Enchaining EDTA-Chelated Lanthanide Molecular Magnets into Ordered 1D Networks

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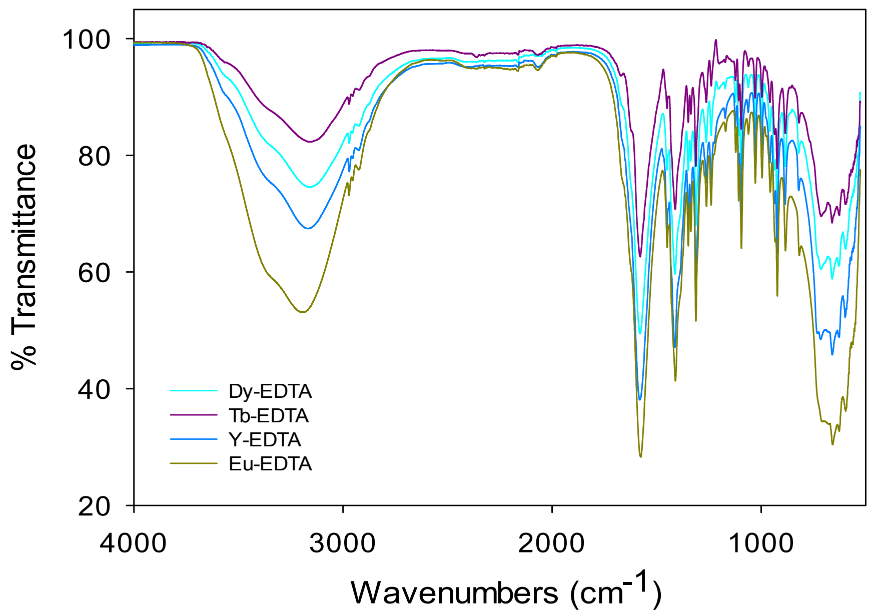

Fig. S1 FTIR spectra of **1-4** for vacuum filtered crystals in the 4000-550 cm^{-1} region.

Table S1. Selected bond distances for complexes **1**-**4**.

Bond	Distance (Å)			
	1	**2**	**3**	**4**
Ln1-O1	2.333(8)	2.358(2)	2.392(3)	2.364(8)
Ln1-O3	2.395(7)	2.397(3)	2.435(3)	2.402(8)
Ln1-O5	2.351(7)	2.355(3)	2.388(3)	2.371(8)
Ln1-O7	2.397(8)	2.400(3)	2.422(4)	2.40(1)
Ln1-O9	2.422(7)	2.380(4)	2.430(4)	2.41(1)
Ln1-O10	2.513(7)	2.430(2)	2.471(3)	2.437(7)
Ln1-O11	2.371(8)	2.520(3)	2.550(3)	2.538(9)
Ln1-N1	2.598(7)	2.655(3)	2.686(3)	2.64(1)
Ln1-N2	2.650(9)	2.611(3)	2.642(4)	2.63(1)
Ln2-O12	-	2.402(3)	2.436(3)	2.409(8)
Ln2-O14	-	2.363(3)	2.394(4)	2.374(9)
Ln2-O16	-	2.392(2)	2.421(3)	2.394(8)
Ln2-O18	-	2.339(2)	2.386(3)	2.341(8)
Ln2-O20	-	2.390(2)	2.425(3)	2.382(7)
Ln2-O21	-	2.448(3)	2.470(4)	2.44(1)
Ln2-O22	-	2.532(3)	2.552(3)	2.513(9)
Ln2-N3	-	2.667(4)	2.688(4)	2.70(1)
Ln2-N4	-	2.614(3)	2.644(4)	2.61(1)

Table S2. Dihedral angles along the edges of coordination polyhedra, used to determine the analogous measurement (AM) of complexes **2-4**. Gd-EDTA was employed as reference.

