

Supporting Information

Impact of Coordination Environment on Magnetic Properties of Single-Molecule Magnets Based on Homo- and Hetero-Dinuclear Terbium(III) Heteroleptic Tris(Crownphthalocyaninate)

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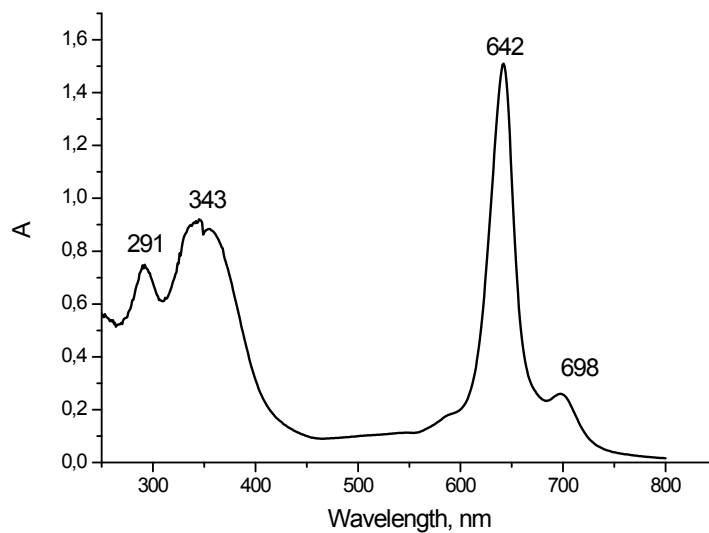


Fig. S1 UV-Vis absorption spectrum of [Tb*,Tb] (1) in chloroform.

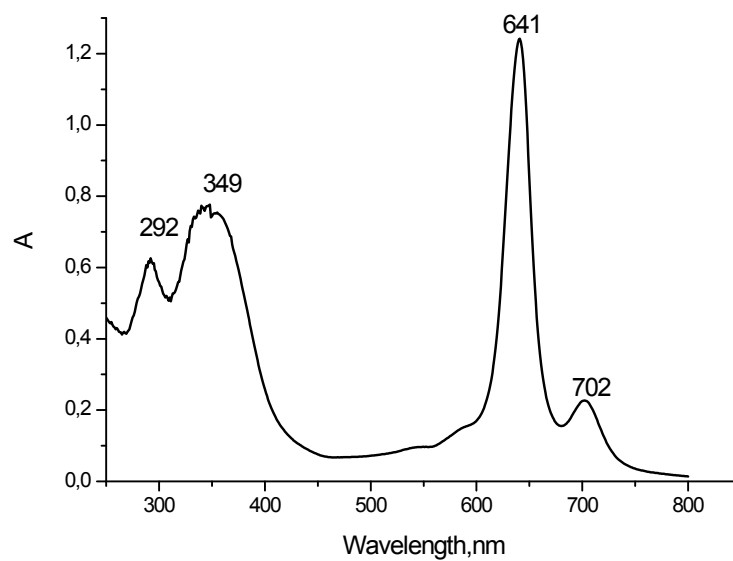


Fig. S2 UV-Vis absorption spectrum of [Tb*,Y] (2) in chloroform.

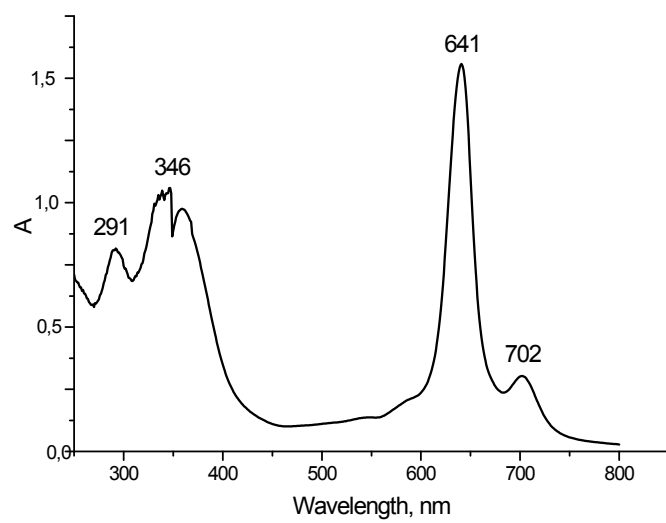


Fig. S3 UV-Vis absorption spectrum of [Y*,Tb] (3) in chloroform.

Complex 1

HR-ESI: found 1148.333 – $[M+3Na]^{3+}$, calculated for $[C_{160}H_{160}N_{24}O_{40}Tb_2+3Na]^{3+}$ - 1148.315

