Supporting Information

2*p*-4*f* one-dimensional chains and two-dimensional networks assembled by multicoordinating nitronyl nitroxide radical ligand

Juan Sun,* Yuqing Fang, Sisi Liao, Tong Luo, Shixun Gao, Zhenhua Qiao, Jie Yang

Hubei Key Laboratory of Pollutant Analysis & Reuse Technology, College of Chemistry and Chemical Engineering, Hubei Normal University, Huangshi 435002, P. R. China. *E-mail: sunjuan@hbnu.edu.cn

Table S1 Selected bond lengths [Å] and angles [°] for **1**.

Bond distances			
Tb(1)-O(6)	2.3824(15)	Tb(1)-O(4)	2.4806(15)
Tb(1)-O(2)	2.4002(16)	Tb(1)-N(3)	2.5274(19)
Tb(1)-O(1)	2.4019(16)	Tb(1)-N(2)	2.5764(19)
Tb(1)-O(3)	2.4042(16)	N(6)-O(9)	1.271(3)
Tb(1)-O(5)	2.4443(16)	N(5)-O(8)	1.288(3)
Tb(1)-O(7)	2.4544(17)		
Angles			
O(6)-Tb(1)-O(2)	137.65(5)	O(3)-Tb(1)-O(4)	68.35(5)
O(6)-Tb(1)-O(1)	141.10(5)	O(5)-Tb(1)-O(4)	125.01(5)
O(2)-Tb(1)-O(1)	70.22(6)	O(7)-Tb(1)-O(4)	128.98(6)
O(6)-Tb(1)-O(3)	136.01(5)	O(6)-Tb(1)-N(3)	76.60(6)
O(2)-Tb(1)-O(3)	70.10(6)	O(2)-Tb(1)-N(3)	74.20(6)
O(1)-Tb(1)-O(3)	70.75(6)	O(1)-Tb(1)-N(3)	141.67(6)
O(6)-Tb(1)-O(5)	72.12(5)	O(3)-Tb(1)-N(3)	84.25(6)
O(2)-Tb(1)-O(5)	108.60(6)	O(5)-Tb(1)-N(3)	133.89(6)
O(1)-Tb(1)-O(5)	72.58(5)	O(7)-Tb(1)-N(3)	70.42(6)
O(3)-Tb(1)-O(5)	141.17(6)	O(4)-Tb(1)-N(3)	69.39(6)
O(6)-Tb(1)-O(7)	73.31(6)	O(6)-Tb(1)-N(2)	81.06(6)
O(2)-Tb(1)-O(7)	68.38(6)	O(2)-Tb(1)-N(2)	140.02(6)
O(1)-Tb(1)-O(7)	108.01(6)	O(1)-Tb(1)-N(2)	71.09(6)
O(3)-Tb(1)-O(7)	135.73(6)	O(3)-Tb(1)-N(2)	88.02(6)
O(5)-Tb(1)-O(7)	68.68(6)	O(5)-Tb(1)-N(2)	68.26(6)
O(6)-Tb(1)-O(4)	67.89(5)	O(7)-Tb(1)-N(2)	134.79(6)
O(2)-Tb(1)-O(4)	126.39(5)	O(4)-Tb(1)-N(2)	69.57(6)
O(1)-Tb(1)-O(4)	123.01(5)	N(3)-Tb(1)-N(2)	138.19(6)

Table S2 Selected bond lengths [Å] and angles [°] for **2**.