Dihedral Angle	Gd-EDTA, Ref	Eu-EDTA, 2	Tb-EDTA, 3	Dy-EDTA, 4
	Gd1	**Eu1**	**Tb1**	**Dy1**
N2-N1-O3^O7-N2-O3	22.075(340)	21.445(157)	21.880(397)	20.902(135)
N2-N1-O3^O1-N2-N1	66.272(357)	66.697(125)	66.770(372)	67.411(123)
N2-N1-O3^O3-N1-O9	66.731(283)	67.090(119)	66.617(364)	67.570(108)
N2-O7-O3^O7-O3-O10	53.199(261)	52.878(124)	53.346(312)	53.438(104)
N2-O7-O3^N2-O7-O5	61.510(253)	61.933(114)	62.031(299)	62.402(106)
O1-N2-N1^N1-O1-O9	58.226(302)	58.057(129)	57.454(342)	58.212(120)
O1-N2-N1^O1-N2-O5	40.494(317)	40.215(127)	41.467(362)	41.02(11)
O5-O1-N2^O11-O1-O5	38.221(253)	38.176(119)	36.871(290)	37.160(107)
O5-O1-N2^O7-O5-N2	59.007(261)	58.771(106)	59.322(314)	58.471(91)
O11-O5-O1^O9-O1-O11	54.455(269)	54.383(125)	55.187(323)	55.482(108)
O11-O5-O1^O11-O10-O5	75.165(241)	75.395(111)	75.10(28)	74.644(92)
O10-O9-O3^O7-O3-O10	54.385(249)	55.212(119)	54.349(311)	54.725(103)
O10-O5-O11^O10-O9-O11	69.787(287)	70.588(125)	69.717(329)	69.884(103)
O9-O10-O11^O11-O1-O9	56.485(288)	56.711(113)	56.709(333)	56.484(97)
O9-O10-O11^O9-O3-O10	50.199(271)	50.142(109)	49.625(307)	49.489(98)
O9-O11-O1^O9-N1-O1	36.301(297)	35.759(131)	35.643(375)	35.183(114)
N1-O9-O1^O9-O3-N1	57.130(337)	56.806(144)	57.272(439)	57.298(111)
O9-O3-N1^O9-O3-O10	35.427(257)	34.768(123)	35.352(346)	35.016(115)
O5-O7-O10^O11-O5-O10	8.541(273)	8.031(124)	9.261(300)	9.097(98)
O5-O7-O10^N2-O5-O7	57.659(275)	57.926(129)	57.158(328)	57.364(109)
O5-O7-O10^O7-O10-O3	65.861(250)	66.589(110)	65.759(270)	66.057(82)
	Gd2	**Eu2**	**Tb2**	**Dy2**
O22-O20-O21^O20-O12-O21	49.254(306)	49.949(106)	48.729(338)	48.511(93)
O22-O20-O21^O20-O14-O22	56.674(315)	56.677(116)	56.159(357)	56.446(102)
O22-O20-O21^O22-O18-O21	70.990(321)	70.733(125)	71.158(346)	71.225(99)
O20-O21-O12^O12-O16-O21	55.559(252)	55.291(111)	55.972(326)	55.594(92)
O20-O21-O12^O20-N3-O12	34.333(297)	34.811(131)	34.164(354)	34.434(102)
O16-O12-O21^O18-O21-O16	66.683(229)	66.610(103)	66.580(285)	66.049(80)
O16-O12-O21^O16-N4-O12	53.449(284)	52.860(124)	53.592(346)	53.564(95)
O18-O16-N4^N4-O16-O12	62.705(283)	61.984(113)	62.655(294)	62.736(98)
O18-O16-N4^N4-O14-O18	58.312(291)	58.730(121)	58.463(300)	58.560(98)
O18-O14-N4^O14-O22-O18	37.998(257)	38.156(125)	38.125(319)	37.603(106)
O18-O14-N4^O14-N3-N4	40.582(335)	40.227(136)	40.000(344)	40.936(122)
O14-N3-N4^N4-N3-O12	68.027(345)	66.751(136)	68.477(340)	68.112(130)
O14-N3-N4^N3-O20-O14	57.472(329)	58.172(123)	58.440(305)	57.501(113)
O20-N3-O12^O14-N3-O20	56.858(349)	56.778(140)	56.738(337)	57.005(112)
O20-N3-O12^N3-N4-O12	67.808(296)	67.148(123)	68.629(345)	67.637(104)
O22-O18-O21^O14-O22-O18	74.594(266)	75.273(126)	74.272(275)	74.286(92)
O18-O16-O21^O18-N4-O16	57.968(307)	57.779(127)	57.703(326)	57.358(101)
O12-N4-N3^O16-O12-N4	19.798(414)	21.467(142)	19.463(393)	20.293(137)
O14-O20-N3^O20-O22-O14	35.739(295)	35.607(133)	35.257(333)	35.387(109)
O18-O21-O16^O21-O22-O18	8.578(279)	7.997(116)	8.704(292)	9.146(93)
O20-O22-O14^O18-O14-O22	54.403(299)	54.577(132)	54.706(315)	55.053(109)
AM	0	0.546842	0.484377	0.55259

Table S3. Dihedral angles (°) along the edges of the coordination polyhedra used to determine the analogous measurement (AM) of polyhedra Dy1 *vs.* Dy2 and Tb1 *vs.* Tb2, within complexes **3**, and **4**.

