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Supporting Information for

Cocrystals of Li^+ Encapsulated Fullerenes and Tb(III) Double-Decker Single Molecule Magnet in a Quasi-Kagome Lattice

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S1. Synthetic details

S1.1 General Considerations

$Li^+@C_{60}\cdot PF_6^-$ was supplied from Idea International Corporation. Other reagents were purchased from Tokyo Chemical Industry Co., Ltd., FUJIFILM Wako Pure Chemical Co., Kanto Chemical Co. Inc. and used without further purification. The heteroleptic double-decker phthalocyanato octaethylporphyrinato terbium(III) complex was synthesized following a previously reported procedure.[1] Phenoxathiin hexachloroantimonate and $Li^+@C_{60}\cdot NTf_2^-$ were prepared according to published procedures.[2, 3] Elemental analysis was performed on J–SCIENCE LAB Co., Ltd. JM−11 microanalyzer.

S1.2 Synthesis of Tb(Pc)(OEP)

A solution of $Tb(OAc)_3\cdot 4H_2O$ (200 mg, 0.49 mmol), phthalonitrile (440 mg, 3.43 mmol) and DBU (0.25 mL, 1.67 mmol) in 1-hexanol (5 mL) was refluxed for 3 h under a N_2 flow. After cooling to room temperature, an excess amount of hexane was added to reaction mixture. The solid was collected by filtration and washed with hexane. The blue solid was obtained and purified by using chromatography over silica gel ($CHCl_3$:MeOH 80:20). The first green fraction contained $Tb(Pc)_2$. The second blue fraction containing Tb(Pc)(OAc) was collected, and the solvent was evaporated. The resulting blue solid was recrystallized from CH_2Cl_2/*n*-hexane to obtain crude Tb(Pc)(OAc) (194 mg, 31.0%).

A mixture of Tb(Pc)(OAc) (116 mg, 0.159 mmol), H_2OEP (85 mg, 0.159 mmol) and DBU (0.5 mL, 3.34 mmol) in 1-octanol (5 mL) was refluxed for 18 h in slow stream of N_2 gas. After removing the volatiles under reduced pressure, $CHCl_3$ (30 mL) and a small amount of MnO_2 were added, and the mixture was stirred for 1 h at room temperature. The obtained mixture was purified by using chromatography over silica gel ($CHCl_3$). The first purple fraction contained unreacted H_2OEP. The second green fraction containing Tb(Pc)(OEP) was collected, and the solvent was evaporated. Black crystals of Tb(Pc)(OEP) were obtained from $CHCl_3$/MeOH (114 mg, 59.5%). ESI-MS (m/z): 1203.43 [M^+], 1226.42[$(M+Na)^+$]; Elemental analysis calcd for Tb(Pc)(OEP)·0.6$CHCl_3$: C 64.574, H 4.787, N 13.175; found: C 64.854, H 4.931, N 13.375.

S1.3 Synthesis of $[Tb(Pc)(OEP)]_3(Li^+@C_{60}\cdot PF_6^-)_2$ (1)

$Li^+@C_{60}\cdot NTf_2^-$ (3.0 mg, 2.98 μmol), Tb(Pc)(OEP) (3.9 mg, 3.24 μmol) and $TBAPF_6$ (2.0 mg, 5.16 μmol) were dissolved in *o*-dichlorobenzene (2 mL), and the solution was sonicated for 3 min. Black crystals were obtained by using vapor diffusion of Et_2O into the o-dichlorobenzene solution (5.0 mg, 94.0% based on $Li^+@C_{60}\cdot NTf_2^-$). Elemental analysis calcd (%) for $[Tb(Pc)(OEP)]_3(Li+@C_{60}\cdot PF_6^-)_{2.3}(o\text{-DCB})_{1.5}(Et_2O)_4$: C 71.04, H 3.68, N 7.93; found: C 71.181, H 3.484, N 7.653.

S1.4 Synthesis of $[Tb(Pc)(OEP)](Li^+@C_{60}\cdot BF_4^-)$ (2)

$Li^+@C_{60}\cdot NTf_2^-$ (3.0 mg, 2.98 μmol), Tb(Pc)(OEP) (3.9 mg, 3.24 μmol) and $TBABF_4$ (1.7 mg, 5.16 μmol) were dissolved in *o*-dichlorobenzene (2 mL), and the solution was sonicated for 3 min. Black crystals were obtained by using vapor diffusion of Et_2O into the o-dichlorobenzene solution (5.0 mg, 94.0% based on $Li^+@C_{60}\cdot NTf_2^-$). Elemental analysis calcd (%) for $[Tb(Pc)(OEP)](Li+@C_{60}\cdot BF_4^-)_{0.7}(o\text{-DCB})_{1.6}(Et_2O)_{0.5}$: C 69.06, H 3.44, N 7.37; found: C 68.939, H 3.435, N 7.599.

S1.5 Synthesis of [Tb(Pc)(OEP)](C_{70})(C_6H_{14}) (3)

Tb(Pc)(OEP) (12.6 mg, 10.5 µmol) and C_{70} (8.7 mg, 10.4 µmol) were dissolved in 1,2,4-trichlorobenzene (2.5 mL), and the solution was sonicated for 1 min. The obtained solution was diffused into hexane to afford black crystals (14.2 mg, 64.1%). Elemental analysis calcd (%) for [Tb(Pc)(OEP)]$(C_{70})_{0.94}(TCB)_{0.1}$: C 79.78, H 3.00, N 8.31; found: C 79.779, H 3.068, N 8.582.

S1.6 Synthesis of [Tb(Pc)(OEP)](C_{60})(C_6H_{14}) (4)

Tb(Pc)(OEP) (24.0 mg, 19.9 µmol) and C_{60} (15 mg, 20.8 µmol) were dissolved in 1,2,4-trichlorobenzene (5 mL), and the solution was sonicated for 1 min. The obtained solution was diffused into hexane to afford black crystals (18.3 mg, 47.7%). Elemental analysis calcd (%) for [Tb(Pc)(OEP)]$(C_{60})_{0.8}(TCB)_{0.25}$: C 76.17, H 3.40, N 9.07;found: C 76.167, H 3.396, N 9.369.

S1.7 Synthesis of [Tb(Pc)(OEP)](C_{60})(Et_2O) (5)

Tb(Pc)(OEP) (12.0 mg, 9.97 µmol) and C_{60} (7.2 mg, 10 µmol) were added in *o*-dichlorobenzene (2 mL) and Et_2O (2 mL). The mixture was sonicated for 1 min to dissolve all materials. The obtained solution was diffused into hexane to afford black crystals (15.0 mg, 76.2%). Elemental analysis calcd (%) for [Tb(Pc)(OEP)]$(C_{60})_{1.1}(Et2O)_{0.75}$: C 80.17, H 3.31, N 8.19;found: C 80.291, H 3.339, N 8.143.

S1.8 Synthesis of TBA^+[Tb(Pc)(OEP)]$^-$

Tb(Pc)(OEP) (12.3 mg, 10.2 µmol) and TBABr (12.4 mg, 38.5 µmol) were suspended in MeOH (3 mL). Hydrazine monohydrate (1.0 mL, 31.6 mmol) was added to the solution, and the solution was sonicated for 5 min. Distilled water was added, and the aqueous phase was extracted with CH_2Cl_2. The organic layer was dried over $MgSO_4$. Deep blue green crystals were obtained from CH_2Cl_2/toluene (9.0 mg, 60.9%). Elemental analysis calcd (%) for [Tb(Pc)(OEP)]$^-$TBA$^+$: C 69.74, H 6.69, N 12.59; found: C 69.529, H 6.782, N 12.860.

S1.9 Synthesis of [Tb(Pc)(OEP)]$^+$$SbCl_6^-$

Tb(Pc)(OEP) (24.0 mg, 19.9 µmol) and phenoxathiin hexachloroantimonate (11 mg, 20.6 µmol) were dissolved in CH_2Cl_2 (5 mL), and the solution was sonicated for 1 min. The obtained solution was diffused into hexane to afford black crystals (29 mg, 89.6%). Elemental analysis calcd (%) for [Tb(Pc)(OEP)]$^+$$SbCl_6^-(CH_2Cl_2)_{0.7}$: C 51.63, H 3.87, N 10.52; found: C 51.562, H 4.155, N 10.481.

S2. X-ray Crystal Structure Analysis

Single crystal X-ray diffraction data were collected on a Rigaku Saturn 724+ CCD and Rigaku HyPix-6000HE detectors using Mo Kα radiation (λ = 0.71069 Å). All non-hydrogen atoms were refined anisotropically using a least-squares method, and hydrogen atoms were fixed at calculated positions and refined using a riding model. SHELXL–2014/7 was used for structure refinement.[4] Squeeze processes were applied for **1** and **2** using PLATON[5] because of the unassignable electron densities on the voids in the crystal packings. Powder X-ray diffraction patterns were recorded using HyPix-6000HE detectors and crushed crystalline samples packed inside a borosilicate glass capillary (diameter: 0.8 mm; length: 80 mm; Hilgenderg). Mercury 4.30 was used for visualizing the structures and simulating PXRD patterns.[6]

S3. Magnetic Properties measurement

Magnetic susceptibility measurements were performed on a Quantum Design SQUID magnetometer (model MPMS–XL and MPMS-3 SQUID magnetometer, Quantum Design, San Diego, CA, USA). Polycrystalline samples were placed in gelatin capsules and fixed with *n*-eicosane. The temperature dependent magnetic susceptibility data were collected from 300 to 1.82 K. Alternating current (ac) measurements were performed in the ac frequency (*v*) range of 0.1–1500 Hz with an ac field amplitude of 3 Oe. All data were corrected for the sample holder, *n*-eicosane, and diamagnetic contributions from the molecules by using Pascal's constants.

AC magnetic susceptibilities were analyzed using generalized Debye model:

$$\chi_M^{'} = \chi_S + (\chi_T - \chi_S)\frac{1 + (2\pi\nu\tau)^{1-\alpha}\sin\left(\frac{1}{2\pi\alpha}\right)}{1 + 2(2\pi\nu\tau)^{1-\alpha}\sin\left(\frac{1}{2\pi\alpha}\right) + (2\pi\tau)^{2-2\alpha}} \quad \text{Eq. S1a}$$

$$\chi_M^{''} = (\chi_T - \chi_S)\frac{\beta(2\pi\nu\tau)^{1-\alpha}\cos\left(\frac{1}{2\pi\alpha}\right)}{1 + 2(2\pi\nu\tau)^{1-\alpha}\sin\left(\frac{1}{2\pi\alpha}\right) + (2\pi\tau)^{2-2\alpha}} \quad \text{Eq. S1b}$$

where χ_s is adiabatic susceptibility, χ_T is isothermal magnetic susceptibility, τ is relaxation time and α is dispersion factor.

