

Supporting Information

Synthesis, crystal structures and magnetic properties of two heterometallic $\{\text{Ln}_8\text{Cr}_4\}$ ($\text{Ln} = \text{Gd}^{3+}$ and Tb^{3+}) complexes with one-dimensional wave chain structure

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1. Structure

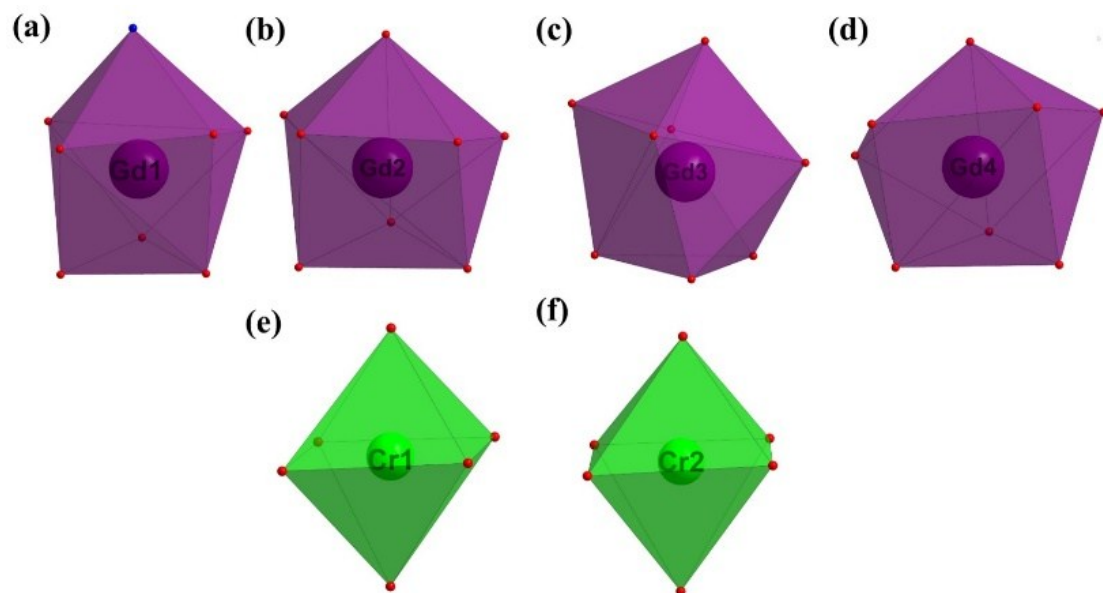


Fig. S1. (a) Coordination polyhedron of Gd1; (b) Coordination polyhedron of Gd2; (c) Coordination polyhedron of Gd3; (d) Coordination polyhedron of Gd4; (e) Coordination polyhedron of Cr1; (f) Coordination polyhedron of Cr2.

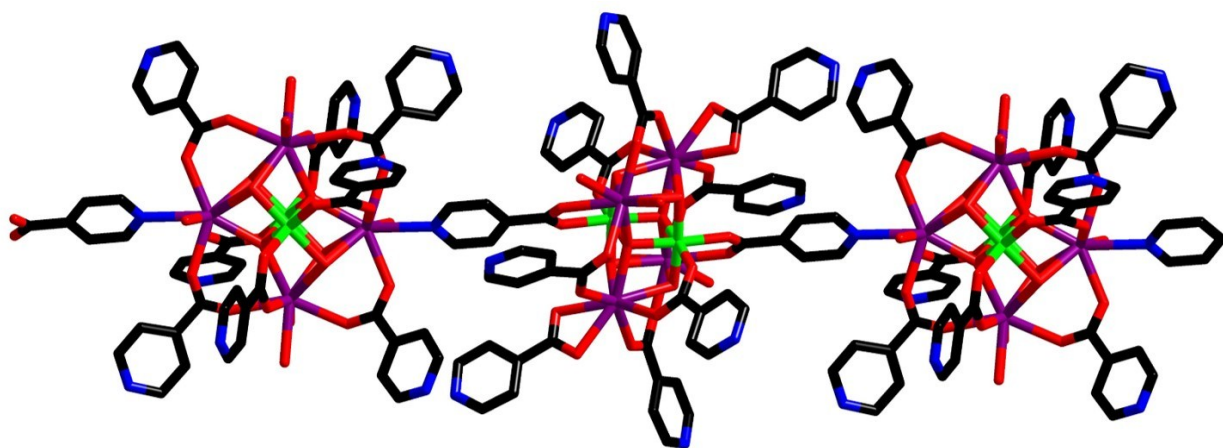


Fig. S2. Ball-and-stick of one-dimensional (1D) chain structure for 1.