Dihedral Angle	Dy1	Tb1
O5-O7-O10^O11-O5-O10	9.097(98)	9.261(300)
N2-N1-O3^O7-N2-O3	20.902(135)	21.880(397)
O9-O3-N1^O9-O3-O10	35.016(115)	35.352(346)
O9-O11-O1^O9-N1-O1	35.183(114)	35.643(375)
O5-O1-N2^O11-O1-O5	37.160(107)	36.871(290)
O1-N2-N1^O1-N2-O5	41.02(11)	41.467(362)
O9-O10-O11^O9-O3-O10	49.489(98)	49.625(307)
N2-O7-O3^O7-O3-O10	53.438(104)	53.346(312)
O10-O9-O3^O7-O3-O10	54.725(103)	54.349(311)
O11-O5-O1^O9-O1-O11	55.482(108)	55.187(323)
O9-O10-O11^O11-O1-O9	56.484(97)	56.709(333)
N1-O9-O1^O9-O3-N1	57.298(111)	57.272(439)
O5-O7-O10^N2-O5-O7	57.364(109)	57.158(328)
O1-N2-N1^N1-O1-O9	58.212(120)	57.454(342)
O5-O1-N2^O7-O5-N2	58.471(91)	59.322(314)
N2-O7-O3^N2-O7-O5	62.402(106)	62.031(299)
O5-O7-O10^O7-O10-O3	66.057(82)	65.759(270)
N2-N1-O3^O1-N2-N1	67.411(123)	66.770(372)
N2-N1-O3^O3-N1-O9	67.570(108)	66.617(364)
O10-O5-O11^O10-O9-O11	69.884(103)	69.717(329)
O11-O5-O1^O11-O10-O5	74.644(92)	75.10(28)
	Dy2	**Tb2**
O18-O21-O16^O21-O22-O18	9.146(93)	8.704(292)
O12-N4-N3^O16-O12-N4	20.293(137)	19.463(393)
O20-O21-O12^O20-N3-O12	34.434(102)	34.164(354)
O14-O20-N3^O20-O22-O14	35.387(109)	35.257(333)
O18-O14-N4^O14-O22-O18	37.603(106)	38.125(319)
O18-O14-N4^O14-N3-N4	40.936(122)	40.000(344)
O22-O20-O21^O20-O12-O21	48.511(93)	48.729(338)
O16-O12-O21^O16-N4-O12	53.564(95)	53.592(346)
O20-O22-O14^O18-O14-O22	55.053(109)	54.706(315)
O20-O21-O12^O12-O16-O21	55.594(92)	55.972(326)
O22-O20-O21^O20-O14-O22	56.446(102)	56.159(357)
O20-N3-O12^O14-N3-O20	57.005(112)	56.738(337)
O18-O16-O21^O18-N4-O16	57.358(101)	57.703(326)
O14-N3-N4^N3-O20-O14	57.501(113)	58.440(305)
O18-O16-N4^N4-O14-O18	58.560(98)	58.463(300)
O18-O16-N4^N4-O16-O12	62.736(98)	62.655(294)
O16-O12-O21^O18-O21-O16	66.049(80)	66.580(285)
O20-N3-O12^N3-N4-O12	67.637(104)	68.629(345)
O14-N3-N4^N4-N3-O12	68.112(130)	68.477(340)
O22-O20-O21^O22-O18-O21	71.225(99)	71.158(346)
O22-O18-O21^O14-O22-O18	74.286(92)	74.272(275)
AM	**0.346301**	**0.78927**

