A series of rare earth complexes with novel 3D non-interpenetrating networks: Synthesisis, structure, magnetic,optical properties.

Xiao-Hua wei[a], Lin-Yan Yang[a], Sheng-Yun Liao, Ming Zhang[a], Jin-Lei Tian[a], Pei-Yao, Du[a], Wen Gu[a,b]*,Xin Liu[a,b]*

[a]Department of Chemistry, Nankai University, Tianjin, China, 300071

[b]Tianjin Key Laboratory of Metal and Molecule Based Material Chemistry, Tianjin , China, 300071

*Correspondence Author. Fax: +86-22-23502779. Tel: 23505020. E-mail: liuxin64@nankai.edu.cn

Supporting Information

Table S1. Selected bonds (Å) and angles (°) for **1**

Bond	Dist	Bond	Dist
O(5)-Pr(1)#1	2.361(7)	O(8)-Pr(1)#2	2.514(7)
O(9)-Pr(1)#3	2.426(8)	O(9)-Pr(1)#2	2.957(8)
O(3)-Pr(1)#4	2.449(7)	O(2)-Pr(1)#5	2.455(7)
Pr(1)-O(5)#1	2.361(7)	Pr(1)-O(6)	2.379(6)
Pr(1)-O(9)#6	2.426(8)	Pr(1)-O(3)#7	2.449(7)
Pr(1)-O(2)#8	2.455(7)	Pr(1)-O(8)#2	2.514(8)
Pr(1)-O(7)	2.627(9)	Pr(1)-O(9)#2	2.957(8)
Angle	(°)	Angle	(°)
Pr(1)#3-O(9)-Pr(1)#2	104.2(2)	O(5)#1-Pr(1)-O(6)	86.4(2)
O(5)#1-Pr(1)-O(9)#6	140.5(3)	O(6)-Pr(1)-O(9)#6	89.2(3)
O(5)#1-Pr(1)-O(3)#7	146.7(3)	O(6)-Pr(1)-O(3)#7	86.0(2)
O(9)#6-Pr(1)-O(3)#7	71.7(3)	O(5)#1-Pr(1)-O(2)#8	77.3(3)
O(6)-Pr(1)-O(2)#8	130.6(3)	O(9)#6-Pr(1)-O(2)#8	76.1(3)
O(3)#7-Pr(1)-O(2)#8	130.4(3)	O(5)#1-Pr(1)-O(8)#2	82.6(2)
O(6)-Pr(1)-O(8)#2	141.3(3)	O(9)#6-Pr(1)-O(8)#2	121.8(3)
O(3)#7-Pr(1)-O(8)#2	83.3(2)	O(2)#8-Pr(1)-O(8)#2	82.7(3)
O(5)#1-Pr(1)-O(7)	73.8(3)	O(6)-Pr(1)-O(7)	71.3(3)
O(9)#6-Pr(1)-O(7)	140.6(3)	O(3)#7-Pr(1)-O(7)	73.0(3)
O(2)#8-Pr(1)-O(7)	142.2(3)	O(8)#2-Pr(1)-O(7)	70.0(3)
O(5)#1-Pr(1)-O(9)#2	116.9(2)	O(6)-Pr(1)-O(9)#2	156.3(2)
O(9)#6-Pr(1)-O(9)#2	75.8(2)	O(3)#7-Pr(1)-O(9)#2	72.1(2)
O(2)#8-Pr(1)-O(9)#2	64.0(2)	O(8)#2-Pr(1)-O(9)#2	46.4(3)
O(7)-Pr(1)-O(9)#2	109.1(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2; #2 -x+2,-y+1,-z+2 #3 x,y-1,z ; #4 -x+3/2,y-1/2,-z+3/2; #5 x-1/2,-y+3/2,z-1/2; #6 x,y+1,z; #7 -x+3/2,y+1/2,-z+3/2; #8 x+1/2,-y+3/2,z+1/2.