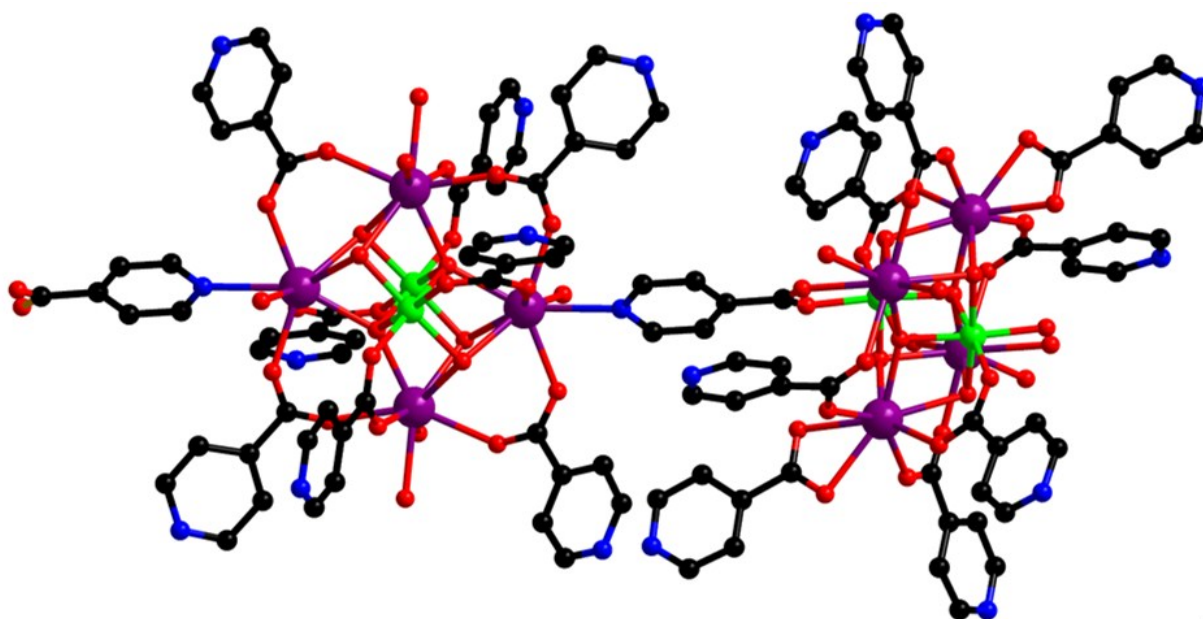


Fig. S3. The unit of compound **1**.

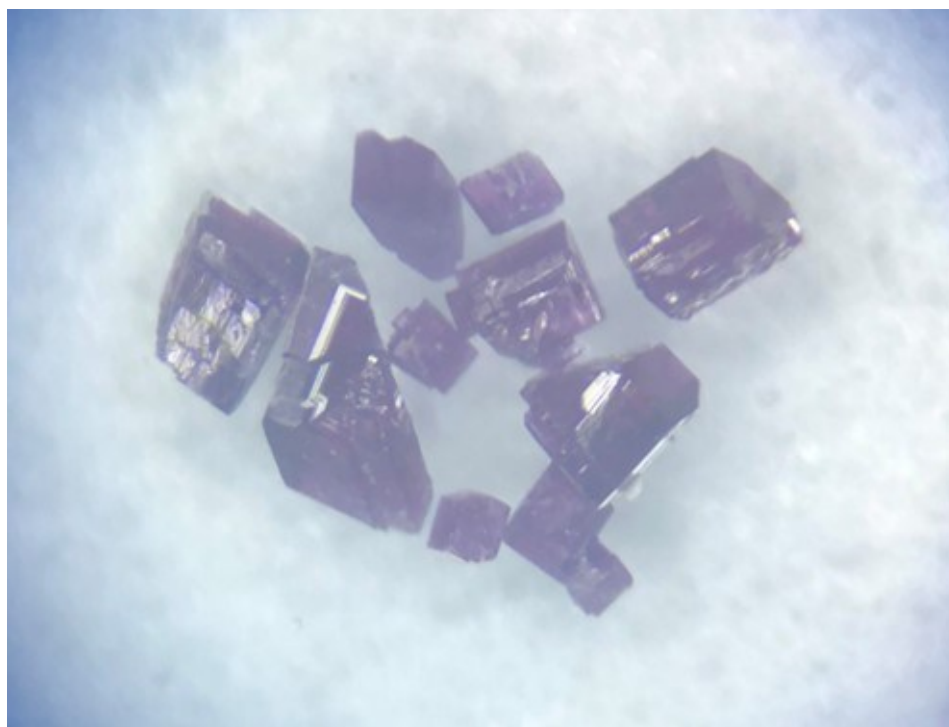


Fig. S4. The image of **1** crystal under optical microscope.

2. IR Spectra

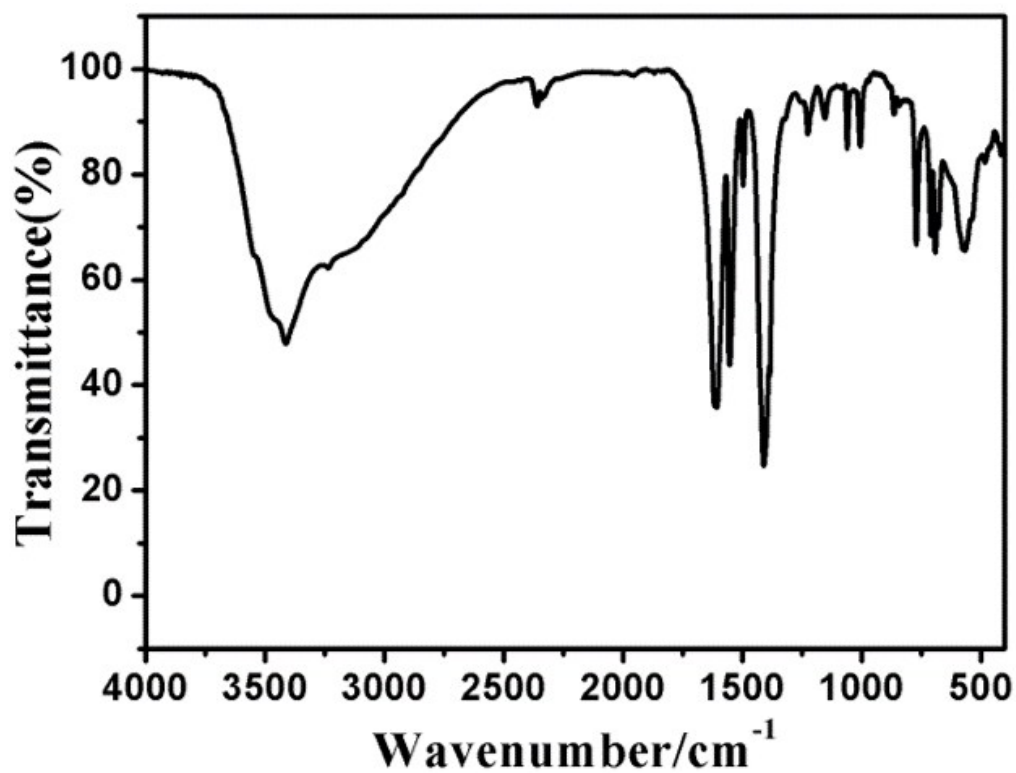


Fig. S5. The IR spectrum of compound 1.