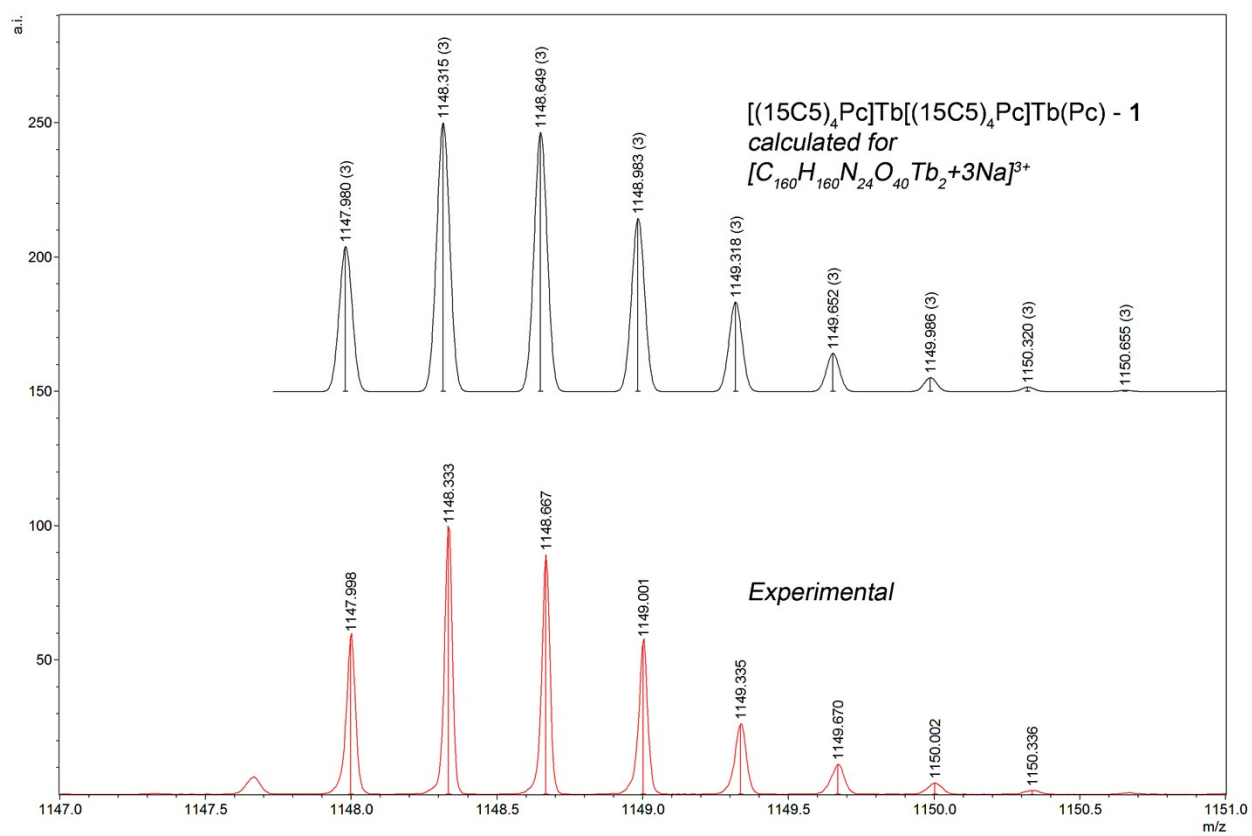


Fig. S4 HR-ESI MS of $[Tb^*,Tb]$ (1).

Complex 2

HR-ESI: found 1124.981 – $[M+3Na]^{3+}$, calculated for $[C_{160}H_{160}N_{24}O_{40}TbY+3Na]^{3+}$ - 1124.975

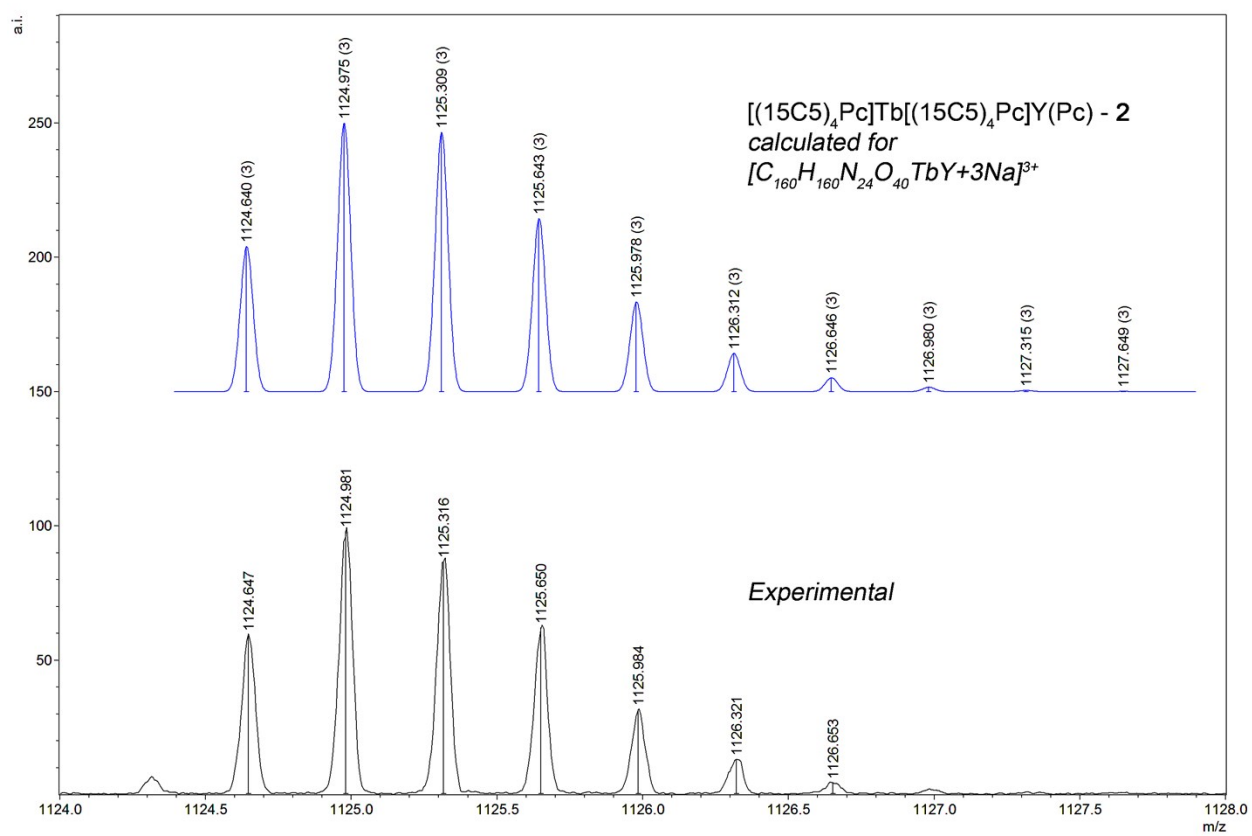


Fig. S5 HR-ESI MS of $[Tb^*,Y] (2)$.

