Electronic Supplementary Information (ESI)

A family of one-dimensional lanthanide complexes bridged by two distinct carboxylate ligands with the Dy analogue displaying magnetic relaxation behaviour

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Table S1 Selected bond lengths (Å) and angles (°) for **3**

Gd(1)–O(1)	2.3167(19)	Gd(1)–O(2)#2	2.3518(18)
Gd(1)–O(4)	2.4820(17)	Gd(1)–O(5)	2.4269(19)
O(1)–Gd(1)–O(1)#1	146.99(10)	O(1)–Gd(1)–O(2)#2	81.16(7)
O(1)–Gd(1)–O(2)#3	106.73(7)	O(1)–Gd(1)–O(4)	77.69(6)
O(1)–Gd(1)–O(4)#1	72.79(7)	O(1)–Gd(1)–O(5)	140.02(7)
O(1)–Gd(1)–O(5)#1	72.36(7)	O(2)#2–Gd(1)–O(2)#3	152.70(10)
O(2)#2–Gd(1)–O(4)	78.72(7)	O(2)#2–Gd(1)–O(4)#1	128.21(7)
O(2)#2–Gd(1)–O(5)	77.84(7)	O(2)#2–Gd(1)–O(5)#1	79.97(7)
O(4)–Gd(1)–O(4)#1	52.69(8)	O(4)–Gd(1)–O(5)	129.65(6)
O(4)–Gd(1)–O(5)#1	145.42(7)	O(5)–Gd(1)–O(5)#1	70.74(9)

Symmetry codes： #1 -x+1, y, -z+3/2, #2 x, -y, z+1/2, #3 -x+1, -y, -z+1

Table S2 Hydrogen bonding geometry for **3**: lengths (Å) and angles (°)

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
O(5)–H(5A)···O(4)#5	0.944(18)	1.81(2)	2.738(2)	167(4)
O(5)–H(5B)···O(3)#6	0.947(19)	1.987(19)	2.667(4)	127(2)
O(5)–H(5B)···O(3)#7	0.947(19)	2.01(4)	2.800(4)	140(5)
O(6)–H(6A)···O(6)#4	0.85	2.64	3.13(4)	118.0
O(6)–H(6B)···O(5)	0.85	2.30	3.134(14)	166.7

Symmetry codes： #1 -x+1, y, -z+3/2, #2 x, -y, z+1/2, #3 -x+1, -y, -z+1, #4 -x+1/2, -y+1/2, -z+2, #5 -x+1, -y, -z+2, #6 x-1/2, y+1/2, z, #7 -x+3/2,y+1/2,-z+3/2

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Table S3 Selected bond lengths (Å) and angles (°) for **5**

Dy(1)–O(1)	2.287(2)	Dy(1)–O(2)#2	2.3127(18)
Dy(1)–O(4)	2.4603(19)	Dy(1)–O(5)	2.418(2)
O(1)–Dy(1)–O(1)#1	147.82(11)	O(1)–Dy(1)–O(2)#2	81.96(8)
O(1)–Dy(1)–O(2)#3	105.79(7)	O(1)–Dy(1)–O(4)	78.17(7)
O(1)–Dy(1)–O(4)#1	73.09(7)	O(1)–Dy(1)–O(5)	139.76(8)
O(1)–Dy(1)–O(5)#1	71.88(7)	O(2)#2–Dy(1)–O(2)#3	152.37(12)
O(2)#2–Dy(1)–O(4)	78.57(7)	O(2)#2–Dy(1)–O(4)#1	128.71(8)
O(2)#2–Dy(1)–O(5)	77.68(8)	O(2)#2–Dy(1)–O(5)#1	79.84(8)
O(4)–Dy(1)–O(4)#1	53.12(8)	O(4)–Dy(1)–O(5)	129.79(6)
O(4)–Dy(1)–O(5)#1	145.09(7)	O(5)–Dy(1)–O(5)#1	70.60(10)

Symmetry codes： #1 -x+1, y, -z+3/2, #2 x, -y, z+1/2, #3 -x+1, -y, -z+1

Table S4 Hydrogen bonding geometry for **5**: lengths (Å) and angles (°)

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
O(5)–H(5A)···O(4)#4	0.945(17)	1.821(18)	2.764(3)	175(4)
O(5)–H(5B)···O(3)#5	0.906(18)	1.943(17)	2.681(5)	137(3)
O(6)–H(6A)···O(5)	1.027(15)	2.074(15)	3.101(10)	178(9)
O(6)–H(6B)···O(6)#6	0.97(2)	2.45(11)	3.09(3)	123(10)