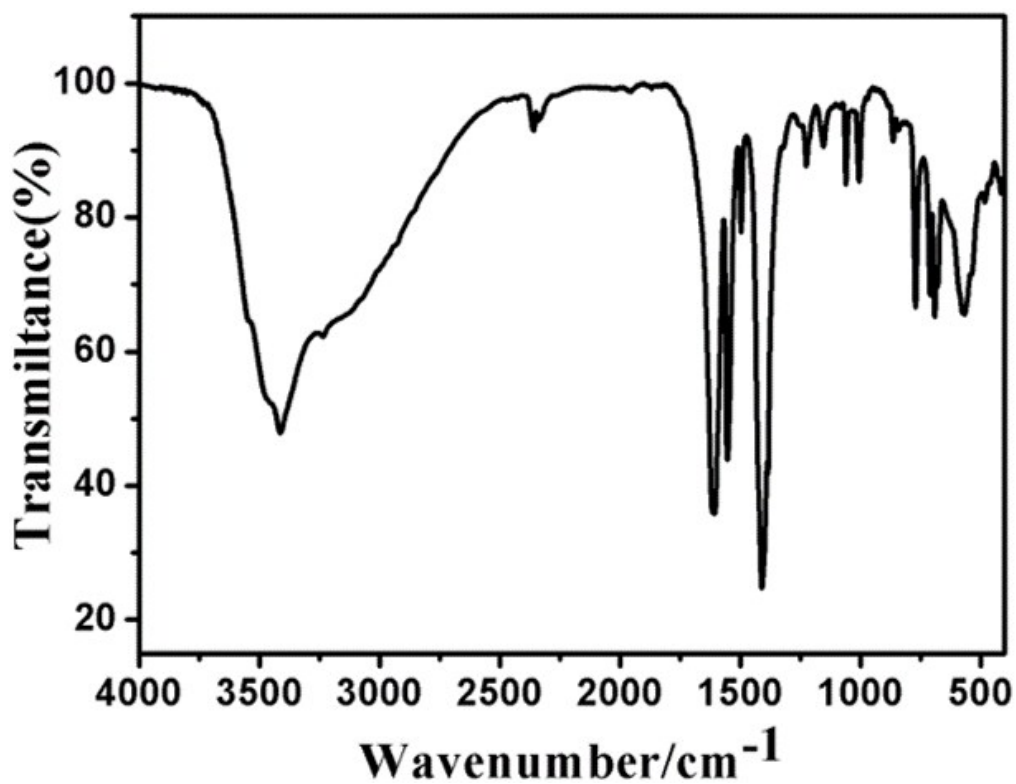


Fig. S6. The IR spectrum of compound 2.

3. Powder X-ray Diffraction (PXRD)

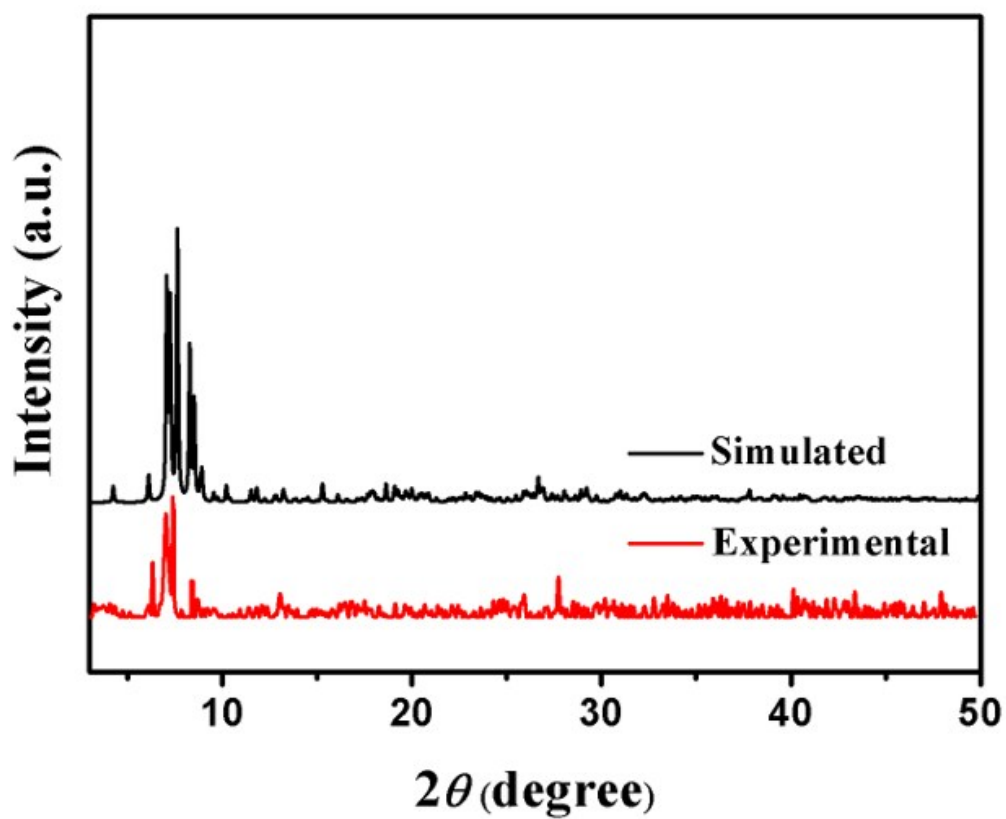


Fig. S7. Experimental and simulated PXRD patterns of 1.