Complex 3

HR-ESI: found 1124.974 – $[M+3Na]^{3+}$, calculated for $[C_{160}H_{160}N_{24}O_{40}TbY+3Na]^{3+}$ - 1124.975

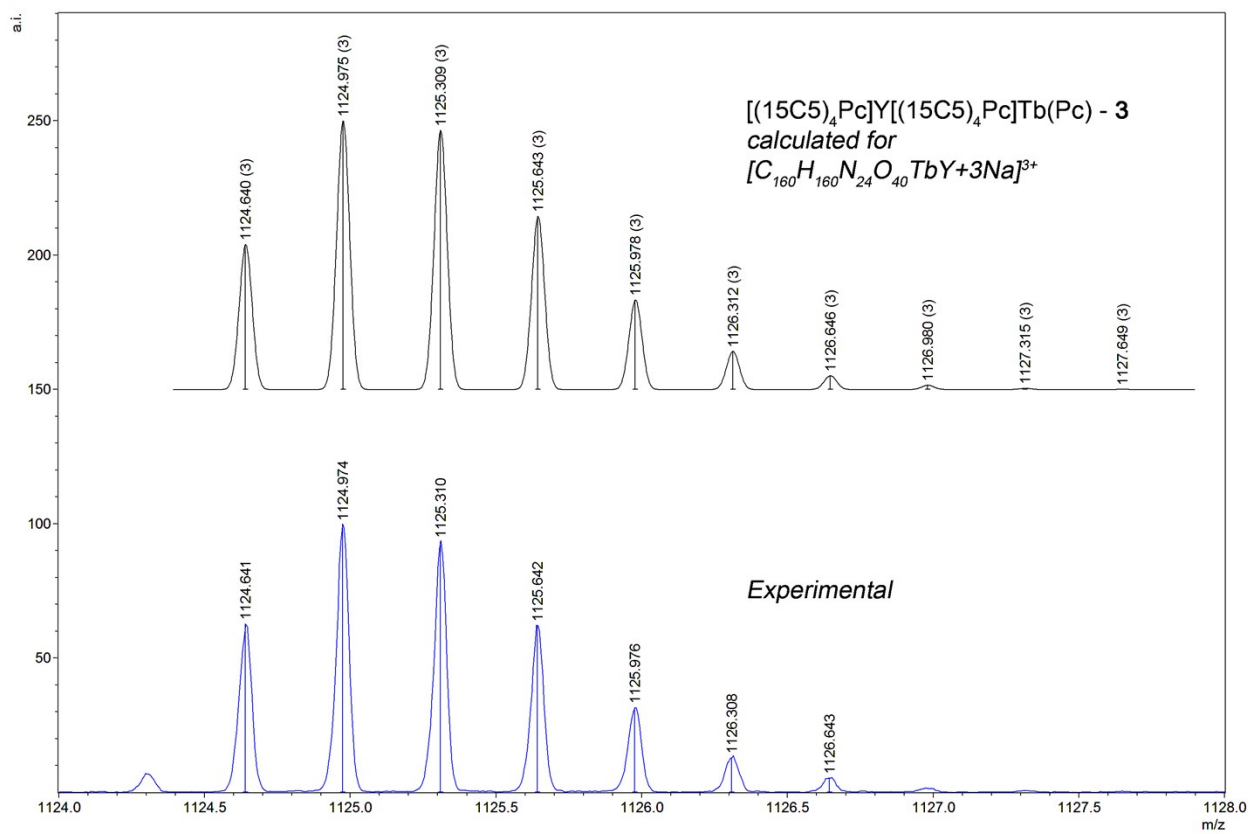


Fig. S6 HR-ESI MS of $[Y^*, Tb] (3)$.

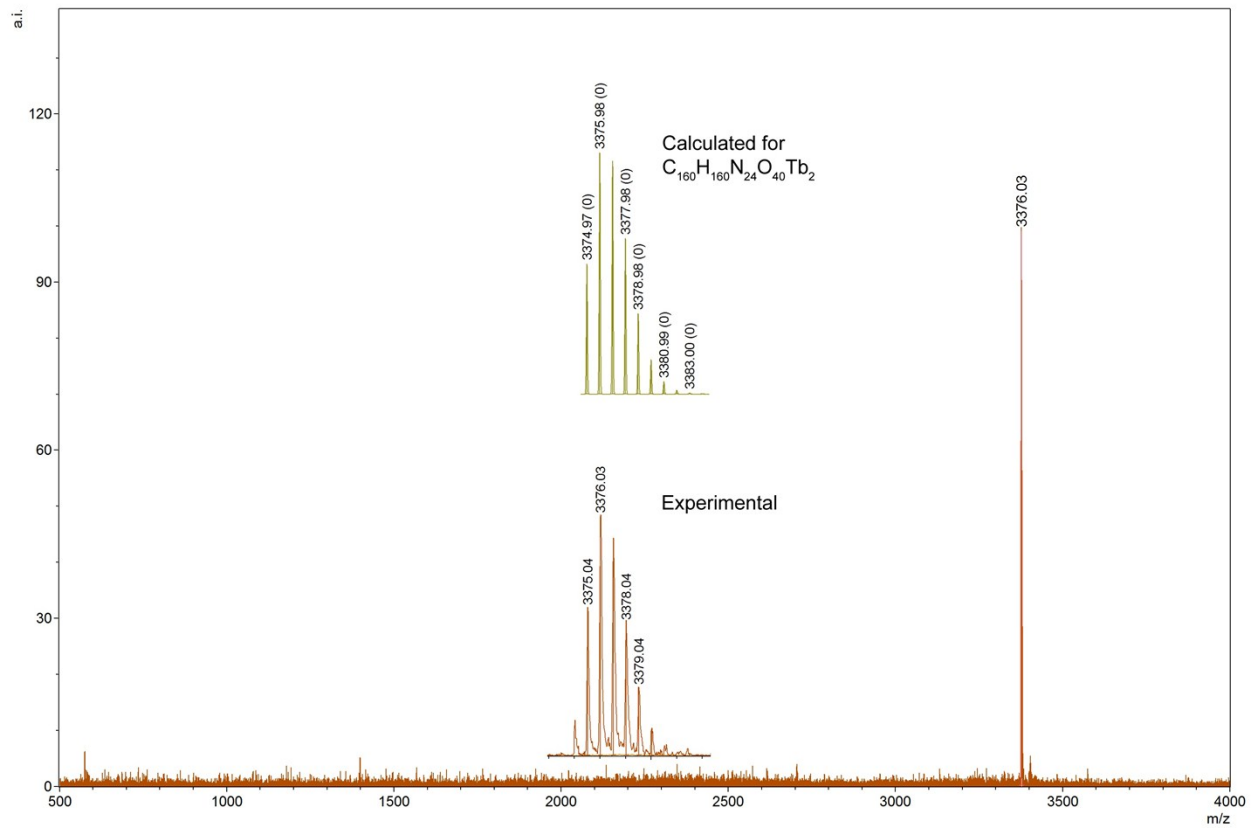


Fig. S7 MALDI-TOF spectrum of [Tb*,Tb] (1).

