Electronic supplementary information

A series of Ln_2 complexes based on 8-hydroxyquinoline derivative: slow magnetization relaxation and photo-luminescent properties

Xiao-Ya Chu,[a] Hong-Xia Zhang,[a] Yi-Xin Chang,[a] Yao-Yao Nie,[a] Jian-Zhong Cui*[a,b] and Hong-Ling Gao*[a,b]

Table S1 Selected bond lengths (Å) and angles (°) for $[Pr_2(hfac)_4L_2]$ (**1**)

Pr(1)-O(5) #1	2.321(2)	Pr(1)-O(3)	2.374(2)
Pr(1)-O(1)	2.376(2)	Pr(1)-O(5)	2.379(2)
Pr(1)-O(2)	2.389(2)	Pr(1)-O(4)	2.400(3)
Pr(1)-N(1)	2.462(3)	Pr(1)-N(2)	2.629(3)
O(5)#1-Pr(1)-O(3)	82.14(9)	O(5)#1-Pr(1)-O(1)	104.75(9)
O(3)-Pr(1)-O(1)	148.62(9)	O(5)#1-Pr(1)-O(5)	72.20(9)
O(3)-Pr(1)-O(5)	132.66(9)	O(1)-Pr(1)-O(5)	77.66(9)
O(5)#1-Pr(1)-O(2)	84.90(9)	O(3)-Pr(1)-O(2)	80.36(9)
O(1)-Pr(1)-O(2)	70.05(8)	O(5)-Pr(1)-O(2)	133.81(8)
O(5)#1-Pr(1)-O(4)	91.43(9)	O(3)-Pr(1)-O(4)	69.82(9)
O(1)-Pr(1)-O(4)	138.93(8)	O(5)-Pr(1)-O(4)	71.76(9)
O(2)-Pr(1)-O(4)	150.17(8)	O(5)#1-Pr(1)-N(1)	139.54(9)
O(3)-Pr(1)-N(1)	123.79(9)	O(1)-Pr(1)-N(1)	70.15(9)
O(5)-Pr(1)-N(1)	67.49(9)	O(2)-Pr(1)-N(1)	126.37(9)
O(4)-Pr(1)-N(1)	73.13(9)	O(5)#1-Pr(1)-N(2)	156.63(9)
O(3)-Pr(1)-N(2)	81.95(9)	O(1)-Pr(1)-N(2)	80.87(9)
O(5)-Pr(1)-N(2)	130.94(9)	O(2)-Pr(1)-N(2)	75.65(9)
O(4)-Pr(1)-N(2)	99.00(9)	N(1)-Pr(1)-N(2)	63.82(1)
O(5)#1-Pr(1)-Pr(1)#1	36.61(6)	O(3)-Pr(1)-Pr(1)#1	109.93(6)
O(1)-Pr(1)-Pr(1)#1	91.24(7)	O(5)-Pr(1)-Pr(1)#1	35.59(5)
O(2)-Pr(1)-Pr(1)#1	112.29(6)	O(4)-Pr(1)-Pr(1)#1	79.58(7)
N(1)-Pr(1)-Pr(1)#1	103.01(7)	N(2)-Pr(1)-Pr(1)#1	166.30(6)

The symmetry code: #1 -x+1, -y, -z+1.

Table S2 Selected bond lengths (Å) and angles (°) for $[Gd_2(hfac)_4L_2]$ (**2**)

Gd(1)-O(5)#1	2.324(2)	Gd(1)-O(3)	2.383(2)
Gd(1)-O(1)	2.387(2)	Gd(1)-O(5)	2.388(2)
Gd(1)-O(2)	2.395(2)	Gd(1)-O(4)	2.406(2)