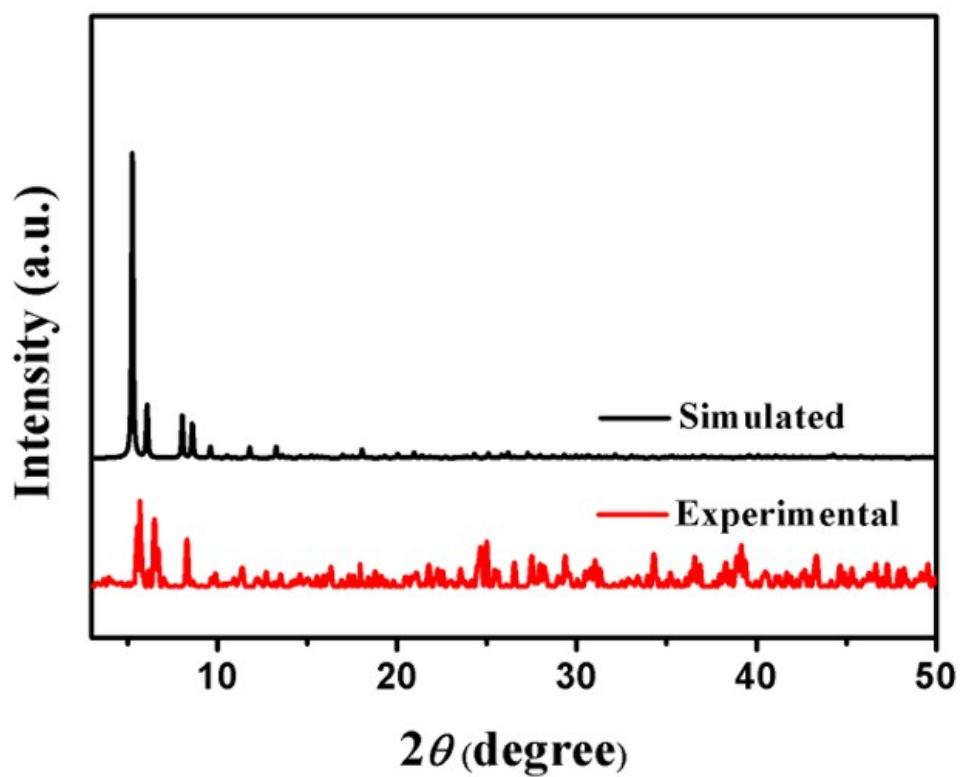


Fig. S8. Experimental and simulated PXRD patterns of 2.

4. Thermogravimetric Analysis (TGA)

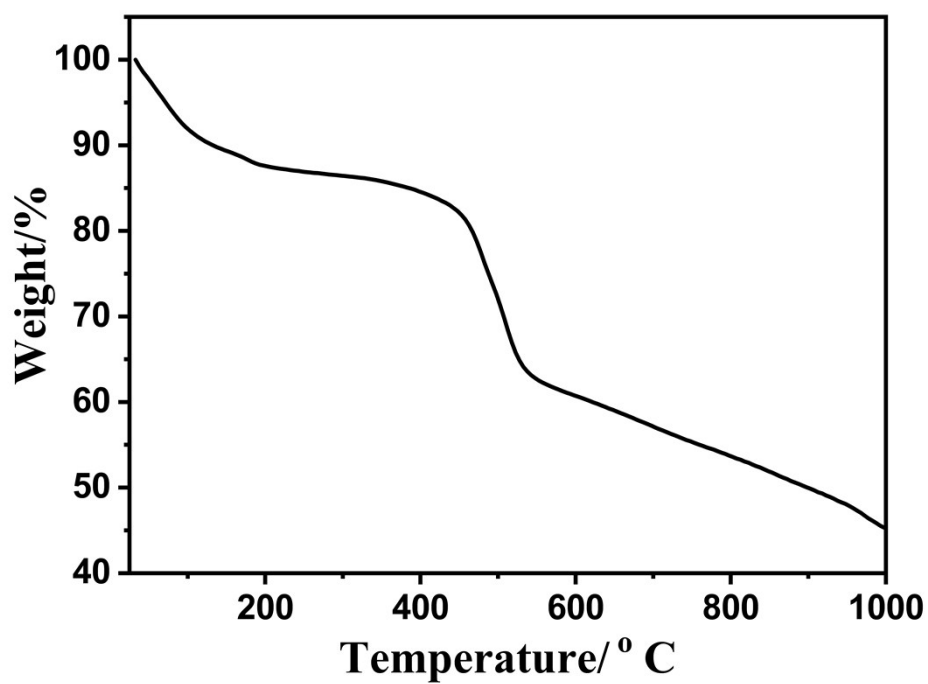


Fig. S9. The TG curve for **1**.

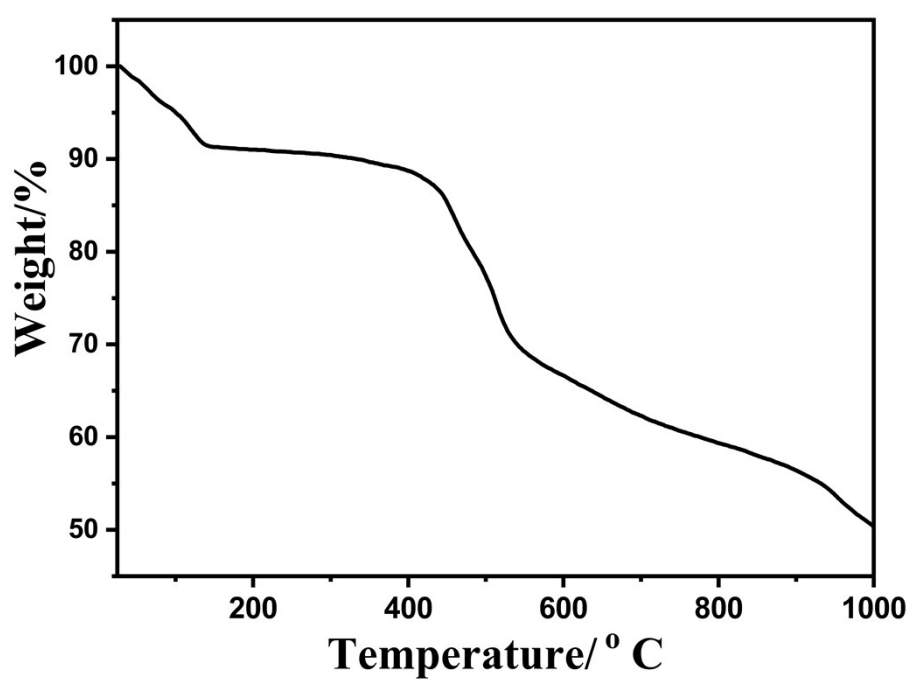


Fig. S10. The TG curve for **2**.