Table S2. Selected bonds (Å) and angles (°) for **2**

Bond	Dist	Bond	Dist
O(1)-Nd(1)#1	2.417(5)	O(2)-Nd(1)#2	2.412(5)
O(6)-Nd(1)#3	2.383(6)	O(6)-Nd(1)#4	2.966(6)
O(10)-Nd(1)	2.594(6)	O(5)-Nd(1)#4	2.461(6)
Nd(1)-O(7)	2.328(4)	Nd(1)-O(8)#5	2.337(5)
Nd(1)-O(6)#6	2.383(6)	Nd(1)-O(2)#7	2.412(5)
Nd(1)-O(1)#1	2.417(5)	Nd(1)-O(5)#8	2.461(6)
Nd(1)-O(6)#8	2.966(6)	O(8)-Nd(1)#5	2.337(5)
Angle	(°)	Angle	(°)
Nd(1)#3-O(6)-Nd(1)#4	104.35(18)	O(7)-Nd(1)-O(8)#5	85.32(16)
O(7)-Nd(1)-O(6)#6	139.62(19)	O(8)#5-Nd(1)-O(6)#6	88.62(18)
O(7)-Nd(1)-O(2)#7	146.91(19)	O(8)#5-Nd(1)-O(2)#7	86.63(17)
O(6)#6-Nd(1)-O(2)#7	72.04(18)	O(7)-Nd(1)-O(1)#1	77.64(18)
O(8)#5-Nd(1)-O(1)#1	130.05(18)	O(6)#6-Nd(1)-O(1)#1	76.10(17)
O(2)#7-Nd(1)-O(1)#1	130.14(17)	O(7)-Nd(1)-O(5)#8	83.18(17)
O(8)#5-Nd(1)-O(5)#8	142.8(2)	O(6)#6-Nd(1)-O(5)#8	122.0(2)
O(2)#7-Nd(1)-O(5)#8	84.06(17)	O(1)#1-Nd(1)-O(5)#8	81.49(19)
O(7)-Nd(1)-O(10)	74.4(2)	O(8)#5-Nd(1)-O(10)	72.19(19)
O(6)#6-Nd(1)-O(10)	140.46(18)	O(2)#7-Nd(1)-O(10)	72.6(2)
O(1)#1-Nd(1)-O(10)	142.30(19)	O(5)#8-Nd(1)-O(10)	70.6(2)
O(7)-Nd(1)-O(6)#8	118.44(15)	O(8)#5-Nd(1)-O(6)#8	155.94(14)
O(6)#6-Nd(1)-O(6)#8	75.65(18)	O(2)#7-Nd(1)-O(6)#8	71.38(15)
O(1)#1-Nd(1)-O(6)#8	64.14(15)	O(5)#8-Nd(1)-O(6)#8	46.55(18)
O(10)-Nd(1)-O(6)#8	108.80(17)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1; #2 x-1/2,y+1/2,z; #3 -x+1/2,y+1,-z+3/2; #4x,-y+3/2,z+1/2; #5 -x+1/2,y+0,-z+3/2; #6 -x+1/2,y-1,-z+3/2 ; #7 x+1/2,y-1/2,z; #8 x,-y+3/2,z-1/2

Table S3. Selected bonds (Å) and angles (°) for **3**

Bond	Dist	Bond	Dist
O(1)-Sm(1)#1	2.435(5)	O(2)-Sm(1)#2	2.375(6)
O(5)-Sm(1)#3	2.311(5)	O(8)-Sm(1)#4	2.386(6)
O(7)-Sm(1)#5	2.418(6)	Sm(1)-O(5)#3	2.311(5)
Sm(1)-O(6)	2.347(5)	Sm(1)-O(2)#6	2.375(6)
Sm(1)-O(8)#7	2.386(6)	Sm(1)-O(7)#5	2.418(6)
Sm(1)-O(1)#8	2.435(5)	Sm(1)-O(9)	2.580(8)
Angle	(°)	Angle	(°)
O(5)#3-Sm(1)-O(6)	83.91(18)	O(5)#3-Sm(1)-O(2)#6	149.1(2)
O(6)-Sm(1)-O(2)#6	87.42(19)	O(5)#3-Sm(1)-O(8)#7	135.7(2)
O(6)-Sm(1)-O(8)#7	87.1(2)	O(2)#6-Sm(1)-O(8)#7	73.1(2)
O(5)#3-Sm(1)-O(7)#5	85.2(2)	O(6)-Sm(1)-O(7)#5	144.7(2)
O(2)#6-Sm(1)-O(7)#5	84.9(2)	O(8)#7-Sm(1)-O(7)#5	123.0(2)
O(5)#3-Sm(1)-O(1)#8	76.7(2)	O(6)-Sm(1)-O(1)#8	128.9(2)
O(2)#6-Sm(1)-O(1)#8	130.0(2)	O(8)#7-Sm(1)-O(1)#8	75.83(19)
O(7)#5-Sm(1)-O(1)#8	80.3(2)	O(5)#3-Sm(1)-O(9)	74.9(2)
O(2)#6-Sm(1)-O(9)	74.2(2)	O(8)#7-Sm(1)-O(9)	142.1(2)
O(7)#5-Sm(1)-O(9)	72.0(2)	O(1)#8-Sm(1)-O(9)	141.5(2)