Bond distances			
Dy(1)-O(6)	2.3712(18)	Dy(1)-O(4)	2.4643(18)
Dy(1)-O(1)	2.3902(18)	Dy(1)-N(3)	2.512(2)
Dy(1)-O(2)	2.392(2)	Dy(1)-N(2)	2.561(2)
Dy(1)-O(3)	2.392(2)	N(6)-O(9)	1.279(4)
Dy(1)-O(5)	2.4339(19)	N(5)-O(8)	1.283(4)
Dy(1)-O(7)	2.450(2)		
Angles			
O(6)-Dy(1)-O(1)	140.91(6)	O(6)-Dy(1)-O(2)	137.45(6)
O(6)-Dy(1)-O(2)	137.41(7)	O(6)-Dy(1)-O(3)	136.30(6)
O(1)-Dy(1)-O(2)	70.37(7)	O(2)-Dy(1)-O(3)	70.11(7)
O(6)-Dy(1)-O(3)	136.30(7)	O(1)-Dy(1)-O(5)	72.26(7)
O(1)-Dy(1)-O(3)	70.77(7)	O(3)-Dy(1)-O(5)	141.11(7)
O(2)-Dy(1)-O(3)	70.18(7)	O(3)-Dy(1)-O(4)	68.65(6)
O(6)-Dy(1)-O(5)	72.33(7)	O(5)-Dy(1)-O(4)	125.48(7)
O(1)-Dy(1)-O(5)	72.29(7)	O(7)-Dy(1)-O(4)	128.93(7)
O(2)-Dy(1)-O(5)	107.86(7)	O(6)-Dy(1)-N(3)	76.51(7)
O(3)-Dy(1)-O(5)	141.15(7)	O(1)-Dy(1)-N(3)	141.90(7)
O(6)-Dy(1)-O(7)	73.40(7)	O(2)-Dy(1)-N(3)	74.24(7)
O(1)-Dy(1)-O(7)	107.92(7)	O(3)-Dy(1)-N(3)	84.45(8)
O(2)-Dy(1)-O(7)	67.90(8)	O(5)-Dy(1)-N(3)	133.54(8)
O(3)-Dy(1)-O(7)	135.35(8)	O(7)-Dy(1)-N(3)	70.13(8)
O(5)-Dy(1)-O(7)	68.47(7)	O(4)-Dy(1)-N(3)	69.47(7)
O(6)-Dy(1)-O(4)	67.89(6)	O(6)-Dy(1)-N(2)	80.75(7)
O(1)-Dy(1)-O(4)	123.15(7)	O(1)-Dy(1)-N(2)	71.18(7)
O(2)-Dy(1)-O(4)	126.66(7)	O(2)-Dy(1)-N(2)	140.40(7)

Table S3 Selected bond lengths [Å] and angles [°] for **3**.

Bond distances			
Pr(1)-O(3)	2.491(10)	Pr(1)-O(7)	2.528(10)
Pr(1)-O(5)	2.473(11)	Pr(1)-N(3)	2.650(11)
Pr(1)-O(6)	2.475(11)	Pr(1)-N(2)	2.679(13)
Pr(1)-O(2)	2.508(11)	O(7)-N(5)	1.281(15)
Pr(1)-O(4)	2.510(11)	N(6)-O(8)	1.261(16)
Pr(1)-O(1)	2.534(11)		
Angles			
O(3)-Pr(1)-O(5)	118.9(4)	O(4)-Pr(1)-O(7)	130.9(3)
O(3)-Pr(1)-O(6)	126.0(3)	O(1)-Pr(1)-O(7)	63.1(3)
O(5)-Pr(1)-O(6)	69.4(4)	O(3)-Pr(1)-N(3)	70.7(4)
O(3)-Pr(1)-O(2)	73.4(3)	O(5)-Pr(1)-N(3)	137.7(4)
O(5)-Pr(1)-O(2)	149.8(4)	O(6)-Pr(1)-N(3)	72.8(4)
O(6)-Pr(1)-O(2)	128.3(4)	O(2)-Pr(1)-N(3)	71.3(4)
O(3)-Pr(1)-O(4)	67.1(3)	O(4)-Pr(1)-N(3)	75.1(4)
O(5)-Pr(1)-O(4)	72.7(4)	O(1)-Pr(1)-N(3)	133.0(4)
O(6)-Pr(1)-O(4)	65.9(4)	O(7)-Pr(1)-N(3)	82.9(4)
O(2)-Pr(1)-O(4)	134.6(3)	O(3)-Pr(1)-N(2)	68.3(4)
O(3)-Pr(1)-O(1)	118.6(3)	O(5)-Pr(1)-N(2)	73.1(4)
O(5)-Pr(1)-O(1)	81.5(4)	O(6)-Pr(1)-N(2)	141.9(4)
O(6)-Pr(1)-O(1)	115.5(4)	O(2)-Pr(1)-N(2)	88.5(4)
O(2)-Pr(1)-O(1)	68.8(3)	O(4)-Pr(1)-N(2)	96.8(4)
O(4)-Pr(1)-O(1)	151.9(4)	O(1)-Pr(1)-N(2)	64.2(4)
O(3)-Pr(1)-O(7)	143.0(3)	O(7)-Pr(1)-N(2)	127.3(4)
O(5)-Pr(1)-O(7)	98.1(4)	N(3)-Pr(1)-N(2)	138.0(4)
O(6)-Pr(1)-O(7)	65.8(3)	N(5)-O(7)-Pr(1)	147.8(9)
O(2)-Pr(1)-O(7)	73.9(3)		

Table S4 Selected bond lengths [Å] and angles [°] for **4**.