For the samples undergoing dual magnetic relaxations, the extended Debye model equations made by connecting two Debye model equations were used.

$$\chi_M^{'} = \chi_S + (\chi_T - \chi_S)\left[\frac{\beta\left\{1 + (2\pi\nu\tau_1)^{1-\alpha_1}\sin\left(\frac{1}{2\pi\alpha_1}\right)\right\}}{1 + 2(2\pi\nu\tau_1)^{1-\alpha_1}\sin\left(\frac{1}{2\pi\alpha_1}\right) + (2\pi\tau_1)^{2-2\alpha_1}} + \frac{(1-\beta)\left\{1 + (2\pi\nu\tau_2)^{1-\alpha_2}\sin\left(\frac{1}{2\pi\alpha_2}\right)\right\}}{1 + 2(2\pi\nu\tau_2)^{1-\alpha_2}\sin\left(\frac{1}{2\pi\alpha_2}\right) + (2\pi\tau_2)^{2-2\alpha_2}}\right] \quad \text{Eq. S2a}$$

$$\chi_M^{''} = (\chi_T - \chi_S)\left[\frac{\beta(2\pi\nu\tau_1)^{1-\alpha_1}\cos\left(\frac{1}{2\pi\alpha_1}\right)}{1 + 2(2\pi\nu\tau_1)^{1-\alpha_1}\sin\left(\frac{1}{2\pi\alpha_1}\right) + (2\pi\tau_1)^{2-2\alpha_1}} + \frac{(1-\beta)\beta(2\pi\nu\tau_2)^{1-\alpha_2}\cos\left(\frac{1}{2\pi\alpha_2}\right)}{1 + 2(2\pi\nu\tau_2)^{1-\alpha_2}\sin\left(\frac{1}{2\pi\alpha_2}\right) + (2\pi\tau_2)^{2-2\alpha_2}}\right] \quad \text{Eq. S2b}$$

In these equations, β is the ratio of two Debye type relaxations.

Table S1. Crystallographic data for **1**–**5**.

	[Tb(Pc)(OEP)]$_3$ (Li$^+$@C$_{60}$·PF$_6^-$)$_2$ (**1**)	[Tb(Pc)(OEP)] (Li$^+$@C$_{60}$·BF$_4^-$) (**2**)	[Tb(Pc)(OEP)](C$_{70}$) (C$_6$H$_{14}$) (**3**)	[Tb(Pc)(OEP)](C$_{60}$) (C$_6$H$_{14}$) (**4**)	[Tb(Pc)(OEP)](C$_{60}$) (Et$_2$O) (**5**)
Formula	$C_{162}H_{90}N_{18}F_6PTb_{1.5}$	$C_{64}H_{30}N_6B_{0.5}F_2Tb_{0.5}$	$C_{72}H_{37}N_6Tb_{0.5}$	$C_{67}H_{37}N_6Tb_{0.5}$	$C_{66}H_{35}N_6O_{0.5}Tb_{0.5}$
Formula weight	5357.72	2018.60	2131.06	2011.06	1974.95
Temperature (K)	100(2)	100(2)	120(2)	120(2)	100(2)
Crystal system	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic
Space Group	$Cmc2_1$	$P2_1/m$	$C2/c$	$C2/m$	$C2/m$
a (Å)	26.9958(6)	15.1885(5)	24.8514(6)	22.8110(2)	22.7366(10)
b (Å)	42.7901(7)	21.4887(6)	15.5073(2)	17.4164(2)	17.3024(11)
c (Å)	23.1133(6)	19.0990(6)	27.2445(6)	22.0814(2)	22.0606(10)
β (°)	90	104.999(3)	118.812(3)	90.9870(10)	90.923(4)
Cell volume (Å^3)	26699.4(10)	6021.2(3)	9199.7(4)	8771.32(15)	8677.5(8)
Z	8	4	4	8	8
R_1 [$I > 2\sigma(I)$]	0.1035	0.0649	0.0278	0.0408	0.1252
wR_2 [$I > 2\sigma(I)$]	0.2520	0.1669	0.0694	0.1071	0.2828
R_1 (all)	0.1415	0.0834	0.0301	0.0437	0.1268
wR_2 (all)	0.2842	0.1749	0.0703	0.1085	0.2837
Goodness of fit	1.008	1.066	1.047	1.060	1.173

Table S2. Selected structural information for **1**–**5**

	1		**2**	**3**	**4**	**5**
	Tb1	Tb2				
Average Tb-N$_{OEP}$ bond distance (Å)	2.440	2.410	2.421	2.427	2.421	2.418
Average Tb-N$_{Pc}$ bond distance (Å)	2.470	2.453	2.439	2.450	2.459	2.446
Tb-OEP plane distance (Å)	1.280	1.272	1.266	1.287	1.285	1.291
Tb-Pc plane distance (Å)	1.440	1.467	1.453	1.459	1.479	1.471
OEP-Pc plane distance (Å)	2.720	2.738	2.739	2.746	2.764	2.762
OEP-Pc twist angle (°)	45.00	43.53	45.00	44.91	43.90	45.00
OEP dihedral angle (°)	11.11	11.16	11.64	11.50	8.965	11.45
Pc dihedral angle (°)	10.47	8.16	10.86	10.18	8.780	8.88

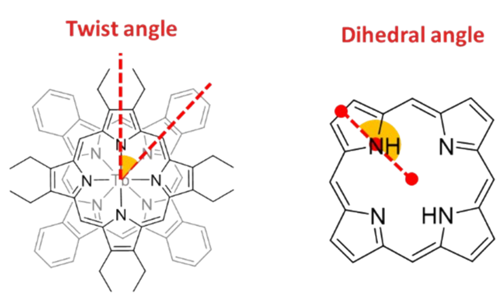

Fig. S1 Representations of twist and dihedral angles.

Table S3. Crystallographic data for the redox series of [Tb(Pc)(OEP)].

	$TBA^+[Tb(Pc)(OEP)]^-$	Tb(Pc)(OEP)	$[Tb(Pc)(OEP)]^+SbCl_6^-$ (CH_2Cl_2)
Formula	$C_{84}H_{60}N_{13}Tb$	$C_{68}H_{60}N_{12}$ Tb	C_{69} $H_{62}Cl_{18}N_{12}SbTb$
Formula weight	1410.37	1204.20	1623.57
Temperature (K)	100(2)	296(2)	100(2)
Crystal system	monoclinic	monoclinic	triclinic
Space Group	$P2_1/n$	$P2_1/n$	$P\bar{1}$
a (Å)	14.9131(7)	15.0313(5)	13.1037(2)
b (Å)	23.0259(9)	17.7925(6)	15.3447(2)
c (Å)	21.9427(10)	21.8637(7)	18.9271(4)
α (°)	90	90	108.8830(10)
β (°)	104.777(5)	96.3300(10)	104.2230(10)
γ (°)	90	90	91.5740(10)
Cell volume (Å^3)	7285.6(6)	5811.7(3)	3466.69(10)
Z	4	4	2
R_1 [$I > 2\sigma(I)$]	0.1001	0.0343	0.0321
wR_2 [$I > 2\sigma(I)$]	0.1691	0.0662	0.0915
R_1 (all)	0.1572	0.0541	0.0875
wR_2 (all)	0.1875	0.0723	0.0887
Goodness of fit	1.185	1.060	1.018

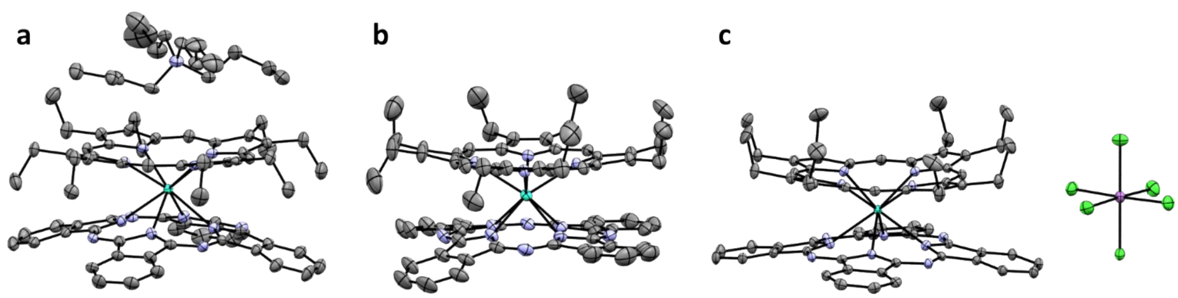

Fig. S2 Crystal structures of (a) $[Tb(Pc)(OEP)]^-TBA^+$, (b) Tb(Pc)(OEP) and (c) $Tb(Pc)(OEP)]^+SbCl_6^-$. Hydrogen atoms and solvent atoms are omitted for clarity. Ellipsoids are drawn at 50% probability (30% for Tb(Pc)(OEP).

Table S4. Selected structural information for the redox series of [Tb(Pc)(OEP)].

	$[Tb(Pc)(OEP)]^-TBA^+$	Tb(Pc)(OEP)	$[Tb(Pc)(OEP)]^+SbCl_6^-$
Average Tb-N_{OEP} bond distance (Å)	2.440	2.428	2.423
Average Tb-N_{Pc} bond distance (Å)	2.478	2.457	2.429
Tb-OEP plane distance (Å)	1.319	1.299	1.301
Tb-Pc plane distance (Å)	1.448	1.483	1.438
OEP-Pc plane distance (Å)	2.807	2.782	2.739
OEP-Pc twist angle (°)	39.71	44.84	40.22
OEP dihedral angle (°)	10.56	10.01	8.548
Pc dihedral angle (°)	15.82	9.517	8.678

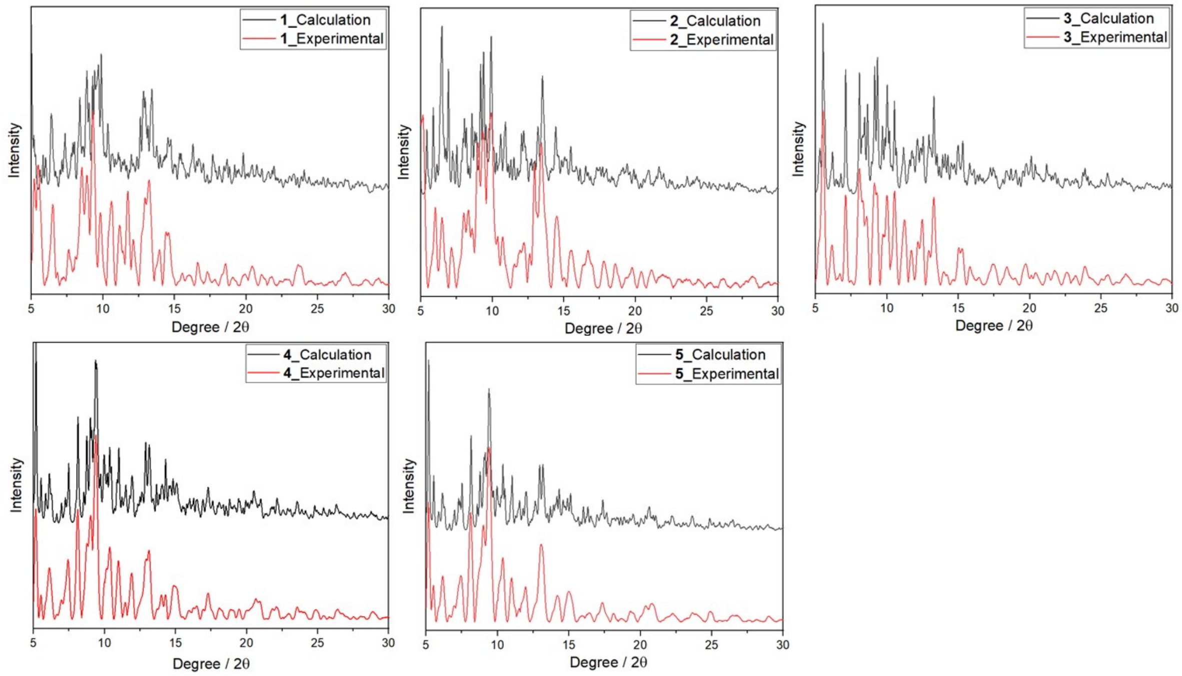

Fig. S3 Experimental and simulated PXRD patterns of **1**–**5**.