Symmetry transformations used to generate equivalent atoms: #1 x+1/2,-y+2,z+1/2; #2 -x+1,y+1/2,-z+1/2; #3 -x+1/2,y+0,-z+1/2; #4 x,y+1,z; #5 -x+1/2,-y+5/2,-z; #6 -x+1,y-1/2,-z+1/2 ; #7 x,y-1,z; #8 x-1/2,-y+2,z-1/2.

Table S4. Selected bonds (Å) and angles (°) for **4**

Bond	Dist	Bond	Dist
O(5)-Eu(1)#1	2.310(6)	O(6)-Eu(1)#2	2.318(6)
Eu(1)-O(5)#3	2.310(6)	Eu(1)-O(6)#2	2.318(6)
Eu(1)-O(8)#4	2.353(8)	Eu(1)-O(2)#5	2.358(8)
Eu(1)-O(1)#6	2.397(7)	Eu(1)-O(9)	2.526(9)
Eu(1)-O(8)	3.003(8)	O(2)-Eu(1)#7	2.358(8)
O(1)-Eu(1)#8	2.397(7)	O(8)-Eu(1)#4	2.353(8)
Angle	(°)	Angle	(°)
O(5)#3-Eu(1)-O(6)#2	83.0(2)	O(5)#3-Eu(1)-O(8)#4	133.2(3)
O(6)#2-Eu(1)-O(8)#4	85.1(3)	O(5)#3-Eu(1)-O(2)#5	150.7(3)
O(6)#2-Eu(1)-O(2)#5	88.0(3)	O(8)#4-Eu(1)-O(2)#5	73.1(3)
O(5)#3-Eu(1)-O(1)#6	75.8(3)	O(6)#2-Eu(1)-O(1)#6	126.4(3)
O(8)#4-Eu(1)-O(1)#6	75.7(2)	O(2)#5-Eu(1)-O(1)#6	130.4(3)
O(5)#3-Eu(1)-O(9)	75.8(3)	O(6)#2-Eu(1)-O(9)	73.7(3)
O(8)#4-Eu(1)-O(9)	142.0(3)	O(2)#5-Eu(1)-O(9)	74.9(3)
O(1)#6-Eu(1)-O(9)	142.1(3)	O(5)#3-Eu(1)-O(8)	120.3(2)
O(6)#2-Eu(1)-O(8)	156.7(2)	O(8)#4-Eu(1)-O(8)	77.7(3)
O(2)#5-Eu(1)-O(8)	72.2(2)	O(1)#6-Eu(1)-O(8)	64.2(2)
O(9)-Eu(1)-O(8)	111.2(2)	O(5)#3-Eu(1)-Eu(1)#4	138.20(19)
O(6)#2-Eu(1)-Eu(1)#4	127.62(18)	O(8)#4-Eu(1)-Eu(1)#4	44.4(2)
O(2)#5-Eu(1)-Eu(1)#4	67.52(18)	O(1)#6-Eu(1)-Eu(1)#4	63.19(17)
O(9)-Eu(1)-Eu(1)#4	134.6(2)	O(8)-Eu(1)-Eu(1)#4	33.26(14)
Eu(1)#4-O(8)-Eu(1)	102.3(3)		

Symmetry transformations used to generate equivalent atoms: #1 x,-y+2,z-1/2; #2 -x+1,-y+2,-z+1; #3 x,-y+2,z+1/2; #4 -x+1,-y+1,-z+1; #5 x+1/2,-y+3/2,z+1/2; #6 -x+1/2,y-1/2,-z+1/2; #7 x-1/2,-y+3/2,z-1/2; #8 -x+1/2,y+1/2,-z+1/2.