Gd(1)-N(1)	2.467(3)	Gd(1)-N(2)	2.635(3)
O(5)#1-Gd(1)-O(3)	82.14(7)	O(5)#1-Gd(1)-O(1)	104.78(8)
O(3)-Gd(1)-O(1)	148.60(8)	O(5)#1-Gd(1)-O(5)	72.07(8)
O(3)-Gd(1)-O(5)	132.59(7)	O(1)-Gd(1)-O(5)	77.73(7)
O(5)#1-Gd(1)-O(2)	84.98(7)	O(3)-Gd(1)-O(2)	80.25(7)
O(1)-Gd(1)-O(2)	70.13(7)	O(5)-Gd(1)-O(2)	133.90(7)
O(5)#1-Gd(1)-O(4)	91.40(7)	O(3)-Gd(1)-O(4)	69.88(7)
O(1)-Gd(1)-O(4)	138.88(7)	O(5)-Gd(1)-O(4)	71.69(7)
O(2)-Gd(1)-O(4)	150.13(7)	O(5)#1-Gd(1)-N(1)	139.52(8)
O(3)-Gd(1)-N(1)	123.86(8)	O(1)-Gd(1)-N(1)	70.07(8)
O(5)-Gd(1)-N(1)	67.59(7)	O(2)-Gd(1)-N(1)	126.32(8)
O(4)-Gd(1)-N(1)	73.17(8)	O(5)#1-Gd(1)-N(2)	156.63(7)
O(3)-Gd(1)-N(2)	82.07(8)	O(1)-Gd(1)-N(2)	80.68(8)
O(5)-Gd(1)-N(2)	131.05(7)	O(2)-Gd(1)-N(2)	75.45(7)
O(4)-Gd(1)-N(2)	99.19(8)	N(1)-Gd(1)-N(2)	63.83(8)
O(5)#1-Gd(1)-Gd(1)#1	36.60(5)	O(3)-Gd(1)-Gd(1)#1	109.92(5)
O(1)-Gd(1)-Gd(1)#1	91.28(6)	O(5)-Gd(1)-Gd(1)#1	35.47(5)
O(2)-Gd(1)-Gd(1)#1	112.41(5)	O(4)-Gd(1)-Gd(1)#1	79.52(6)
N(1)-Gd(1)-Gd(1)#1	103.00(6)	N(2)-Gd(1)-Gd(1)#1	166.26(6)

The symmetry code: #1 -x+1, -y, -z+1.

Table S3 Selected bond lengths (Å) and angles (°) for $[Tb_2(hfac)_4L_2]$ (**3**)

Tb(1)-O(1)#1	2.302(2)	Tb(1)-O(4)	2.363(2)
Tb(1)-O(2)	2.364(2)	Tb(1)-O(1)	2.378(2)
Tb(1)-O(3)	2.379(2)	Tb(1)-O(5)	2.389(2)
Tb(1)-N(1)	2.452(3)	Tb(1)-N(2)	2.629(3)
O(1)#1-Tb(1)-O(4)	81.71(8)	O(1)#1-Tb(1)-O(2)	105.39(8)
O(4)-Tb(1)-O(2)	148.37(8)	O(1)#1-Tb(1)-O(1)	72.32(9)
O(4)-Tb(1)-O(1)	132.96(8)	O(2)-Tb(1)-O(1)	77.59(8)
O(1)#1-Tb(1)-O(3)	84.58(8)	O(4)-Tb(1)-O(3)	79.59(8)
O(2)-Tb(1)-O(3)	70.67(8)	O(1)-Tb(1)-O(3)	133.81(8)
O(1)#1-Tb(1)-O(5)	90.92(8)	O(4)-Tb(1)-O(5)	70.21(8)
O(2)-Tb(1)-O(5)	138.77(8)	O(1)-Tb(1)-O(5)	71.70(8)
O(3)-Tb(1)-O(5)	149.80(8)	O(1)#1-Tb(1)-N(1)	140.03(8)
O(4)-Tb(1)-N(1)	123.62(9)	O(2)-Tb(1)-N(1)	70.16(9)
O(1)-Tb(1)-N(1)	67.92(8)	O(3)-Tb(1)-N(1)	126.85(8)
O(5)-Tb(1)-N(1)	73.13(8)	O(1)#1-Tb(1)-N(2)	155.95(8)
O(4)-Tb(1)-N(2)	81.72(9)	O(2)-Tb(1)-N(2)	80.60(9)

O(1)-Tb(1)-N(2)	131.50(8)	O(3)-Tb(1)-N(2)	75.37(8)
O(5)-Tb(1)-N(2)	99.71(8)	N(1)-Tb(1)-N(2)	64.02(9)
O(1)#1-Tb(1)-Tb(1)#1	36.84(6)	O(4)-Tb(1)-Tb(1)#1	109.94(6)
O(2)-Tb(1)-Tb(1)#1	91.52(6)	O(1)-Tb(1)-Tb(1)#1	35.48(5)
O(3)-Tb(1)-Tb(1)#1	112.22(6)	O(5)-Tb(1)-Tb(1)#1	79.18(6)
N(1)-Tb(1)-Tb(1)#1	103.32(7)	N(2)-Tb(1)-Tb(1)#1	166.73(6)

The symmetry code: #1 -x+2, -y, -z+1.