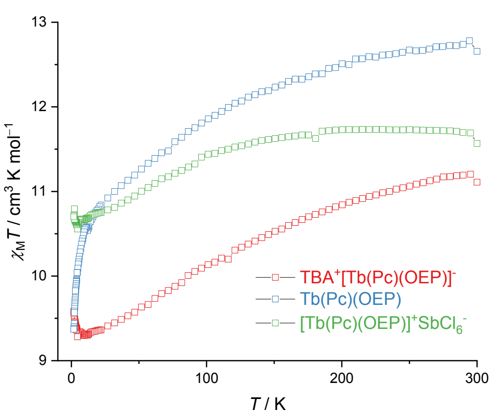

Fig. S4 $\chi_M T$ vs T plots for the redox series of Tb(Pc)(OEP) complexes.

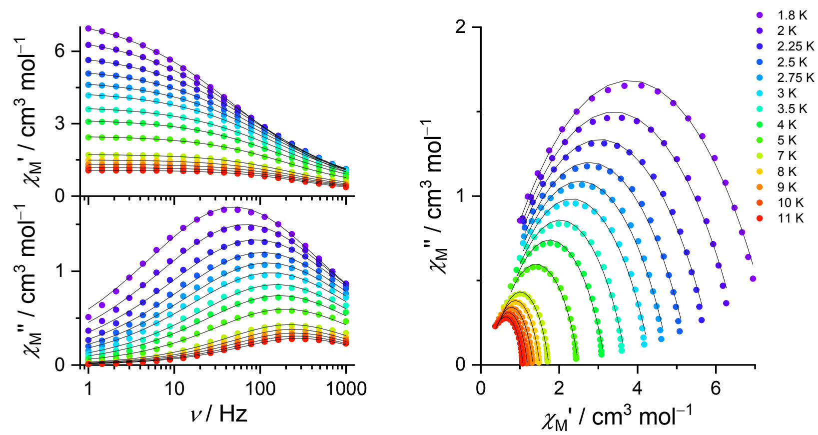

Fig. S5 AC magnetic susceptibilities for **1** in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

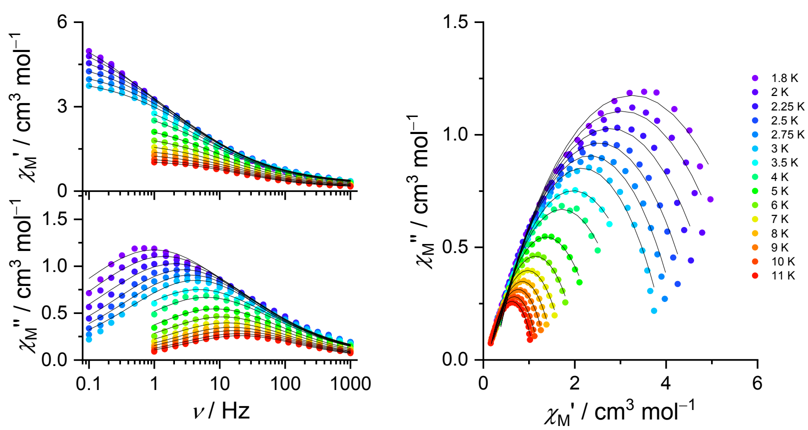

Fig. S6 AC magnetic susceptibilities for **1** in a 2 kOe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

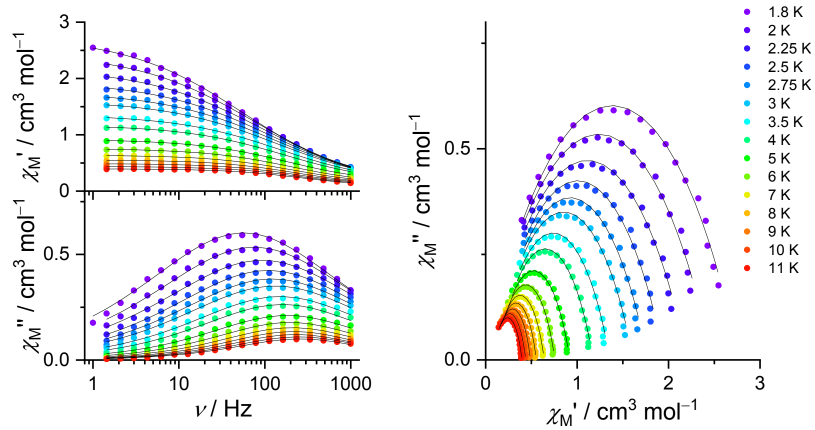

Fig. S7 AC magnetic susceptibilities for **2** in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

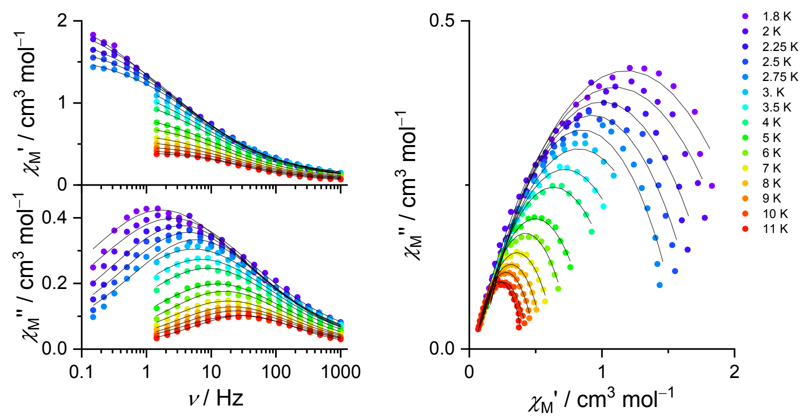

Fig. S8 AC magnetic susceptibilities for **2** in a 2 kOe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

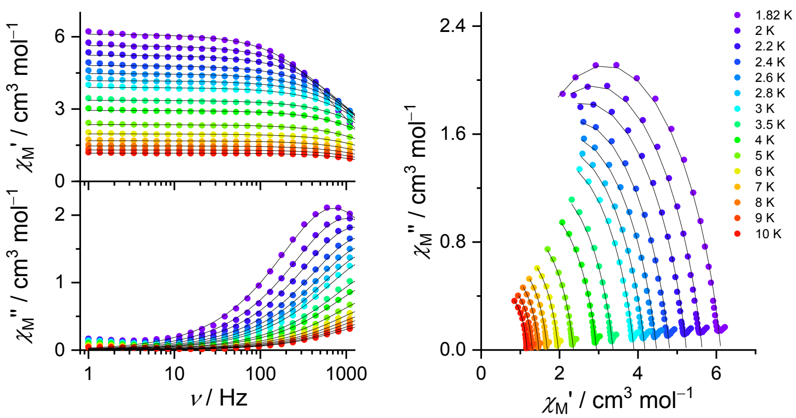

Fig. S9 AC magnetic susceptibilities for **3** in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

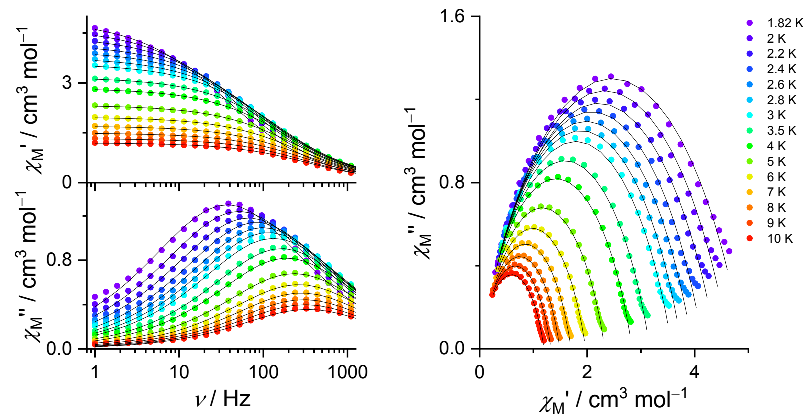

Fig. S10 AC magnetic susceptibilities for **3** in a 2 kOe dc magnetic field. Solid curves represent fits using Eq. S1.

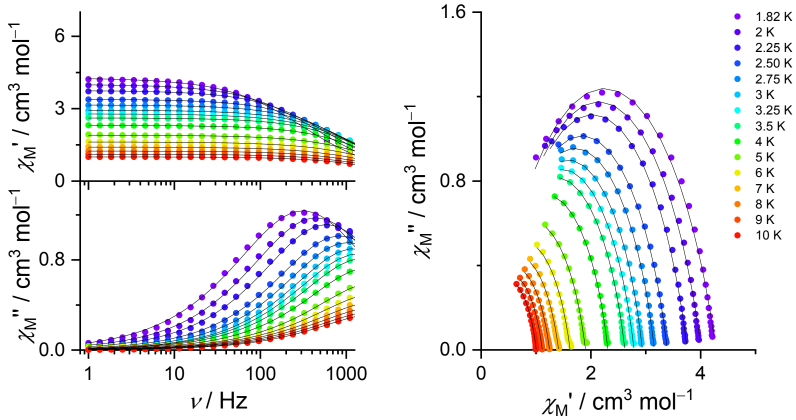

Fig. S11 AC magnetic susceptibilities for **4** in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1.

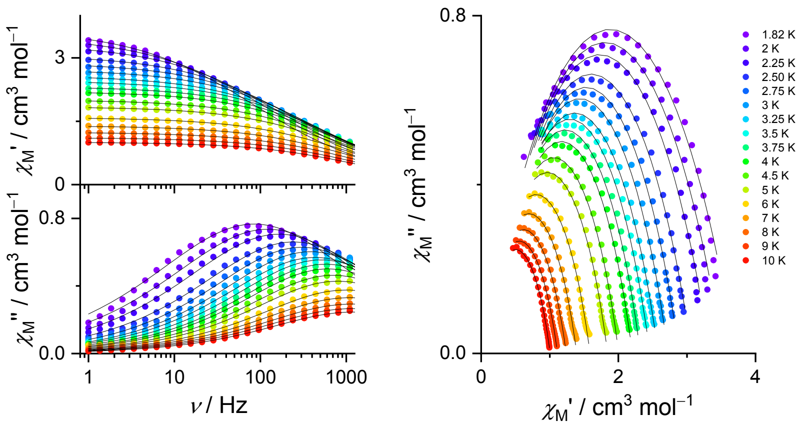

Fig. S12 AC magnetic susceptibilities for **4** in a 2 kOe dc magnetic field. Solid curves represent fits using Eq. S1.