Table S5. Selected bonds (Å) and angles (°) for **5**

Bond	Dist	Bond	Dist
O(7)-Gd(1)#1	2.379(9)	O(1)-Gd(1)#3	2.424(10)
O(3)-Gd(1)#4	2.319(7)	O(4)-Gd(1)#5	2.322(8)
Gd(1)-O(2)#4	2.328(9)	Gd(1)-O(3)#2	2.319(7)
Gd(1)-O(4)#6	2.322(8)	Gd(1)-O(7)#1	2.379(9)
Gd(1)-O(8)	2.378(10)	Gd(1)-O(1)#7	2.424(10)
Gd(1)-O(9)	2.841(6)	O(9)-Gd(1)#8	2.841(6)
Angle	(°)	Angle	(°)
O(2)#4-Gd(1)-O(3)#2	85.4(3)	O(2)#4-Gd(1)-O(4)#6	141.4(4)
O(3)#2-Gd(1)-O(4)#6	88.2(3)	O(2)#4-Gd(1)-O(7)#1	77.8(3)
O(3)#2-Gd(1)-O(7)#1	135.4(4)	O(4)#6-Gd(1)-O(7)#1	80.5(3)
O(2)#4-Gd(1)-O(8)	73.1(4)	O(3)#2-Gd(1)-O(8)	84.3(3)
O(4)#6-Gd(1)-O(8)	143.9(3)	O(7)#1-Gd(1)-O(8)	127.7(3)
O(2)#4-Gd(1)-O(1)#7	123.3(3)	O(3)#2-Gd(1)-O(1)#7	143.5(4)
O(4)#6-Gd(1)-O(1)#7	81.6(3)	O(7)#1-Gd(1)-O(1)#7	77.3(4)
O(8)-Gd(1)-O(1)#7	83.8(3)	O(2)#4-Gd(1)-O(9)	72.5(3)
O(3)#2-Gd(1)-O(9)	69.1(3)	O(4)#6-Gd(1)-O(9)	69.8(3)
O(7)#1-Gd(1)-O(9)	66.5(3)	O(8)-Gd(1)-O(9)	137.6(3)
O(1)#7-Gd(1)-O(9)	136.5(2)	Gd(1)#8-O(9)-Gd(1)	121.3(4)

Symmetry transformations used to generate equivalent atoms:#1 -x+2,-y+1,-z+2; #2 -x+3/2,y-1/2,-z+3/2; #3 x-1/2,-y+1/2,z-1/2; #4 -x+3/2,y+1/2,-z+3/2; #5 x-1/2,y+1/2,z; #6 x+1/2,y-1/2,z; #7 x+1/2,-y+1/2,z+1/2; #8 -x+2,y,-z+3/2 .