5. Magnetic property

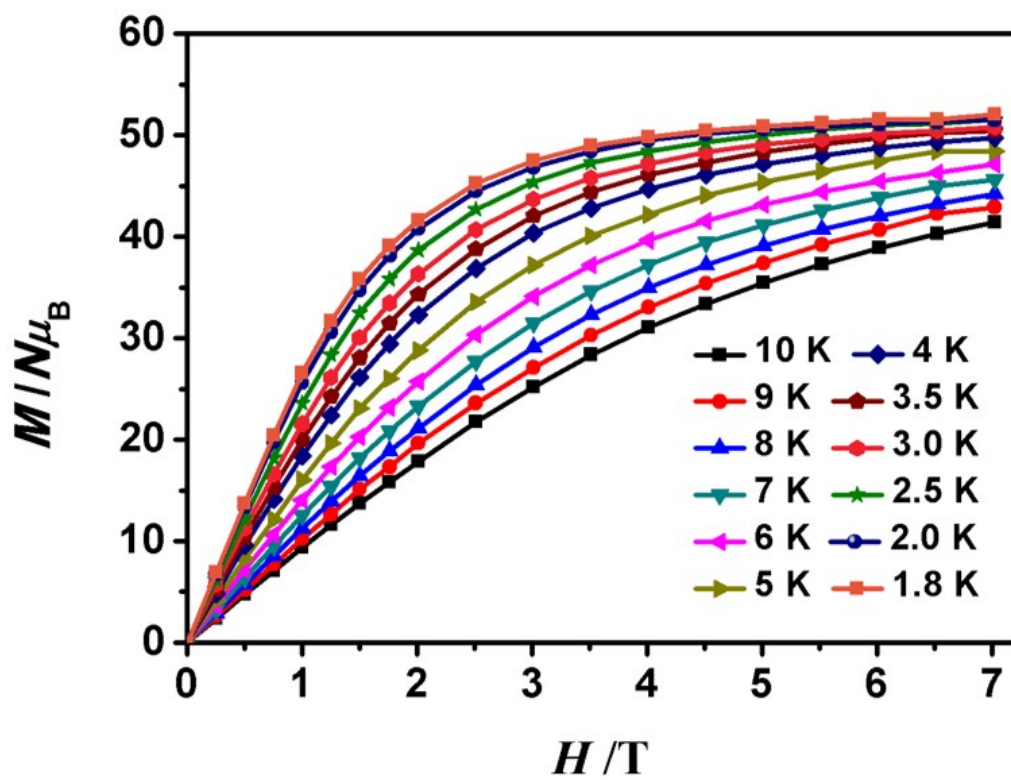


Fig. S11. Field-dependent experimental magnetization plots for **1** from 1.8 -10 K.

Table S1. Bond lengths (Å) of main metal atoms for complex **1**.

Gd(1)-O(6)	2.378(4)	Cr(1)-O(2)	2.005(4)
Gd(1)-O(11)#1	2.395(5)	Cr(1)-O(3)#2	2.036(4)
Gd(1)-O(13)	2.429(5)	Cr(1)-O(5)#2	2.044(4)
Gd(1)-O(3W)	2.445(5)	Cr(2)-O(6)	1.988(4)
Gd(1)-O(12)	2.448(5)	Cr(2)-O(6)#1	1.992(4)
Gd(1)-O(10)	2.449(5)	Cr(2)-O(10)	2.012(4)
Gd(1)-O(7)#1	2.507(5)	Cr(2)-O(9)	2.016(5)
Gd(1)-N(1)#2	2.674(6)	Cr(2)-O(7)	2.028(4)
Gd(2)-O(1)#2	2.372(4)	Cr(2)-O(8)	2.057(5)
Gd(2)-O(15)	2.396(5)		
Gd(2)-O(16)#2	2.418(5)		
Gd(2)-O(4W)	2.425(5)		
Gd(2)-O(4)#2	2.461(4)		
Gd(2)-O(14)	2.482(5)		
Gd(2)-O(2)	2.484(5)		
Gd(2)-O(5W)	2.498(5)		
Gd(3)-O(6)#1	2.367(5)		
Gd(3)-O(17)	2.414(5)		
Gd(3)-O(19)	2.426(5)		
Gd(3)-O(1W)	2.441(5)		
Gd(3)-O(18)	2.462(5)		
Gd(3)-O(2W)	2.487(5)		
Gd(3)-O(10)	2.488(5)		
Gd(3)-O(7)#1	2.493(5)		
Gd(4)-O(1)	2.361(4)		
Gd(4)-O(20)	2.427(5)		
Gd(4)-O(23)	2.442(5)		
Gd(4)-O(21)	2.461(5)		
Gd(4)-O(2)	2.473(4)		
Gd(4)-O(4)#2	2.496(5)		
Gd(4)-O(22)	2.514(6)		
Gd(4)-O(24)	2.577(5)		
Cr(1)-O(4)	1.974(4)		
Cr(1)-O(1)	1.992(4)		
Cr(1)-O(1)#2	1.994(4)		

Table S2. Bond angles (°) of main metal atoms for complex **1**.