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

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Table S5 Continuous shape measures (CShM) for **5** using SHAPE 2.1

	5
OP-8	27.572
HPY-8	22.288
HBPY-8	12.278
CU-8	9.305
SAPR-8	1.741
TDD-8	2.361
JGBF-8	11.809
JETBPY-8	27.677
JBTPR-8	2.467
BTPR-8	2.172
JSD-8	2.968
TT-8	10.163
ETBPY-8	24.032

OP-8 = (D_{8h}) Octagon

HPY-8 = (C_{7v}) Heptagonal pyramid

HBPY-8 = (D_{6h}) Hexagonal bipyramid

CU-8 = (O_h) Cube

SAPR-8 = (D_{4d}) Square antiprism

TDD-8 = (D_{2d}) Triangular dodecahedron

JGBF-8 = (D_{2d}) Johnson gyrobifastigium J26

JETBPY-8 = (D_{3h}) Johnson elongated triangular bipyramid J14

JBTPR-8 = (C_{2v}) Biaugmented trigonal prism J50

BTPR-8 = (C_{2v}) Biaugmented trigonal prism

JSD-8 = (D_{2d}) Snub diphenoid J84

TT-8 = (T_d) Triakis tetrahedron

ETBPY-8 = (D_{3h}) Elongated trigonal bipyramid

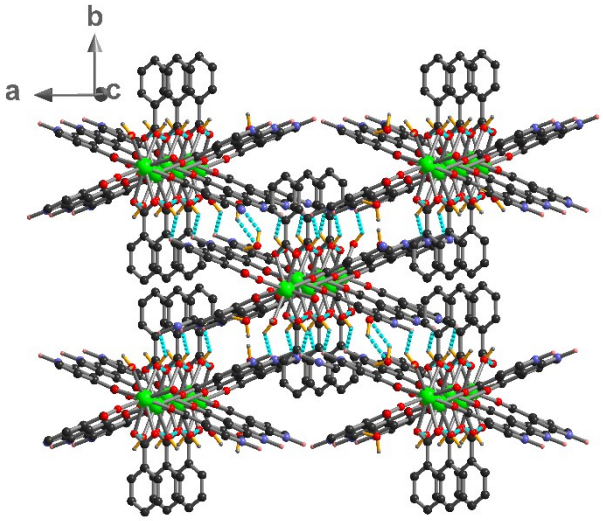

Fig. S1 View of the packing diagram of complex **5** along the *c*-axis.

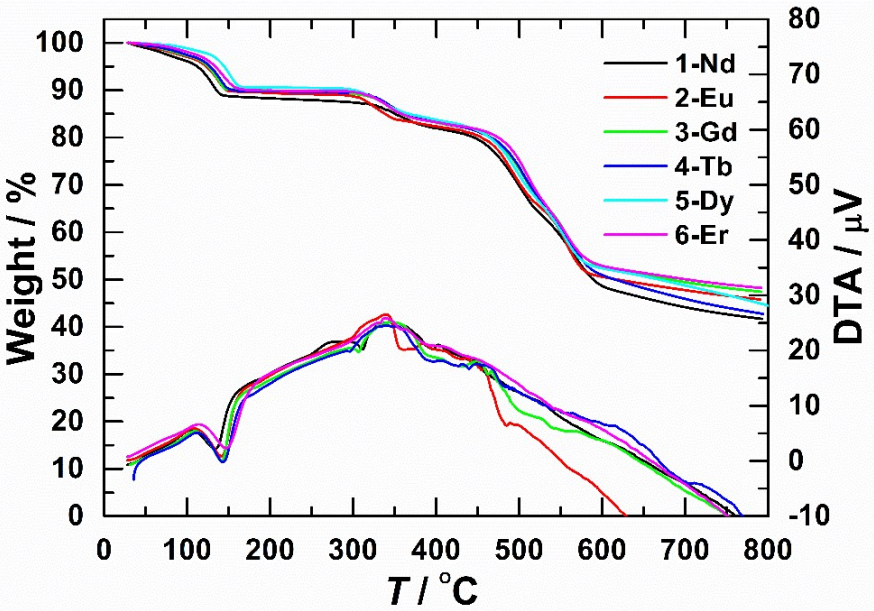

Fig. S2 The TG–DTA curves for complexes **1**–**6**.

