Supporting Information for:

In situ hydrothermal synthesis of dysprosium(III) single-molecule magnet with lanthanide salt as catalyst

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Table S1 Selected bond distances (Å) and angles (°) for complexes **1** and **3-6**

Complex 1[(a)]			
Gd(1)-O(8)#1	2.2852(19)	Gd(1)-O(7)	2.339(2)
Gd(1)-O(3W)	2.3420	Gd(1)-O(9)	2.3938(19)
Gd(1)-O(6W)	2.3988	Gd(1)-O(5W)	2.4353
Gd(1)-O(4W)	2.4385	Gd(1)-O(10)	2.6240(9)
O(8)#1-Gd(1)-O(7)	97.96(7)	O(8)#1-Gd(1)-O(3W)	93.53(7)
O(7)-Gd(1)-O(3W)	73.12(6)	O(8)#1-Gd(1)-O(9)	133.26(7)
O(7)-Gd(1)-O(9)	121.42(7)	O(3W)-Gd(1)-O(9)	76.88(6)
O(8)#1-Gd(1)-O(6W)	87.14(6)	O(7)-Gd(1)-O(6W)	142.29(6)
O(3W)-Gd(1)-O(6W)	144.2	O(9)-Gd(1)-O(6W)	76.81(6)
O(8)#1-Gd(1)-O(5W)	76.38(6)	O(7)-Gd(1)-O(5W)	74.23(6)
O(3W)-Gd(1)-O(5W)	144.0	O(9)-Gd(1)-O(5W)	134.55(6)
O(6W)-Gd(1)-O(5W)	70.8	O(8)#1-Gd(1)-O(4W)	155.57(6)
O(7)-Gd(1)-O(4W)	76.24(6)	O(3W)-Gd(1)-O(4W)	107.0
O(9)-Gd(1)-O(4W)	66.23(5)	O(6W)-Gd(1)-O(4W)	83.8
O(5W)-Gd(1)-O(4W)	79.2	O(8)#1-Gd(1)-O(10)	81.88(6)
O(7)-Gd(1)-O(10)	145.03(6)	O(3W)-Gd(1)-O(10)	72.00(3)
O(9)-Gd(1)-O(10)	51.51(5)	O(6W)-Gd(1)-O(10)	72.65(3)
O(5W)-Gd(1)-O(10)	137.96(4)	O(4W)-Gd(1)-O(10)	116.59(3)
Complex 3[(b)]			
Eu(1)-O(8)#1	2.289(3)	Eu(1)-O(7)	2.351(3)
Eu(1)-O(4W)	2.358(4)	Eu(1)-O(9)	2.403(3)
Eu(1)-O(6W)	2.415(3)	Eu(1)-O(5W)	2.448(3)
Eu(1)-O(3W)	2.459(3)	Eu(1)-O(10)	2.635(3)
O(8)#1-Eu(1)-O(7)	98.92(10)	O(8)#1-Eu(1)-O(4W)	93.95(14)
O(7)-Eu(1)-O(4W)	73.13(12)	O(8)#1-Eu(1)-O(9)	133.11(10)
O(7)-Eu(1)-O(9)	120.97(10)	O(4W)-Eu(1)-O(9)	76.99(11)
O(8)#1-Eu(1)-O(6W)	86.55(12)	O(7)-Eu(1)-O(6W)	142.35(12)
O(4W)-Eu(1)-O(6W)	144.04(13)	O(9)-Eu(1)-O(6W)	76.68(11)
O(8)#1-Eu(1)-O(5W)	76.49(12)	O(7)-Eu(1)-O(5W)	73.97(12)