O(6)-Gd(1)-O(11)#1	79.02(16)	O(4W)-Gd(2)-O(4)#2	142.31(14)
O(6)-Gd(1)-O(13)	140.36(14)	O(1)#2-Gd(2)-O(14)	80.53(14)
O(11)#1-Gd(1)-O(13)	140.55(15)	O(15)-Gd(2)-O(14)	111.41(16)
O(6)-Gd(1)-O(3W)	110.81(15)	O(16)#2-Gd(2)-O(14)	78.96(15)
O(11)#1-Gd(1)-O(3W)	74.51(18)	O(4W)-Gd(2)-O(14)	141.34(16)
O(13)-Gd(1)-O(3W)	88.41(17)	O(4)#2-Gd(2)-O(14)	73.51(16)
O(6)-Gd(1)-O(12)	81.75(16)	O(1)#2-Gd(2)-O(2)	69.07(13)
O(11)#1-Gd(1)-O(12)	76.43(18)	O(15)-Gd(2)-O(2)	77.98(16)
O(13)-Gd(1)-O(12)	102.31(16)	O(16)#2-Gd(2)-O(2)	118.03(16)
O(3W)-Gd(1)-O(12)	145.13(14)	O(4W)-Gd(2)-O(2)	80.25(15)
O(6)-Gd(1)-O(10)	70.01(12)	O(4)#2-Gd(2)-O(2)	69.17(15)
O(11)#1-Gd(1)-O(10)	140.59(15)	O(14)-Gd(2)-O(2)	138.05(12)
O(13)-Gd(1)-O(10)	72.95(13)	O(1)#2-Gd(2)-O(5W)	141.94(14)
O(3W)-Gd(1)-O(10)	139.02(15)	O(15)-Gd(2)-O(5W)	73.34(19)
O(12)-Gd(1)-O(10)	75.57(15)	O(16)#2-Gd(2)-O(5W)	81.08(19)
O(6)-Gd(1)-O(7)#1	69.35(14)	O(4W)-Gd(2)-O(5W)	81.46(16)
O(11)#1-Gd(1)-O(7)#1	122.37(14)	O(4)#2-Gd(2)-O(5W)	114.33(16)
O(13)-Gd(1)-O(7)#1	84.48(14)	O(14)-Gd(2)-O(5W)	65.87(14)
O(3W)-Gd(1)-O(7)#1	73.73(14)	O(2)-Gd(2)-O(5W)	148.96(14)
O(12)-Gd(1)-O(7)#1	139.64(14)	O(6)#1-Gd(3)-O(17)	82.20(14)
O(10)-Gd(1)-O(7)#1	68.50(12)	O(6)#1-Gd(3)-O(19)	76.03(14)
O(6)-Gd(1)-N(1)#2	147.67(15)	O(17)-Gd(3)-O(19)	78.06(18)
O(11)#1-Gd(1)-N(1)#2	72.87(18)	O(6)#1-Gd(3)-O(1W)	115.42(16)
O(13)-Gd(1)-N(1)#2	68.66(16)	O(17)-Gd(3)-O(1W)	144.22(15)
O(3W)-Gd(1)-N(1)#2	76.86(19)	O(19)-Gd(3)-O(1W)	76.79(18)
O(12)-Gd(1)-N(1)#2	76.49(19)	O(6)#1-Gd(3)-O(18)	139.01(14)
O(10)-Gd(1)-N(1)#2	125.48(15)	O(17)-Gd(3)-O(18)	106.44(17)
O(7)#1-Gd(1)-N(1)#2	140.40(16)	O(19)-Gd(3)-O(18)	144.65(15)
O(1)#2-Gd(2)-O(15)	139.02(16)	O(1W)-Gd(3)-O(18)	81.09(19)
O(1)#2-Gd(2)-O(16)#2	75.18(15)	O(6)#1-Gd(3)-O(2W)	145.77(15)
O(15)-Gd(2)-O(16)#2	144.21(15)	O(17)-Gd(3)-O(2W)	71.97(18)
O(1)#2-Gd(2)-O(4W)	119.85(15)	O(19)-Gd(3)-O(2W)	76.92(18)
O(15)-Gd(2)-O(4W)	75.85(16)	O(1W)-Gd(3)-O(2W)	77.84(19)
O(16)#2-Gd(2)-O(4W)	75.95(15)	O(18)-Gd(3)-O(2W)	71.66(18)
O(1)#2-Gd(2)-O(4)#2	69.41(13)	O(6)#1-Gd(3)-O(10)	70.44(13)
O(15)-Gd(2)-O(4)#2	76.65(15)	O(17)-Gd(3)-O(10)	72.71(15)

O(16)#2-Gd(2)-O(4)#2	137.90(14)	O(2)-Gd(4)-O(24)	122.54(18)
O(1W)-Gd(3)-O(10)	141.23(14)	O(4)#2-Gd(4)-O(24)	141.63(16)
O(18)-Gd(3)-O(10)	74.17(17)	O(19)-Gd(3)-O(10)	137.78(15)
O(2W)-Gd(3)-O(10)	120.15(16)	O(22)-Gd(4)-O(24)	51.43(17)
O(6)#1-Gd(3)-O(7)#1	69.85(12)	O(4)-Cr(1)-O(1)	87.92(17)
O(17)-Gd(3)-O(7)#1	137.50(16)	O(4)-Cr(1)-O(1)#2	89.62(17)
O(19)-Gd(3)-O(7)#1	122.55(14)	O(1)-Cr(1)-O(1)#2	83.34(18)
O(1W)-Gd(3)-O(7)#1	78.05(16)	O(4)-Cr(1)-O(2)	175.08(15)
O(18)-Gd(3)-O(7)#1	78.32(14)	O(1)-Cr(1)-O(2)	88.09(16)
O(2W)-Gd(3)-O(7)#1	143.85(15)	O(1)#2-Cr(1)-O(2)	87.05(17)
O(10)-Gd(3)-O(7)#1	68.13(12)	O(4)-Cr(1)-O(3)#2	93.69(18)
O(1)-Gd(4)-O(20)	141.34(15)	O(1)-Cr(1)-O(3)#2	94.29(19)
O(1)-Gd(4)-O(23)	83.77(16)	O(1)#2-Cr(1)-O(3)#2	175.87(16)
O(20)-Gd(4)-O(23)	98.35(17)	O(2)-Cr(1)-O(3)#2	89.49(17)
O(1)-Gd(4)-O(21)	76.33(16)	O(4)-Cr(1)-O(5)#2	92.85(17)
O(20)-Gd(4)-O(21)	142.26(15)	O(1)-Cr(1)-O(5)#2	177.60(16)
O(23)-Gd(4)-O(21)	80.30(17)	O(1)#2-Cr(1)-O(5)#2	94.38(19)
O(1)-Gd(4)-O(2)	70.13(13)	O(2)-Cr(1)-O(5)#2	91.02(17)
O(20)-Gd(4)-O(2)	84.36(16)	O(3)#2-Cr(1)-O(5)#2	87.9(2)
O(23)-Gd(4)-O(2)	138.62(15)	O(6)-Cr(2)-O(6)#1	82.92(15)
O(21)-Gd(4)-O(2)	121.41(17)	O(6)-Cr(2)-O(10)	87.64(15)
O(1)-Gd(4)-O(4)#2	70.25(13)	O(6)#1-Cr(2)-O(10)	88.82(16)
O(20)-Gd(4)-O(4)#2	73.68(14)	O(6)-Cr(2)-O(9)	93.17(16)
O(23)-Gd(4)-O(4)#2	72.44(16)	O(6)#1-Cr(2)-O(9)	175.44(16)
O(21)-Gd(4)-O(4)#2	138.52(15)	O(10)-Cr(2)-O(9)	93.37(18)
O(2)-Gd(4)-O(4)#2	68.79(15)	O(6)-Cr(2)-O(7)	87.78(14)
O(1)-Gd(4)-O(22)	115.34(15)	O(6)#1-Cr(2)-O(7)	87.57(17)
O(20)-Gd(4)-O(22)	83.84(17)	O(10)-Cr(2)-O(7)	174.49(15)
O(23)-Gd(4)-O(22)	146.10(17)	O(9)-Cr(2)-O(7)	89.94(18)
O(21)-Gd(4)-O(22)	77.86(17)	O(6)-Cr(2)-O(8)	179.30(17)
O(2)-Gd(4)-O(22)	75.26(16)	O(6)#1-Cr(2)-O(8)	96.38(16)
O(4)#2-Gd(4)-O(22)	138.92(14)	O(10)-Cr(2)-O(8)	92.26(16)
O(1)-Gd(4)-O(24)	146.83(16)	O(9)-Cr(2)-O(8)	87.53(17)
O(20)-Gd(4)-O(24)	71.59(18)	O(7)-Cr(2)-O(8)	92.28(15)
O(23)-Gd(4)-O(24)	96.93(19)		
O(21)-Gd(4)-O(24)	71.17(19)		