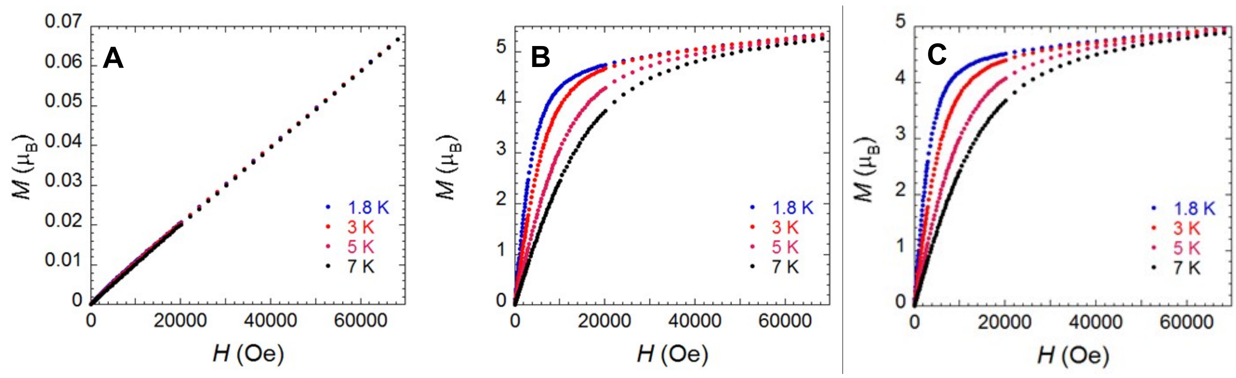

Fig. S2 Field dependence of the magnetisation of: (a) **2**, (b) **3** and (c) **4** at indicated temperatures.

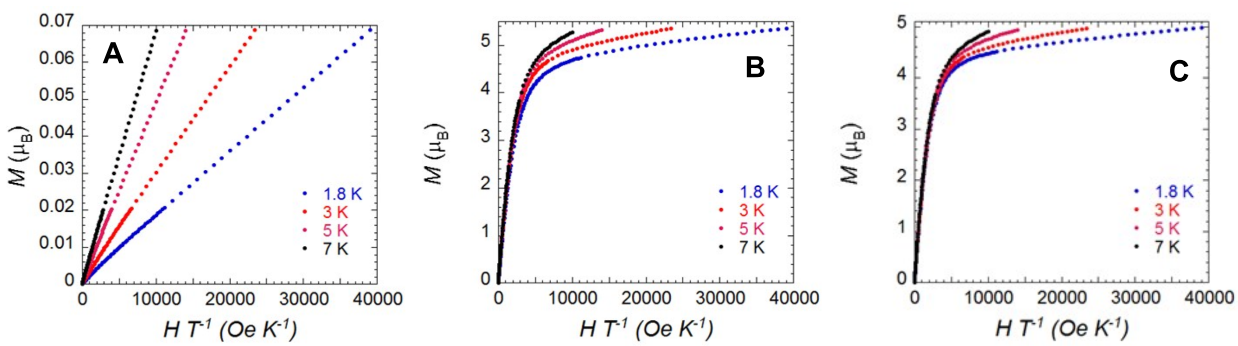

Fig. S3 M vs. HT^{-1} plot for: (a) **2**, (b) **3** and (c) **4** at indicated temperatures.