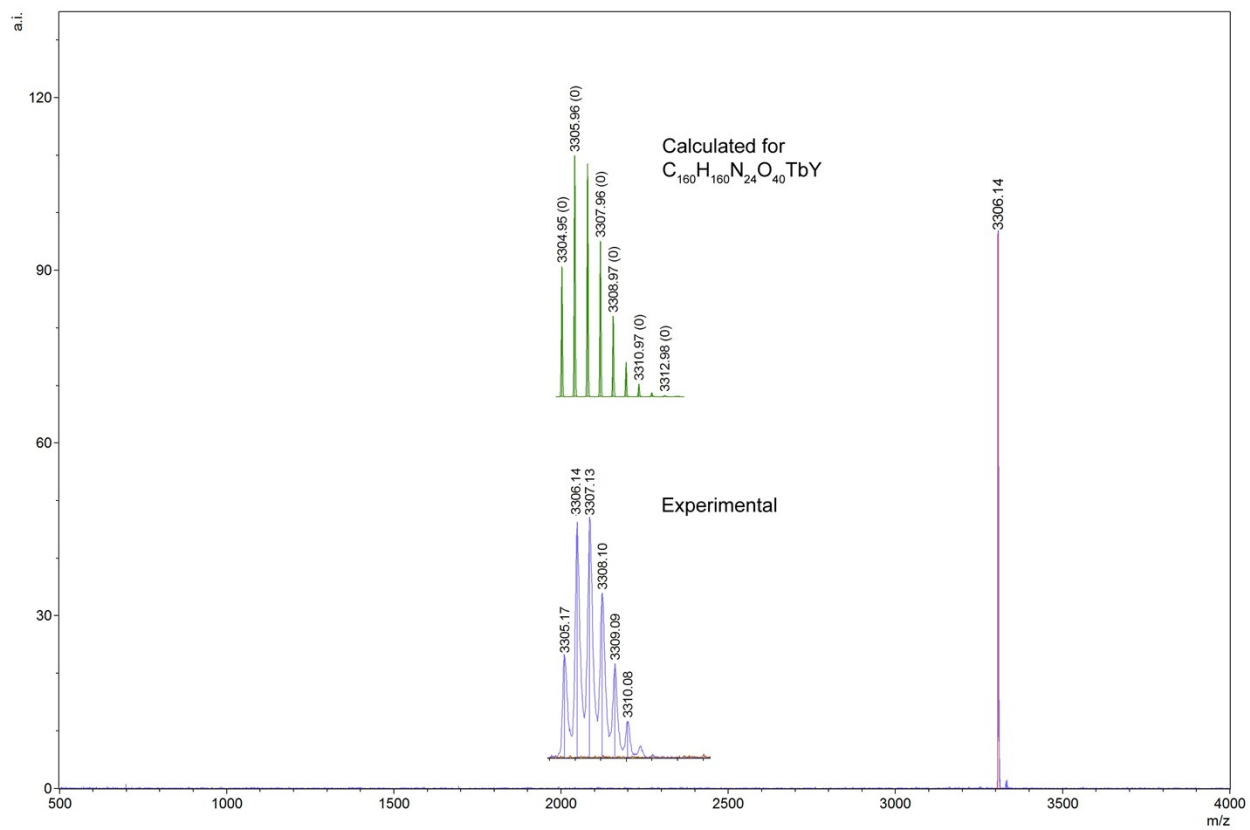


Fig. S8 MALDI-TOF spectrum of $[Tb^*,Y]$ (**2**).