Table S4 Selected bond lengths (Å) and angles (°) for $[Dy_2(hfac)_4L_2]$ (**4**)

Dy(1)-O(1)#1	2.2924(18)	Dy(1)-O(2)	2.352(2)
Dy(1)-O(4)	2.355(2)	Dy(1)-O(3)	2.363(6)
Dy(1)-O(1)	2.366(0)	Dy(1)-O(5)	2.369(2)
Dy(1)-N(1)	2.436(2)	Dy(1)-N(2)	2.615(2)
O(1)#1-Dy(1)-O(2)	104.59(7)	O(1)#1-Dy(1)-O(4)	82.13(7)
O(2)-Dy(1)-O(4)	148.29(7)	O(1)#1-Dy(1)-O(3)	84.24(7)
O(2)-Dy(1)-O(3)	70.66(7)	O(4)-Dy(1)-O(3)	79.44(7)
O(1)#1-Dy(1)-O(1)	72.04(7)	O(2)-Dy(1)-O(1)	77.47(7)
O(4)-Dy(1)-O(1)	133.06(7)	O(3)-Dy(1)-O(1)	133.62(6)
O(1)#1-Dy(1)-O(5)	91.65(7)	O(2)-Dy(1)-O(5)	138.74(7)
O(4)-Dy(1)-O(5)	70.40(7)	O(3)-Dy(1)-O(5)	149.84(7)
O(1)-Dy(1)-O(5)	71.89(7)	O(1)#1-Dy(1)-N(1)	140.00(7)
O(2)-Dy(1)-N(1)	70.41(8)	O(4)-Dy(1)-N(1)	123.65(7)
O(3)-Dy(1)-N(1)	126.95(7)	O(1)-Dy(1)-N(1)	68.13(7)
O(5)-Dy(1)-N(1)	72.87(8)	O(1)#1-Dy(1)-N(2)	155.65(7)
O(2)-Dy(1)-N(2)	81.27(7)	O(4)-Dy(1)-N(2)	81.20(7)
O(3)-Dy(1)-N(2)	75.36(7)	O(1)-Dy(1)-N(2)	132.06(7)
O(5)-Dy(1)-N(2)	99.29(7)	N(1)-Dy(1)-N(2)	64.35(8)
O(1)#1-Dy(1)-Dy(1)#1	36.68(5)	O(2)-Dy(1)-Dy(1)#1	90.97(5)
O(4)-Dy(1)-Dy(1)#1	110.21(5)	O(3)-Dy(1)-Dy(1)#1	111.84(5)
O(1)-Dy(1)-Dy(1)#1	35.36(4)	O(5)-Dy(1)-Dy(1)#1	79.76(5)
N(1)-Dy(1)-Dy(1)#1	103.42(6)	N(2)-Dy(1)-Dy(1)#1	167.13(5)

The symmetry code: #1 -x+2, -y, -z+1.

Table S5 Selected bond lengths (Å) and angles (°) for $[Ho_2(hfac)_4L_2]$ (**5**)

Ho(1)-O(5)#1	2.276(2)	Ho(1)-O(3)	2.336(2)
Ho(1)-O(1)	2.341(2)	Ho(1)-O(5)	2.350(2)
Ho(1)-O(2)	2.352(2)	Ho(1)-O(4)	2.361(2)
Ho(1)-N(1)	2.419(3)	Ho(1)-N(2)	2.598(3)

