

Electronic Supplementary Materials (ESI) for RSC Advances
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Electronic Supplementary Information (ESI)

A simple route to 1D ferromagnetic Dy-containing compound showing magnetic relaxation behaviour

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Synthesis of [Dy(4-NBz)₃](H₂O) (**3**)

It was described that complex **3** could be synthesized from potentially explosive Dy(ClO₄)₃·6H₂O instead of Dy(NO₃)₃·6H₂O or DyCl₃·6H₂O with 4-NBz in the absence of any additives (*Inorg. Chem. Commun.*, 2011, **14**, 778-780). Here a simple improved method was applied to produce complex **3** under hydrothermal conditions from non-explosive and easily available materials, Dy(NO₃)₃·6H₂O, by finely tuning the acidity of the reaction mixture with alkalescent triethylamine. A mixture of Dy(NO₃)₃·6H₂O (0.1142 g, 0.25 mmol), 4-NBz (0.0835 g, 0.5 mmol), TEA (triethylamine, 0.1 mL), and H₂O (10 mL) was added in a 25 mL capacity stainless-steel reactor lined with Teflon and heated at 150 °C for 3 days, and then cooled to room temperature overnight. Pale yellow block-shaped crystals of **3** were isolated from the yellow mother liquid. The yield (0.0505 g) was about 29.8% based on Dy^{III} ion. The single-crystal X-ray diffraction analysis reveals that the structure of **3** obtained from Dy(NO₃)₃·6H₂O is the same as that from Dy(ClO₄)₃·6H₂O. Anal. (%) Calcd for C₂₁H₁₄N₃O₁₃Dy: C, 37.16; H, 2.08; N, 6.19. Found: C, 36.92; H, 2.20; N, 6.12. IR (cm⁻¹, KBr pellet): 3603 (s), 3496 (s), 3110 (w), 1662 (m), 1609 (s), 1567 (vs), 1526 (vs), 1429 (vs), 1348 (vs), 1316 (s), 1107 (m), 1014 (w), 878 (m), 844 (m), 796 (s), 727 (s), 516 (m).

Table S1 Selected bond lengths (Å) and angles (°) for **1**

Y(1)-O(1)	2.336(2)	Y(1)-O(2)#1	2.278(2)
Y(1)-O(3)	2.285(2)	Y(1)-O(4)#2	2.377(2)
Y(1)-O(5)	2.369(2)	Y(1)-O(6)#2	2.296(2)
Y(1)-O(7)	2.432(2)	Y(1)-O(8)	2.496(2)
O(1)-Y(1)-O(4)#2	139.94(6)	O(1)-Y(1)-O(5)	142.52(6)
O(1)-Y(1)-O(7)	73.18(7)	O(1)-Y(1)-O(8)	72.64(7)
O(2)#1-Y(1)-O(1)	100.06(6)	O(2)#1-Y(1)-O(3)	144.31(7)
O(2)#1-Y(1)-O(4)#2	79.31(6)	O(2)#1-Y(1)-O(5)	79.03(6)
O(2)#1-Y(1)-O(6)#2	142.12(6)	O(2)#1-Y(1)-O(7)	72.95(6)
O(2)#1-Y(1)-O(8)	71.41(7)	O(3)-Y(1)-O(1)	81.91(6)
O(3)-Y(1)-O(4)#2	121.59(6)	O(3)-Y(1)-O(5)	78.45(6)
O(3)-Y(1)-O(6)#2	73.42(6)	O(3)-Y(1)-O(7)	73.66(6)
O(3)-Y(1)-O(8)	140.44(7)	O(4)#2-Y(1)-O(7)	140.79(7)
O(4)#2-Y(1)-O(8)	69.27(6)	O(5)-Y(1)-O(4)#2	77.22(6)
O(5)-Y(1)-O(7)	70.79(6)	O(5)-Y(1)-O(8)	138.48(6)
O(6)#2-Y(1)-O(1)	77.89(6)	O(6)#2-Y(1)-O(4)#2	79.03(6)
O(6)#2-Y(1)-O(5)	125.18(6)	O(6)#2-Y(1)-O(7)	138.55(6)
O(6)#2-Y(1)-O(8)	71.98(6)	O(7)-Y(1)-O(8)	124.32(6)