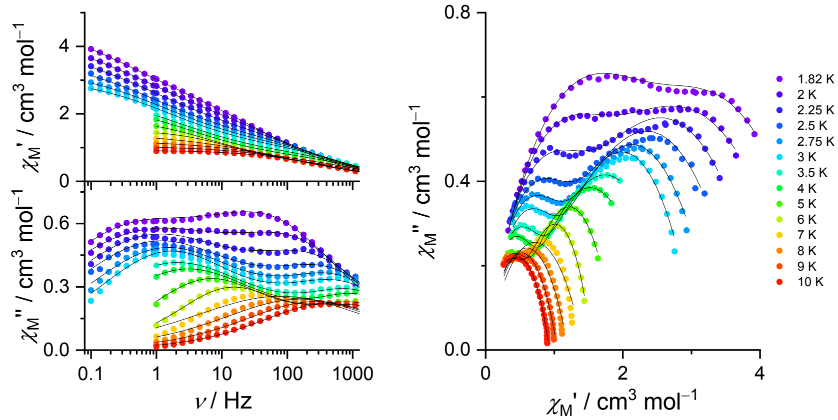

Fig. S13 AC magnetic susceptibilities for **5** in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S2a and S2b.

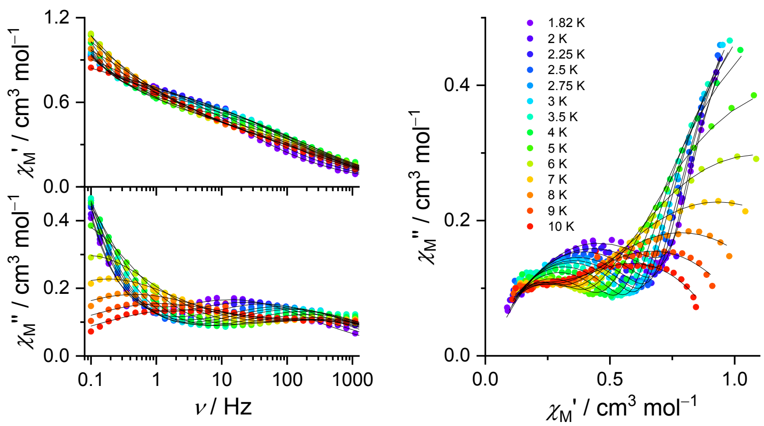

Fig. S14 AC magnetic susceptibilities for **5** in a 3 kOe dc magnetic field. Solid curves represent fits using Eq. S2a and S2b.

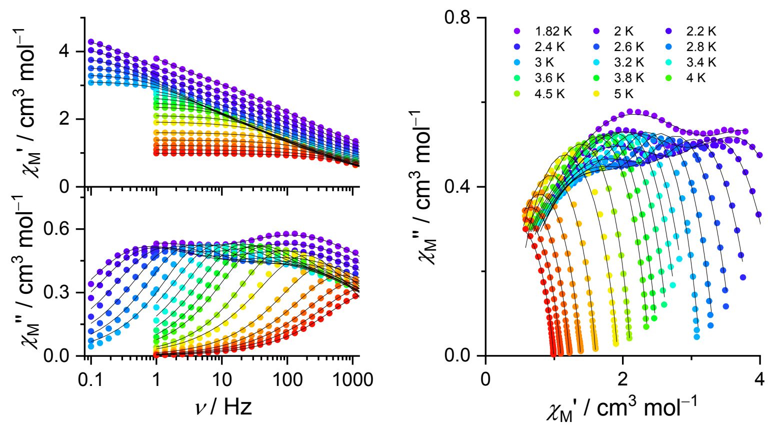

Fig. S15 AC magnetic susceptibilities for Tb(Pc)(OEP) in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S2a and S2b.

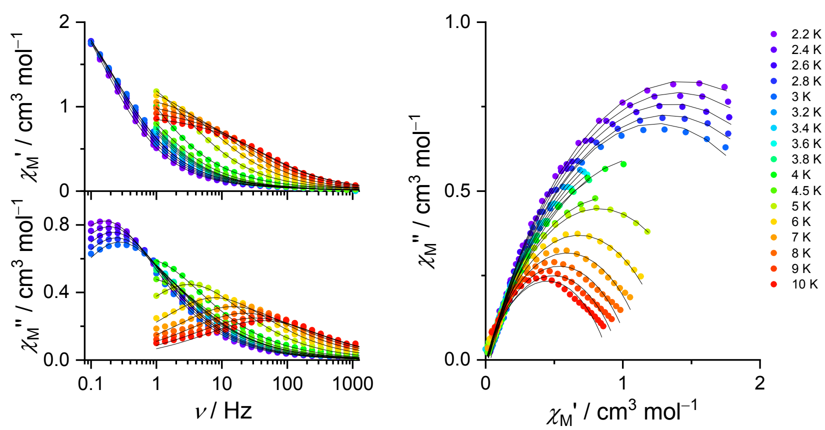

Fig. S16 AC magnetic susceptibilities for Tb(Pc)(OEP) in a 3 kOe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

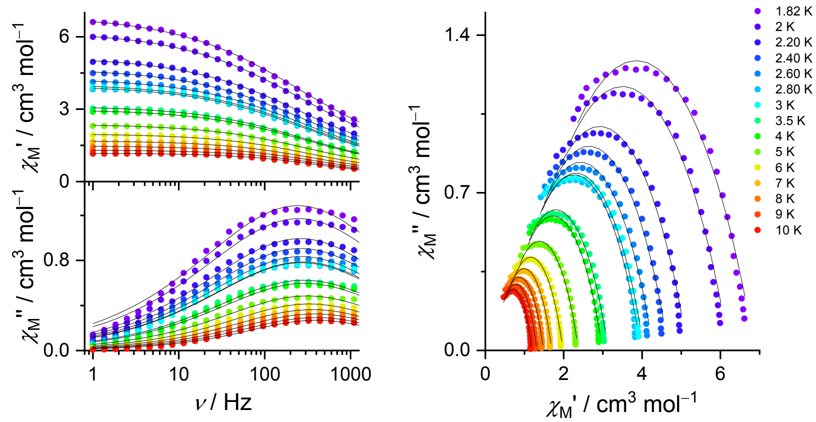

Fig. S17 AC magnetic susceptibilities for TBA$^+$[Tb(Pc)(OEP)]$^-$ in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

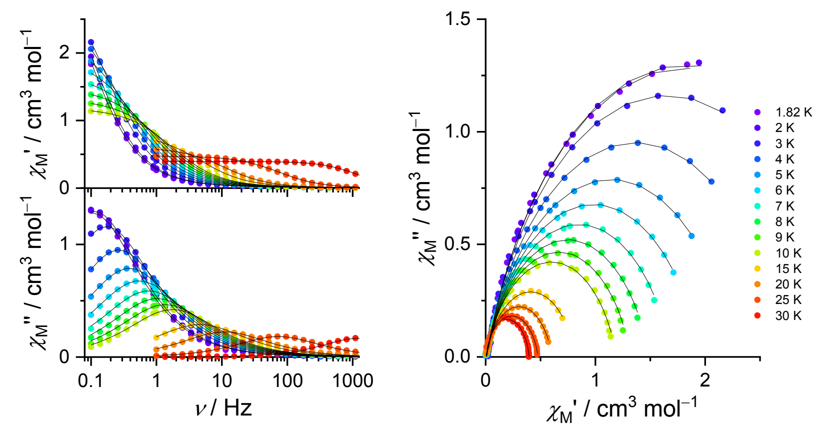

Fig. S18 AC magnetic susceptibilities for TBA$^+$[Tb(Pc)(OEP)]$^-$ in a 3 kOe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

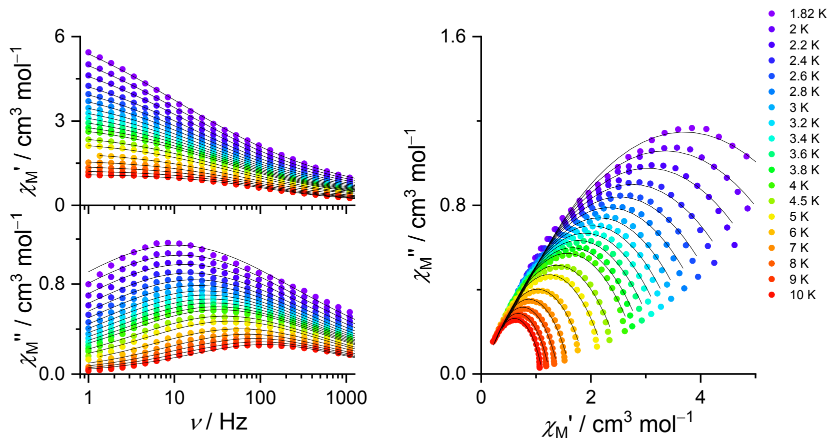

Fig. S19 AC magnetic susceptibilities for $[Tb(Pc)(OEP)]^{+}SbCl_6^{-}$ in a 0 Oe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

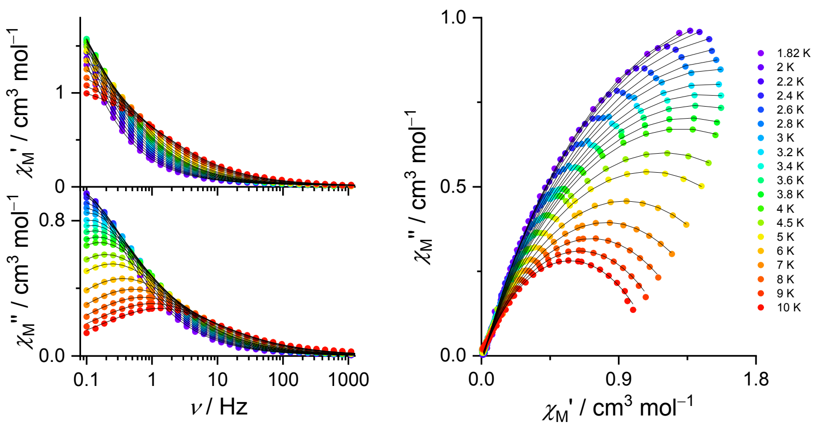

Fig. S20 AC magnetic susceptibilities for $[Tb(Pc)(OEP)]^{+}SbCl_6^{-}$ in a 3 kOe dc magnetic field. Solid curves represent fits using Eq. S1a and S1b.

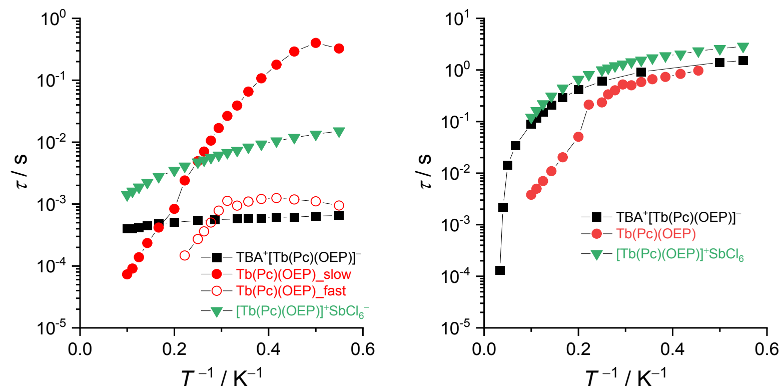

Fig. S21 τ vs T^{-1} plots for redox series of Tb(Pc)(OEP) in 0 Oe (left) and 3 kOe (right) dc bias fields.

