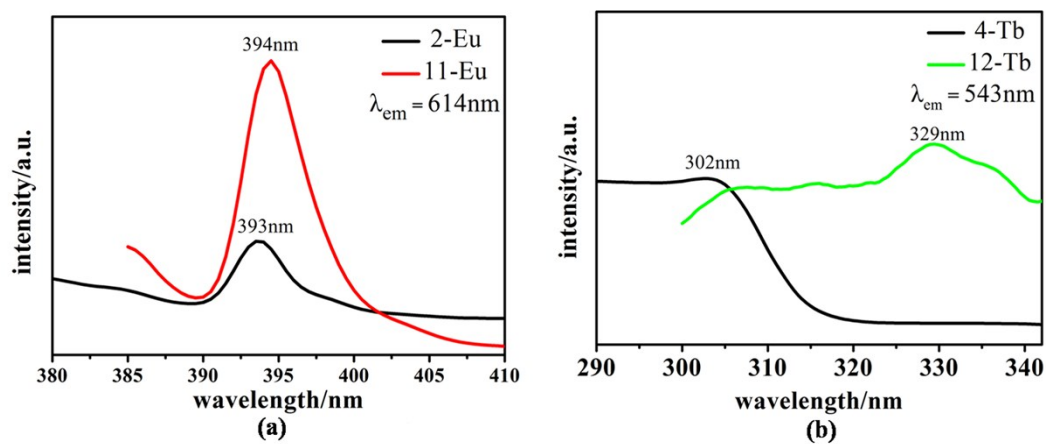


Table S3. Corresponding CIE coordinates of Tb³⁺-doped **2-Eu** with different molar

Sample	10%	30%	50%	60%	70%
CIE (x,y)	(0.262,0.534)	(0.266,0.495)	(0.289,0.449)	(0.328,0.414)	(0.358,0.384)
Sample	80%	90%	95%	98%	
CIE (x,y)	(0.388,0.363)	(0.402,0.354)	(0.410,0.342)	(0.415,0.325)	

ratios excited at 365 nm.

Table S4. The CIE coordinates of emissions for the doping molar ratio of Tb^{3+} is 70% excited at different wavelengths.

excitation wavelength (nm)	345	365	380	390
CIE (x,y)	(0.362,0.439)	(0.358,0.384)	(0.344,0.369)	(0.332,0.337)

Figure S4. PXRD patterns of 4-Tb and after immersing in Fe^{3+} aqueous solution.

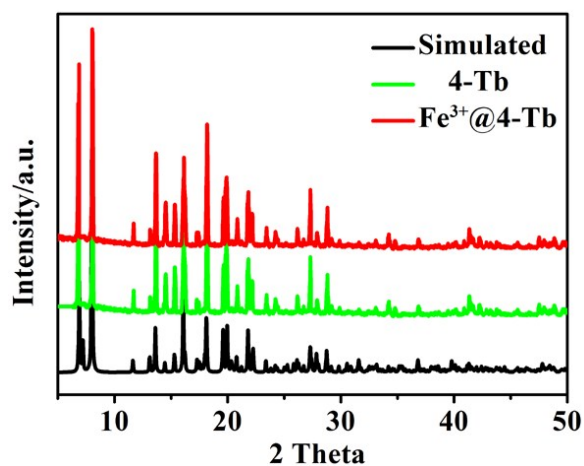


Figure S5. The UV-vis absorption spectrum of the Fe^{3+} , H_4dpstc and 4-Tb in 0.01M Fe^{3+} aqueous solution.