Symmetry codes: #1 -x, -y, -z, #2 -x+1, -y, -z

Table S2 Hydrogen bonding geometry for **1**: lengths (Å) and angles (°)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(71)...O(16)#3	0.924(18)	2.29(3)	3.090(3)	145(3)
O(7)-H(72)...O(8)#1	0.912(17)	1.91(2)	2.799(3)	165(3)
O(8)-H(81)...O(15)#4	0.913(17)	2.18(3)	2.956(3)	143(3)
O(8)-H(82)...O(9)	0.949(18)	1.92(3)	2.782(4)	150(4)
O(9)-H(92)...O(18)#5	0.97(2)	2.48(6)	3.187(4)	129(6)
O(9)-H(92)...O(20)#6	0.97(2)	2.60(6)	3.326(5)	132(6)

Symmetry codes: #1 -x, -y, -z, #2 -x+1, -y, -z, #3 -x+1, -y+1, -z, #4 x, y-1, z, #5 x, y, z+1, #6 x-1, y, z+1.

Table S3 Selected bond lengths (Å) and angles (°) for **2**

Dy(1)-O(1)	2.350(2)	Dy(1)-O(2)#1	2.292(2)
Dy(1)-O(3)	2.301(2)	Dy(1)-O(4)#2	2.387(2)
Dy(1)-O(5)	2.382(2)	Dy(1)-O(6)#2	2.311(2)
Dy(1)-O(7)	2.438(3)	Dy(1)-O(8)	2.512(3)
O(1)-Dy(1)-O(4)#2	139.92(9)	O(1)-Dy(1)-O(5)	141.95(9)
O(1)-Dy(1)-O(7)	72.81(9)	O(1)-Dy(1)-O(8)	72.86(9)
O(2)#1-Dy(1)-O(1)	99.95(9)	O(2)#1-Dy(1)-O(3)	144.12(9)
O(2)#1-Dy(1)-O(4)#2	79.12(9)	O(2)#1-Dy(1)-O(5)	78.83(9)
O(2)#1-Dy(1)-O(6)#2	142.20(9)	O(2)#1-Dy(1)-O(7)	72.72(9)
O(2)#1-Dy(1)-O(8)	71.50(9)	O(3)-Dy(1)-O(1)	81.98(9)
O(3)-Dy(1)-O(4)#2	121.90(8)	O(3)-Dy(1)-O(5)	78.28(8)
O(3)-Dy(1)-O(6)#2	73.52(9)	O(3)-Dy(1)-O(7)	73.78(9)
O(3)-Dy(1)-O(8)	140.60(9)	O(4)#2-Dy(1)-O(7)	140.82(9)
O(4)#2-Dy(1)-O(8)	68.90(8)	O(5)-Dy(1)-O(4)#2	77.74(9)
O(5)-Dy(1)-O(7)	70.58(9)	O(5)-Dy(1)-O(8)	138.57(8)
O(6)#2-Dy(1)-O(1)	77.73(9)	O(6)#2-Dy(1)-O(4)#2	79.42(9)
O(6)#2-Dy(1)-O(5)	125.82(8)	O(6)#2-Dy(1)-O(7)	138.35(8)
O(6)#2-Dy(1)-O(8)	71.85(9)	O(7)-Dy(1)-O(8)	124.15(9)

Symmetry codes: #1 -x, -y, -z, #2 -x+1, -y, -z

Table S4 Hydrogen bonding geometry for **2**: lengths (Å) and angles (°)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(7)-H(71)...O(9)#1	0.941(19)	2.61(4)	3.205(5)	121(3)
O(7)-H(71)...O(16)#3	0.941(19)	2.32(3)	3.092(4)	139(4)
O(7)-H(72)...O(2)	0.940(19)	2.60(4)	3.180(4)	120(3)
O(7)-H(72)...O(8)#1	0.940(19)	1.88(2)	2.796(4)	163(4)
O(8)-H(81)...O(15)#4	0.942(19)	2.17(3)	2.956(4)	140(4)
O(8)-H(82)...O(9)	0.950(19)	1.83(3)	2.760(6)	165(6)
O(9)-H(92)...O(18)#5	0.96(2)	2.49(6)	3.194(6)	131(6)
O(9)-H(92)...O(20)#6	0.96(2)	2.61(5)	3.321(8)	132(6)

Symmetry codes: #1 -x, -y, -z, #2 -x+1, -y, -z, #3 -x+1, -y+1, -z, #4 x, y-1, z, #5 x, y, z+1, #6 x-1, y, z+1.