O(5)#1- Ho(1)-O(3)	82.27(8)	O(5)#1- Ho(1)-O(1)	104.57(8)
O(3)-Ho(1)-O(1)	148.22(9)	O(5)#1-Ho(1)-O(5)	71.94(8)
O(3)-Ho(1)-O(5)	133.34(8)	O(1)-Ho(1)-O(5)	77.25(8)
O(5)#1-Ho(1)-O(2)	83.96(8)	O(3)-Ho(1)-O(2)	79.19(8)
O(1)-Ho(1)-O(2)	70.93(8)	O(5)-Ho(1)-O(2)	133.38(8)
O(5)#1-Ho(1)-O(4)	91.90(8)	O(3)-Ho(1)-O(4)	70.70(8)
O(1)-Ho(1)-O(4)	138.42(8)	O(5)-Ho(1)-O(4)	72.00(8)
O(2)-Ho(1)-O(4)	149.88(8)	O(5)#1-Ho(1)-N(1)	140.29(9)
O(3)-Ho(1)-N(1)	123.41(9)	O(1)-Ho(1)-N(1)	70.41(9)
O(5)-Ho(1)-N(1)	68.52(9)	O(2)-Ho(1)-N(1)	127.07(9)
O(4)-Ho(1)-N(1)	72.64(9)	O(5)#1-Ho(1)-N(2)	155.06(8)
O(3)-Ho(1)-N(2)	80.54(9)	O(1)-Ho(1)-N(2)	81.60(9)
O(5)-Ho(1)-N(2)	132.74(8)	O(2)-Ho(1)-N(2)	75.17(8)
O(4)-Ho(1)-N(2)	99.27(9)	N(1)-Ho(1)-N(2)	64.65(9)
O(5)#1-Ho(1)-Ho(1)#1	36.64(6)	O(3)-Ho(1)-Ho(1)#1	110.43(6)
O(1)-Ho(1)-Ho(1)#1	90.82(7)	O(5)-Ho(1)-Ho(1)#1	35.30(5)
O(2)-Ho(1)-Ho(1)#1	111.54(6)	O(4)-Ho(1)-Ho(1)#1	79.99(6)
N(1)-Ho(1)-Ho(1)#1	103.75(7)	N(2)-Ho(1)-Ho(1)#1	167.73(6)

The symmetry code: #1 -x+1, -y, -z+1.

Table S6 Selected bond lengths (Å) and angles (°) for $[Er_2(hfac)_4L_2]$ (**6**)

Er(1)-O(5)#1	2.277(2)	Er(1)-O(3)	2.329(2)
Er(1)-O(1)	2.331(2)	Er(1)-O(2)	2.344(2)
Er(1)-O(5)	2.347(2)	Er(1)-O(4)	2.353(2)
Er(1)-N(1)	2.417(3)	Er(1)-N(2)	2.597(3)
O(5)#1- Er(1)-O(3)	82.26(8)	O(5)#1- Er(1)-O(1)	104.57(8)
O(3)-Er(1)-O(1)	148.26(8)	O(5)#1-Er(1)-O(2)	83.81(8)
O(3)-Er(1)-O(2)	78.91(8)	O(1)-Er(1)-O(2)	71.26(8)
O(5)#1-Er(1)-O(5)	71.95(8)	O(3)-Er(1)-O(5)	133.43(8)
O(1)-Er(1)-O(5)	77.11(9)	O(2)-Er(1)-O(5)	133.47(8)
O(5)#1-Er(1)-O(4)	91.85(8)	O(3)-Er(1)-O(4)	70.97(8)
O(1)-Er(1)-O(4)	138.15(8)	O(2)-Er(1)-O(4)	149.88(8)
O(5)-Er(1)-O(4)	71.88(8)	O(5)#1-Er(1)-N(1)	140.46(8)
O(3)-Er(1)-N(1)	123.34(9)	O(1)-Er(1)-N(1)	70.36(9)
O(2)-Er(1)-N(1)	127.18(8)	O(5)-Er(1)-N(1)	68.69(8)
O(4)-Er(1)-N(1)	72.58(8)	O(5)#1-Er(1)-N(2)	154.80(8)
O(3)-Er(1)-N(2)	80.33(8)	O(1)-Er(1)-N(2)	81.75(8)
O(2)-Er(1)-N(2)	75.08(8)	O(5)-Er(1)-N(2)	132.98(8)

O(4)-Er(1)-N(2)	99.47(8)	N(1)-Er(1)-N(2)	64.73(9)
O(5)#1-Er(1)-Er(1)#1	36.60(5)	O(3)-Er(1)-Er(1)#1	110.46(6)
O(1)-Er(1)-Er(1)#1	90.73(6)	O(2)-Er(1)-Er(1)#1	111.42(6)
O(5)-Er(1)-Er(1)#1	35.35(5)	O(4)-Er(1)-Er(1)#1	79.90(6)
N(1)-Er(1)-Er(1)#1	103.97(7)	N(2)-Er(1)-Er(1)#1	168.00(6)

The symmetry code: #1 -x+1, -y, -z+1.