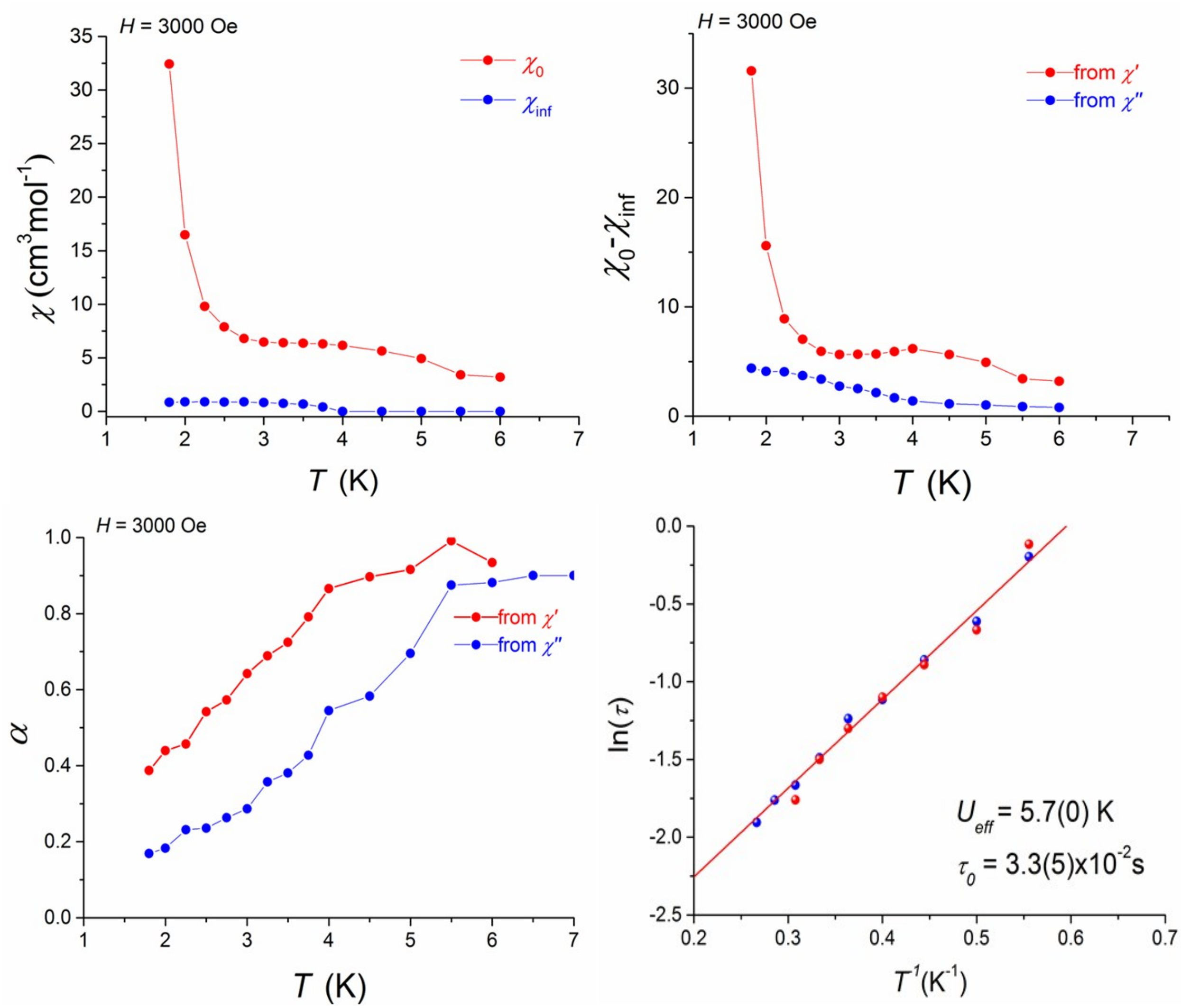

Fig. S4 Data obtained from generalized Debye fits of χ' and χ'' frequency dependent ac data under 3000 Oe applied dc field for **3**. Temperature dependence of χ_0 and χ_{inf} (top left), χ_0-χ_{inf} (top right), and α (bottom left). Relaxation times of the magnetization ln(τ) vs. T^{-1} for **3** (Arrhenius plot using χ'(red) and χ'' (blue) ac data) under 3000 Oe applied dc field (bottom right). The solid red line corresponds to the fit of the data.