Table S5 δ ($^\circ$) and φ ($^\circ$) values for **2** and **3**^a

	2		3		DD	BTP	SAP
δ_1	O5-[O3-O4#2]-O6#2	3.87	O1-[O2-O7]-O6#5	5.71	29.5	0.0	0.0
δ_2	O7-[O1-O2#1]-O8	17.34	O2#5-[O3-O5]-O4#1	2.75	29.5	21.8	0.0
δ_3	O6#2-[O1-O3]-O7	44.68	O1-[O4#1-O7]-O3	51.97	29.5	48.2	52.4
δ_4	O5-[O2#1-O4#2]-O8	44.39	O6#5-[O2#5-O2]-O5	54.75	29.5	48.2	52.4
φ_1	O3-O6#2-O8-O2#1	23.40	O7-O2#5-O1-O5	37.38	0.0	14.1	24.5
φ_2	O1-O7-O5-O4#2	27.22	O2-O4#1-O6#5-O3	23.32	0.0	14.1	24.5

^a The meaning of the dihedral angles δ (A[BC]D) and φ (A-B-C-D) is the same as defined in *Cryst. Eng. Comm.*, 2014, **16**, 585-590.

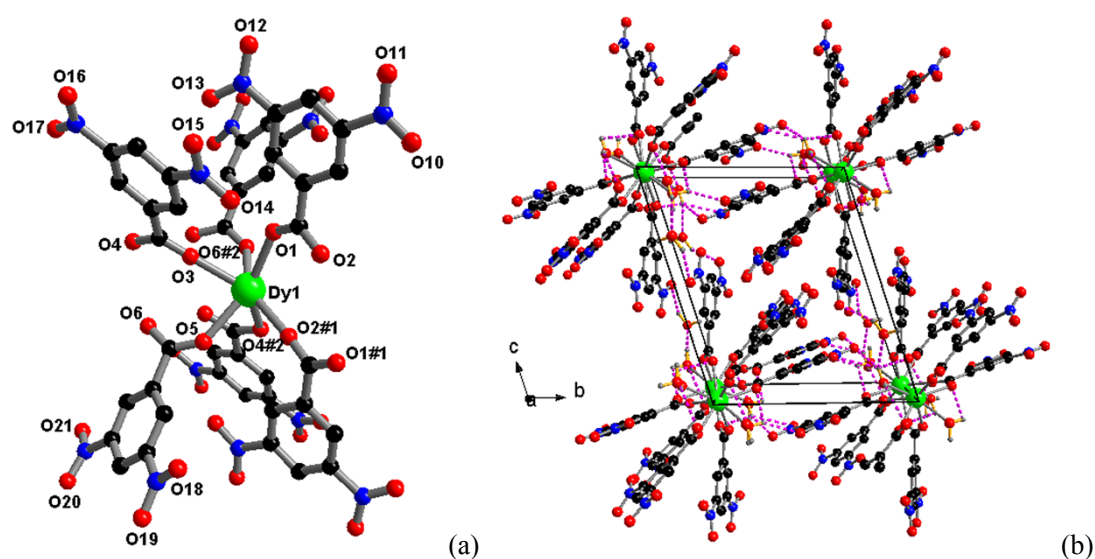


Fig. S1 (a) View of the coordination environment with coordinated and lattice water molecules omitted. (b) View of the packing diagram of complex **2** along the *a*-axis.