Table S5. Fitting parameters for **1** in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S5.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.80	0.00E+00	3.36E-02	7.58E+00	2.55E-02	3.22E-03	4.74E-05	4.67E-01	4.19E-03
2.00	4.31E-02	4.11E-02	6.74E+00	2.58E-02	2.36E-03	4.61E-05	4.64E-01	5.30E-03
2.25	8.04E-02	4.59E-02	6.00E+00	2.41E-02	1.79E-03	4.30E-05	4.60E-01	6.18E-03
2.50	1.70E-01	4.69E-02	5.36E+00	2.21E-02	1.51E-03	4.14E-05	4.48E-01	6.96E-03
2.75	2.22E-01	4.63E-02	4.84E+00	2.00E-02	1.31E-03	3.93E-05	4.38E-01	7.50E-03
3.00	2.71E-01	4.73E-02	4.36E+00	1.92E-02	1.20E-03	4.07E-05	4.29E-01	8.52E-03
3.50	3.15E-01	3.95E-02	3.73E+00	1.47E-02	1.04E-03	3.41E-05	4.07E-01	8.42E-03
4.00	3.33E-01	3.65E-02	3.18E+00	1.28E-02	9.47E-04	3.34E-05	3.90E-01	9.26E-03
5.00	3.15E-01	2.96E-02	2.50E+00	9.47E-03	8.24E-04	2.94E-05	3.63E-01	9.73E-03
7.00	2.76E-01	1.93E-02	1.74E+00	5.65E-03	7.08E-04	2.28E-05	3.20E-01	9.54E-03
8.00	2.54E-01	1.57E-02	1.51E+00	4.47E-03	6.71E-04	1.99E-05	3.02E-01	9.09E-03
9.00	2.28E-01	1.36E-02	1.33E+00	3.71E-03	6.29E-04	1.80E-05	2.93E-01	8.81E-03
10.0	2.11E-01	1.25E-02	1.19E+00	3.30E-03	5.99E-04	1.73E-05	2.81E-01	9.07E-03
11.0	1.85E-01	1.09E-02	1.08E+00	2.79E-03	5.66E-04	1.55E-05	2.74E-01	8.62E-03

Table S6. Fitting parameters for **1** in a dc magnetic field of 2 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S6.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.80	1.50E-01	2.65E-02	6.36E+00	8.81E-02	1.59E-01	8.65E-03	5.40E-01	7.97E-03
2.00	1.69E-01	2.61E-02	5.89E+00	7.15E-02	1.12E-01	5.30E-03	5.30E-01	7.93E-03
2.25	1.81E-01	2.62E-02	5.35E+00	5.90E-02	7.76E-02	3.34E-03	5.18E-01	8.23E-03
2.50	2.25E-01	2.25E-02	4.84E+00	4.28E-02	5.64E-02	1.97E-03	4.96E-01	7.66E-03
2.75	2.25E-01	2.21E-02	4.44E+00	3.72E-02	4.49E-02	1.52E-03	4.82E-01	7.98E-03
3.00	2.37E-01	1.90E-02	4.09E+00	2.91E-02	3.72E-02	1.09E-03	4.70E-01	7.33E-03
3.50	1.83E-01	9.71E-03	3.75E+00	3.24E-02	3.37E-02	9.88E-04	4.91E-01	5.15E-03
4.00	1.72E-01	1.00E-02	3.26E+00	2.80E-02	2.57E-02	7.31E-04	4.80E-01	5.73E-03
5.00	1.67E-01	8.45E-03	2.57E+00	1.92E-02	1.86E-02	4.52E-04	4.57E-01	5.82E-03
6.00	1.53E-01	8.54E-03	2.13E+00	1.66E-02	1.46E-02	3.74E-04	4.43E-01	6.82E-03
7.00	1.45E-01	6.58E-03	1.80E+00	1.14E-02	1.23E-02	2.58E-04	4.29E-01	6.07E-03
8.00	1.33E-01	6.40E-03	1.57E+00	1.01E-02	1.05E-02	2.27E-04	4.24E-01	6.53E-03
9.00	1.20E-01	7.04E-03	1.40E+00	1.05E-02	9.59E-03	2.45E-04	4.21E-01	7.85E-03
10.0	1.15E-01	5.49E-03	1.24E+00	7.42E-03	8.21E-03	1.73E-04	4.08E-01	6.82E-03
11.0	1.15E-01	6.37E-03	1.13E+00	8.18E-03	7.58E-03	1.96E-04	3.95E-01	8.72E-03

Table S7. Fitting parameters for **2** in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S7.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.80	0.00E+00	2.14E-02	2.77E+00	1.49E-02	2.81E-03	7.10E-05	4.77E-01	6.88E-03
2.00	0.00E+00	2.32E-02	2.47E+00	1.50E-02	2.11E-03	6.22E-05	4.80E-01	7.88E-03
2.25	2.04E-02	2.40E-02	2.20E+00	1.36E-02	1.72E-03	5.83E-05	4.80E-01	8.63E-03
2.50	6.04E-02	2.55E-02	1.96E+00	1.29E-02	1.46E-03	5.92E-05	4.64E-01	1.03E-02
2.75	8.08E-02	2.27E-02	1.77E+00	1.07E-02	1.31E-03	5.26E-05	4.56E-01	1.01E-02
3.00	9.22E-02	2.14E-02	1.61E+00	9.53E-03	1.20E-03	5.02E-05	4.50E-01	1.03E-02
3.50	1.17E-01	2.04E-02	1.36E+00	8.34E-03	1.06E-03	5.00E-05	4.26E-01	1.20E-02
4.00	1.29E-01	1.58E-02	1.17E+00	6.15E-03	9.89E-04	4.15E-05	4.06E-01	1.11E-02
5.00	1.25E-01	1.21E-02	9.20E-01	4.33E-03	8.74E-04	3.53E-05	3.78E-01	1.11E-02
6.00	1.19E-01	9.50E-03	7.56E-01	3.26E-03	8.15E-04	3.10E-05	3.51E-01	1.11E-02
7.00	1.11E-01	7.79E-03	6.40E-01	2.56E-03	7.61E-04	2.76E-05	3.32E-01	1.09E-02
8.00	1.07E-01	6.47E-03	5.54E-01	2.09E-03	7.33E-04	2.52E-05	3.07E-01	1.10E-02
9.00	9.85E-02	6.04E-03	4.89E-01	1.89E-03	6.96E-04	2.49E-05	2.94E-01	1.17E-02
10.0	8.58E-02	5.35E-03	4.38E-01	1.58E-03	6.43E-04	2.23E-05	2.90E-01	1.12E-02
11.0	8.15E-02	4.22E-03	3.96E-01	1.23E-03	6.24E-04	1.88E-05	2.78E-01	9.90E-03

Table S8. Fitting parameters for **2** in a dc magnetic field of 2 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S8.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.80	5.15E-02	1.24E-02	2.32E+00	3.52E-02	9.30E-02	5.48E-03	5.44E-01	9.21E-03
2.00	3.02E-02	1.35E-02	2.16E+00	3.09E-02	6.28E-02	3.47E-03	5.44E-01	9.57E-03
2.25	8.03E-02	1.10E-02	1.92E+00	2.13E-02	4.58E-02	1.97E-03	5.05E-01	9.14E-03
2.50	8.90E-02	1.07E-02	1.76E+00	1.81E-02	3.57E-02	1.44E-03	4.88E-01	9.44E-03
2.75	9.18E-02	9.67E-03	1.61E+00	1.42E-02	2.74E-02	9.80E-04	4.71E-01	9.09E-03
3.00	6.12E-02	4.12E-03	1.59E+00	1.47E-02	2.97E-02	9.53E-04	5.15E-01	4.96E-03
3.50	6.79E-02	4.93E-03	1.37E+00	1.49E-02	2.27E-02	8.21E-04	4.93E-01	6.67E-03
4.00	7.22E-02	4.49E-03	1.19E+00	1.17E-02	1.81E-02	5.76E-04	4.73E-01	6.81E-03
5.00	6.52E-02	3.15E-03	9.29E-01	6.43E-03	1.26E-02	2.79E-04	4.51E-01	5.72E-03
6.00	6.62E-02	3.99E-03	7.78E-01	6.96E-03	9.94E-03	2.83E-04	4.14E-01	8.63E-03
7.00	5.73E-02	2.79E-03	6.60E-01	4.47E-03	8.74E-03	1.93E-04	4.22E-01	6.73E-03
8.00	5.57E-02	2.41E-03	5.70E-01	3.50E-03	7.51E-03	1.53E-04	4.08E-01	6.63E-03
9.00	4.98E-02	2.06E-03	5.04E-01	2.73E-03	6.50E-03	1.20E-04	3.94E-01	6.27E-03
10.0	4.87E-02	3.18E-03	4.55E-01	4.03E-03	6.08E-03	1.89E-04	4.06E-01	1.04E-02
11.0	4.81E-02	2.47E-03	4.10E-01	2.81E-03	5.14E-03	1.25E-04	3.41E-01	9.39E-03

Table S9. Fitting parameters for **3** in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S59.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	1.93E-01	9.83E-02	6.11E+00	1.55E-02	2.20E-04	7.08E-06	2.12E-01	9.69E-03
2.00	9.97E-02	1.38E-01	5.64E+00	1.56E-02	1.55E-04	7.46E-06	2.16E-01	1.22E-02
2.20	2.70E-02	1.80E-01	5.24E+00	1.54E-02	1.20E-04	7.91E-06	2.20E-01	1.46E-02
2.40	0.00E+00	2.25E-01	4.81E+00	1.50E-02	9.59E-05	8.54E-06	2.19E-01	1.74E-02
2.60	0.00E+00	2.66E-01	4.47E+00	1.49E-02	8.27E-05	9.25E-06	2.17E-01	2.02E-02
2.80	0.00E+00	2.90E-01	4.18E+00	1.40E-02	7.35E-05	9.49E-06	2.15E-01	2.19E-02
3.00	0.00E+00	3.03E-01	3.90E+00	1.32E-02	6.74E-05	9.66E-06	2.12E-01	2.33E-02
3.50	0.00E+00	3.47E-01	3.37E+00	1.16E-02	5.50E-05	1.04E-05	2.13E-01	2.70E-02
4.00	0.00E+00	5.37E-01	2.95E+00	1.38E-02	4.42E-05	1.50E-05	2.32E-01	4.12E-02
5.00	0.00E+00	2.87E-01	2.36E+00	8.20E-03	4.92E-05	1.07E-05	2.04E-01	2.97E-02
6.00	0.00E+00	2.52E-01	1.97E+00	6.75E-03	4.70E-05	1.07E-05	2.04E-01	3.01E-02
7.00	0.00E+00	2.15E-01	1.69E+00	5.68E-03	4.70E-05	1.05E-05	1.94E-01	3.00E-02
8.00	5.93E-02	1.68E-01	1.47E+00	4.95E-03	5.15E-05	1.04E-05	1.76E-01	2.99E-02
9.00	1.62E-01	1.25E-01	1.30E+00	4.33E-03	5.87E-05	1.06E-05	1.55E-01	3.01E-02
10.0	1.55E-01	1.10E-01	1.17E+00	3.86E-03	5.92E-05	1.06E-05	1.52E-01	3.01E-02