Table S6. Selected bonds (Å) and angles (°) for **6**

Bond	Dist	Bond	Dist
O(1)-Tb(1)#1	2.357(7)	O(2)-Tb(1)#2	2.318(7)
O(8)-Tb(1)#3	2.265(6)	O(6)-Tb(1)#4	2.373(7)
O(5)-Tb(1)#5	2.305(8)	Tb(1)-O(8)#3	2.265(6)
Tb(1)-O(7)	2.297(6)	Tb(1)-O(5)#6	2.305(8)
Tb(1)-O(2)#7	2.318(7)	Tb(1)-O(1)#8	2.357(7)
Tb(1)-O(6)#4	2.373(7)	Tb(1)-O(9)	2.494(9)
	Angle	(°)	Angle
O(8)#3-Tb(1)-O(7)	83.2(2)	O(8)#3-Tb(1)-O(5)#6	133.6(3)
O(7)-Tb(1)-O(5)#6	85.7(3)	O(8)#3-Tb(1)-O(2)#7	149.9(3)
O(7)-Tb(1)-O(2)#7	87.2(2)	O(5)#6-Tb(1)-O(2)#7	73.5(3)
O(8)#3-Tb(1)-O(1)#8	77.0(3)	O(7)-Tb(1)-O(1)#8	130.0(3)
O(5)#6-Tb(1)-O(1)#8	76.4(3)	O(2)#7-Tb(1)-O(1)#8	129.2(3)
O(8)#3-Tb(1)-O(6)#4	87.0(2)	O(7)-Tb(1)-O(6)#4	145.8(3)
O(5)#6-Tb(1)-O(6)#4	123.4(3)	O(2)#7-Tb(1)-O(6)#4	85.1(3)
O(1)#8-Tb(1)-O(6)#4	78.6(3)	O(8)#3-Tb(1)-O(9)	76.5(3)
O(7)-Tb(1)-O(9)	73.8(3)	O(5)#6-Tb(1)-O(9)	141.6(3)
O(2)#7-Tb(1)-O(9)	73.4(3)	O(1)#8-Tb(1)-O(9)	141.2(3)
O(6)#4-Tb(1)-O(9)	72.1(3)	C(21)-O(7)-Tb(1)	144.5(6)

Symmetry transformations used to generate equivalent atoms: #1 x+1/2,-y+1,z+1/2; #2 -x+1,y-1/2,-z+1/2; #3 -x+1/2,y+0,-z+1/2; #4 -x+1/2,-y+1/2,-z; #5 x,y-1,z; #6 x,y+1,z; #7 -x+1,y+1/2,-z+1/2; #8 x-1/2,-y+1,z-1/2

Table S7. Selected bonds (Å) and angles (°) for **7**

Bond	Dist.	Bond	Dist
O(7)-Dy(1)#1	2.341(4)	O(2)-Dy(1)#2	2.299(4)
O(1)-Dy(1)#3	2.361(4)	O(3)-Dy(1)#4	2.297(4)
O(4)-Dy(1)#5	2.247(4)	Dy(1)-O(4)#6	2.247(4)
Dy(1)-O(8)	2.293(4)	Dy(1)-O(3)#2	2.297(4)
Dy(1)-O(2)#4	2.299(4)	Dy(1)-O(7)#1	2.341(4)
Dy(1)-O(1)#7	2.361(4)	Dy(1)-O(10)	2.467(5)
Angle	(°)	Angle	(°)
O(4)#6-Dy(1)-O(8)	151.72(17)	O(4)#6-Dy(1)-O(3)#2	80.89(15)
O(8)-Dy(1)-O(3)#2	89.41(16)	O(4)#6-Dy(1)-O(2)#4	129.28(17)
O(8)-Dy(1)-O(2)#4	75.20(16)	O(3)#2-Dy(1)-O(2)#4	83.73(16)
O(4)#6-Dy(1)-O(7)#1	76.02(16)	O(8)-Dy(1)-O(7)#1	129.39(15)
O(3)#2-Dy(1)-O(7)#1	127.17(17)	O(2)#4-Dy(1)-O(7)#1	75.82(15)
O(4)#6-Dy(1)-O(1)#7	89.63(15)	O(8)-Dy(1)-O(1)#7	84.59(16)
O(3)#2-Dy(1)-O(1)#7	147.86(17)	O(2)#4-Dy(1)-O(1)#7	124.60(17)
O(7)#1-Dy(1)-O(1)#7	78.98(16)	O(4)#6-Dy(1)-O(10)	75.42(18)
O(8)-Dy(1)-O(10)	76.39(17)	O(3)#2-Dy(1)-O(10)	74.44(17)
O(2)#4-Dy(1)-O(10)	144.09(17)	O(7)#1-Dy(1)-O(10)	140.01(17)

Symmetry transformations used to generate equivalent atoms:#1 -x+2,-y+1,-z+2; #2 -x+3/2,y-1/2,-z+3/2; #3 x-1/2,-y+1/2,z-1/2; #4 -x+3/2,y+1/2,-z+3/2; #5 x-1/2,y+1/2,z; #6 x+1/2,y-1/2,z; #7 x+1/2,-y+1/2,z+1/2.