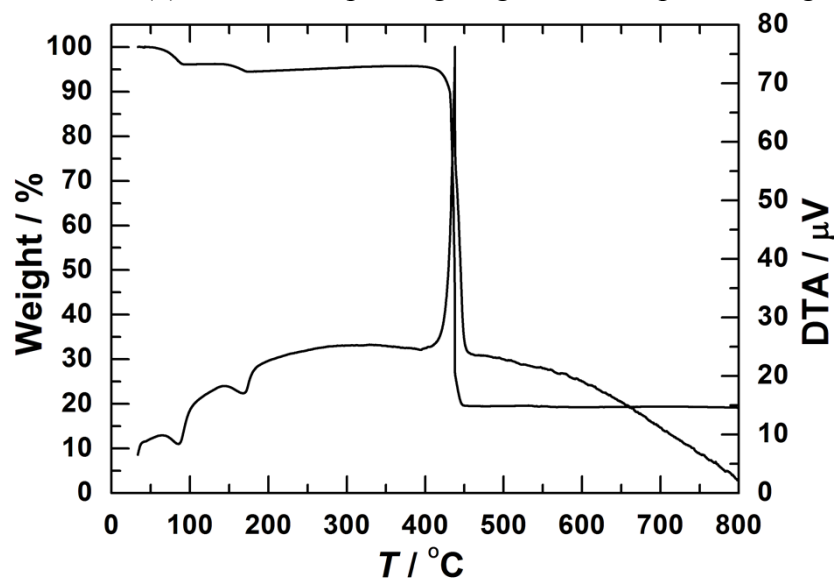


Fig. S2 The TG-DTA curves for complex **2**.

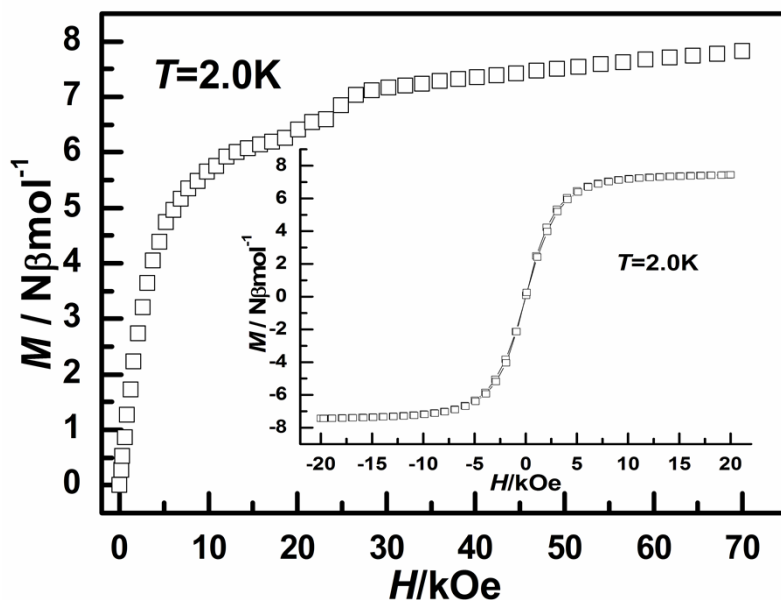


Fig. S3 Field dependence of the magnetization of compound 2 at 2.0 K. Inset: the hysteresis loop plot of compound 2 measured at 2.0 K.

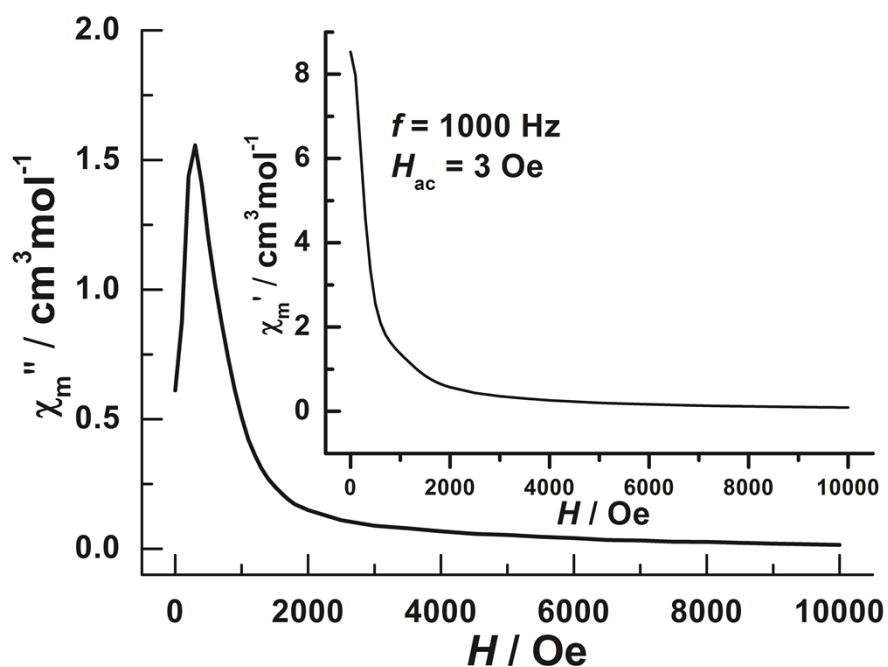


Fig. S4 Field dependence of the in-phase (χ' , inset) and out-of-phase (χ'') ac susceptibility for 2 with $f = 1000\text{ Hz}$.

