Electronic Supplementary Information

Squaring the cube: A Family of Octametallic Lanthanide Complexes Including a Dy_8 Single-Molecule Magnet

Ming Fang,[a,b] Hanhua Zhao,[a] Andrey V. Prosvirin,[a] Dawid Pinkowicz,[a,c] Bin Zhao,*[,b] Peng Cheng,[b] Wolfgang Wernsdorfer[d] and Euan K. Brechin,*[,e] and Kim R. Dunbar,*[a]

[a] *Department of Chemistry, Texas A&M University, College Station, TX 77842-3012, USA*
[b] *Department of Chemistry and Key Laboratory of Advanced Energy Materials Chemistry, Ministry of Education, Nankai University, Tianjin 300071, P. R. China*
[c] *Faculty of Chemistry, Jagiellonian University, Ingardena 3, 30-060 Kraków, Poland*
[d] *Institut Néel, CNRS and Université Joseph Fournier, BP 166, 25 Avenue des Martyrs, 38042 Grenoble Cedex 9, France*
[e] *EaStChem School of Chemistry, The University of Edinburgh, West Mains Road, Edinburgh, Scotland, EH9 3JJ, UK*
** corresponding author email: dunbar@mail.chem.tamu.edu, zhaobin@nankai.edu.cn, ebrechin@staffmail.ed.ac.uk*

Electronic Supplementary Information Table of Contents:

Figure S1a. Asymmetric unit (top) and packing diagrams along *c* (middle) and *a* (bottom) crystallographic directions for compound **6**. Dy_8 units highlighted in green.

Figure S1b. Coordination mode of the Sao^{2-} ligand in **1 – 8**.

Table S1. Selected bond distances (Å) and angles (deg) for **1 – 8**.

Table S2. Selected parameters obtained by fitting Cole-Cole plots of **6** with the Debye model.

Figure S2. Sweep rate dependence of the magnetic hysteresis in compound **6** (microSQUID data) at 0.5 K (top) and 30 mK (bottom).

Figure S2. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 1000 Oe.

Figure S3. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 2000 Oe.

Figure S4. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 3000 Oe.

Figure S5. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 4000 Oe

Figure S1a. Asymmetric unit with labeling scheme (top) and packing diagrams along *c* (middle) and *a* (bottom) directions for compound **6**. Dy_8 units highlighted in green.

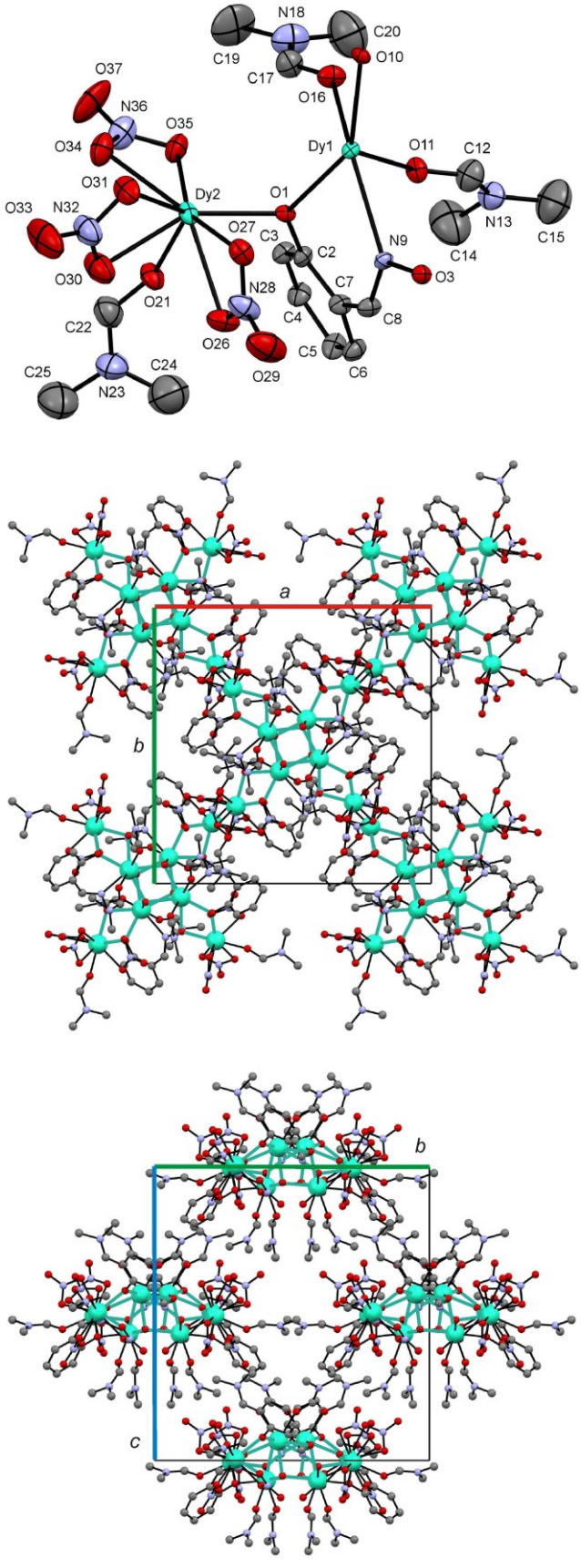

Figure S1b. Coordination mode of the Sao^{2-} ligand in **6** (**1-8** is exacly the same).

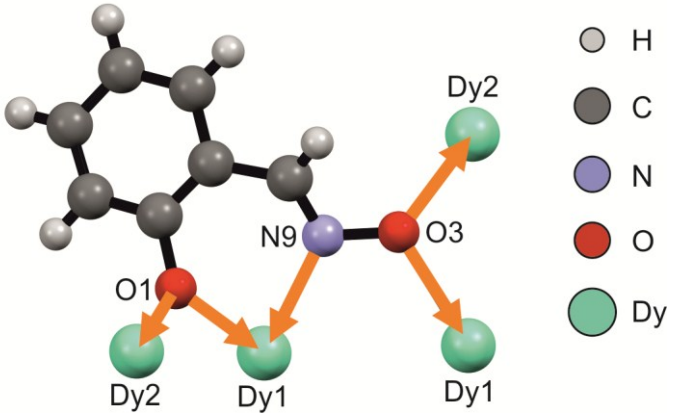

Table S1. Selected bond distances (Å) and angles (deg) for **1 – 8**.