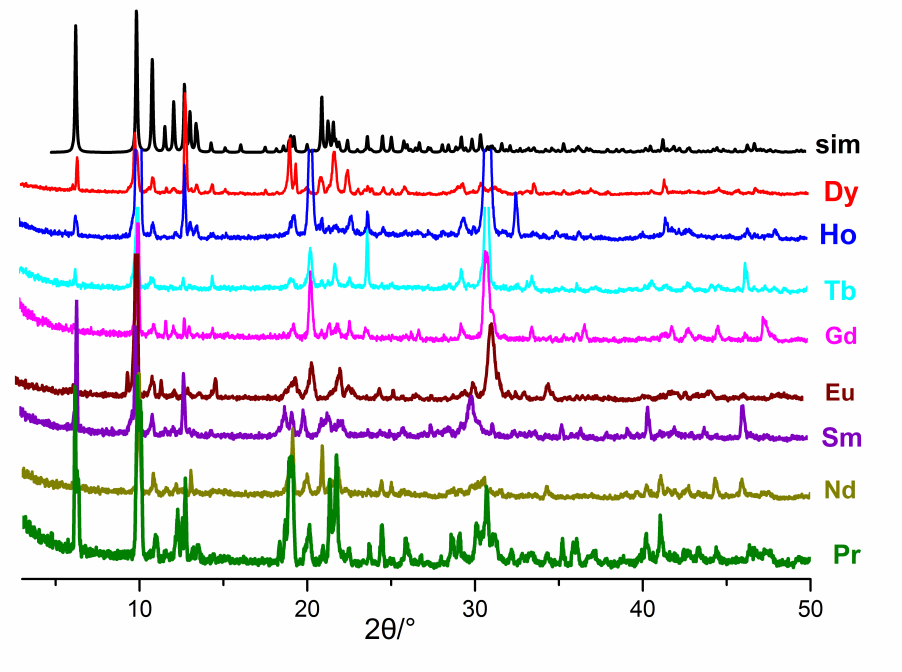


Figure S1. XRPD patterns of **1-7** compared with a simulated pattern.