Table S7 Selected bond lengths (Å) and angles (°) for $[Lu_2(hfac)_4L_2]$ (**7**)

Lu(1)-O(5)#1	2.242(2)	Lu(1)-O(2)	2.315(2)
Lu(1)-O(4)	2.326(2)	Lu(1)-O(3)	2.304(2)
Lu(1)-O(1)	2.301(2)	Lu(1)-O(5)	2.323(2)
Lu(1)-N(1)	2.381(3)	Lu(1)-N(2)	2.579(3)
O(5)#1-Lu(1)-O(2)	83.22(8)	O(5)#1-Lu(1)-O(4)	92.12(8)
O(2)-Lu(1)-O(4)	149.45(7)	O(5)#1-Lu(1)-O(3)	82.60(8)
O(2)-Lu(1)-O(5)	133.16(7)	O(1)-Lu(1)-O(3)	147.96(8)
O(5)#1-Lu(1)-O(1)	104.14(8)	O(2)-Lu(1)-O(1)	71.92(8)
O(4)-Lu(1)-O(1)	138.01(7)	O(3)-Lu(1)-O(1)	147.96(8)
O(5)#1-Lu(1)-O(5)	71.56(8)	O(2)-Lu(1)-O(5)	133.16(7)
O(4)-Lu(1)-O(5)	72.09(7)	O(3)-Lu(1)-O(5)	133.92(7)
O(1)-Lu(1)-O(5)	76.81(8)	O(5)#1-Lu(1)-N(1)	140.92(8)
O(2)-Lu(1)-N(1)	127.66(8)	O(4)-Lu(1)-N(1)	72.40(8)
O(3)-Lu(1)-N(1)	122.95(8)	O(1)-Lu(1)-N(1)	70.69(8)
O(5)-Lu(1)-N(1)	69.56(8)	O(5)#1-Lu(1)-N(2)	153.88(8)
O(2)-Lu(1)-N(2)	74.80(8)	O(4)-Lu(1)-N(2)	99.62(8)
O(3)-Lu(1)-N(2)	79.21(8)	O(1)-Lu(1)-N(2)	82.49(8)
O(5)-Lu(1)-N(2)	134.28(7)	N(1)-Lu(1)-N(2)	65.20(8)
O(5)#1-Lu(1)-Lu(1)#1	36.52(5)	O(2)-Lu(1)-Lu(1)#1	110.95(5)
O(4)-Lu(1)-Lu(1)#1	80.18(6)	O(3)-Lu(1)-Lu(1)#1	110.93(6)
O(1)-Lu(1)-Lu(1)#1	90.27(6)	O(5)-Lu(1)-Lu(1)#1	35.04(5)
N(1)-Lu(1)-Lu(1)#1	104.52(6)	N(2)-Lu(1)-Lu(1)#1	168.93(6)

The symmetry code: #1 -x, -y, -z.

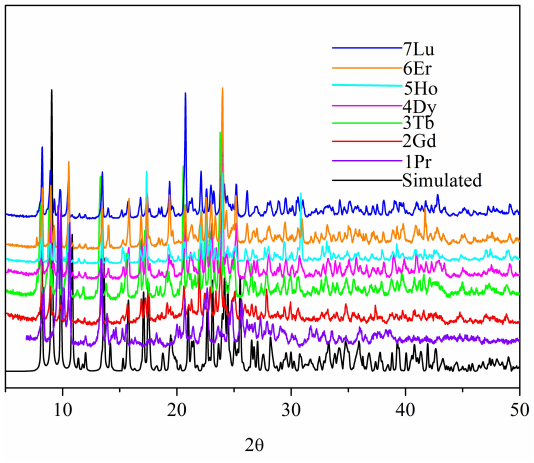

Fig. S1 PXRD patterns of complexes **1-7**.

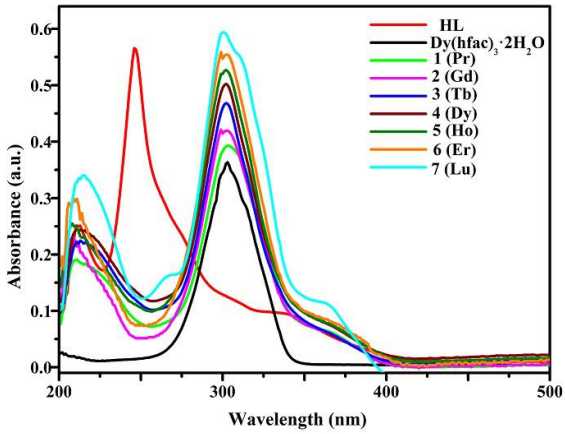

Fig. S2 UV-vis absorption spectra of the ligand HL, $Dy(hfac)_3 \cdot 2H_2O$ and complexes **1-7** in methanol solution.