Bond distances			
Nd(1)-O(6)	2.462(6)	Nd(1)-O(1)	2.517(6)
Nd(1)-O(5)	2.468(6)	Nd(1)-N(3)	2.617(6)
Nd(1)-O(2)	2.479(6)	Nd(1)-N(2)	2.657(7)
Nd(1)-O(3)	2.497(5)	O(7)-N(5)	1.298(8)
Nd(1)-O(4)	2.503(6)	N(6)-O(8)	1.270(8)
Nd(1)-O(7)	2.509(5)		
Angles			
O(6)-Nd(1)-O(5)	69.54(18)	O(4)-Nd(1)-O(1)	151.33(18)
O(6)-Nd(1)-O(2)	129.21(18)	O(7)-Nd(1)-O(1)	63.20(17)
O(5)-Nd(1)-O(2)	149.24(18)	O(6)-Nd(1)-N(3)	72.91(19)
O(6)-Nd(1)-O(3)	126.18(18)	O(5)-Nd(1)-N(3)	138.04(19)
O(5)-Nd(1)-O(3)	118.78(19)	O(2)-Nd(1)-N(3)	71.68(19)
O(2)-Nd(1)-O(3)	72.79(19)	O(3)-Nd(1)-N(3)	70.93(19)
O(6)-Nd(1)-O(4)	65.35(19)	O(4)-Nd(1)-N(3)	75.03(19)
O(5)-Nd(1)-O(4)	72.84(19)	O(7)-Nd(1)-N(3)	82.99(19)
O(2)-Nd(1)-O(4)	134.61(18)	O(1)-Nd(1)-N(3)	133.55(19)
O(3)-Nd(1)-O(4)	67.68(19)	O(6)-Nd(1)-N(2)	141.35(19)
O(6)-Nd(1)-O(7)	65.99(18)	O(5)-Nd(1)-N(2)	72.44(19)
O(5)-Nd(1)-O(7)	98.04(18)	O(2)-Nd(1)-N(2)	88.15(19)
O(2)-Nd(1)-O(7)	74.57(18)	O(3)-Nd(1)-N(2)	68.29(19)
O(3)-Nd(1)-O(7)	143.15(18)	O(4)-Nd(1)-N(2)	97.02(19)
O(4)-Nd(1)-O(7)	130.54(18)	O(7)-Nd(1)-N(2)	127.19(18)
O(6)-Nd(1)-O(1)	115.30(18)	O(1)-Nd(1)-N(2)	64.00(19)
O(5)-Nd(1)-O(1)	80.64(19)	N(3)-Nd(1)-N(2)	138.3(2)
O(2)-Nd(1)-O(1)	69.31(18)	N(5)-O(7)-Nd(1)	147.6(4)
O(3)-Nd(1)-O(1)	118.53(18)		

Table S5 SHAPE analysis for the Ln coordination spheres.

Compound	JCSAPR-9	CSAPR-9	TCTPR-9	MFF-9
1 Tb	1.383	**0.232**	1.284	0.797
2 Dy	1.398	**0.239**	1.328	0.776
3 Pr	3.020	1.627	2.156	**1.144**
4 Nd	2.924	1.584	2.145	**1.113**

JCSAPR-9 = Capped square antiprism J10 (C_{4v}); CSAPR-9 = Spherical capped square antiprism (C_{4v}); TCTPR-9 = Spherical tricapped trigonal prism (D_{3h}); MFF-9 = Muffin (C_s).

Table S6 Distances (Å) and angles (°) for the hydrogen bonds in **1–2**.