1					
Nd(1)-O(1)	2.379(5)	O(1)-Nd(1)-O(11)	85.3(2	O(11)-Nd(1)-O(10)#1	116.8(2)
Nd(1)-O(11)	2.408(8)	O(1)-Nd(1)-O(10)#1	146.73(17)	O(11)-Nd(1)-O(16)	72.2(3)
Nd(1)-O(10)#1	2.421(5)	O(1)-Nd(1)-O(16)	88.3(3)	O(11)-Nd(1)-O(10)	76.9(2)
Nd(1)-O(16)	2.442(10)	O(1)-Nd(1)-O(10)	142.28(17)	O(11)-Nd(1)-O(10)#2	141.6(2)
Nd(1)-O(10)	2.450(5)	O(1)-Nd(1)-O(10)#2	106.91(18)	O(11)-Nd(1)-O(26)	141.2(2)
Nd(1)-O(10)#2	2.450(5)	O(1)-Nd(1)-O(26)	67.51(17)	O(11)-Nd(1)-N(9)	76.4(3)
Nd(1)-O(26)	2.476(5)	O(1)-Nd(1)-N(9)	69.80(19)		
Nd(1)-N(9)	2.650(6)				
Nd(2)-O(1)	2.370(6)	O(1)-Nd(2)-O(21)	91.3(3)	O(21)-Nd(2)-O(26)	150.8(3)
Nd(2)-O(21)	2.400(11)	O(1)-Nd(2)-O(26)	68.78(18)	O(21)-Nd(2)-O(32)	72.1(4)
Nd(2)-O(26)	2.408(5)	O(1)-Nd(2)-O(32)	151.7(3)	O(21)-Nd(2)-O(38)	74.6(4)
Nd(2)-O(32)	2.540(11)	O(1)-Nd(2)-O(38)	78.5(3)	O(21)-Nd(2)-O(28)	123.4(3)
Nd(2)-O(38)	2.548(10)	O(1)-Nd(2)-O(28)	80.5(2)	O(21)-Nd(2)-O(33)	121.4(4)
Nd(2)-O(28)	2.562(7)	O(1)-Nd(2)-O(33)	144.8(3)	O(21)-Nd(2)-O(36)	86.4(4)
Nd(2)-O(33)	2.544(11)	O(1)-Nd(2)-O(36)	126.8(3)	O(21)-Nd(2)-O(29)	74.5(3)
Nd(2)-O(36)	2.554(10)	O(1)-Nd(2)-O(29)	78.6(3)		
Nd(2)-O(29)	2.568(9)	Nd(1)-O(10)-Nd(1)#3	104.62(19)		
Nd(1)-Nd(1)#2	3.8775(7)	Nd(1)#2-Nd(1)-Nd(1)#3	59.516(6)	Nd(1)#3-Nd(1)-Nd(2)	114.751(18)
Nd(1)-Nd(1)#3	3.8775(7)	Nd(1)#2-Nd(1)-Nd(1)#1	59.513(6)	Nd(1)#1-Nd(1)-Nd(2)	150.423(13)
Nd(1)-Nd(1)#1	3.9341(9)	Nd(1)#3-Nd(1)-Nd(1)#1	59.516(6)	Nd(1)#1-O(10)-Nd(1)	107.74(18)
Nd(1)-Nd(2)	3.9436(8)	Nd(1)#2-Nd(1)-Nd(2)	91.723(14)	Nd(1)#1-O(10)-Nd(1)#3	105.52(19)
2					
Sm(1)-O(10)	2.347(6)	O(10)-Sm(1)-O(15)	84.3(3)	O(15)-Sm(1)-O(38)	118.4(3)
Sm(1)-O(15)	2.387(15)	O(10)-Sm(1)-O(38)	145.3(2)	O(15)-Sm(1)-O(38)#1	141.2(3)
Sm(1)-O(38)	2.400(6)	O(10)-Sm(1)-O(38)#1	107.5(2)	O(15)-Sm(1)-O(25)	72.6(4)
Sm(1)-O(38)#1	2.414(6)	O(10)-Sm(1)-O(25)	87.6(3)	O(15)-Sm(1)-O(38)#2	77.2(3)
Sm(1)-O(25)	2.415(10)	O(10)-Sm(1)-O(38)#2	143.4(2)	O(15)-Sm(1)-O(9)	140.8(3)
Sm(1)-O(38)#2	2.431(6)	O(10)-Sm(1)-O(9)	67.1(2)	O(15)-Sm(1)-N(8)#1	75.6(3)
Sm(1)-O(9)	2.467(6)	O(10)-Sm(1)-N(8)#1	70.8(2)		
Sm(1)-N(8)#1	2.617(8)				