Table S10. Fitting parameters for **3** in a dc magnetic field of 2 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S10.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	0.00E+00	1.93E-02	4.92E+00	1.96E-02	4.25E-03	6.15E-05	3.80E-01	5.03E-03
2.00	0.00E+00	2.22E-02	4.66E+00	1.88E-02	3.10E-03	5.00E-05	3.76E-01	5.60E-03
2.20	0.00E+00	2.58E-02	4.42E+00	1.88E-02	2.39E-03	4.46E-05	3.74E-01	6.40E-03
2.40	0.00E+00	2.39E-02	4.17E+00	1.54E-02	1.93E-03	3.36E-05	3.62E-01	6.00E-03
2.60	0.00E+00	2.25E-02	3.96E+00	1.31E-02	1.62E-03	2.69E-05	3.57E-01	5.67E-03
2.80	0.00E+00	2.22E-02	3.77E+00	1.19E-02	1.39E-03	2.35E-05	3.52E-01	5.68E-03
3.00	0.00E+00	2.54E-02	3.58E+00	1.24E-02	1.21E-03	2.40E-05	3.52E-01	6.52E-03
3.50	0.00E+00	2.06E-02	3.17E+00	8.86E-03	9.69E-04	1.70E-05	3.38E-01	5.70E-03
4.00	0.00E+00	1.86E-02	2.84E+00	7.31E-03	8.37E-04	1.44E-05	3.33E-01	5.52E-03
5.00	0.00E+00	1.74E-02	2.33E+00	5.99E-03	6.82E-04	1.30E-05	3.28E-01	5.91E-03
6.00	0.00E+00	1.62E-02	1.97E+00	5.17E-03	6.05E-04	1.25E-05	3.23E-01	6.29E-03
7.00	0.00E+00	1.47E-02	1.70E+00	4.43E-03	5.58E-04	1.19E-05	3.18E-01	6.44E-03
8.00	0.00E+00	1.32E-02	1.49E+00	3.81E-03	5.24E-04	1.14E-05	3.16E-01	6.46E-03
9.00	0.00E+00	1.25E-02	1.33E+00	3.54E-03	5.03E-04	1.15E-05	3.11E-01	6.88E-03
10.0	0.00E+00	1.41E-02	1.20E+00	3.79E-03	4.71E-04	1.35E-05	3.16E-01	8.29E-03

Table S11. Fitting parameters for **4** in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S11.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	2.18E-01	2.77E-02	4.28E+00	7.92E-03	5.06E-04	8.29E-06	3.02E-01	5.04E-03
2.00	2.74E-01	2.88E-02	4.01E+00	6.49E-03	3.60E-04	6.30E-06	2.84E-01	5.12E-03
2.25	2.98E-01	2.89E-02	3.75E+00	5.26E-03	2.72E-04	4.95E-06	2.70E-01	5.02E-03
2.50	2.85E-01	2.49E-02	3.39E+00	3.32E-03	1.90E-04	3.21E-06	2.63E-01	4.12E-03
2.75	2.69E-01	2.82E-02	3.16E+00	3.09E-03	1.54E-04	3.11E-06	2.55E-01	4.57E-03
3.00	2.41E-01	3.03E-02	2.94E+00	2.80E-03	1.30E-04	2.97E-06	2.51E-01	4.82E-03
3.25	1.80E-01	2.82E-02	2.79E+00	2.25E-03	1.13E-04	2.53E-06	2.60E-01	4.29E-03
3.50	1.44E-01	3.47E-02	2.62E+00	2.44E-03	1.00E-04	2.88E-06	2.58E-01	5.21E-03
4.00	1.04E-01	4.08E-02	2.31E+00	2.42E-03	8.63E-05	3.22E-06	2.53E-01	6.32E-03
5.00	0.00E+00	8.21E-02	1.90E+00	3.68E-03	6.65E-05	5.97E-06	2.77E-01	1.25E-02
6.00	0.00E+00	8.32E-02	1.62E+00	3.53E-03	6.30E-05	6.82E-06	2.87E-01	1.44E-02
7.00	0.00E+00	6.04E-02	1.41E+00	2.49E-03	6.09E-05	5.56E-06	2.94E-01	1.17E-02
8.00	0.00E+00	3.43E-02	1.25E+00	1.40E-03	6.07E-05	3.55E-06	2.90E-01	7.54E-03
9.00	0.00E+00	1.89E-02	1.11E+00	7.66E-04	6.08E-05	2.15E-06	2.81E-01	4.66E-03
10.0	0.00E+00	1.69E-02	1.00E+00	6.80E-04	6.13E-05	2.09E-06	2.64E-01	4.68E-03

Table S12. Fitting parameters for **4** in a dc magnetic field of 2 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S12.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	6.85E-02	2.54E-02	3.70E+00	1.58E-02	1.87E-03	4.37E-05	4.90E-01	5.83E-03
2.00	9.27E-02	2.73E-02	3.52E+00	1.37E-02	1.30E-03	3.37E-05	4.83E-01	6.04E-03
2.25	1.21E-01	2.66E-02	3.33E+00	1.10E-02	9.66E-04	2.54E-05	4.72E-01	5.83E-03
2.50	1.41E-01	2.47E-02	3.07E+00	7.95E-03	6.54E-04	1.71E-05	4.60E-01	5.33E-03
2.75	1.71E-01	2.54E-02	2.89E+00	7.06E-03	5.25E-04	1.49E-05	4.47E-01	5.61E-03
3.00	1.51E-01	2.76E-02	2.73E+00	6.53E-03	4.15E-04	1.34E-05	4.42E-01	5.97E-03
3.25	1.50E-01	2.62E-02	2.58E+00	5.69E-03	3.68E-04	1.19E-05	4.42E-01	5.74E-03
3.50	1.24E-01	3.13E-02	2.46E+00	6.01E-03	3.10E-04	1.23E-05	4.35E-01	6.78E-03
3.75	1.27E-01	3.55E-02	2.32E+00	6.23E-03	2.76E-04	1.30E-05	4.28E-01	7.91E-03
4.00	1.40E-01	3.00E-02	2.20E+00	5.03E-03	2.60E-04	1.09E-05	4.23E-01	6.99E-03
4.50	1.10E-01	2.96E-02	2.01E+00	4.44E-03	2.25E-04	1.01E-05	4.20E-01	7.12E-03
5.00	9.06E-02	3.00E-02	1.84E+00	4.10E-03	1.99E-04	9.78E-06	4.20E-01	7.44E-03
6.00	1.97E-02	3.41E-02	1.59E+00	3.92E-03	1.60E-04	1.01E-05	4.30E-01	8.54E-03
7.00	0.00E+00	3.23E-02	1.39E+00	3.45E-03	1.46E-04	9.89E-06	4.35E-01	8.70E-03
8.00	0.00E+00	2.65E-02	1.24E+00	2.72E-03	1.38E-04	8.69E-06	4.37E-01	7.82E-03
9.00	0.00E+00	1.67E-02	1.11E+00	1.69E-03	1.37E-04	5.98E-06	4.32E-01	5.51E-03
10.0	0.00E+00	1.13E-02	1.01E+00	1.11E-03	1.34E-04	4.26E-06	4.20E-01	4.13E-03

Table S13. Fitting parameters for **5** in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S13.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ_1 / s	SD_χ_T	α_1	SD_α_1	τ_2 / s	SD_τ_2	α_2	SD_α_2	β	SD_β
1.82	5.74E-04	1.25E-02	4.93E+00	7.58E-02	4.90E-01	4.84E-02	5.49E-01	2.48E-02	2.45E-03	2.06E-04	4.66E-01	1.30E-02	5.55E-01	3.98E-02
2.00	0.00E+00	1.41E-02	4.68E+00	7.81E-02	2.54E-01	3.07E-02	6.05E-01	2.11E-02	1.03E-03	7.31E-05	4.01E-01	2.47E-02	7.09E-01	4.04E-02
2.25	0.00E+00	2.75E-02	4.18E+00	6.18E-02	1.97E-01	1.85E-02	5.68E-01	1.99E-02	5.67E-04	4.49E-05	3.88E-01	3.27E-02	7.06E-01	3.62E-02
2.50	0.00E+00	4.10E-02	3.81E+00	5.38E-02	1.67E-01	1.34E-02	5.54E-01	1.87E-02	3.44E-04	2.76E-05	3.67E-01	4.23E-02	7.19E-01	3.43E-02
2.75	0.00E+00	3.93E-02	3.38E+00	2.81E-02	1.24E-01	6.74E-03	5.18E-01	1.29E-02	2.57E-04	1.76E-05	3.59E-01	3.55E-02	6.99E-01	2.54E-02
3.00	0.00E+00	5.27E-02	3.08E+00	2.38E-02	1.08E-01	6.03E-03	4.75E-01	1.40E-02	2.26E-04	2.07E-05	3.75E-01	4.24E-02	6.71E-01	2.94E-02
3.50	0.00E+00	1.78E-02	2.82E+00	3.02E-02	8.29E-02	2.42E-03	5.27E-01	9.58E-03	1.39E-04	5.30E-06	2.98E-01	2.08E-02	7.44E-01	1.45E-02
4.00	0.00E+00	2.33E-02	2.46E+00	2.35E-02	5.57E-02	1.45E-03	4.96E-01	1.00E-02	1.20E-04	6.68E-06	2.66E-01	2.73E-02	7.38E-01	1.67E-02
5.00	0.00E+00	3.57E-02	1.87E+00	1.12E-02	2.63E-02	8.33E-04	3.79E-01	1.16E-02	1.25E-04	1.09E-05	3.31E-01	3.97E-02	3.47E-01	2.67E-02
6.00	0.00E+00	3.31E-02	1.53E+00	5.43E-03	1.30E-02	4.91E-04	3.20E-01	1.07E-02	1.29E-04	1.03E-05	3.25E-01	4.24E-02	6.08E-01	3.02E-02
7.00	0.00E+00	3.55E-02	1.31E+00	4.28E-03	6.58E-03	3.93E-04	3.16E-01	1.25E-02	1.19E-04	1.02E-05	2.72E-01	5.61E-02	4.00E-01	4.13E-02
8.00	0.00E+00	3.07E-02	1.15E+00	2.78E-03	3.36E-03	2.55E-04	3.32E-01	1.11E-02	1.05E-04	7.97E-06	2.28E-01	6.07E-02	6.13E-01	4.72E-02
9.00	0.00E+00	3.02E-02	1.02E+00	2.03E-03	2.31E-03	3.08E-04	3.27E-01	1.48E-02	1.24E-04	1.14E-05	2.83E-01	6.78E-02	5.25E-01	8.04E-02
10.00	0.00E+00	3.85E-02	9.17E-01	1.90E-03	1.55E-03	5.17E-04	3.41E-01	2.75E-02	1.38E-04	3.52E-05	3.16E-01	9.89E-02	4.42E-01	1.95E-01