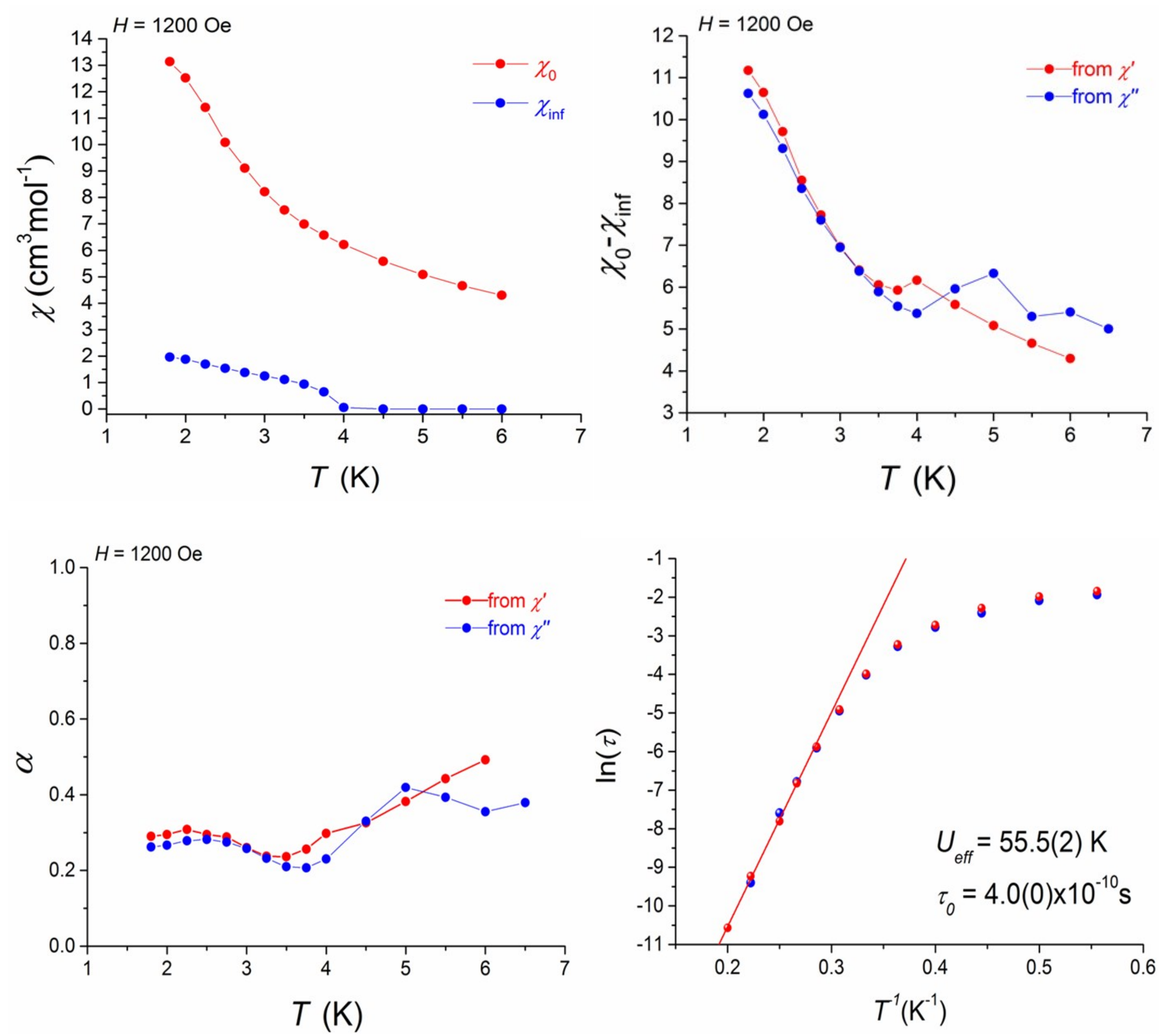

Fig. S5 Data obtained from generalized Debye fits of χ' and χ'' frequency dependent ac data under 1200 Oe applied dc field for **4**. Temperature dependence of χ_0 and χ_{inf} (top left), χ_0-χ_{inf} (top right), and α (bottom left). Relaxation times of the magnetization ln(τ) vs. T^{-1} for **2** (Arrhenius plot using χ'(red) and χ'' (blue) ac data) under 1200 Oe applied dc field (bottom right). The solid red line corresponds to the fit of the data.

Table S4. *Cole-Cole* fitting values using a generalized Debye model for ac susceptibility data of **4** under 1200 Oe applied dc field.

T **(K)**	***τ*** **(s)**	***α***	X_{inf}	X_0
6	0.000001739	0.72055	0	2.21193
5.5	0.000003238	0.67703	0	2.64156
5	0.000003631	0.69226	0	2.8015
4.5	0.000083010	0.65324	0.64556	3.60222
4	0.000503393	0.46878	1.4722	5.08173
3.75	0.001129997	0.41435	1.69645	5.60608
3.5	0.002739993	0.3676	1.8774	6.13707
3.25	0.007119981	0.3529	2.07863	6.66517
3	0.018079981	0.34831	2.29181	7.23623
2.75	0.037900158	0.36606	2.57326	7.85101
2.5	0.062090021	0.38118	2.87758	8.58645
2.25	0.089829666	0.39885	3.26144	9.50147
2	0.124259892	0.38299	3.51166	10.50988
1.8	0.144830672	0.38273	3.6697	11.04093