Sm(2)-O(10)	2.330(7)	O(10)-Sm(2)-O(20)	92.0(3)	O(20)-Sm(2)-O(9)	150.6(3)
Sm(2)-O(20)	2.384(11)	O(10)-Sm(2)-O(9)	68.8(2)	O(20)-Sm(2)-O(31)	72.0(4)
Sm(2)-O(9)	2.380(6)	O(10)-Sm(2)-O(31)	152.0(3)	O(20)-Sm(2)-O(28)	84.4(4)
Sm(2)-O(31)	2.505(12)	O(10)-Sm(2)-O(28)	126.0(3)	O(20)-Sm(2)-O(34)	123.8(4)
Sm(2)-O(28)	2.509(11)	O(10)-Sm(2)-O(34)	81.2(3)	O(20)-Sm(2)-O(27)	73.7(4)
Sm(2)-O(34)	2.525(10)	O(10)-Sm(2)-O(27)	78.1(3)	O(20)-Sm(2)-O(35)	74.5(4)
Sm(2)-O(27)	2.529(11)	O(10)-Sm(2)-O(35)	80.2(3)	O(20)-Sm(2)-O(30)	121.4(4)
Sm(2)-O(35)	2.534(10)	O(10)-Sm(2)-O(30)	144.6(3)		
Sm(2)-O(30)	2.523(12)	Sm(1)#3-O(38)-Sm(1)#2	104.7(2)		
Sm(1)-Sm(1)#1	3.8311(9)	Sm(1)#1-Sm(1)-Sm(1)#3	60.957(16)	Sm(1)#3-Sm(1)-Sm(2)	91.747(17)
Sm(1)-Sm(1)#3	3.8311(9)	Sm(1)#1-Sm(1)-Sm(1)#2	59.521(8)	Sm(1)#2-Sm(1)-Sm(2)	150.351(16)
Sm(1)-Sm(1)#2	3.8865(10)	Sm(1)#3-Sm(1)-Sm(1)#2	59.521(8)	Sm(1)-O(38)-Sm(1)#3	105.5(2)
Sm(1)-Sm(2)	3.8948(8)	Sm(1)#1-Sm(1)-Sm(2)	115.14(2)	Sm(1)-O(38)-Sm(1)#2	107.1(2)
3					
Eu(2)-O(1)	2.338(6)	O(1)-Eu(2)-O(11)	84.2(2)	O(11)-Eu(2)-O(10)#1	118.1(3)
Eu(2)-O(11)	2.376(9)	O(1)-Eu(2)-O(10)#1	145.5(2)	O(11)-Eu(2)-O(10)#2	141.5(3)
Eu(2)-O(10)#1	2.386(6)	O(1)-Eu(2)-O(10)#2	107.8(2)	O(11)-Eu(2)-O(16)	72.5(4)
Eu(2)-O(10)#2	2.400(6)	O(1)-Eu(2)-O(16)	87.6(3)	O(11)-Eu(2)-O(10)	77.3(3)
Eu(2)-O(16)	2.399(10)	O(1)-Eu(2)-O(10)	143.4(2)	O(11)-Eu(2)-O(2)	140.7(3)
Eu(2)-O(10)	2.410(6)	O(1)-Eu(2)-O(2)	66.9(2)	O(11)-Eu(2)-N(9)#3	75.5(3)
Eu(2)-O(2)	2.451(7)	O(1)-Eu(2)-N(9)#3	70.7(2)		
Eu(2)-N(9)#3	2.594(8)				
Eu(1)-O(1)	2.321(7)	O(1)-Eu(1)-O(2)	68.6(2)	O(2)-Eu(1)-O(21)	150.0(3)
Eu(1)-O(2)	2.366(7)	O(1)-Eu(1)-O(21)	91.7(3)	O(2)-Eu(1)-O(30)	90.2(3)