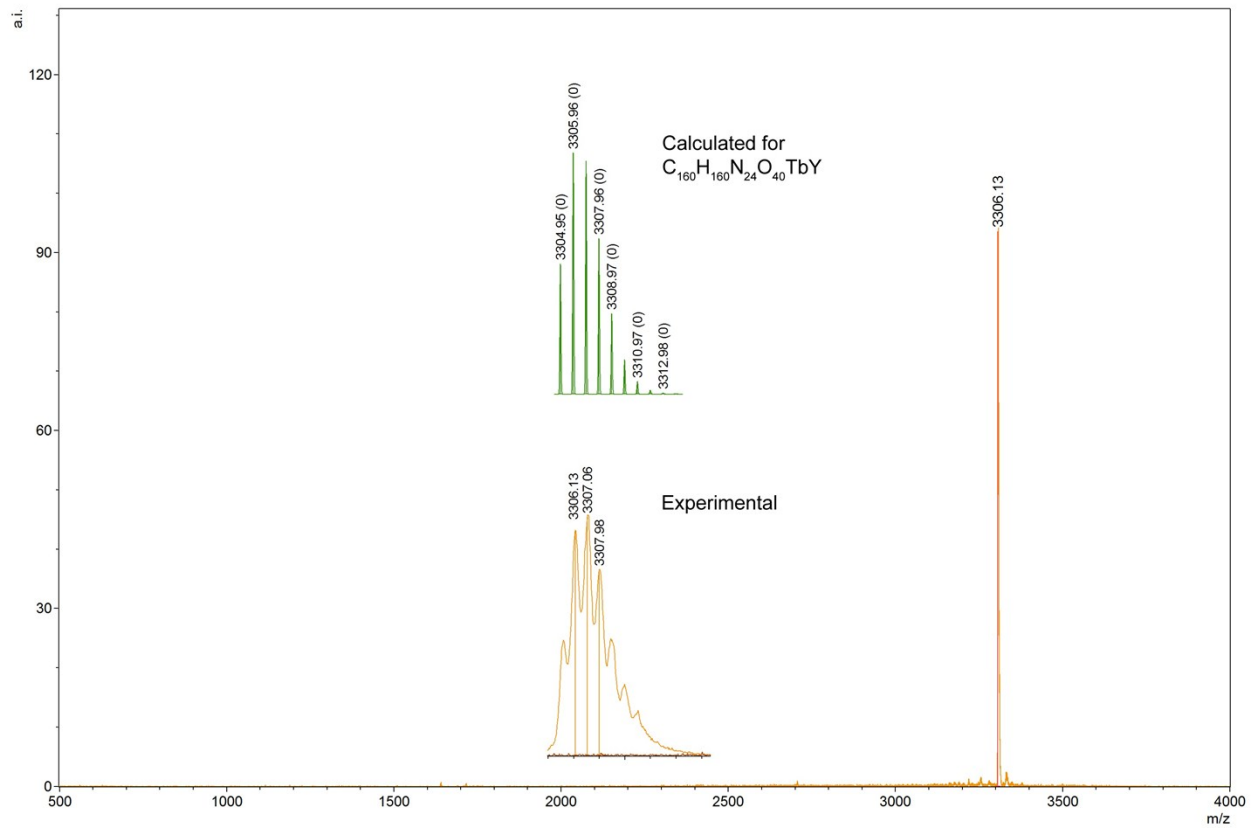


Fig. S9 MALDI-TOF mass spectrum of [Y*,Tb] (3).

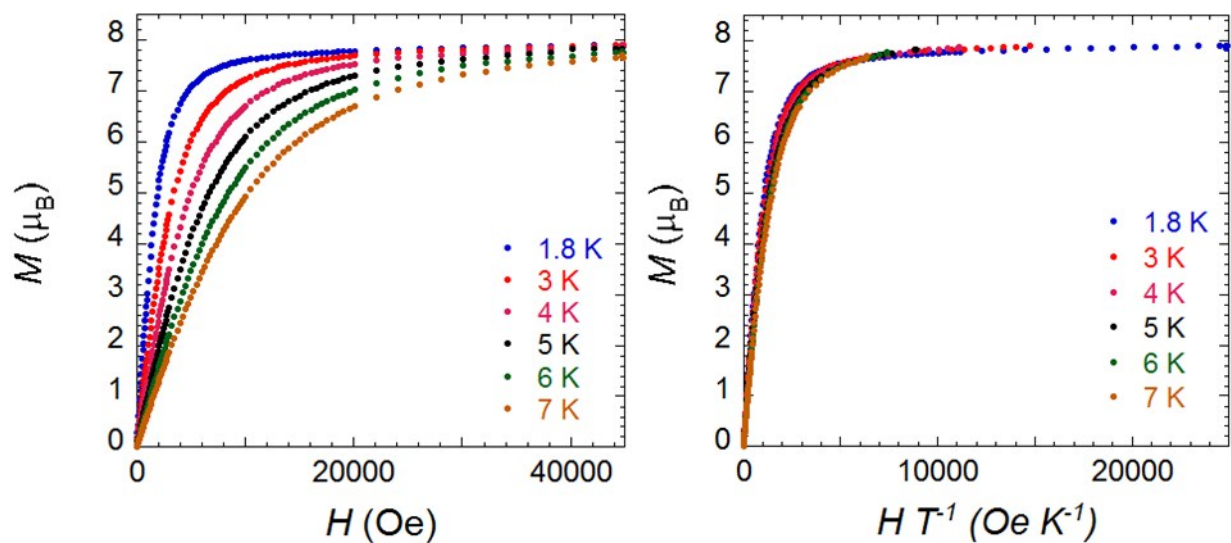


Fig. S10 Field dependence of the magnetization (left) and M vs. HT^{-1} plot (right) of **1** at indicated temperatures.

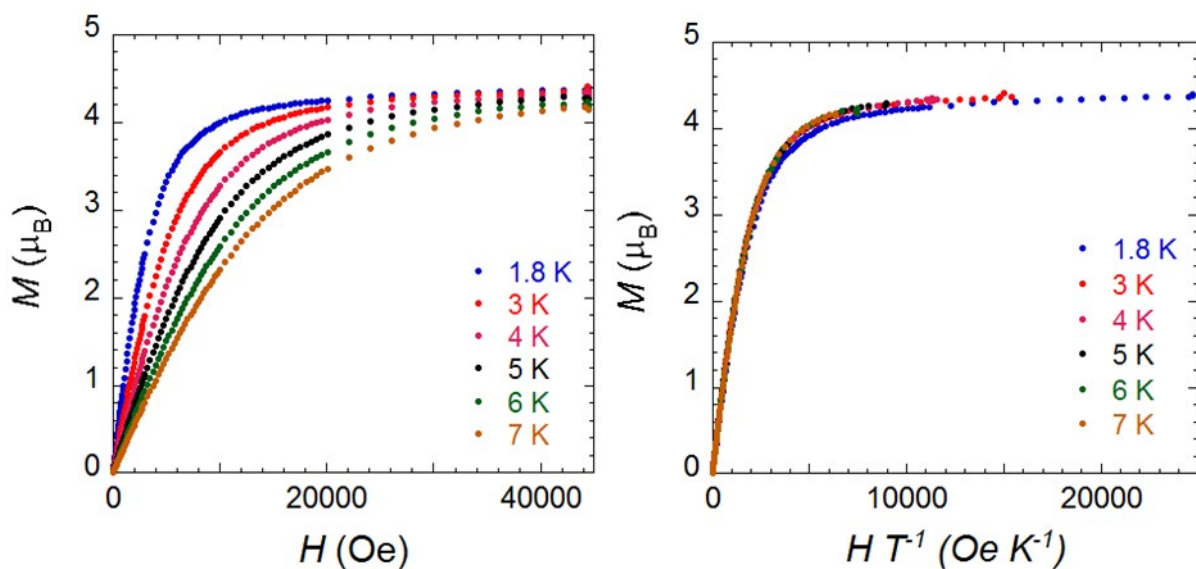


Fig. S11 Field dependence of the magnetization (left) and M vs. HT^{-1} plot (right) of **2** at indicated temperatures.