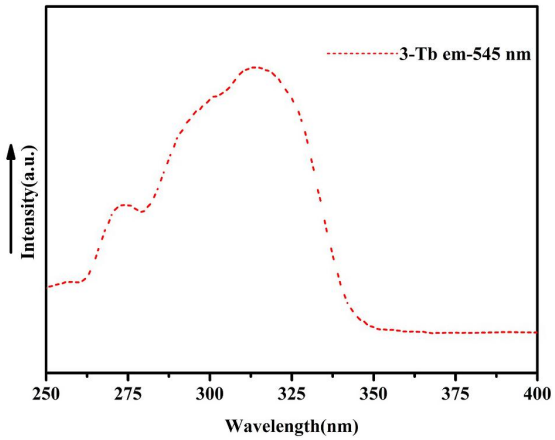

Fig. S3 Room temperature excitation spectrum of **3** (λ_{em} = 545 nm) in the methanol solution.

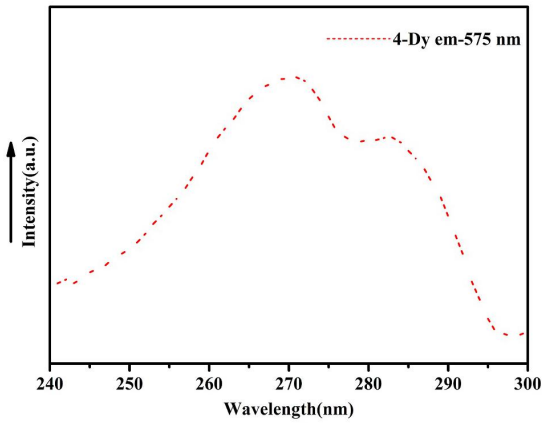

Fig. S4 Room temperature excitation spectrum of **4** (λ_{em} = 575 nm) in the methanol solution.

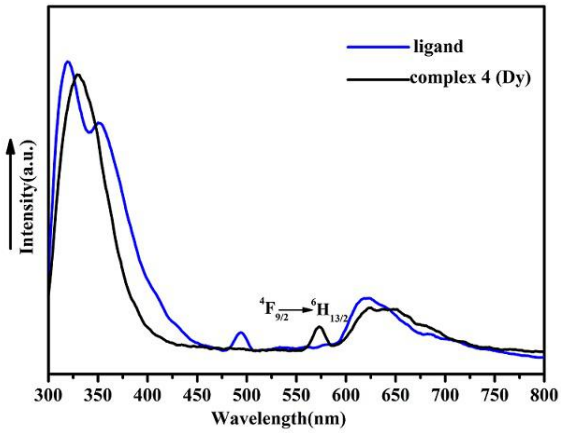

Fig. S5 The emission spectrum of the ligand and complex **4** in methanol solution.

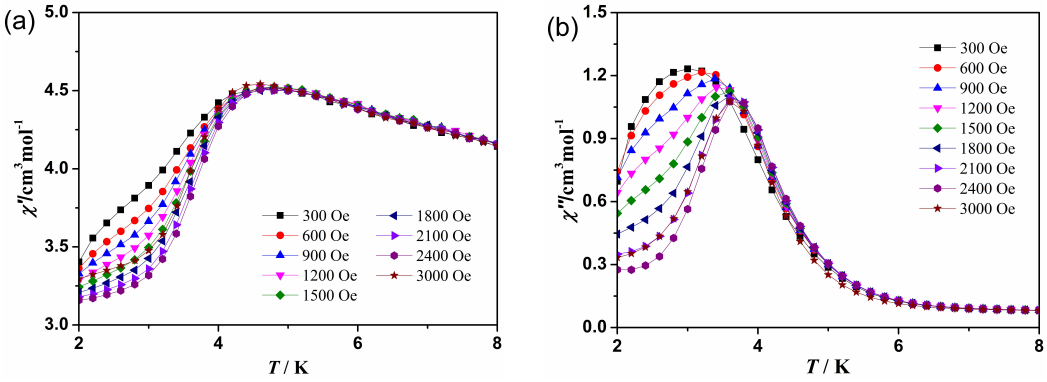

Fig. S6 The temperature dependency of the *ac* susceptibility was measured on powder samples **4** in the applied *dc* field from 300 to 3000 Oe at 2311 Hz.