Eu(1)-O(21)	2.375(11)	O(1)-Eu(1)-O(30)	126.3(3)	O(2)-Eu(1)-O(31)	81.0(3)
Eu(1)-O(30)	2.474(11)	O(1)-Eu(1)-O(31)	77.7(3)	O(2)-Eu(1)-O(26)	134.3(3)
Eu(1)-O(31)	2.504(11)	O(1)-Eu(1)-O(26)	152.1(3)	O(2)-Eu(1)-O(27)	83.3(3)
Eu(1)-O(26)	2.507(12)	O(1)-Eu(1)-O(27)	144.3(3)	O(2)-Eu(1)-O(34)	76.9(3)
Eu(1)-O(27)	2.505(13)	O(1)-Eu(1)-O(34)	81.8(3)	O(2)-Eu(1)-O(35)	120.6(3)
Eu(1)-O(34)	2.509(11)	O(1)-Eu(1)-O(35)	79.4(3)		
Eu(1)-O(35)	2.515(11)	Eu(2)#3-O(10)-Eu(2)	104.6(2)		
Eu(2)-Eu(2)#3	3.8052(8)	Eu(2)#3-Eu(2)-Eu(2)#2	61.040(15)	Eu(2)#2-Eu(2)-Eu(1)	91.846(16)
Eu(2)-Eu(2)#2	3.8052(8)	Eu(2)#3-Eu(2)-Eu(2)#1	59.480(7)	Eu(2)#1-Eu(2)-Eu(1)	150.460(16)
Eu(2)-Eu(2)#1	3.8648(10)	Eu(2)#2-Eu(2)-Eu(2)#1	59.480(7)	Eu(2)#1-O(10)-Eu(2)#3	105.3(2)
Eu(2)-Eu(1)	3.8778(8)	Eu(2)#3-Eu(2)-Eu(1)	115.08(2)	Eu(2)#1-O(10)-Eu(2)	107.4(2)
4					
Gd(1)-O(1)	2.338(6)	O(1)-Gd(1)-O(34)	83.9(3)	O(34)-Gd(1)-O(28)#1	118.0(3)
Gd(1)-O(34)	2.372(8)	O(1)-Gd(1)-O(28)#1	145.4(2)	O(34)-Gd(1)-O(28)#2	141.8(3)
Gd(1)-O(28)#1	2.388(6)	O(1)-Gd(1)-O(28)#2	107.9(2)	O(34)-Gd(1)-O(29)	72.3(4)
Gd(1)-O(28)#2	2.392(6)	O(1)-Gd(1)-O(29)	87.2(3)	O(34)-Gd(1)-O(28)	77.4(3)
Gd(1)-O(29)	2.393(9)	O(1)-Gd(1)-O(28)	143.38(19)	O(34)-Gd(1)-O(10)	140.0(3)
Gd(1)-O(28)	2.411(6)	O(1)-Gd(1)-O(10)	66.3(2)	O(34)-Gd(1)-N(9)	75.6(3)
Gd(1)-O(10)	2.445(6)	O(1)-Gd(1)-N(9)	70.8(2)		
Gd(1)-N(9)	2.602(7)				
Gd(2)-O(1)	2.320(6)	O(1)-Gd(2)-O(23)	91.8(2)	O(23)-Gd(2)-O(10)	149.9(3)
Gd(2)-O(23)	2.362(7)	O(1)-Gd(2)-O(10)	68.30(19)	O(23)-Gd(2)-O(16)	72.3(3)
Gd(2)-O(10)	2.344(6)	O(1)-Gd(2)-O(16)	150.9(3)	O(23)-Gd(2)-O(12)	83.0(3)
Gd(2)-O(16)	2.484(9)	O(1)-Gd(2)-O(12)	127.4(3)	O(23)-Gd(2)-O(19)	124.3(3)
Gd(2)-O(12)	2.471(9)	O(1)-Gd(2)-O(19)	82.1(2)	O(23)-Gd(2)-O(15)	121.8(3)