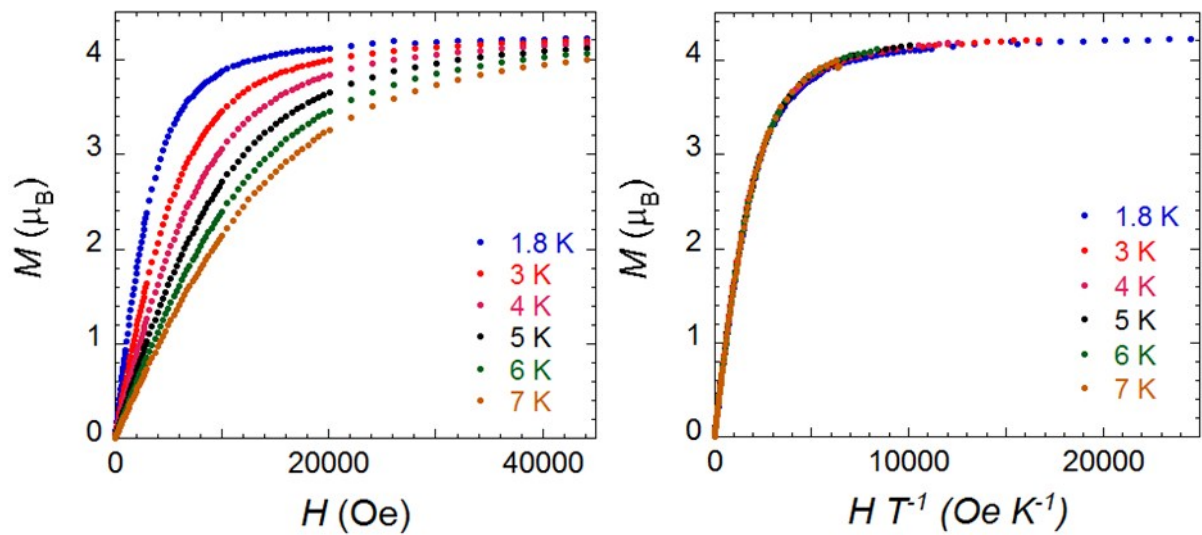


Fig. S12 Field dependence of the magnetization (left) and M vs. HT^{-1} plot (right) of **3** at indicated temperatures.