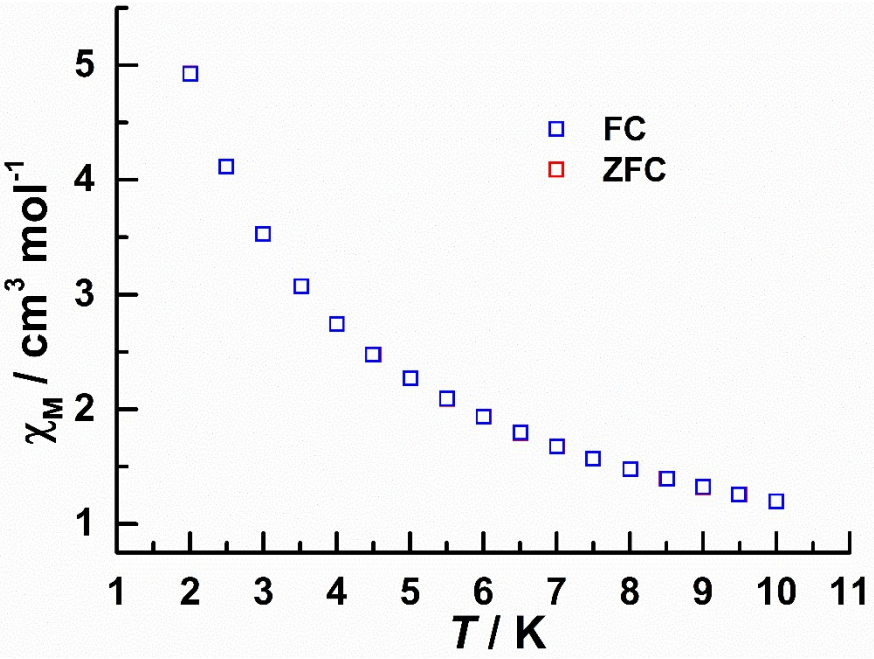

Fig. S3 The zero-field-cooled/field-cooled (ZFC-FC) magnetic susceptibility χ_M under a 20 Oe dc field in warm mode for **5**.

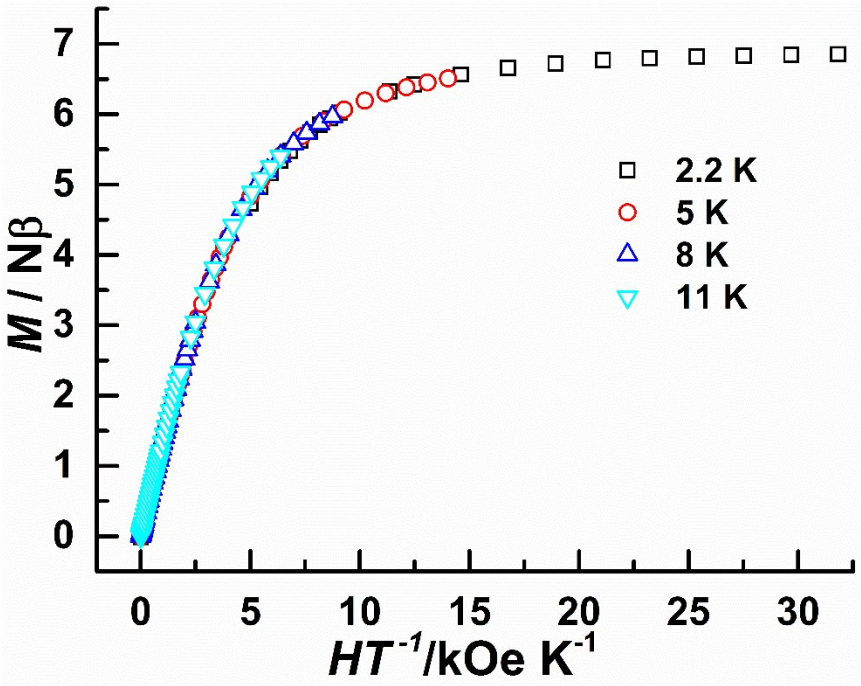

Fig. S4 Field dependence of the magnetization for compound **3** at 2.2, 5, 8, 11 K.