D–H···A	Compounds	d(D–H)	d(H···A)	d(D···A)	<(DHA)
O7-H7B···O7	**1 Tb**	0.853	1.982	2.778	154.99
O7-H7B···O7	**2 Dy**	0.862	1.963	2.771	155.54

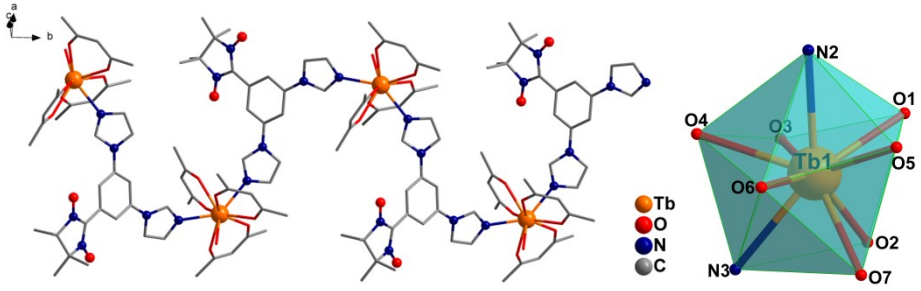

Fig. S1 (left) 1D structure of compound **1**. (right) The coordination polyhedra for Tb center (all F atoms, H atoms and Et_2O solvent molecules are omitted).

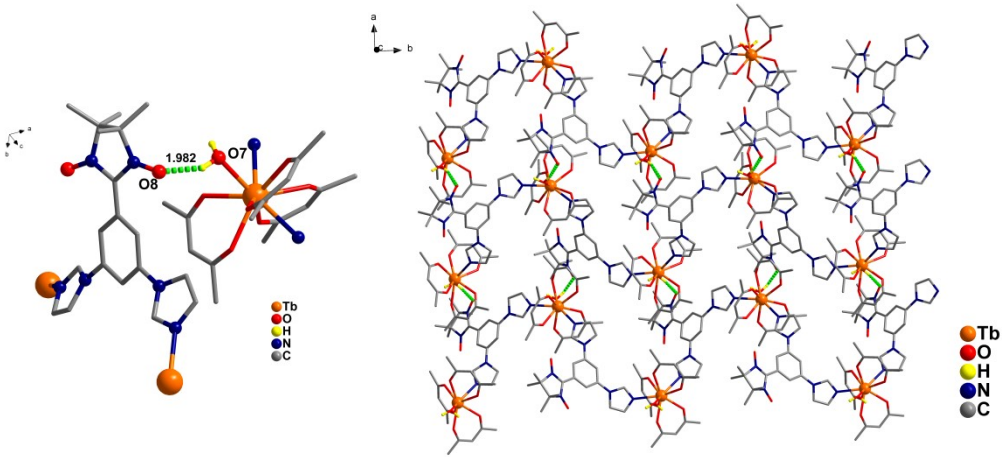

Fig. S2 (left) The hydrogen-bonded Tb–O_{water}–H···O_{rad} motif in compound **1**. (right) 2D layer structure results from the hydrogen-bonding interactions in **1** (all F atoms, partial H atoms and Et_2O solvent molecules are omitted).

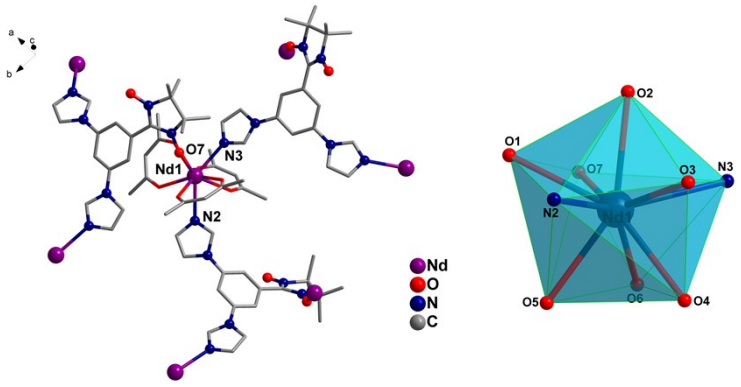

Fig. S3. (left) View of coordination environment of Nd(III) ion in compound **4**. (right) Coordination polyhedra of the Nd(III) ions (all F and H atoms are omitted).