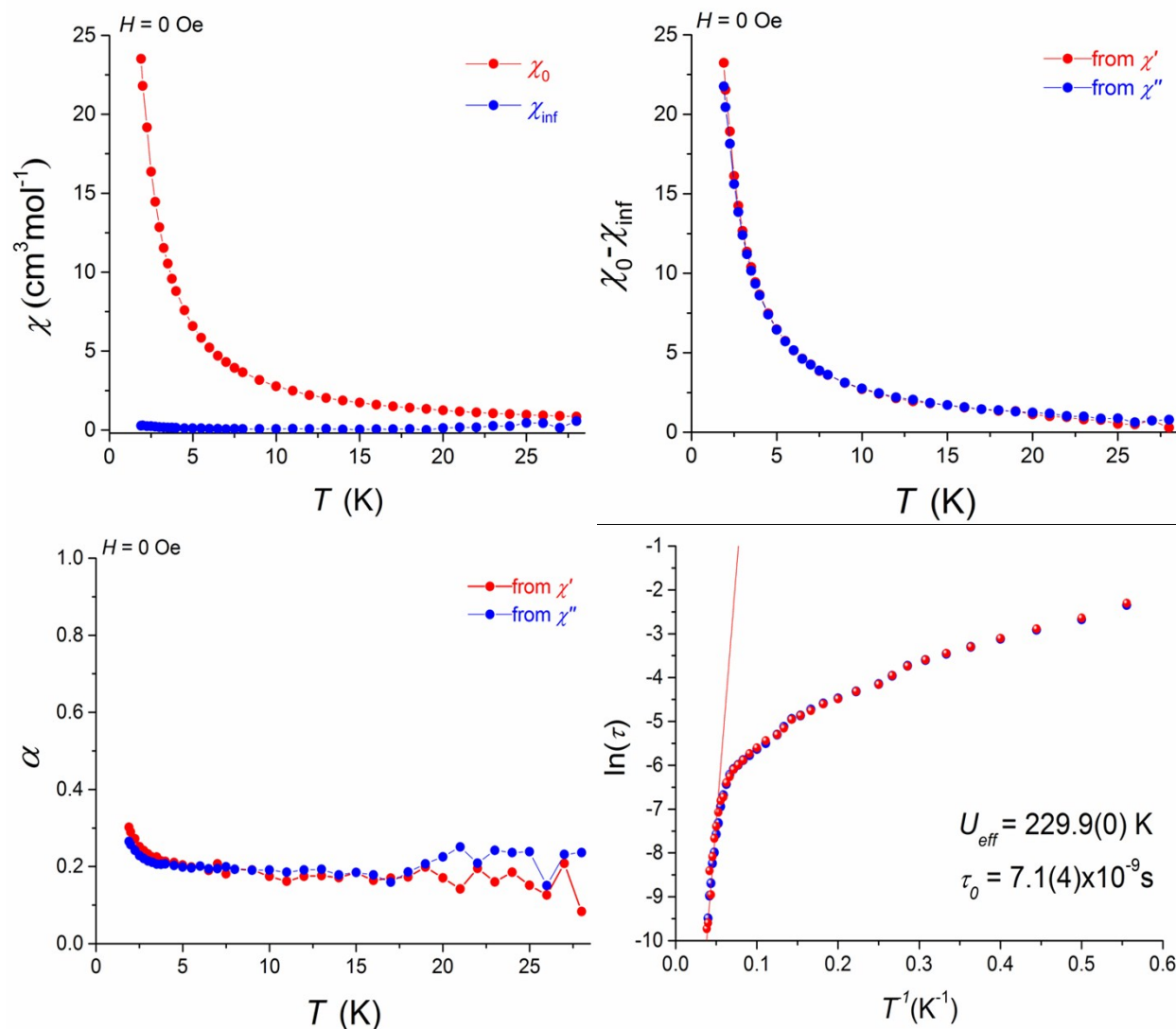


Fig. S13 Data obtained from generalized Debye fits of χ' and χ'' frequency dependent ac data **1**. Temperature dependence of χ_0 and χ_{inf} (top left), $\chi_0 - \chi_{\text{inf}}$ (top right), and α (bottom left). Relaxation times of the magnetization $\ln(\tau)$ vs. T^{-1} for **1** (Arrhenius plot using χ' (red) and χ'' (blue) ac data) under 0 Oe applied dc field (bottom right). The solid red line corresponds to the fit of the data.

Table S1. Fitting values from Cole-Cole plot for **1** under 0 Oe applied dc field.

T (K)	τ (s)	α	X_S	X_T
24	0.00017985	0.38462	0.23544	0.86573
23	0.00035068	0.23646	0.22963	0.96151
22	0.00044249	0.27251	0.21626	1.00100
21	0.00062282	0.26694	0.17962	1.04777
20	0.00081929	0.25809	0.17979	1.11288
19	0.00089111	0.26055	0.15262	1.21000
18	0.00130159	0.22149	0.15656	1.26941
17	0.00149722	0.21996	0.17093	1.35526
16	0.00177027	0.21831	0.17046	1.35618
15	0.00199297	0.21018	0.17326	1.45384
14	0.00221499	0.21166	0.18911	1.69036
13	0.0024853	0.23832	0.23447	1.82545
12	0.002888	0.22425	0.24583	2.00049
11	0.00350962	0.19601	0.25189	2.27613
10	0.00396596	0.20678	0.28858	2.52376
9	0.00450744	0.22423	0.35304	2.86017
8	0.00547219	0.22416	0.39111	3.29238
7.5	0.00592504	0.23301	0.43514	3.54052
7	0.00657247	0.23747	0.47205	3.85004
6.5	0.00768218	0.23495	0.51735	4.22236
6	0.00850233	0.24317	0.57813	4.65519
5.5	0.01007128	0.24464	0.6723	5.21374
5	0.011773	0.24811	0.75771	5.86022
4.5	0.01396308	0.26849	0.90901	6.68588
4	0.01734291	0.26824	1.06888	7.75803
3.75	0.01997734	0.26593	1.161	8.44211
3.5	0.02256522	0.28542	1.33596	9.18394
3.25	0.02598269	0.28728	1.47357	10.05497
3	0.03100923	0.29933	1.70565	11.1297
2.75	0.03751467	0.3172	2.01524	12.39333
2.5	0.04686485	0.33325	2.3966	13.903
2.25	0.06263439	0.36597	3.02747	15.9682
2	0.07999911	0.40328	3.7613	17.76293
1.9	0.09387486	0.42089	4.19594	18.817