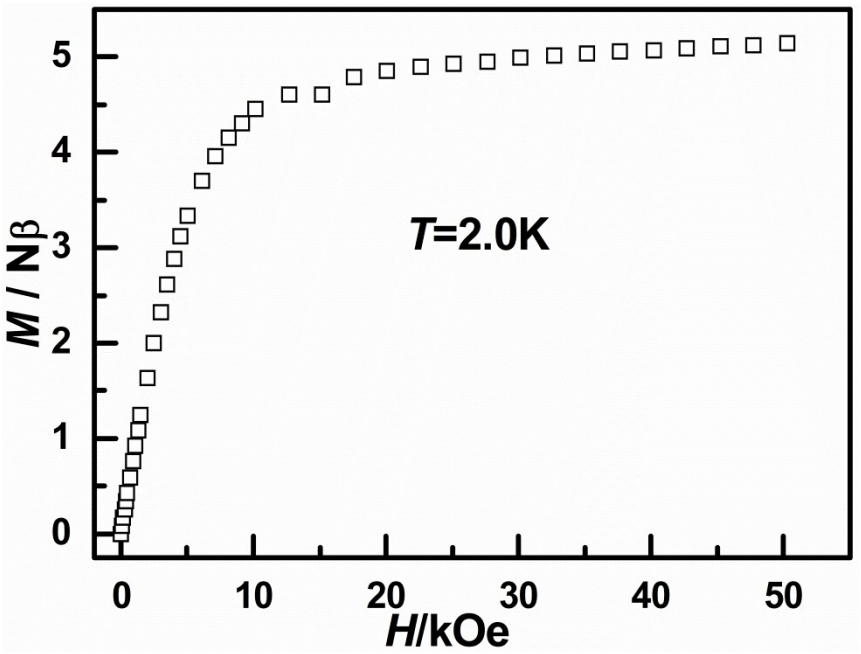

Fig. S5 Field dependence of the magnetization for compound **5** at 2.0 K.

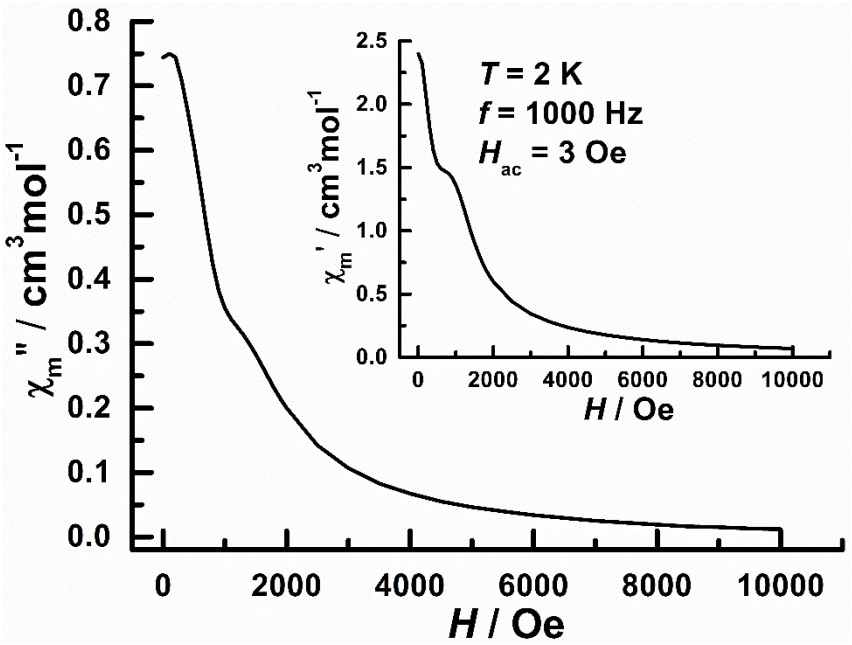

Fig. S6 Field dependence of the in-phase (χ', inset) and out-of-phase (χ'') ac susceptibilities for **5** with f = 1000 Hz.