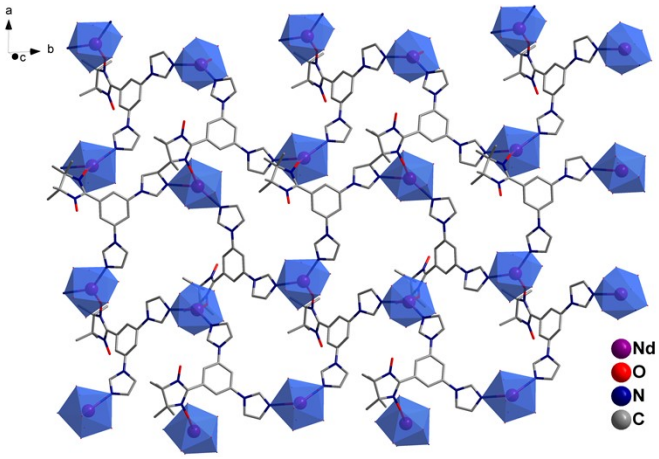

Fig. S4 2D structure of compound **4** (all F atoms, H atoms and hfac molecules are omitted).

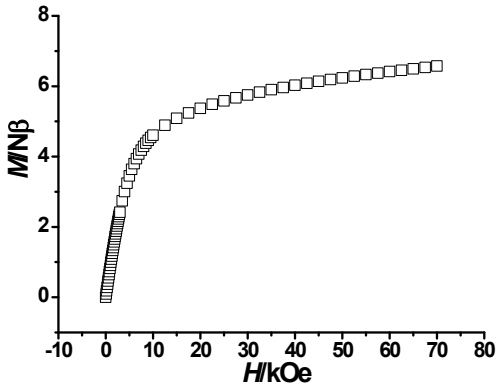

Fig. S5 *M* versus *H* curve for compound **1** at 2.0 K.

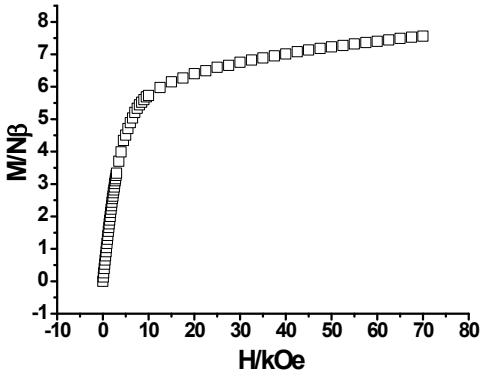

Fig. S6 *M* versus *H* curve for compound **2** at 2.0 K.

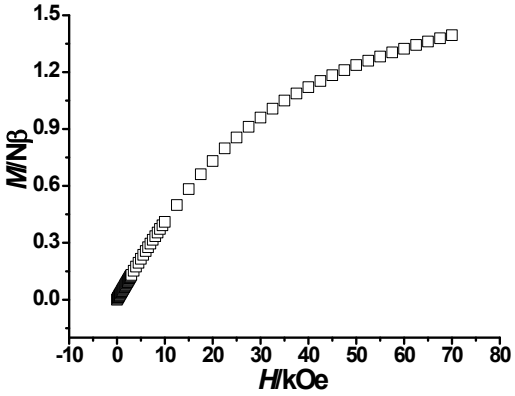

Fig. S7 *M* versus *H* curve for compound **3** at 2.0 K.

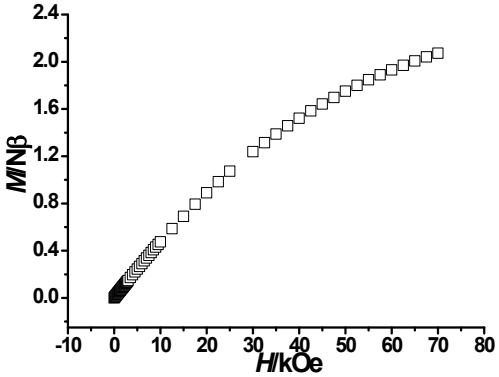

Fig. S8 *M* versus *H* curve for compound **4** at 2.0 K.