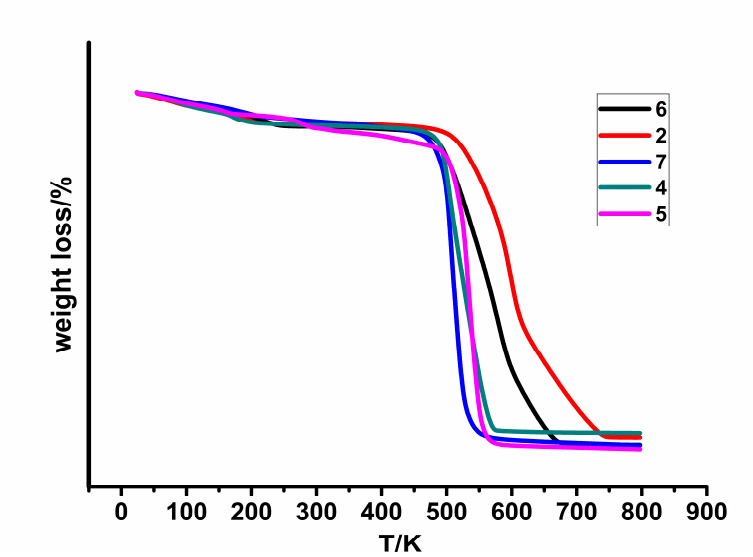


Figure S2. TG curves for compounds **2**, **4**, **5**, **6**, **7**

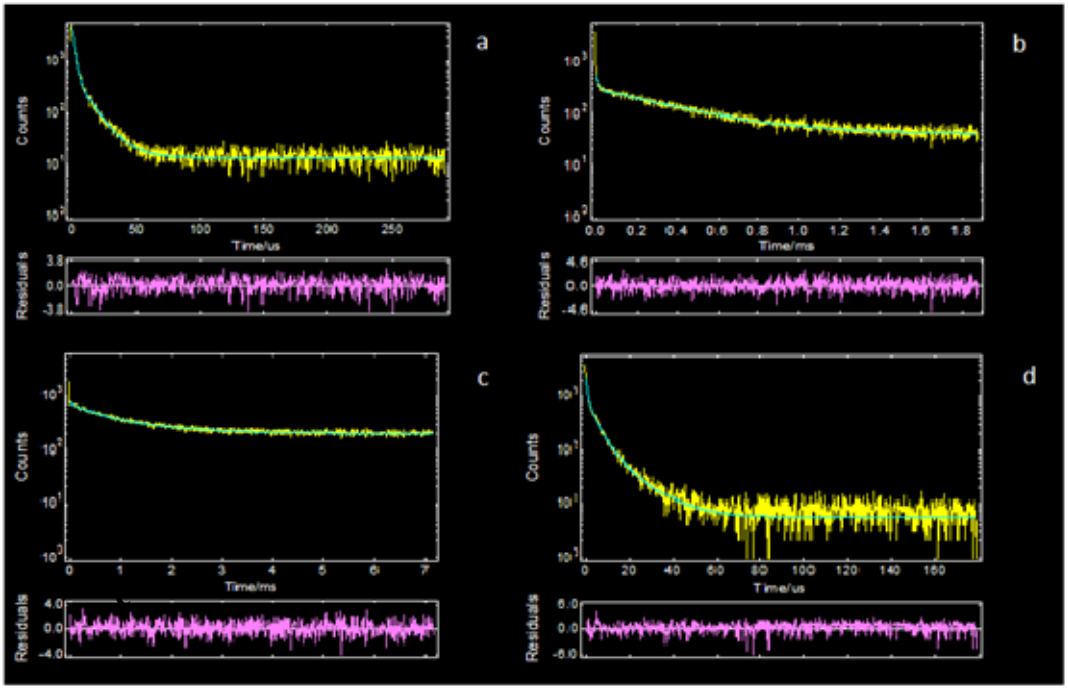
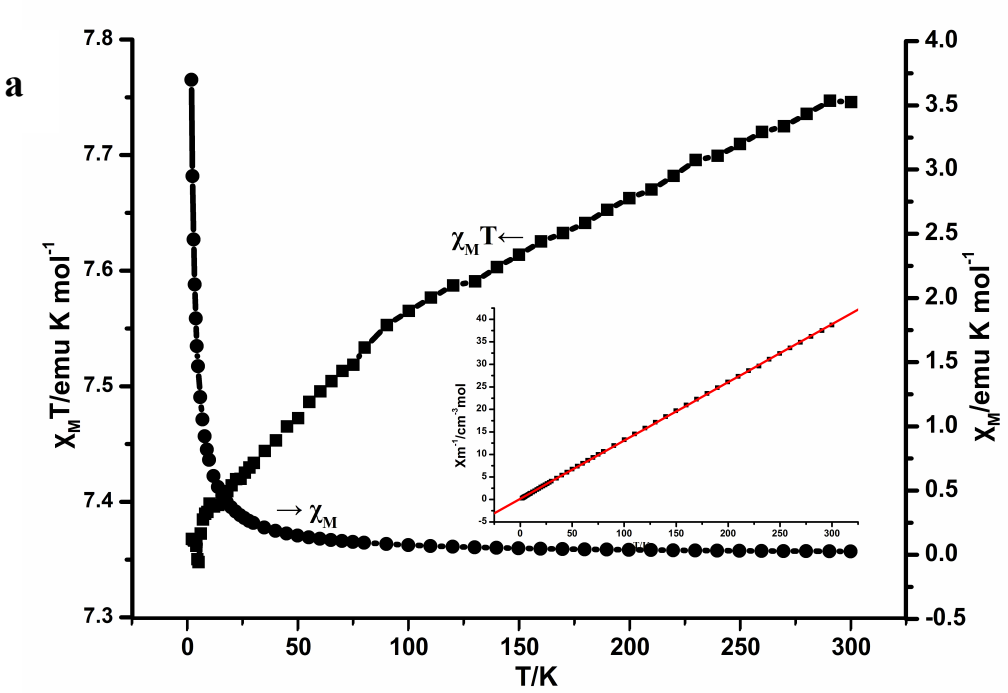


Figure S3. Luminescence decay curves for complexes **2**(a), **3**(b), **4**(c), **5**(d) were obtained in the solid state at 298 K. The scattering points are experimental data and the solid lines are the fitting results.