Table S3. Bond lengths (Å) of main metal atoms for complex **2**.

Tb(1)-O(6)	2.318(3)	Cr(1)-O(2)	1.978(3)
Tb(1)-O(11)#1	2.338(4)	Cr(1)-O(3)#2	1.998(3)
Tb(1)-O(13)	2.378(4)	Cr(1)-O(5)#2	2.000(4)
Tb(1)-O(3W)	2.385(4)	Cr(2)-O(6)#1	1.952(3)
Tb(1)-O(10)	2.401(3)	Cr(2)-O(6)	1.959(3)
Tb(1)-O(12)	2.402(3)	Cr(2)-O(10)	1.967(3)
Tb(1)-O(7)#1	2.452(3)	Cr(2)-O(9)	1.987(3)
Tb(1)-N(1)#2	2.622(4)	Cr(2)-O(7)	1.991(3)
Tb(2)-O(1)#2	2.331(3)	Cr(2)-O(8)	2.019(4)
Tb(2)-O(15)	2.356(4)		
Tb(2)-O(4W)	2.360(4)		
Tb(2)-O(16)#2	2.372(4)		
Tb(2)-O(4)#2	2.395(3)		
Tb(2)-O(2)	2.415(3)		
Tb(2)-O(14)	2.429(3)		
Tb(2)-O(5W)	2.445(4)		
Tb(3)-O(6)#1	2.319(3)		
Tb(3)-O(17)	2.352(4)		
Tb(3)-O(19)	2.367(4)		
Tb(3)-O(1W)	2.389(4)		
Tb(3)-O(18)	2.390(4)		
Tb(3)-O(10)	2.430(3)		
Tb(3)-O(7)#1	2.440(3)		
Tb(3)-O(2W)	2.443(4)		
Tb(4)-O(1)	2.308(3)		
Tb(4)-O(20)	2.366(3)		
Tb(4)-O(23)	2.372(4)		
Tb(4)-O(21)	2.397(4)		
Tb(4)-O(2)	2.422(3)		
Tb(4)-O(4)#2	2.422(3)		
Tb(4)-O(22)	2.430(4)		
Tb(4)-O(24)	2.528(5)		
Cr(1)-O(1)	1.950(3)		
Cr(1)-O(1)#2	1.951(3)		
Cr(1)-O(4)	1.959(3)		

Table S4. Bond angles (°) of main metal atoms for complex **2**.

O(6)-Tb(1)-O(11)#1	78.80(12)	O(15)-Tb(2)-O(14)	111.45(13)
O(6)-Tb(1)-O(13)	140.47(12)	O(4W)-Tb(2)-O(14)	140.58(13)
O(11)#1-Tb(1)-O(13)	140.66(13)	O(16)#2-Tb(2)-O(14)	78.97(13)
O(6)-Tb(1)-O(3W)	110.02(13)	O(4)#2-Tb(2)-O(14)	74.21(11)
O(11)#1-Tb(1)-O(3W)	74.51(15)	O(2)-Tb(2)-O(14)	138.51(11)
O(13)-Tb(1)-O(3W)	88.81(15)	O(1)#2-Tb(2)-O(5W)	141.53(12)
O(6)-Tb(1)-O(10)	70.45(11)	O(15)-Tb(2)-O(5W)	72.96(14)
O(11)#1-Tb(1)-O(10)	140.68(12)	O(4W)-Tb(2)-O(5W)	81.45(14)
O(13)-Tb(1)-O(10)	72.68(12)	O(16)#2-Tb(2)-O(5W)	81.31(14)
O(3W)-Tb(1)-O(10)	138.81(13)	O(4)#2-Tb(2)-O(5W)	114.16(13)
O(6)-Tb(1)-O(12)	81.94(11)	O(2)-Tb(2)-O(5W)	148.68(12)
O(11)#1-Tb(1)-O(12)	76.10(15)	O(14)-Tb(2)-O(5W)	65.50(12)
O(13)-Tb(1)-O(12)	102.49(13)	O(6)#1-Tb(3)-O(17)	82.46(12)
O(3W)-Tb(1)-O(12)	145.11(14)	O(6)#1-Tb(3)-O(19)	76.57(12)
O(10)-Tb(1)-O(12)	75.86(12)	O(17)-Tb(3)-O(19)	77.70(15)
O(6)-Tb(1)-O(7)#1	69.82(11)	O(6)#1-Tb(3)-O(1W)	115.67(14)
O(11)#1-Tb(1)-O(7)#1	122.94(13)	O(17)-Tb(3)-O(1W)	143.45(14)
O(13)-Tb(1)-O(7)#1	83.80(12)	O(19)-Tb(3)-O(1W)	76.48(14)
O(3W)-Tb(1)-O(7)#1	73.41(12)	O(6)#1-Tb(3)-O(18)	139.09(12)
O(10)-Tb(1)-O(7)#1	68.34(11)	O(17)-Tb(3)-O(18)	106.40(14)
O(12)-Tb(1)-O(7)#1	139.95(11)	O(19)-Tb(3)-O(18)	144.06(14)
O(1)#2-Tb(2)-O(15)	139.82(12)	O(1W)-Tb(3)-O(18)	81.07(14)
O(1)#2-Tb(2)-O(4W)	119.69(13)	O(6)#1-Tb(3)-O(10)	70.10(11)
O(15)-Tb(2)-O(4W)	76.10(14)	O(17)-Tb(3)-O(10)	72.95(13)
O(1)#2-Tb(2)-O(16)#2	74.82(12)	O(19)-Tb(3)-O(10)	137.75(12)
O(15)-Tb(2)-O(16)#2	143.75(13)	O(1W)-Tb(3)-O(10)	141.73(12)
O(4W)-Tb(2)-O(16)#2	75.17(14)	O(18)-Tb(3)-O(10)	74.58(12)
O(1)#2-Tb(2)-O(4)#2	69.98(11)	O(6)#1-Tb(3)-O(7)#1	69.90(10)
O(15)-Tb(2)-O(4)#2	76.58(12)	O(17)-Tb(3)-O(7)#1	137.87(12)
O(4W)-Tb(2)-O(4)#2	142.43(13)	O(19)-Tb(3)-O(7)#1	123.09(13)
O(16)#2-Tb(2)-O(4)#2	138.50(12)	O(1W)-Tb(3)-O(7)#1	78.47(13)
O(1)#2-Tb(2)-O(2)	69.76(11)	O(18)-Tb(3)-O(7)#1	78.31(12)
O(15)-Tb(2)-O(2)	77.95(13)	O(10)-Tb(3)-O(7)#1	68.09(11)
O(4W)-Tb(2)-O(2)	80.53(13)	O(6)#1-Tb(3)-O(2W)	145.88(13)
O(16)#2-Tb(2)-O(2)	118.07(12)	O(17)-Tb(3)-O(2W)	71.66(15)
O(4)#2-Tb(2)-O(2)	68.89(11)	O(19)-Tb(3)-O(2W)	76.48(16)