Table S14. Fitting parameters for **5** in a dc magnetic field of 3 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S14.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ_1 / s	SD_χ_T	α_1	SD_α_1	τ_2 / s	SD_τ_2	α_2	SD_α_2	β	SD_β
1.82	1.22E-02	6.21E-03	2.11E+00	1.50E-01	4.91E+00	7.64E-01	0.00E+00	3.12E-02	1.01E-02	5.63E-04	5.32E-01	1.03E-02	5.94E-01	3.47E-02
2.00	3.39E-03	1.07E-02	1.96E+00	1.46E-01	4.06E+00	6.83E-01	0.00E+00	3.86E-02	6.37E-03	4.45E-04	5.42E-01	1.52E-02	5.73E-01	3.97E-02
2.25	9.39E-03	1.13E-02	2.26E+00	2.10E-01	5.25E+00	1.09E+00	9.79E-02	3.45E-02	3.36E-03	2.03E-04	5.12E-01	1.63E-02	6.65E-01	3.74E-02
2.50	0.00E+00	1.04E-02	2.70E+00	2.66E-01	7.72E+00	1.71E+00	1.77E-01	2.59E-02	1.99E-03	9.67E-05	5.12E-01	1.39E-02	7.35E-01	3.05E-02
2.75	0.00E+00	9.35E-03	3.01E+00	2.76E-01	9.60E+00	2.00E+00	2.27E-01	2.01E-02	1.44E-03	6.03E-05	5.02E-01	1.25E-02	7.76E-01	2.38E-02
3.00	0.00E+00	1.17E-02	3.19E+00	3.59E-01	1.12E+01	3.01E+00	2.75E-01	2.25E-02	1.07E-03	5.48E-05	4.85E-01	1.58E-02	8.00E-01	2.63E-02
3.50	0.00E+00	1.12E-02	3.27E+00	2.93E-01	1.20E+01	2.75E+00	3.31E-01	1.75E-02	7.31E-04	3.66E-05	4.69E-01	1.54E-02	8.22E-01	1.95E-02
4.00	0.00E+00	1.50E-02	2.62E+00	1.67E-01	6.72E+00	1.22E+00	3.50E-01	1.86E-02	5.84E-04	4.09E-05	4.73E-01	2.08E-02	7.92E-01	1.92E-02
5.00	0.00E+00	1.14E-02	2.18E+00	6.35E-02	3.82E+00	3.74E-01	4.31E-01	1.18E-02	4.30E-04	2.45E-05	4.54E-01	1.84E-02	7.87E-01	1.25E-02
6.00	0.00E+00	1.31E-02	1.77E+00	3.76E-02	1.69E+00	1.26E-01	4.83E-01	1.25E-02	3.52E-04	2.46E-05	4.38E-01	2.50E-02	7.71E-01	1.54E-02
7.00	0.00E+00	1.43E-02	1.54E+00	3.33E-02	8.56E-01	6.42E-02	5.49E-01	1.46E-02	2.78E-04	2.37E-05	3.84E-01	3.67E-02	7.89E-01	2.04E-02
8.00	0.00E+00	2.03E-02	1.31E+00	3.27E-02	3.65E-01	2.85E-02	5.70E-01	2.23E-02	2.61E-04	3.50E-05	3.76E-01	6.51E-02	7.84E-01	3.80E-02
9.00	0.00E+00	2.11E-02	1.14E+00	2.68E-02	1.62E-01	1.97E-02	5.86E-01	2.64E-02	2.52E-04	4.07E-05	3.62E-01	8.95E-02	7.89E-01	5.45E-02
10.00	0.00E+00	2.21E-02	9.91E-01	1.96E-02	9.36E-02	2.03E-02	5.66E-01	3.11E-02	3.04E-04	5.69E-05	4.00E-01	9.33E-02	7.36E-01	7.87E-02

Table S15. Fitting parameters for [Tb(Pc)(OEP)] in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S15.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ_1 / s	SD_χ_T	α_1	SD_α_1	τ_2 / s	SD_τ_2	α_2	SD_α_2	β	SD_β
1.82	2.51E-01	4.99E-02	4.94E+00	1.27E-01	3.26E-01	6.51E-02	3.54E-01	6.72E-02	9.46E-04	1.16E-04	6.14E-01	1.46E-02	2.57E-01	5.15E-02
2.00	1.26E-01	5.70E-02	4.73E+00	1.60E-02	4.00E-01	1.30E-02	3.26E-01	2.42E-02	1.10E-03	8.93E-05	6.42E-01	1.34E-02	2.32E-01	2.43E-02
2.20	1.40E-01	6.32E-02	4.36E+00	1.98E-02	2.91E-01	8.63E-03	2.67E-01	2.73E-02	1.18E-03	1.14E-04	6.38E-01	1.64E-02	2.23E-01	2.74E-02
2.40	1.81E-01	6.49E-02	3.97E+00	2.61E-02	1.78E-01	4.77E-03	2.07E-01	3.22E-02	1.25E-03	1.54E-04	6.25E-01	2.04E-02	2.21E-01	3.26E-02
2.60	2.56E-01	5.68E-02	3.65E+00	2.35E-02	1.07E-01	2.90E-03	1.63E-01	3.41E-02	1.21E-03	1.68E-04	5.93E-01	2.31E-02	2.43E-01	3.63E-02
2.80	3.11E-01	4.96E-02	3.37E+00	1.89E-02	1.10E-03	1.68E-04	5.56E-01	2.58E-02	6.55E-02	1.99E-03	1.40E-01	3.53E-02	7.28E-01	4.08E-02
3.00	3.43E-01	4.48E-02	3.15E+00	1.54E-02	3.89E-02	1.37E-03	1.27E-01	3.75E-02	9.41E-04	1.62E-04	5.20E-01	2.87E-02	2.98E-01	4.71E-02
3.20	2.47E-01	4.72E-02	3.04E+00	4.72E-02	2.65E-02	6.72E-04	1.16E-01	5.61E-02	1.12E-03	3.36E-04	5.60E-01	3.19E-02	2.41E-01	6.63E-02
3.40	2.78E-01	5.08E-02	2.86E+00	3.35E-02	1.69E-02	6.35E-04	1.45E-01	5.62E-02	7.84E-04	2.71E-04	5.14E-01	4.28E-02	3.08E-01	8.90E-02
3.60	2.55E-01	5.22E-02	2.69E+00	2.21E-02	1.06E-02	4.97E-04	1.69E-01	4.74E-02	5.02E-04	1.71E-04	4.86E-01	4.91E-02	3.68E-01	9.56E-02
3.80	2.45E-01	4.91E-02	2.52E+00	1.43E-02	7.03E-03	3.52E-04	1.74E-01	3.92E-02	3.61E-04	1.13E-04	4.57E-01	5.24E-02	4.16E-01	9.37E-02
4.00	2.35E-01	4.19E-02	2.39E+00	8.64E-03	4.94E-03	2.20E-04	1.78E-01	2.90E-02	2.72E-04	6.99E-05	4.32E-01	4.99E-02	4.62E-01	8.10E-02
4.50	1.36E-01	1.75E-02	2.12E+00	2.87E-03	2.41E-03	4.25E-05	1.65E-01	1.11E-02	1.47E-04	1.84E-05	4.35E-01	1.71E-02	4.84E-01	2.93E-02
5.00	3.88E-01	1.77E-02	1.93E+00	7.09E-03	8.35E-04	2.40E-05	2.95E-01	1.02E-02					1	
6.00	2.97E-01	1.05E-02	1.61E+00	2.68E-03	4.17E-04	7.39E-06	2.63E-01	5.78E-03					1	
7.00	1.95E-01	9.41E-03	1.38E+00	1.51E-03	2.35E-04	4.03E-06	2.72E-01	4.45E-03					1	
8.00	8.06E-02	1.17E-02	1.22E+00	1.14E-03	1.38E-04	3.16E-06	2.97E-01	4.36E-03					1	
9.00	0.00E+00	1.36E-02	1.10E+00	8.79E-04	9.07E-05	2.56E-06	3.14E-01	4.20E-03					1	
10.0	0.00E+00	1.51E-02	9.92E-01	7.72E-04	7.31E-05	2.46E-06	3.06E-01	4.61E-03					1	

Table S16. Fitting parameters for [Tb(Pc)(OEP)] in a dc magnetic field of 3 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S16.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
2.20	1.81E-02	1.81E-03	2.88E+00	1.71E-02	9.71E-01	1.43E-02	3.34E-01	2.76E-03
2.40	1.64E-02	2.23E-03	2.79E+00	2.14E-02	8.37E-01	1.62E-02	3.39E-01	3.48E-03
2.60	1.49E-02	2.01E-03	2.70E+00	1.74E-02	7.32E-01	1.21E-02	3.45E-01	3.07E-03
2.80	1.25E-02	1.78E-03	2.63E+00	1.44E-02	6.60E-01	9.50E-03	3.55E-01	2.68E-03
3.00	3.51E-02	6.05E-03	2.46E+00	4.37E-02	5.82E-01	2.65E-02	3.33E-01	9.54E-03
3.20	1.24E-02	2.01E-03	2.44E+00	8.54E-02	5.03E-01	4.11E-02	3.58E-01	6.75E-03
3.40	2.06E-03	3.88E-03	2.50E+00	1.61E-01	5.22E-01	8.17E-02	3.82E-01	1.22E-02
3.60	6.90E-03	2.02E-03	2.28E+00	6.49E-02	4.02E-01	2.79E-02	3.72E-01	6.21E-03
3.80	8.70E-03	2.66E-03	2.12E+00	7.13E-02	3.35E-01	2.76E-02	3.69E-01	8.08E-03
4.00	1.90E-02	3.15E-03	2.31E+00	5.72E-02	2.34E-01	1.51E-02	3.86E-01	7.13E-03
4.50	4.65E-03	1.83E-03	1.81E+00	3.06E-02	2.12E-01	9.15E-03	3.75E-01	5.13E-03
5.00	1.79E-02	2.80E-03	1.63E+00	1.36E-02	5.05E-02	1.09E-03	3.55E-01	4.92E-03
6.00	6.26E-03	3.84E-03	1.35E+00	9.91E-03	2.03E-02	4.06E-04	3.61E-01	5.93E-03
7.00	0.00E+00	6.47E-03	1.19E+00	1.14E-02	1.09E-02	3.12E-04	3.77E-01	9.22E-03
8.00	0.00E+00	9.61E-03	1.08E+00	1.31E-02	7.00E-03	2.76E-04	3.94E-01	1.30E-02
9.00	0.00E+00	1.20E-02	9.89E-01	1.33E-02	4.96E-03	2.36E-04	4.05E-01	1.56E-02
10.0	0.00E+00	1.09E-02	9.03E-01	1.04E-02	3.78E-03	1.64E-04	3.92E-01	1.47E-02

Table S17. Fitting parameters for $TBA^+[Tb(Pc)(OEP)]^-$ in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S17.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	8.37E-01	1.03E-01	6.87E+00	3.34E-02	6.55E-04	3.63E-05	4.87E-01	1.03E-02
2.00	7.76E-01	9.61E-02	6.23E+00	3.06E-02	6.38E-04	3.62E-05	4.83E-01	1.06E-02
2.20	6.72E-01	7.57E-02	5.17E+00	2.36E-02	6.19E-04	3.28E-05	4.69E-01	1.03E-02
2.40	6.25E-01	6.92E-02	4.68E+00	2.13E-02	6.09E-04	3.25E-05	4.64E-01	1.05E-02
2.60	5.76E-01	6.44E-02	4.29E+00	1.95E-02	5.96E-04	3.21E-05	4.61E-01	1.06E-02
2.80	5.54E-01	6.03E-02	3.97E+00	1.82E-02	5.91E-04	3.20E-05	4.55E-01	1.09E-02
3.00	5.70E-01	6.23E-02	4.05E+00	1.85E-02	5.77E-04	3.20E-05	4.59E-01	1.09E-02
3.50	4.59E-01	4.92E-02	3.13E+00	1.43E-02	5.57E-04	3.09E-05	4.43E-01	1.13E-02
4.00	4.64E-01	4.50E-02	2.99E+00	1.28E-02	5.43E-04	2.89E-05	4.37E-01	1.10E-02
5.00	3.83E-01	3.67E-02	2.38E+00	9.98E-03	5.07E-04	2.72E-05	4.22E-01	1.14E-02
6.00	3.36E-01	3.13E-02	1.98E+00	8.20E-03	4.79E-04	2.58E-05	4.06E-01	1.18E-02
7.00	2.86E-01	2.85E-02	1.69E+00	7.11E-03	4.44E-04	2.49E-05	3.93E-01	1.25E-02
8.00	2.54E-01	2.51E-02	1.48E+00	6.01E-03	4.18E-04	2.30E-05	3.77E-01	1.26E-02
9.00	2.37E-01	2.30E-02	1.31E+00	5.40E-03	4.03E-04	2.25E-05	3.62E-01	1.33E-02
10.00	2.34E-01	1.82E-02	1.18E+00	4.27E-03	3.98E-04	1.93E-05	3.40E-01	1.23E-02