O(4W)-Eu(1)-O(5W)	143.73(13)	O(9)-Eu(1)-O(5W)	134.45(12)
O(6W)-Eu(1)-O(5W)	71.20(13)	O(8)#1-Eu(1)-O(3W)	155.49(11)
O(7)-Eu(1)-O(3W)	75.73(11)	O(4W)-Eu(1)-O(3W)	106.90(14)
O(9)-Eu(1)-O(3W)	66.07(10)	O(6W)-Eu(1)-O(3W)	84.01(13)
O(5W)-Eu(1)-O(3W)	79.06(11)	O(8)#1-Eu(1)-O(10)	82.00(10)
O(7)-Eu(1)-O(10)	145.07(11)	O(4W)-Eu(1)-O(10)	71.98(12)
O(9)-Eu(1)-O(10)	51.29(9)	O(6W)-Eu(1)-O(10)	72.50(12)
O(5W)-Eu(1)-O(10)	138.53(11)	O(3W)-Eu(1)-O(10)	116.26(10)
Complex 4[(c)]			
Tb(1)-O(7)	2.375(2)	Tb(1)-O(8)	2.625(2)
Tb(1)-O(9)	2.266(2)	Tb(1)#1-O(10)	2.3275(9)
Tb(1)-O(4W)	2.3818	Tb(1)-O(5W)	2.4286
Tb(1)-O(6W)	2.4153	Tb(1)-O(10)#1	2.3275(9)
O(9)-Tb(1)-O(3W)	93.08(7)	O(9)-Tb(1)-O(10)#1	97.20(6)
O(3W)-Tb(1)-O(10)#1	72.93(4)	O(9)-Tb(1)-O(7)	133.14(8)
O(3W)-Tb(1)-O(7)	76.76(6)	O(10)#1-Tb(1)-O(7)	121.83(6)
O(9)-Tb(1)-O(4W)	87.59(7)	O(3W)-Tb(1)-O(4W)	144.1
O(10)#1-Tb(1)-O(4W)	142.560(18)	O(7)-Tb(1)-O(4W)	76.84(6)
O(9)-Tb(1)-O(6W)	76.58(6)	O(3W)-Tb(1)-O(6W)	144.0
O(10)#1-Tb(1)-O(6W)	74.33(4)	O(7)-Tb(1)-O(6W)	134.74(6)
O(4W)-Tb(1)-O(6W)	70.7	O(9)-Tb(1)-O(5W)	155.96(7)
O(3W)-Tb(1)-O(5W)	106.7	O(10)#1-Tb(1)-O(5W)	76.39(4)
O(7)-Tb(1)-O(5W)	66.53(6)	O(4W)-Tb(1)-O(5W)	84.3
O(6W)-Tb(1)-O(5W)	79.4	O(9)-Tb(1)-O(8)	81.43(7)
O(3W)-Tb(1)-O(8)	72.04(6)	O(10)#1-Tb(1)-O(8)	144.80(6)
O(7)-Tb(1)-O(8)	51.80(7)	O(4W)-Tb(1)-O(8)	72.63(6)
O(6W)-Tb(1)-O(8)	137.67(6)	O(5W)-Tb(1)-O(8)	117.22(5)
Complex 5[(d)]			
Sm(1)-O(1)	2.357(2)	Sm(1)-O(3W)	2.485(2)
Sm(1)#1-O(2)	2.307(2)	Sm(1)-O(4W)	2.367(3)
Sm(1)-O(5)	2.645(3)	Sm(1)-O(5W)	2.431(3)
Sm(1)-O(6)	2.414(2)	Sm(1)-O(6W)	2.446(3)
O(2)#1-Sm(1)-O(1)	100.32(9)	O(2)#1-Sm(1)-O(4W)	94.92(12)
O(1)-Sm(1)-O(4W)	73.15(10)	O(2)#1-Sm(1)-O(6)	132.78(9)
O(1)-Sm(1)-O(6)	120.32(8)	O(4W)-Sm(1)-O(6)	76.74(10)
O(2)#1-Sm(1)-O(5W)	86.14(10)	O(1)-Sm(1)-O(5W)	142.02(11)
O(4W)-Sm(1)-O(5W)	144.11(11)	O(6)-Sm(1)-O(5W)	76.47(9)
O(2)#1-Sm(1)-O(6W)	76.80(10)	O(1)-Sm(1)-O(6W)	73.92(10)
O(4W)-Sm(1)-O(6W)	143.88(11)	O(6)-Sm(1)-O(6W)	134.10(10)
O(5W)-Sm(1)-O(6W)	71.26(11)	O(2)#1-Sm(1)-O(3W)	155.53(10)
O(1)-Sm(1)-O(3W)	75.38(9)	O(4W)-Sm(1)-O(3W)	106.45(11)
O(6)-Sm(1)-O(3W)	65.61(9)	O(5W)-Sm(1)-O(3W)	83.45(11)
O(6W)-Sm(1)-O(3W)	78.89(10)	O(2)#1-Sm(1)-O(5)	81.87(8)
O(1)-Sm(1)-O(5)	145.07(9)	O(4W)-Sm(1)-O(5)	71.94(10)