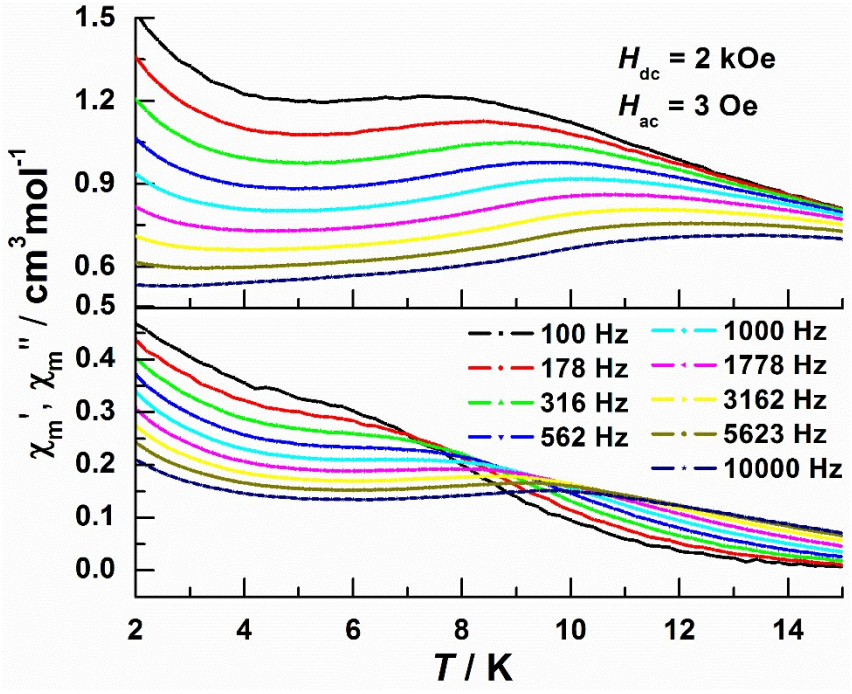

Fig. S7 Temperature dependence of χ' and χ'' ac susceptibility components under a 2 kOe dc field for **5**.

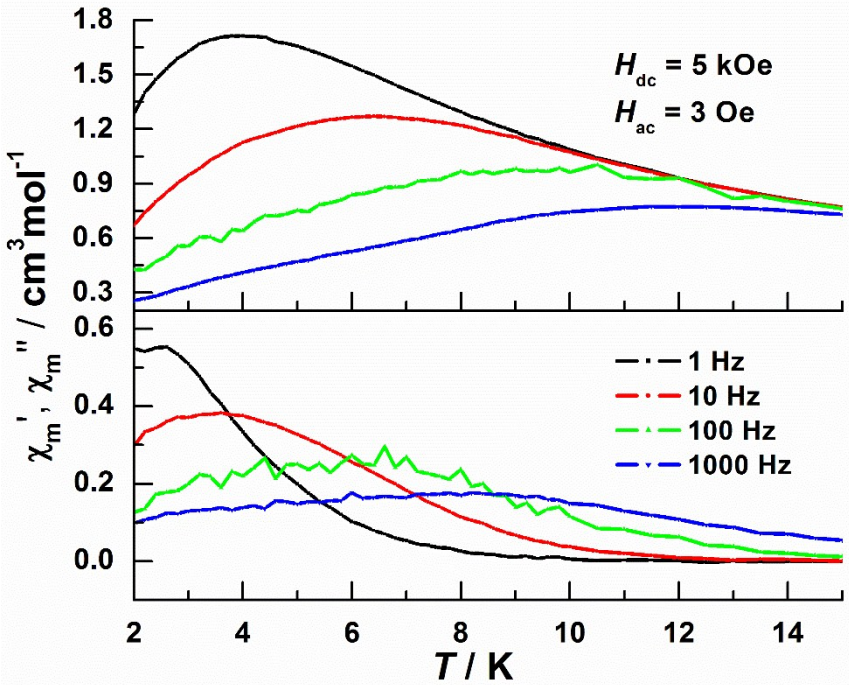

Fig. S8 Temperature dependence of χ' and χ'' ac susceptibility components under a 5 kOe dc field for **5**.