Gd(2)-O(19)	2.508(8)	O(1)-Gd(2)-O(15)	144.5(3)	O(23)-Gd(2)-O(11)	72.6(3)
Gd(2)-O(15)	2.499(10)	O(1)-Gd(2)-O(11)	78.1(3)	O(23)-Gd(2)-O(20)	74.4(3)
Gd(2)-O(11)	2.501(11)	O(1)-Gd(2)-O(20)	78.5(3)		
Gd(2)-O(20)	2.548(10)	Gd(1)#3-O(28)-Gd(1)	105.2(2)		
Gd(1)-Gd(1)#2	3.7975(12)	Gd(1)#2-Gd(1)-Gd(1)#3	61.17(2)	Gd(1)#3-Gd(1)-Gd(2)	115.11(3)
Gd(1)-Gd(1)#3	3.7974(12)	Gd(1)#2-Gd(1)-Gd(1)#1	59.417(10)	Gd(1)#1-Gd(1)-Gd(2)	150.510(15)
Gd(1)-Gd(1)#1	3.8641(12)	Gd(1)#3-Gd(1)-Gd(1)#1	59.418(11)	Gd(1)#1-O(28)-Gd(1)#3	104.50(2)
Gd(1)-Gd(2)	3.8754(11)	Gd(1)#2-Gd(1)-Gd(2)	91.92(2)	Gd(1)#1-O(28)-Gd(1)	107.2(2)
5					
Tb(1)-O(1)	2.315(6)	O(1)-Tb(1)-O(14)	83.7(2)	O(14)-Tb(1)-O(3)	118.2(2)
Tb(1)-O(14)	2.340(7)	O(1)-Tb(1)-O(3)	145.0(2)	O(14)-Tb(1)-O(13)	71.6(3)
Tb(1)-O(3)	2.364(6)	O(1)-Tb(1)-O(13)	86.8(3)	O(14)-Tb(1)-O(3)#1	141.7(2)
Tb(1)-O(13)	2.366(8)	O(1)-Tb(1)-O(3)#1	108.1(2)	O(14)-Tb(1)-O(3)#2	77.4(2)
Tb(1)-O(3)#1	2.375(6)	O(1)-Tb(1)-O(3)#2	143.7(2)	O(14)-Tb(1)-O(2)	140.1(2)
Tb(1)-O(3)#2	2.393(6)	O(1)-Tb(1)-O(2)	66.7(2)	O(14)-Tb(1)-N(1)	75.9(2)
Tb(1)-O(2)	2.427(6)	O(1)-Tb(1)-N(1)	70.6(2)		
Tb(1)-N(1)	2.571(7)				
Tb(2)-O(1)	2.298(7)	O(1)-Tb(2)-O(15)	92.1(3)	O(15)-Tb(2)-O(2)	149.9(3)
Tb(2)-O(15)	2.317(11)	O(1)-Tb(2)-O(2)	68.5(2)	O(15)-Tb(2)-O(8)	72.6(4)
Tb(2)-O(2)	2.337(7)	O(1)-Tb(2)-O(8)	150.3(3)	O(15)-Tb(2)-O(4)	124.8(3)
Tb(2)-O(8)	2.441(9)	O(1)-Tb(2)-O(4)	82.6(2)	O(15)-Tb(2)-O(10)	81.8(4)
Tb(2)-O(4)	2.475(7)	O(1)-Tb(2)-O(10)	127.7(3)	O(15)-Tb(2)-O(7)	121.4(4)
Tb(2)-O(10)	2.461(9)	O(1)-Tb(2)-O(7)	144.9(3)	O(15)-Tb(2)-O(11)	73.7(3)
Tb(2)-O(7)	2.502(9)	O(1)-Tb(2)-O(11)	78.0(3)	O(15)-Tb(2)-O(5)	74.5(3)
Tb(2)-O(11)	2.499(9)	O(1)-Tb(2)-O(5)	78.0(3)		
Tb(2)-O(5)	2.531(9)	Tb(1)#3-O(3)-Tb(1)#2	104.2(2)		
Tb(1)-Tb(1)#3	3.7627(11)	Tb(1)#3-Tb(1)-Tb(1)#1	61.119(19)	Tb(1)#1-Tb(1)-Tb(2)	115.22(3)
Tb(1)-Tb(1)#1	3.7626(11)	Tb(1)#3-Tb(1)-Tb(1)#2	59.438(10)	Tb(1)#2-Tb(1)-Tb(2)	150.475(17)
Tb(1)-Tb(1)#2	3.8262(11)	Tb(1)#1-Tb(1)-Tb(1)#2	59.440(9)	Tb(1)-O(3)-Tb(1)#3	105.1(2)
Tb(1)-Tb(2)	3.8364(10)	Tb(1)#3-Tb(1)-Tb(2)	91.912(19)	Tb(1)-O(3)-Tb(1)#2	107.1(2)
6					
Dy(1)-O(1)	2.303(7)	O(1)-Dy(1)-O(11)	83.4(4)	O(11)-Dy(1)-O(10)	117.4(3)
Dy(1)-O(11)	2.330(11)	O(1)-Dy(1)-O(10)	145.1(3)	O(11)-Dy(1)-O(10)#1	142.2(3)
Dy(1)-O(10)	2.345(7)	O(1)-Dy(1)-O(10)#1	108.5(3)	O(11)-Dy(1)-O(16)	72.2(5)
Dy(1)-O(10)#1	2.367(7)	O(1)-Dy(1)-O(16)	86.6(4)	O(11)-Dy(1)-O(10)#2	77.3(4)
Dy(1)-O(16)	2.367(12)	O(1)-Dy(1)-O(10)#2	143.6(2)	O(11)-Dy(1)-O(3)	139.9(4)
Dy(1)-O(10)#2	2.384(7)	O(1)-Dy(1)-O(3)	66.5(3)	O(11)-Dy(1)-N(9)	75.8(4)
Dy(1)-O(3)	2.411(8)	O(1)-Dy(1)-N(9)	71.1(3)		
Dy(1)-N(9)	2.546(8)				
Dy(2)-O(1)	2.296(8)	O(1)-Dy(2)-O(3)	68.3(2)	O(3)-Dy(2)-O(21)	149.8(4)
Dy(2)-O(3)	2.311(8)	O(1)-Dy(2)-O(21)	91.4(4)	O(3)-Dy(2)-O(30)	134.4(4)
Dy(2)-O(21)	2.326(12)	O(1)-Dy(2)-O(30)	151.1(4)	O(3)-Dy(2)-O(34)	92.0(4)
Dy(2)-O(30)	2.426(13)	O(1)-Dy(2)-O(34)	126.9(3)	O(3)-Dy(2)-O(27)	77.5(3)
Dy(2)-O(34)	2.422(11)	O(1)-Dy(2)-O(27)	82.9(3)	O(3)-Dy(2)-O(31)	83.3(3)
Dy(2)-O(27)	2.471(9)	O(1)-Dy(2)-O(31)	144.5(3)	O(3)-Dy(2)-O(35)	81.0(3)
Dy(2)-O(31)	2.472(9)	O(1)-Dy(2)-O(35)	77.4(3)	O(3)-Dy(2)-O(26)	121.0(3)
Dy(2)-O(35)	2.480(11)	O(1)-Dy(2)-O(26)	78.5(3)		
Dy(2)-O(26)	2.522(11)	Dy(1)#3-O(10)-Dy(1)#2	103.7(2)		
Dy(1)-Dy(1)#3	3.7354(18)	Dy(1)#3-Dy(1)-Dy(1)#1	61.24(3)	Dy(1)#1-Dy(1)-Dy(2)	114.95(4)