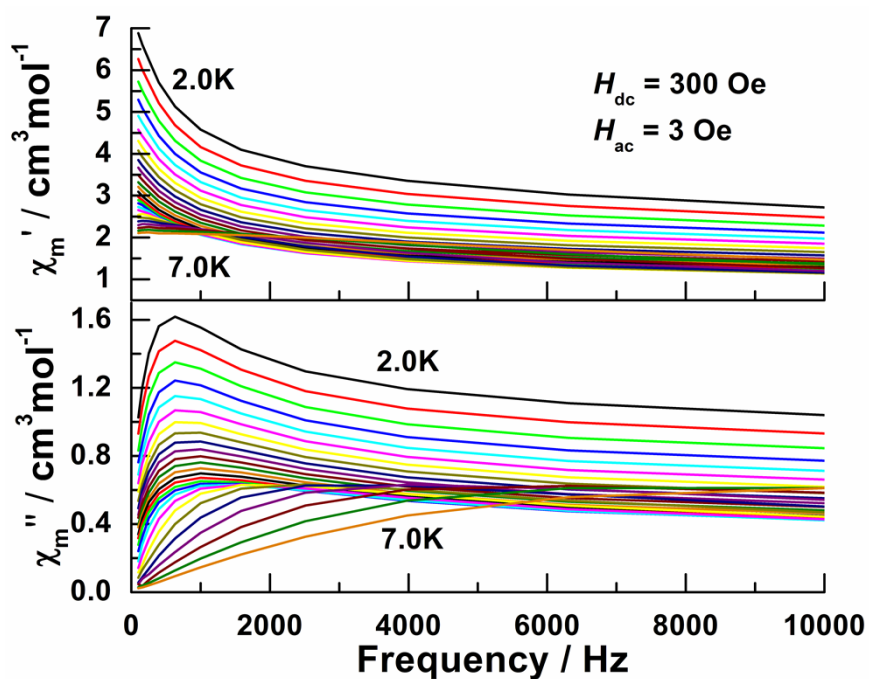


Fig. S5 Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility from 2.0 K to 7.0 K at an interval of 0.2 K under 300 Oe dc field for **2**.

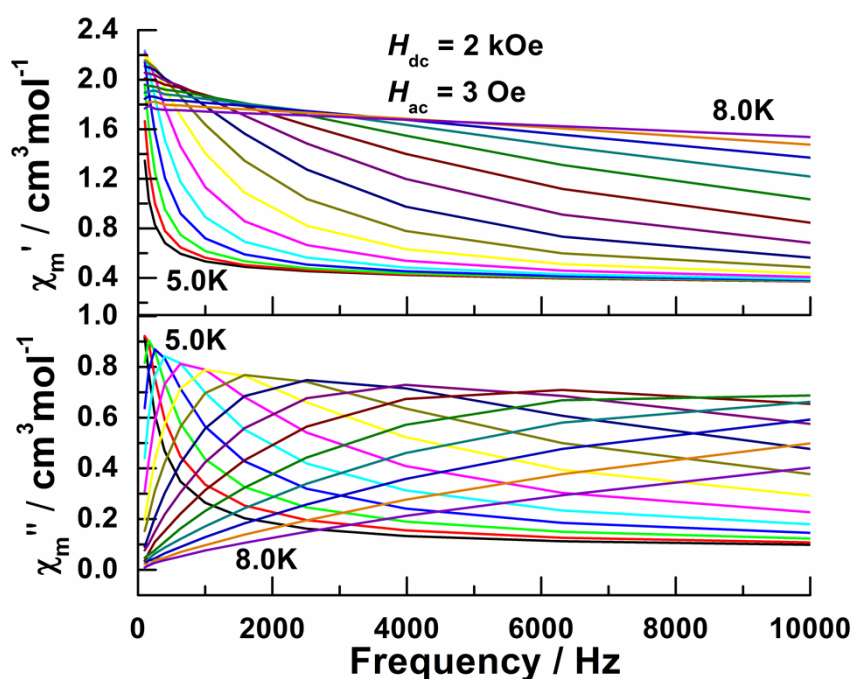


Fig. S6 Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility from 5.0 K to 8.0 K at an interval of 0.2 K under 2 kOe dc field for **2**.