Table S18. Fitting parameters for $TBA^+[Tb(Pc)(OEP)]^-$ in a dc magnetic field of 3 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S18.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	8.04E-03	2.33E-03	3.62E+00	3.63E-02	1.52E+00	2.91E-02	2.13E-01	3.90E-03
2.00	7.80E-03	1.94E-03	3.66E+00	2.78E-02	1.41E+00	2.05E-02	2.13E-01	3.09E-03
3.00	5.31E-03	1.31E-03	3.30E+00	1.23E-02	9.16E-01	6.75E-03	2.17E-01	1.88E-03
4.00	6.73E-03	8.86E-04	2.73E+00	5.81E-03	6.02E-01	2.63E-03	2.22E-01	1.30E-03
5.00	5.78E-03	8.10E-04	2.28E+00	4.04E-03	4.12E-01	1.56E-03	2.27E-01	1.25E-03
6.00	6.99E-03	1.18E-03	1.96E+00	4.68E-03	2.91E-01	1.55E-03	2.26E-01	1.91E-03
7.00	6.62E-03	1.58E-03	1.69E+00	5.16E-03	2.08E-01	1.47E-03	2.24E-01	2.72E-03
8.00	8.22E-03	1.72E-03	1.49E+00	4.75E-03	1.54E-01	1.19E-03	2.20E-01	3.14E-03
9.00	7.95E-03	1.82E-03	1.32E+00	4.36E-03	1.16E-01	9.67E-04	2.15E-01	3.53E-03
10.0	7.04E-03	1.88E-03	1.19E+00	4.00E-03	9.02E-02	8.00E-04	2.12E-01	3.85E-03
15.0	2.21E-03	1.20E-03	8.20E-01	3.98E-03	3.44E-02	3.51E-04	2.15E-01	3.96E-03
20.0	2.55E-03	9.93E-04	6.06E-01	1.87E-03	1.43E-02	1.04E-04	1.87E-01	3.47E-03
25.0	0.00E+00	2.02E-03	4.77E-01	1.48E-03	2.17E-03	2.45E-05	1.69E-01	5.67E-03
30.0	0.00E+00	7.99E-03	3.96E-01	8.21E-04	1.30E-04	4.09E-06	1.08E-01	9.75E-03

Table S19. Fitting parameters for $[Tb(Pc)(OEP)]^{+}SbCl_6^{-}$ in the absence of dc magnetic field obtained from fitting the ac magnetic susceptibilities in Fig. S19.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	1.71E-01	5.37E-02	7.24E+00	1.13E-01	1.52E-02	9.06E-04	6.01E-01	9.04E-03
2.00	1.77E-01	4.89E-02	6.53E+00	9.60E-02	1.34E-02	7.43E-04	5.91E-01	9.10E-03
2.20	1.84E-01	4.34E-02	5.90E+00	7.98E-02	1.19E-02	5.97E-04	5.81E-01	8.91E-03
2.40	1.76E-01	4.11E-02	5.32E+00	7.05E-02	1.04E-02	5.09E-04	5.71E-01	9.26E-03
2.60	1.80E-01	3.75E-02	4.86E+00	6.01E-02	9.26E-03	4.20E-04	5.61E-01	9.20E-03
2.80	1.76E-01	3.51E-02	4.48E+00	5.29E-02	8.28E-03	3.59E-04	5.52E-01	9.28E-03
3.00	1.72E-01	3.18E-02	4.13E+00	4.46E-02	7.35E-03	2.93E-04	5.44E-01	8.99E-03
3.20	1.69E-01	3.09E-02	3.86E+00	4.14E-02	6.78E-03	2.70E-04	5.36E-01	9.31E-03
3.40	1.59E-01	2.93E-02	3.61E+00	3.71E-02	6.15E-03	2.37E-04	5.30E-01	9.30E-03
3.60	1.58E-01	2.75E-02	3.38E+00	3.31E-02	5.63E-03	2.10E-04	5.24E-01	9.23E-03
3.80	1.50E-01	2.59E-02	3.16E+00	2.95E-02	5.14E-03	1.86E-04	5.18E-01	9.17E-03
4.00	1.46E-01	2.44E-02	2.98E+00	2.65E-02	4.76E-03	1.67E-04	5.10E-01	9.11E-03
4.50	1.38E-01	2.21E-02	2.62E+00	2.20E-02	4.09E-03	1.41E-04	4.98E-01	9.26E-03
5.00	1.28E-01	2.00E-02	2.33E+00	1.82E-02	3.51E-03	1.18E-04	4.86E-01	9.22E-03
6.00	1.02E-01	1.69E-02	1.94E+00	1.45E-02	2.77E-03	8.84E-05	4.75E-01	9.09E-03
7.00	1.04E-01	1.56E-02	1.64E+00	1.08E-02	2.23E-03	7.49E-05	4.47E-01	9.67E-03
8.00	9.98E-02	1.41E-02	1.42E+00	8.84E-03	1.87E-03	6.39E-05	4.29E-01	9.97E-03
9.00	9.72E-02	1.27E-02	1.25E+00	7.27E-03	1.61E-03	5.45E-05	4.12E-01	1.01E-02
10.0	9.30E-02	1.18E-02	1.12E+00	6.25E-03	1.41E-03	4.83E-05	3.96E-01	1.03E-02

Table S20. Fitting parameters for $[Tb(Pc)(OEP)]^{+}SbCl_6^{-}$ in a dc magnetic field of 3 kOe obtained from fitting the ac magnetic susceptibilities in Fig. S20.

T / K	χ_S / cm^3 mol^{-1}	SD_χ_S	χ_T / cm^3 mol^{-1}	SD_χ_T	τ / s	SD_τ	α	SD_α
1.82	1.65E-02	1.33E-03	3.48E+00	4.06E-02	2.87E+00	7.67E-02	3.30E-01	2.92E-03
2.00	1.50E-02	1.14E-03	3.47E+00	3.13E-02	2.59E+00	5.43E-02	3.34E-01	2.37E-03
2.20	1.47E-02	9.14E-04	3.43E+00	2.25E-02	2.33E+00	3.60E-02	3.36E-01	1.82E-03
2.40	1.42E-02	1.01E-03	3.32E+00	2.17E-02	2.03E+00	3.16E-02	3.39E-01	1.94E-03
2.60	1.21E-02	1.10E-03	3.26E+00	2.17E-02	1.88E+00	3.07E-02	3.49E-01	2.05E-03
2.80	1.23E-02	8.51E-04	3.17E+00	1.54E-02	1.71E+00	2.07E-02	3.56E-01	1.55E-03
3.00	1.22E-02	1.13E-03	3.10E+00	1.85E-02	1.55E+00	2.35E-02	3.61E-01	1.99E-03
3.20	1.02E-02	8.11E-04	2.99E+00	1.25E-02	1.43E+00	1.55E-02	3.70E-01	1.42E-03
3.40	1.04E-02	9.67E-04	2.90E+00	1.36E-02	1.29E+00	1.60E-02	3.74E-01	1.67E-03
3.60	8.73E-03	1.09E-03	2.82E+00	1.44E-02	1.20E+00	1.64E-02	3.83E-01	1.86E-03
3.80	8.47E-03	1.09E-03	2.71E+00	1.33E-02	1.09E+00	1.46E-02	3.88E-01	1.85E-03
4.00	7.53E-03	1.00E-03	2.61E+00	1.15E-02	9.99E-01	1.21E-02	3.94E-01	1.70E-03
4.50	5.18E-03	1.35E-03	2.39E+00	1.32E-02	8.13E-01	1.29E-02	4.06E-01	2.29E-03
5.00	6.16E-03	7.67E-04	2.19E+00	6.39E-03	6.54E-01	5.57E-03	4.11E-01	1.30E-03
6.00	3.75E-03	9.28E-04	1.88E+00	5.95E-03	4.44E-01	4.25E-03	4.22E-01	1.59E-03
7.00	4.81E-03	1.20E-03	1.64E+00	6.11E-03	3.10E-01	3.59E-03	4.27E-01	2.11E-03
8.00	3.21E-03	1.29E-03	1.44E+00	5.36E-03	2.21E-01	2.58E-03	4.29E-01	2.33E-03
9.00	6.64E-03	1.56E-03	1.28E+00	5.40E-03	1.62E-01	2.17E-03	4.25E-01	2.94E-03
10.0	8.10E-03	1.95E-03	1.15E+00	5.75E-03	1.21E-01	1.96E-03	4.19E-01	3.83E-03

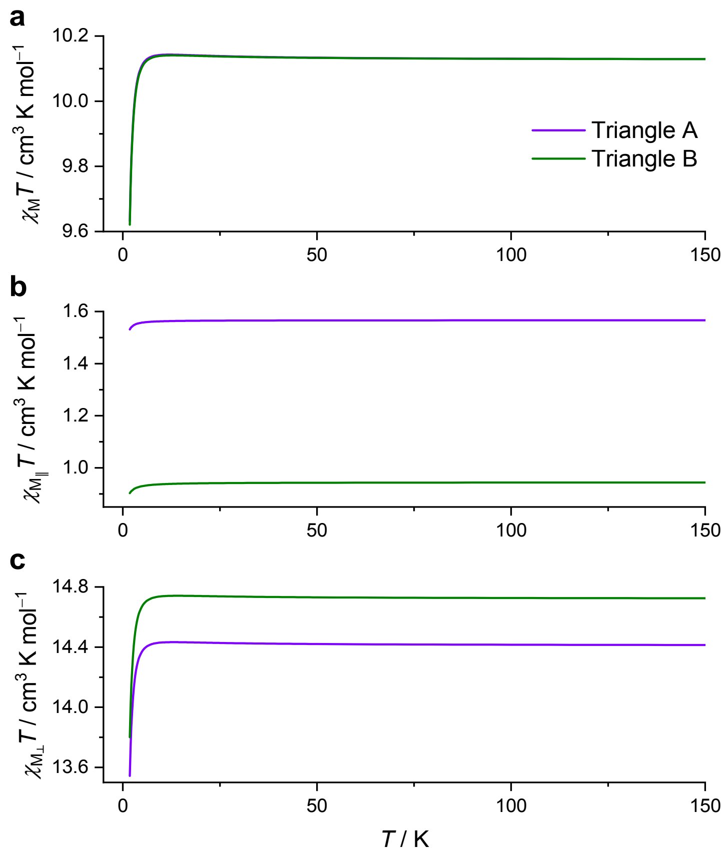

Fig. S22 Calculated $\chi_M T$ values for triangles A and B in a 0.1 T field.

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