Dy(1)-Dy(1)#1	3.7354(18)	Dy(1)#3-Dy(1)-Dy(1)#2	59.381(17)	Dy(1)#2-Dy(1)-Dy(2)	150.74(2)
Dy(1)-Dy(1)#2	3.8052(18)	Dy(1)#1-Dy(1)-Dy(1)#2	59.380(17)	Dy(1)-O(10)-Dy(1)#3	104.9(3)
Dy(1)-Dy(2)	3.8162(16)	Dy(1)#3-Dy(1)-Dy(2)	92.11(3)	Dy(1)-O(10)-Dy(1)#2	107.1(3)
7					
Ho(1)-O(1)	2.303(7)	O(1)-Ho(1)-O(33)	83.4(4)	O(33)-Ho(1)-O(38)#1	142.3(4)
Ho(1)-O(33)	2.313(11)	O(1)-Ho(1)-O(38)#1	109.2(3)	O(33)-Ho(1)-O(38)#2	117.7(4)
Ho(1)-O(38)#1	2.334(8)	O(1)-Ho(1)-O(38)#2	145.1(3)	O(33)-Ho(1)-O(28)	72.1(5)
Ho(1)-O(38)#2	2.338(8)	O(1)-Ho(1)-O(28)	86.3(4)	O(33)-Ho(1)-O(38)	77.9(4)
Ho(1)-O(28)	2.364(13)	O(1)-Ho(1)-O(38)	144.0(3)	O(33)-Ho(1)-O(10)	139.7(4)
Ho(1)-O(38)	2.372(8)	O(1)-Ho(1)-O(10)	66.2(3)	O(33)-Ho(1)-N(9)	76.2(4)
Ho(1)-O(10)	2.397(8)	O(1)-Ho(1)-N(9)	71.2(3)		
Ho(1)-N(9)	2.555(10)				
Ho(2)-O(1)	2.281(8)	O(1)-Ho(2)-O(23)	91.8(4)	O(23)-Ho(2)-O(10)	149.6(5)
Ho(2)-O(23)	2.306(12)	O(1)-Ho(2)-O(10)	68.1(3)	O(23)-Ho(2)-O(16)	73.7(5)
Ho(2)-O(10)	2.303(8)	O(1)-Ho(2)-O(16)	150.0(4)	O(23)-Ho(2)-O(11)	124.4(5)
Ho(2)-O(16)	2.431(13)	O(1)-Ho(2)-O(11)	83.3(3)	O(23)-Ho(2)-O(20)	81.8(5)
Ho(2)-O(11)	2.451(11)	O(1)-Ho(2)-O(20)	127.0(4)	O(23)-Ho(2)-O(19)	72.0(5)
Ho(2)-O(20)	2.447(13)	O(1)-Ho(2)-O(19)	77.3(3)	O(23)-Ho(2)-O(15)	123.2(5)
Ho(2)-O(19)	2.460(12)	O(1)-Ho(2)-O(15)	143.5(4)	O(23)-Ho(2)-O(12)	73.8(5)
Ho(2)-O(15)	2.473(10)	O(1)-Ho(2)-O(12)	78.0(4)		
Ho(2)-O(12)	2.521(11)	Ho(1)#3-O(38)-Ho(1)	104.5(3)		
Ho(1)-Ho(1)#3	3.7215(9)	Ho(1)#3-Ho(1)-Ho(1)#2	59.340(9)	Ho(1)#2-Ho(1)-Ho(2)	150.924(19)
Ho(1)-Ho(1)#2	3.7956(10)	Ho(1)#3-Ho(1)-Ho(1)#1	59.340(9)	Ho(1)#1-Ho(1)-Ho(2)	92.337(19)
Ho(1)-Ho(1)#1	3.7215(9)	Ho(1)#2-Ho(1)-Ho(1)#1	59.341(9)	Ho(1)#2-O(38)-Ho(1)#3	105.5(3)
Ho(1)-Ho(2)	3.8058(8)	Ho(1)#3-Ho(1)-Ho(2)	115.13(2)	Ho(1)#2-O(38)-Ho(1)	107.4(3)
8					
Er(1)-O(3)	2.308(7)	O(3)-Er(1)-O(14)	83.8(4)	O(14)-Er(1)-O(13)	117.0(3)
Er(1)-O(14)	2.336(11)	O(3)-Er(1)-O(13)	145.2(2)	O(14)-Er(1)-O(13)#1	142.8(3)
Er(1)-O(13)	2.336(7)	O(3)-Er(1)-O(13)#1	108.8(2)	O(14)-Er(1)-O(19)	71.9(5)
Er(1)-O(13)#1	2.337(7)	O(3)-Er(1)-O(19)	86.2(4)	O(14)-Er(1)-O(13)#2	77.5(3)
Er(1)-O(19)	2.354(13)	O(3)-Er(1)-O(13)#2	143.7(2)	O(14)-Er(1)-O(12)	139.9(3)
Er(1)-O(13)#2	2.356(7)	O(3)-Er(1)-O(12)	66.3(2)	O(14)-Er(1)-N(11)	76.4(4)
Er(1)-O(12)	2.383(7)	O(3)-Er(1)-N(11)	71.1(3)		
Er(1)-N(11)	2.524(9)				
Er(2)-O(3)	2.260(7)	O(3)-Er(2)-O(24)	91.0(4)	O(24)-Er(2)-O(12)	148.8(4)
Er(2)-O(24)	2.295(14)	O(3)-Er(2)-O(12)	68.3(3)	O(24)-Er(2)-O(38)	80.8(5)
Er(2)-O(12)	2.309(8)	O(3)-Er(2)-O(38)	126.9(4)	O(24)-Er(2)-O(34)	74.5(5)
Er(2)-O(38)	2.397(11)	O(3)-Er(2)-O(34)	149.9(4)	O(24)-Er(2)-O(40)	71.6(5)
Er(2)-O(34)	2.419(14)	O(3)-Er(2)-O(40)	77.6(3)	O(24)-Er(2)-O(31)	124.5(5)
Er(2)-O(40)	2.459(11)	O(3)-Er(2)-O(31)	83.9(3)	O(24)-Er(2)-O(35)	123.5(5)
Er(2)-O(31)	2.467(9)	O(3)-Er(2)-O(35)	144.2(4)	O(24)-Er(2)-O(30)	73.7(5)
Er(2)-O(35)	2.471(14)	O(3)-Er(2)-O(30)	77.9(4)		
Er(2)-O(30)	2.480(11)	Er(1)#3-O(13)-Er(1)#2	104.3(3)		
Er(1)-Er(1)#3	3.7066(10)	Er(1)#3-Er(1)-Er(1)#1	61.255(19)	Er(1)#1-Er(1)-Er(2)	114.89(3)
Er(1)-Er(1)#1	3.7067(10)	Er(1)#3-Er(1)-Er(1)#2	59.372(9)	Er(1)#2-Er(1)-Er(2)	151.06(2)
Er(1)-Er(1)#2	3.7769(12)	Er(1)#1-Er(1)-Er(1)#2	59.371(9)	Er(1)-O(13)-Er(1)#3	105.0(3)
Er(1)-Er(2)	3.7914(10)	Er(1)#3-Er(1)-Er(2)	92.39(2)	Er(1)-O(13)-Er(1)#2	107.2(3)