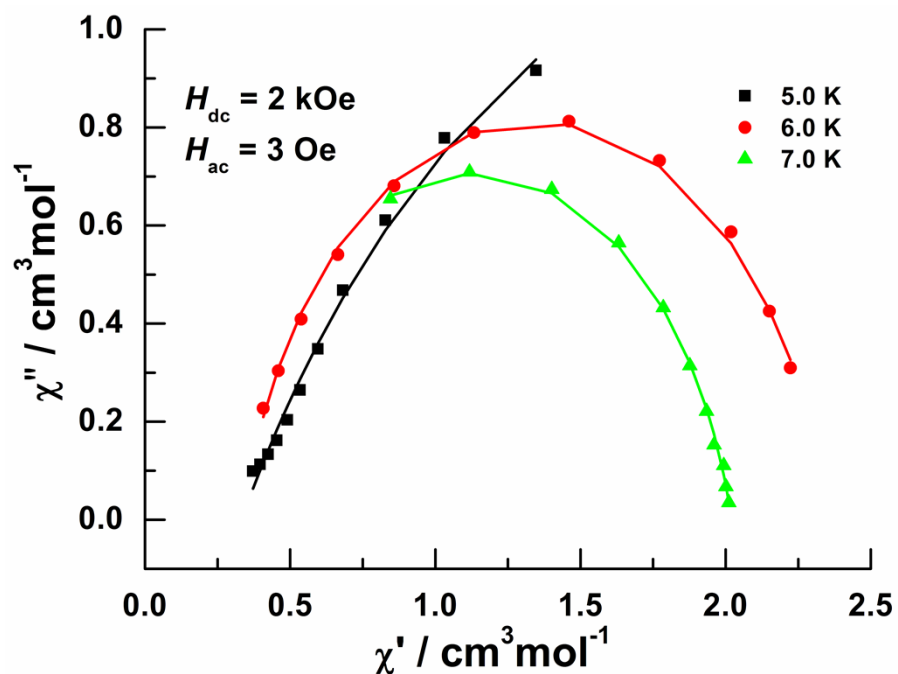


Fig. S7 The Cole–Cole plots of χ'' vs. χ' at 5.0, 6.0 and 7.0 K for compound 2 under 2 kOe dc field. The solid lines are the least-square fitting of the data to a distribution of single relaxation processes.