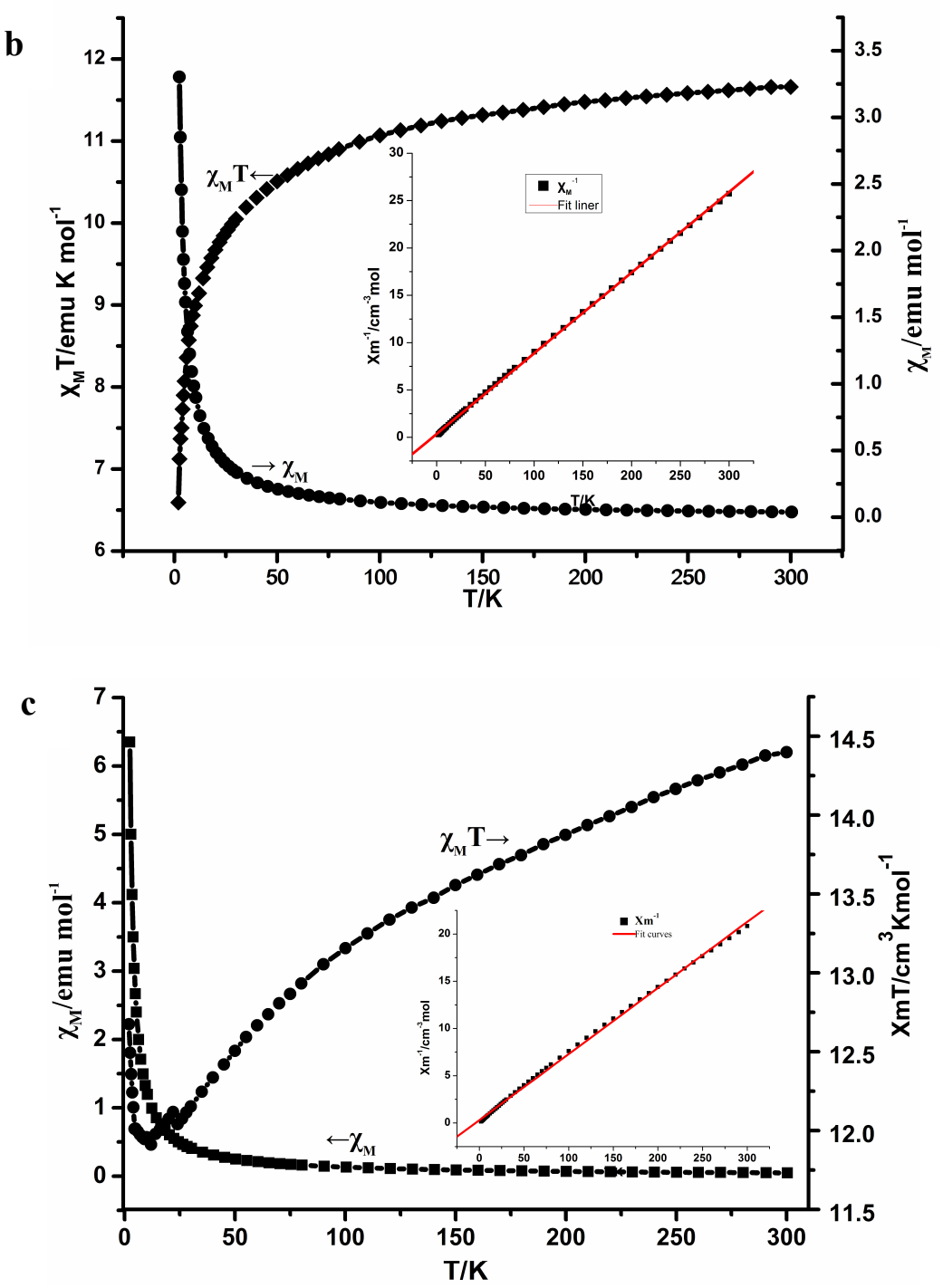


Figure. S4 Temperature dependence of the $\chi_M T$(◆) product and χ_M(●) for **7**(a), **4**(b), **5**(c)