Table S2. Selected parameters obtained by fitting Cole-Cole plots for **6** with the Debye model.

T / K	τ / s	α
1.8	0.003371	0.226
1.9	0.003829	0.230
2.0	0.004406	0.235
2.1	0.005048	0.240

Figure S2. Sweep rate dependence of the magnetic hysteresis in compound **6** (microSQUID data) at 0.5 K (top) and 30 mK (bottom).

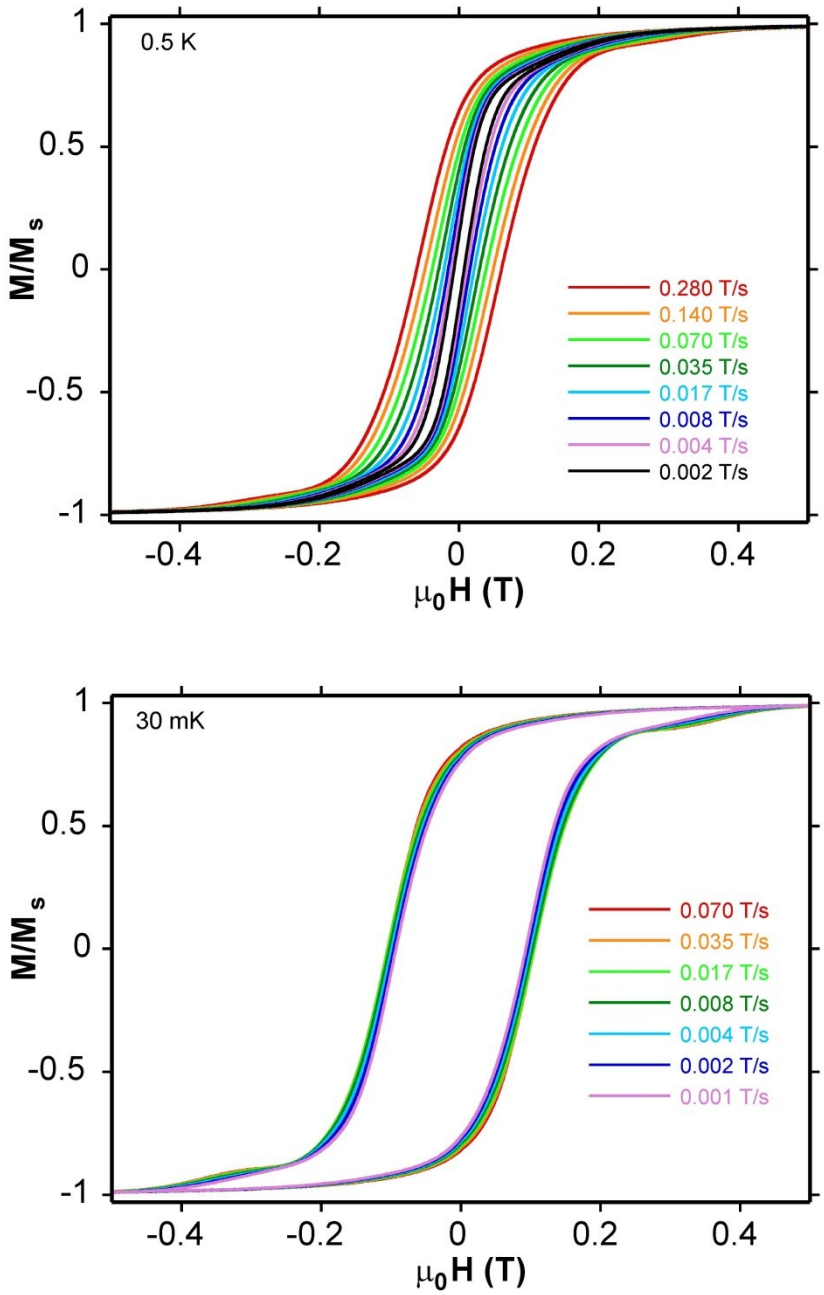

Figure S3. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 1000 Oe.

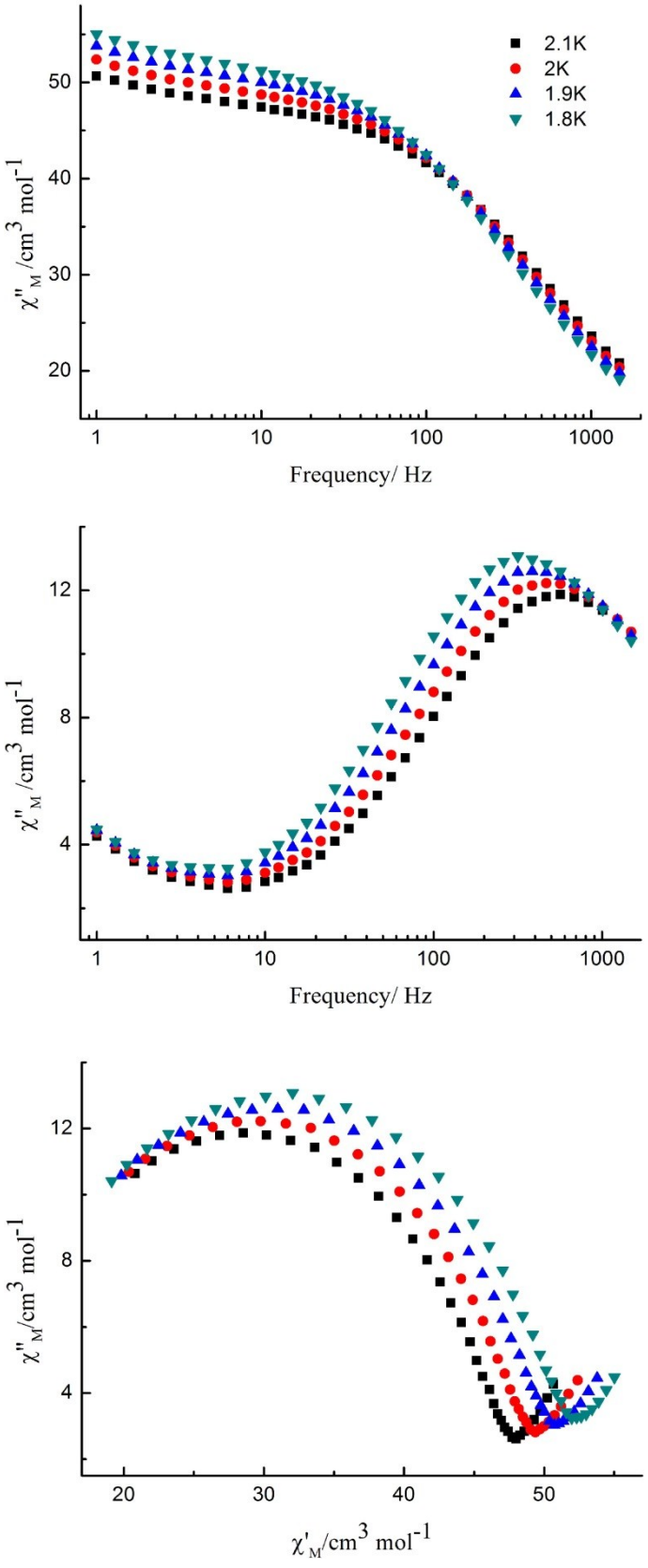

Figure S4. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 2000 Oe.