O(1)#2-Tb(2)-O(14)	80.45(11)	O(1)-Cr(1)-O(2)	87.59(13)
O(18)-Tb(3)-O(2W)	71.45(15)	O(1W)-Tb(3)-O(2W)	77.44(16)
O(10)-Tb(3)-O(2W)	120.30(15)	O(1)#2-Cr(1)-O(2)	87.43(13)
O(7)#1-Tb(3)-O(2W)	143.70(13)	O(4)-Cr(1)-O(2)	174.20(14)
O(6)#1-Tb(3)-Cr(2)	35.42(7)	O(1)-Cr(1)-O(3)#2	94.17(14)
O(1)-Tb(4)-O(20)	141.61(12)	O(1)#2-Cr(1)-O(3)#2	176.31(15)
O(1)-Tb(4)-O(23)	84.05(13)	O(4)-Cr(1)-O(3)#2	93.86(14)
O(20)-Tb(4)-O(23)	99.29(14)	O(2)-Cr(1)-O(3)#2	89.98(14)
O(1)-Tb(4)-O(21)	76.58(12)	O(1)-Cr(1)-O(5)#2	177.23(14)
O(20)-Tb(4)-O(21)	141.77(14)	O(1)#2-Cr(1)-O(5)#2	94.29(14)
O(23)-Tb(4)-O(21)	79.52(15)	O(4)-Cr(1)-O(5)#2	93.07(15)
O(1)-Tb(4)-O(2)	70.11(11)	O(2)-Cr(1)-O(5)#2	91.39(15)
O(20)-Tb(4)-O(2)	83.89(12)	O(3)#2-Cr(1)-O(5)#2	88.40(15)
O(23)-Tb(4)-O(2)	139.09(13)	O(6)#1-Cr(2)-O(6)	82.99(14)
O(21)-Tb(4)-O(2)	121.93(13)	O(6)#1-Cr(2)-O(10)	88.28(13)
O(1)-Tb(4)-O(4)#2	70.41(10)	O(6)-Cr(2)-O(10)	87.83(13)
O(20)-Tb(4)-O(4)#2	73.99(12)	O(6)#1-Cr(2)-O(9)	175.66(15)
O(23)-Tb(4)-O(4)#2	73.43(13)	O(6)-Cr(2)-O(9)	93.27(14)
O(21)-Tb(4)-O(4)#2	138.89(12)	O(10)-Cr(2)-O(9)	93.79(14)
O(2)-Tb(4)-O(4)#2	68.33(11)	O(6)#1-Cr(2)-O(7)	87.73(13)
O(1)-Tb(4)-O(22)	115.42(14)	O(6)-Cr(2)-O(7)	87.38(13)
O(20)-Tb(4)-O(22)	82.98(15)	O(10)-Cr(2)-O(7)	174.10(14)
O(23)-Tb(4)-O(22)	145.38(16)	O(9)-Cr(2)-O(7)	89.91(14)
O(21)-Tb(4)-O(22)	77.96(15)	O(6)#1-Cr(2)-O(8)	96.01(14)
O(2)-Tb(4)-O(22)	75.51(14)	O(6)-Cr(2)-O(8)	178.98(14)
O(4)#2-Tb(4)-O(22)	138.61(13)	O(10)-Cr(2)-O(8)	92.37(14)
O(1)-Tb(4)-O(24)	147.01(14)	O(9)-Cr(2)-O(8)	87.72(15)
O(20)-Tb(4)-O(24)	71.03(15)	O(7)-Cr(2)-O(8)	92.36(14)
O(23)-Tb(4)-O(24)	96.63(16)		
O(21)-Tb(4)-O(24)	71.18(15)		
O(2)-Tb(4)-O(24)	122.37(14)		
O(4)#2-Tb(4)-O(24)	141.44(14)		
O(22)-Tb(4)-O(24)	51.13(16)		
O(1)-Cr(1)-O(1)#2	83.10(14)		
O(1)-Cr(1)-O(4)	87.79(13)		
O(1)#2-Cr(1)-O(4)	88.54(13)		