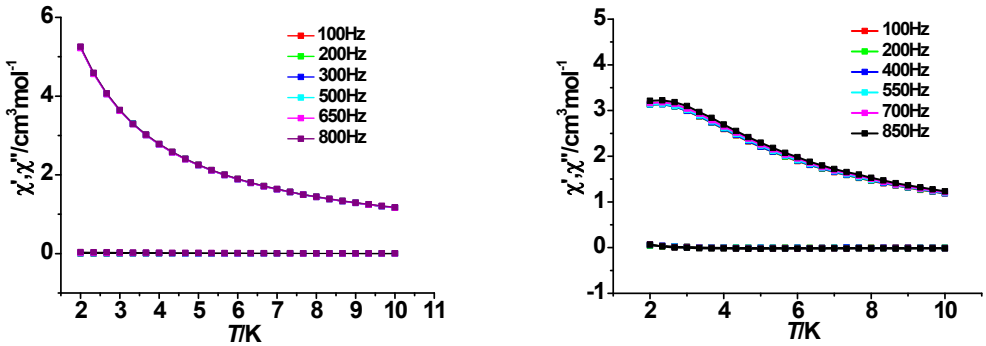

Fig. S9 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility in zero field (left) and 2500 Oe dc field (right) for compound **1**.

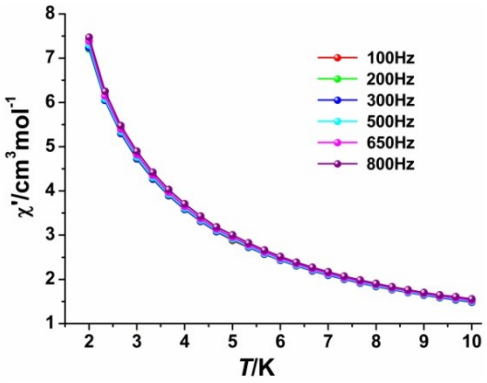

Fig. S10 Temperature dependence of the in-phase component of the ac magnetic susceptibility in zero field for compound **2**.

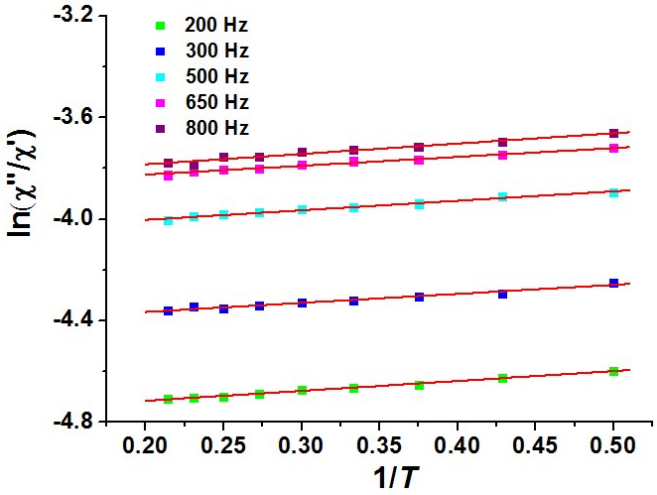

Fig. S11 Plots of ln(χ″/χ′) versus 1/*T* of **2**, the solid line represents the fitting results.

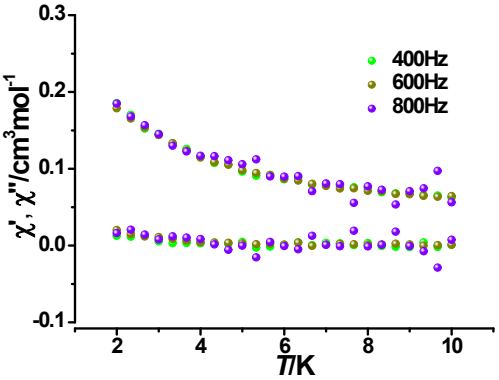

Fig. S12 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility under 3000 Oe dc field for compound **3**.

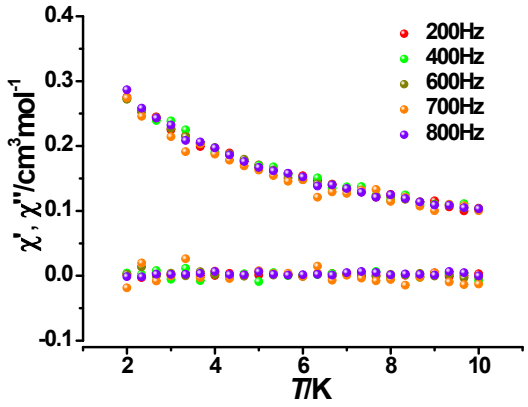

Fig. S13 Temperature dependence of the in-phase and out-of-phase components of the ac magnetic susceptibility under 3000 Oe dc field for compound **4**.