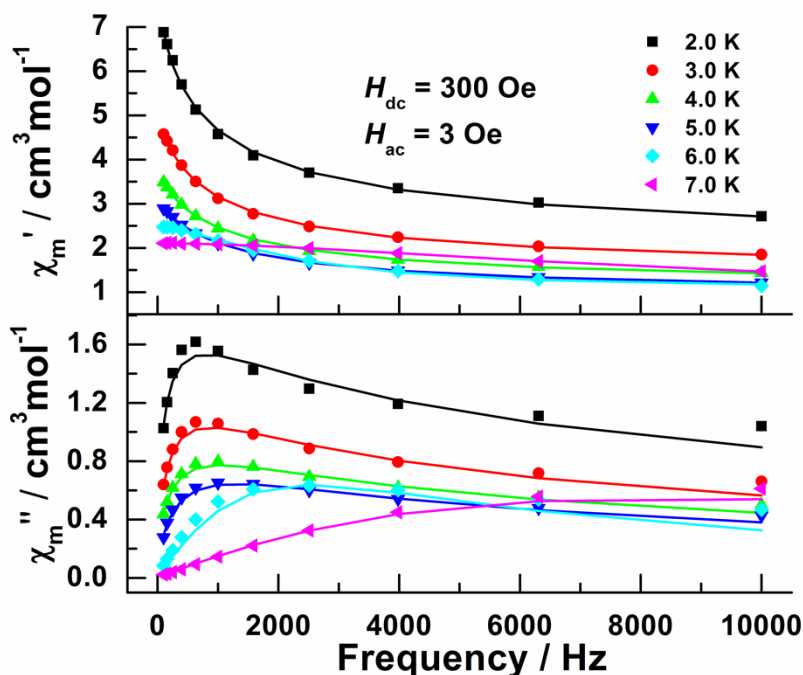


Fig. S8 Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility at 2.0, 3.0, 4.0, 5.0, 6.0 and 7.0 K for **2** under 300 Oe dc field. The solid lines are the least-square fitting of the data to single relaxation processes as the generalized Debye model described.

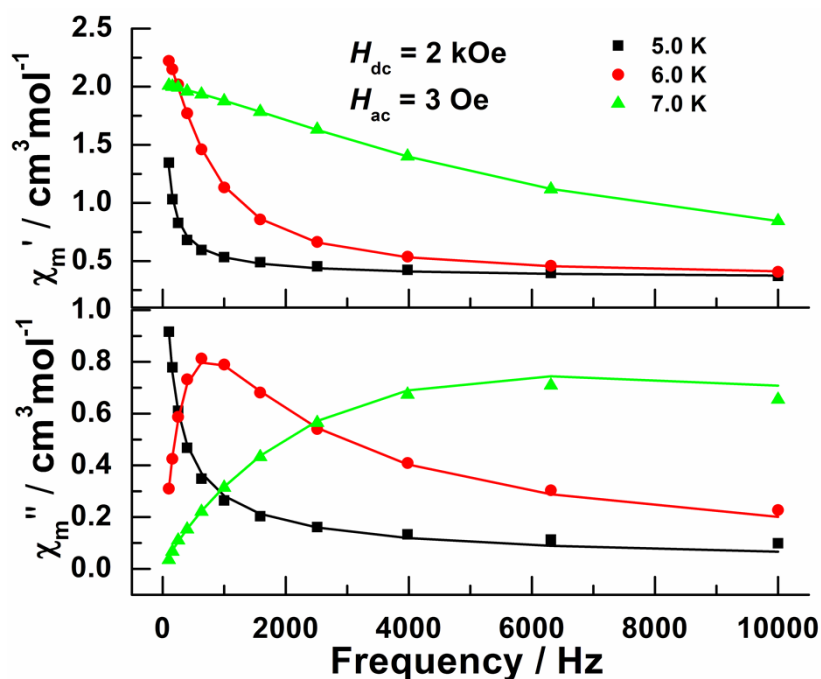


Fig. S9 Frequency dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility at 5.0, 6.0 and 7.0 K for **2** under 2 kOe dc field. The solid lines are least-square fitting of the data to single relaxation processes as the generalized Debye model described.

Table S6 Relaxation parameters from the best fitting of the Cole–Cole diagrams by the generalized Debye model and from the least-square fitting of the frequency dependence of χ' and χ'' under 300 Oe dc field for **2**.

$T(K)$	$\chi_s(\text{cm}^3 \text{mol}^{-1})$	$\chi_T(\text{cm}^3 \text{mol}^{-1})$	$\tau(\text{s})$	α
2.0	1.73	8.24	2.0×10^{-4}	0.44
3.0	1.32	5.29	1.8×10^{-4}	0.39
4.0	1.00	3.92	1.6×10^{-4}	0.38
5.0	0.89	3.15	1.3×10^{-4}	0.34
6.0	1.08	2.44	6.3×10^{-5}	0.04
7.0	0.93	2.11	1.8×10^{-5}	0.05

Table S7 Relaxation parameters from the best fitting of the Cole–Cole diagrams by the generalized Debye model and from the least-square fitting of the frequency dependence of χ' and χ'' under 2 kOe dc field for **2**.

$T(K)$	$\chi_s(\text{cm}^3 \text{mol}^{-1})$	$\chi_T(\text{cm}^3 \text{mol}^{-1})$	$\tau(\text{s})$	α
5.0	0.33	4.58	6.5×10^{-3}	0.34
6.0	0.35	2.36	2.1×10^{-4}	0.14
7.0	0.16	2.02	2.4×10^{-5}	0.14