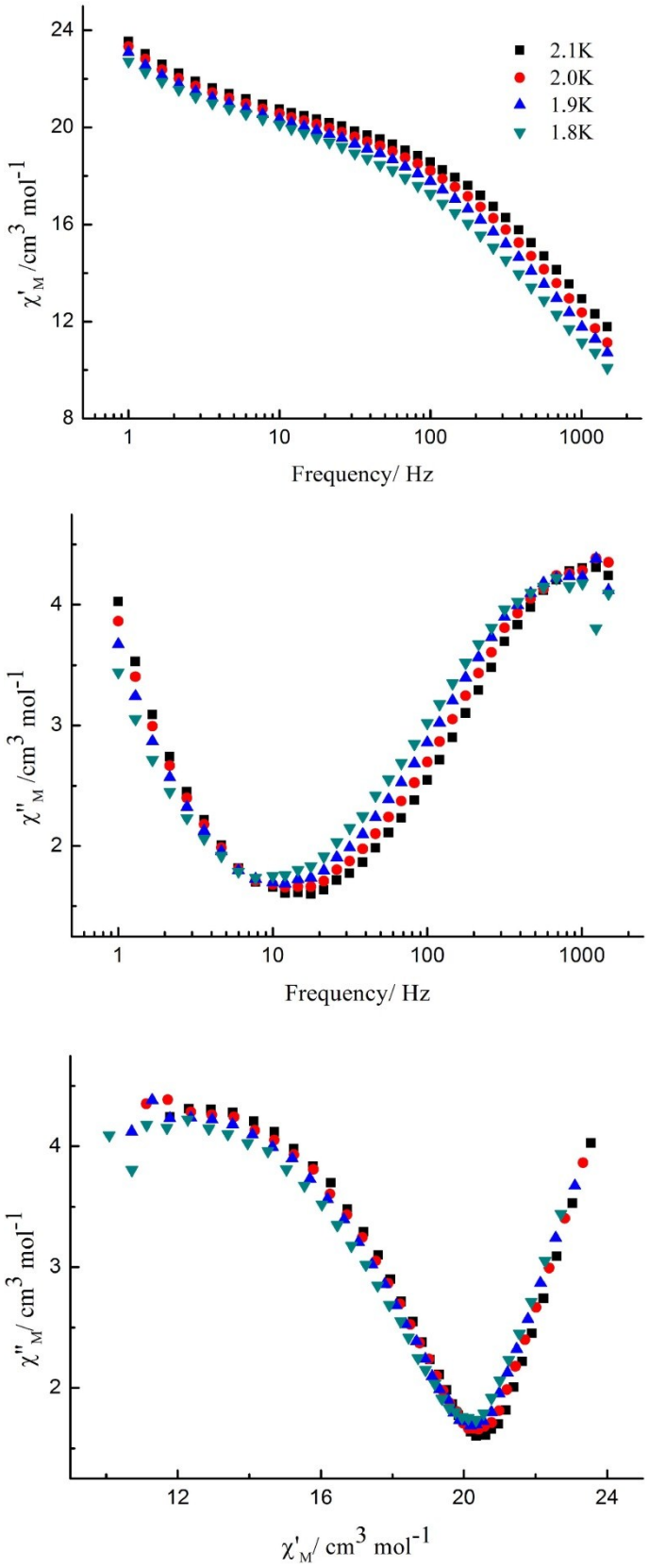

Figure S5. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 3000 Oe.

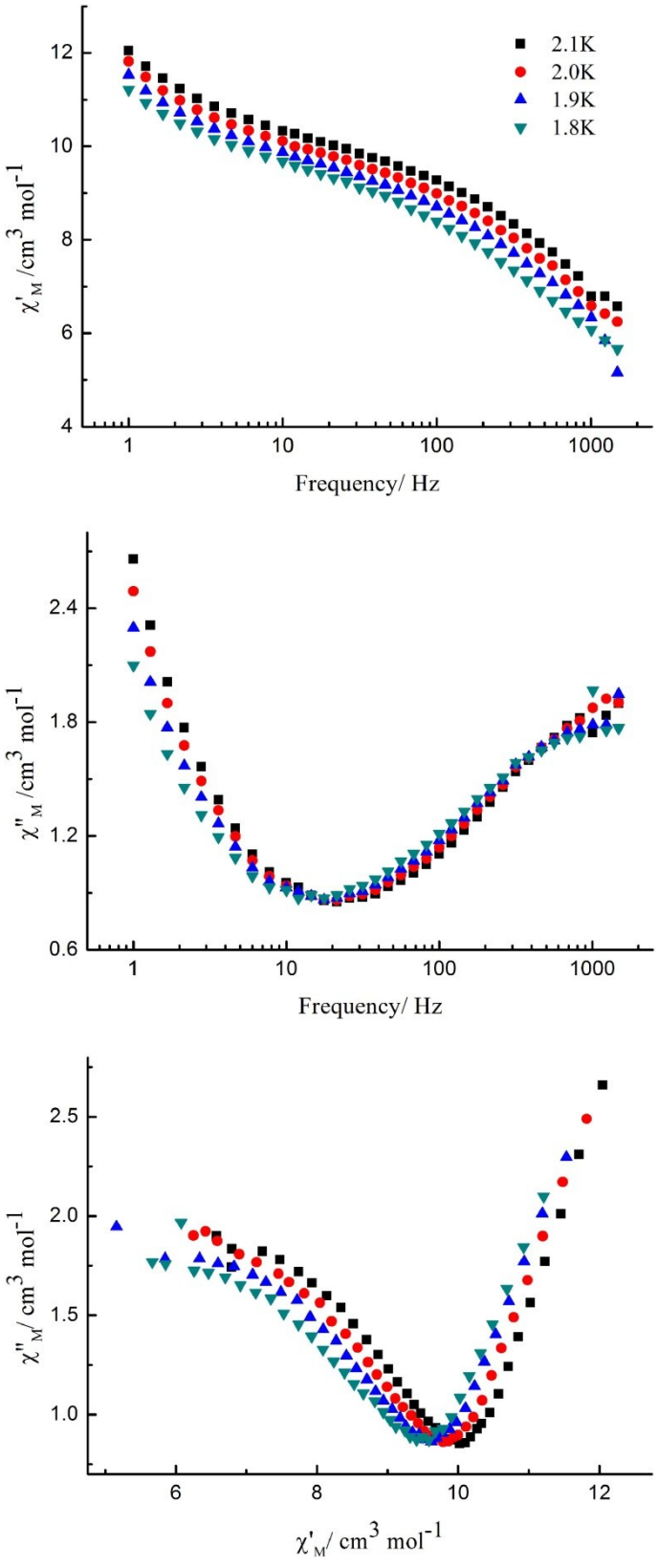

Figure S6. Frequency dependence of the in-phase χ' (top) and out-of-phase χ'' (middle) *ac* susceptibilities and Cole-Cole plots (bottom) for **6** in H_{dc}= 4000 Oe.