O(6)-Sm(1)-O(5)	51.16(8)	O(5W)-Sm(1)-O(5)	72.72(10)
O(6W)-Sm(1)-O(5)	138.98(10)	O(3W)-Sm(1)-O(5)	115.69(8)
Complex 6[(e)]			
Er(1)-O(10)#1	2.2293(12)	Er(1)-O(3W)	2.2891(14)
Er(1)-O(9)	2.298(3)	Er(1)-O(5W)	2.3406(13)
Er(1)-O(8)	2.341(3)	Er(1)-O(4W)	2.3732(12)
Er(1)-O(6W)	2.3914(15)	Er(1)-O(7)	2.603(3)
O(10)#1-Er(1)-O(3W)	92.12(4)	O(10)#1-Er(1)-O(9)	95.72(8)
O(3W)-Er(1)-O(9)	72.77(8)	O(10)#1-Er(1)-O(5W)	88.40(4)
O(3W)-Er(1)-O(5W)	144.24(5)	O(9)-Er(1)-O(5W)	142.74(8)
O(10)#1-Er(1)-O(8)	132.88(7)	O(3W)-Er(1)-O(8)	76.78(8)
O(9)-Er(1)-O(8)	122.83(10)	O(5W)-Er(1)-O(8)	76.86(8)
O(10)#1-Er(1)-O(4W)	156.209(17)	O(3W)-Er(1)-O(4W)	106.8
O(9)-Er(1)-O(4W)	76.92(8)	O(5W)-Er(1)-O(4W)	84.5
O(8)-Er(1)-O(4W)	67.24(8)	O(10)#1-Er(1)-O(6W)	76.14(5)
O(3W)-Er(1)-O(6W)	144.10(6)	O(9)-Er(1)-O(6W)	74.79(8)
O(5W)-Er(1)-O(6W)	70.3	O(8)-Er(1)-O(6W)	135.38(8)
O(4W)-Er(1)-O(6W)	80.1	O(10)#1-Er(1)-O(7)	80.71(7)
O(3W)-Er(1)-O(7)	71.93(8)	O(9)-Er(1)-O(7)	144.34(11)
O(5W)-Er(1)-O(7)	72.89(8)	O(8)-Er(1)-O(7)	52.23(9)
O(4W)-Er(1)-O(7)	118.41(7)□	O(6W)-Er(1)-O(7)	136.63(8)

Symmetry codes: (a) #1: -*x* + 1, -*y* + 2, -*z* + 1; (b) #1: -*x* + 1, -*y* + 1, -*z* + 2; (c) #1: -*x* + 1, -*y* + 2, -*z* ; (d) #1: -*x*, -*y* + 1, -*z* + 2; (e) #1: -*x* + 1, -*y*, -*z*.

Table S2. Analysis of Cole-Cole plot of complex **2**

T (K)	χ_0 (cm^3/mol)	χ_{inf} (cm^3/mol)	α	R^2
1.8	15.659(56)	1.109(40)	0.267(7)	0.974
2.0	13.756(49)	1.035(37)	0.266(8)	0.971
2.2	12.538(45)	0.993(35)	0.265(8)	0.970
2.4	10.805(39)	0.909(32)	0.263(8)	0.967
2.7	9.496(34)	0.880(30)	0.255(9)	0.964
3.0	8.469(28)	0.881(29)	0.236(9)	0.960
3.3	7.621(20)	0.905(27)	0.201(9)	0.961