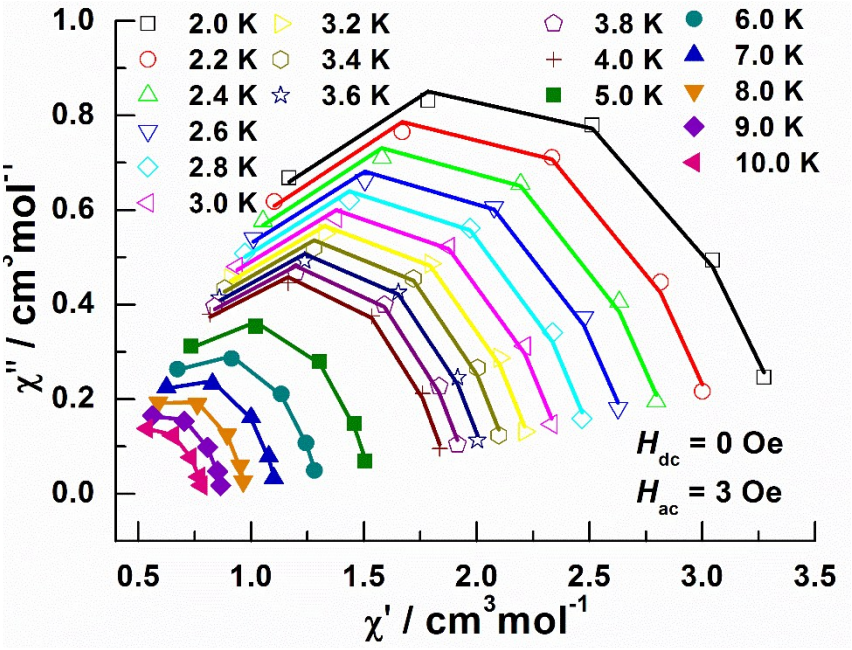

Fig. S9 The Cole–Cole plots of χ'' vs. χ' at 2.0−4.0 K (0.2 K interval) and 4.0−10.0 K (1.0 K interval) for compound **5** under a 0 Oe dc field. The solid lines are the least-square fitting of the data to a distribution of single relaxation processes.

Table S6 Relaxation parameters from the best fitting of the Cole–Cole diagrams by the generalized Debye model under a zero dc field for **5**.

T(K)	χ_S(cm^3 mol^{-1})	χ_T(cm^3 mol^{-1})	τ (s)	α
2.0	0.49	3.45	6.4×10^{-5}	0.33
2.2	0.50	3.15	6.4×10^{-5}	0.31
2.4	0.50	2.93	6.2×10^{-5}	0.31
2.6	0.48	2.75	6.1×10^{-5}	0.31
2.8	0.49	2.57	5.9×10^{-5}	0.30
3.0	0.48	2.43	5.8×10^{-5}	0.30
3.2	0.47	2.30	5.6×10^{-5}	0.29
3.4	0.47	2.18	5.5×10^{-5}	0.28
3.6	0.46	2.07	5.3×10^{-5}	0.28
3.8	0.46	1.98	5.2×10^{-5}	0.28
4.0	0.45	1.89	5.0×10^{-5}	0.28
5.0	0.43	1.54	4.4×10^{-5}	0.26
6.0	0.40	1.31	3.7×10^{-5}	0.27
7.0	0.39	1.12	3.3×10^{-5}	0.24
8.0	0.38	0.98	3.0×10^{-5}	0.24
9.0	0.37	0.87	2.6×10^{-5}	0.25
10.0	0.35	0.79	2.2×10^{-5}	0.28

Table S7 Relaxation parameters from the best fitting of the Cole–Cole diagrams by the generalized Debye model under 1 kOe dc field for **5**.

T(K)	χ_S(cm^3 mol^{-1})	χ_T(cm^3 mol^{-1})	τ (s)	α
5.0	0.09	3.09	8.8×10^{-4}	0.74
6.0	0.23	2.34	2.4×10^{-4}	0.68
7.0	0.34	1.89	1.1×10^{-4}	0.61
8.0	0.45	1.58	5.9×10^{-5}	0.50
9.0	0.51	1.38	3.8×10^{-5}	0.40
10.0	0.56	1.23	2.8×10^{-5}	0.31
11.0	0.61	1.12	2.3×10^{-5}	0.24

Table S8 Relaxation parameters from the best fitting of the Cole–Cole diagrams by the generalized Debye model under a 2 kOe dc field for **5**.

T(K)	χ_S(cm^3 mol^{-1})	χ_T(cm^3 mol^{-1})	τ (s)	α
7.0	0.30	2.24	2.4×10^{-3}	0.66
8.0	0.34	1.70	4.4×10^{-4}	0.61
9.0	0.35	1.43	1.5×10^{-4}	0.57
10.0	0.35	1.28	5.6×10^{-5}	0.57
11.0	0.41	1.13	3.5×10^{-5}	0.41
12.0	0.45	1.03	2.2×10^{-5}	0.48