3.6	6.893(11)	0.953(23)	0.149(8)	0.972
3.8	6.461(8)	0.992(23)	0.112(7)	0.978
4.0	6.090(4)	1.019(20)	0.085(5)	0.990
4.2	5.768(3)	1.045(29)	0.068(6)	0.992
4.4	5.485(3)	1.027(40)	0.069(6)	0.994
4.6	5.219(2)	1.045(76)	0.061(8)	0.989
4.8	4.993(3)	1.198(75)	0.050(0)	0.979
5.0	4.770(1)	1.514(52)	0.032(0)	0.990

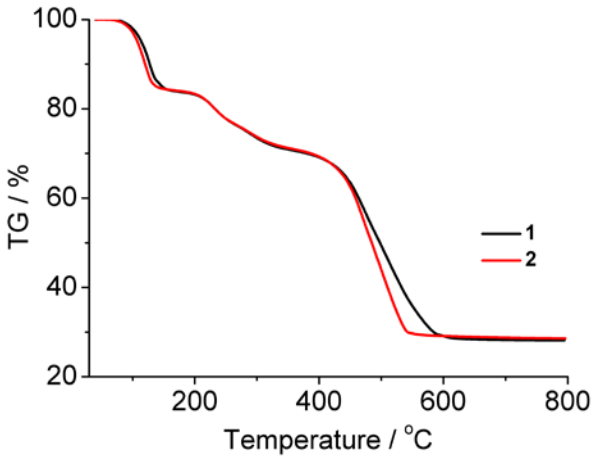

Figure S1. TGA trace of complexes **1** - **2**.

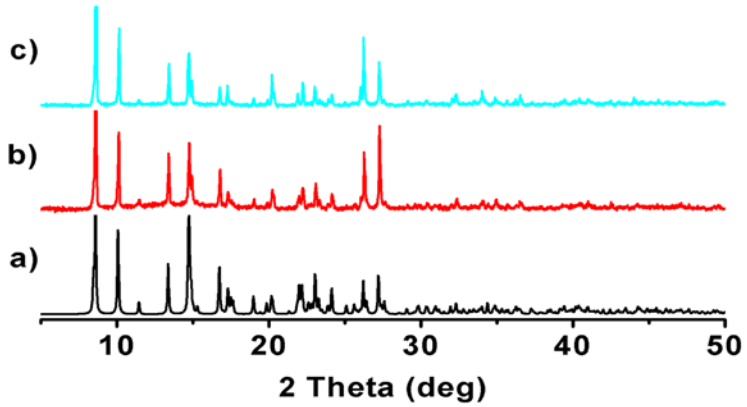

Figure S2. PXRD patterns (a) simulated based on the X-ray single crystal diffraction data of **2**, (b) for as-synthesized **1**, (c) for as-synthesized **2**.

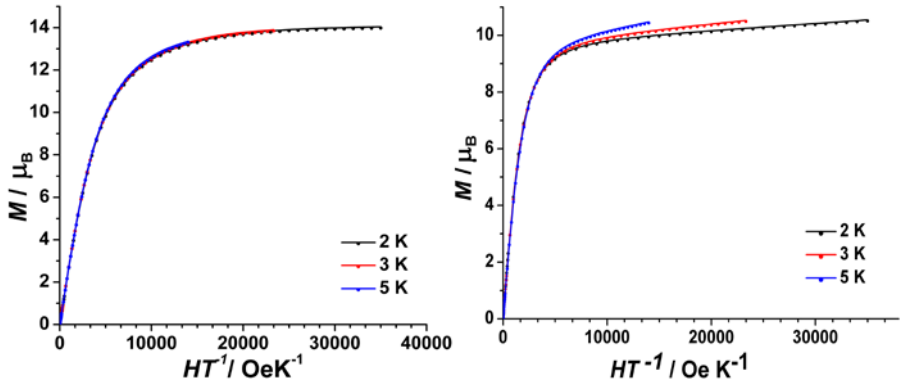

Figure S3. Plots of *M vs. H/T* measured between 2 and 5 K for complexes **1** and **2**.