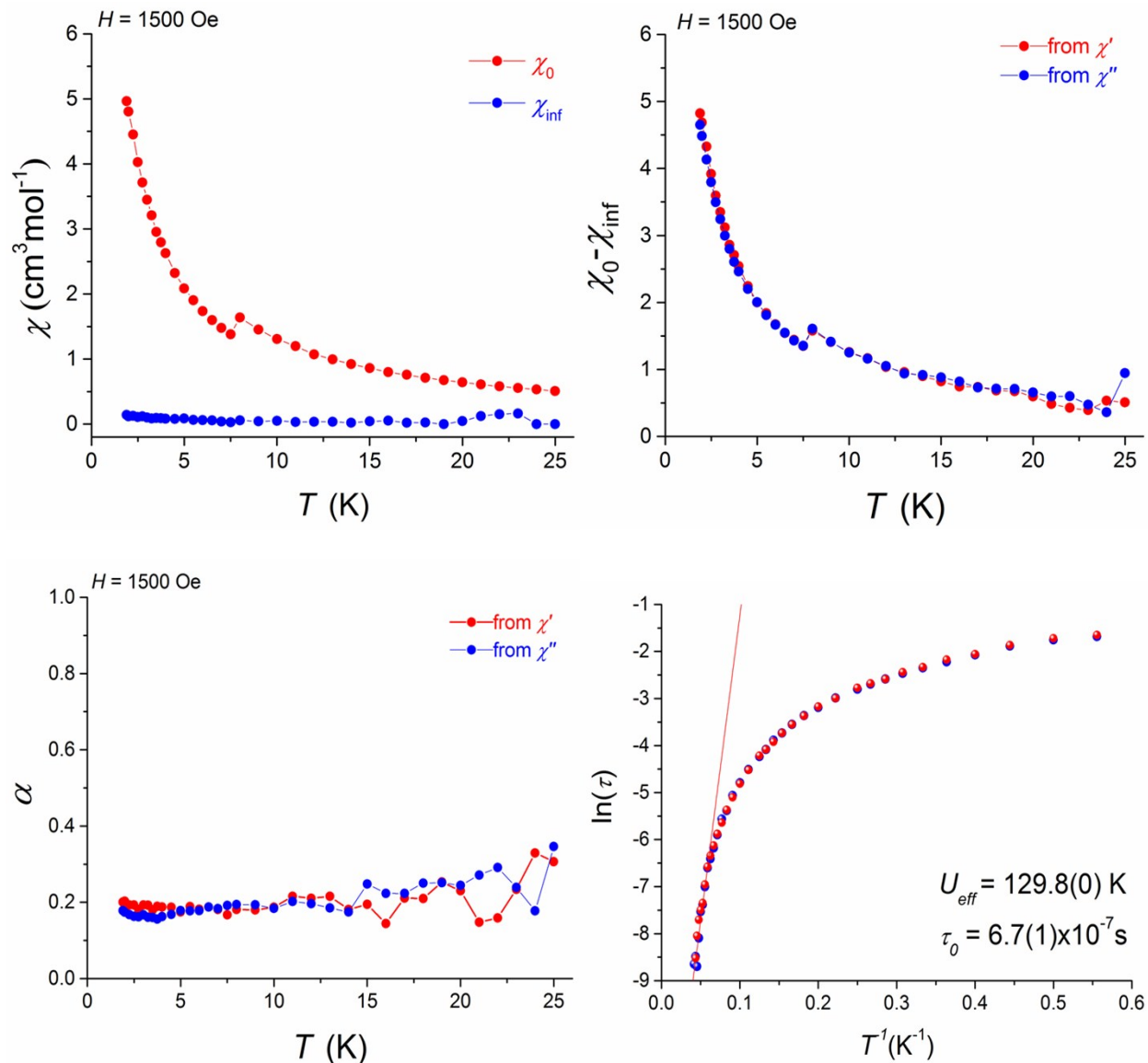


Fig. S14 | Data obtained from generalized Debye fits of χ' and χ'' frequency dependent ac data under 1500 Oe applied dc field for **2**. Temperature dependence of χ_0 and χ_{inf} (top left), $\chi_0 - \chi_{\text{inf}}$ (top right), and α (bottom left). Relaxation times of the magnetization $\ln(\tau)$ vs. T^{-1} for **2** (Arrhenius plot using χ' (red) and χ'' (blue) ac data) under 1500 Oe applied dc field (bottom right). The solid red line corresponds to the fit of the data.

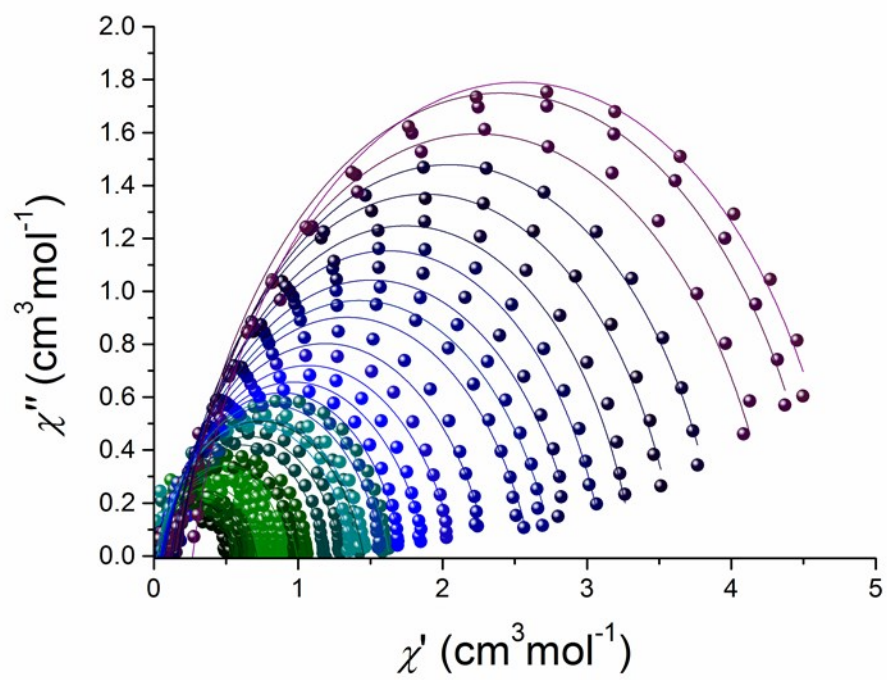


Fig. S15 Cole-Cole plot for ac susceptibility data of **2** under 1500 Oe applied dc field. Solid lines are the best fit to the generalized Debye model.

Table S2. Fitting values from Cole-Cole plot for **2** under 1500 Oe applied dc field.

T (K)	τ (s)	α	X_S	X_T
23	0.00014977	0.15928	0.17738	0.52183
22	0.00027271	0.30407	0.11102	0.51405
21	0.00032813	0.26009	0.12069	0.55084
20	0.00038903	0.28247	0.09301	0.5702
19	0.00049347	0.21264	0.0645	0.59267
18	0.00069644	0.27368	0.09816	0.63257
17	0.00103199	0.26022	0.10392	0.67556
16	0.00130364	0.26654	0.09402	0.71531
15	0.00161582	0.26469	0.10605	0.76815
14	0.00217307	0.22953	0.09874	0.83778
13	0.00260201	0.27187	0.1387	0.88181
12	0.00353311	0.24632	0.1371	0.95873
11	0.00453866	0.25611	0.15077	1.06345
10	0.00588136	0.27991	0.17285	1.1559
9	0.00794643	0.26993	0.18341	1.29193
8	0.01124812	0.23777	0.19949	1.47155
7.5	0.0126867	0.24631	0.15265	1.2367
7	0.01442855	0.2712	0.18781	1.31504
6.5	0.018128	0.23603	0.1985	1.43507
6	0.02176318	0.23712	0.21648	1.55674
5.5	0.02485139	0.27177	0.25414	1.68526
5	0.03009696	0.2755	0.28737	1.85429
4.5	0.03617997	0.27144	0.31371	2.06206
4	0.04475436	0.2753	0.35594	2.32135
3.75	0.04988592	0.26583	0.37075	2.4738
3.5	0.05609293	0.24743	0.37359	2.64286
3.25	0.06802268	0.19896	0.37395	2.86753
3	0.07921552	0.17492	0.40127	3.08494
2.75	0.09191493	0.1812	0.40775	3.35258
2.5	0.10455368	0.17506	0.45469	3.6347
2.25	0.12356619	0.19358	0.5205	3.96503
2	0.14627561	0.17693	0.5208	4.28468
1.9	0.15862855	0.17128	0.60458	4.45011

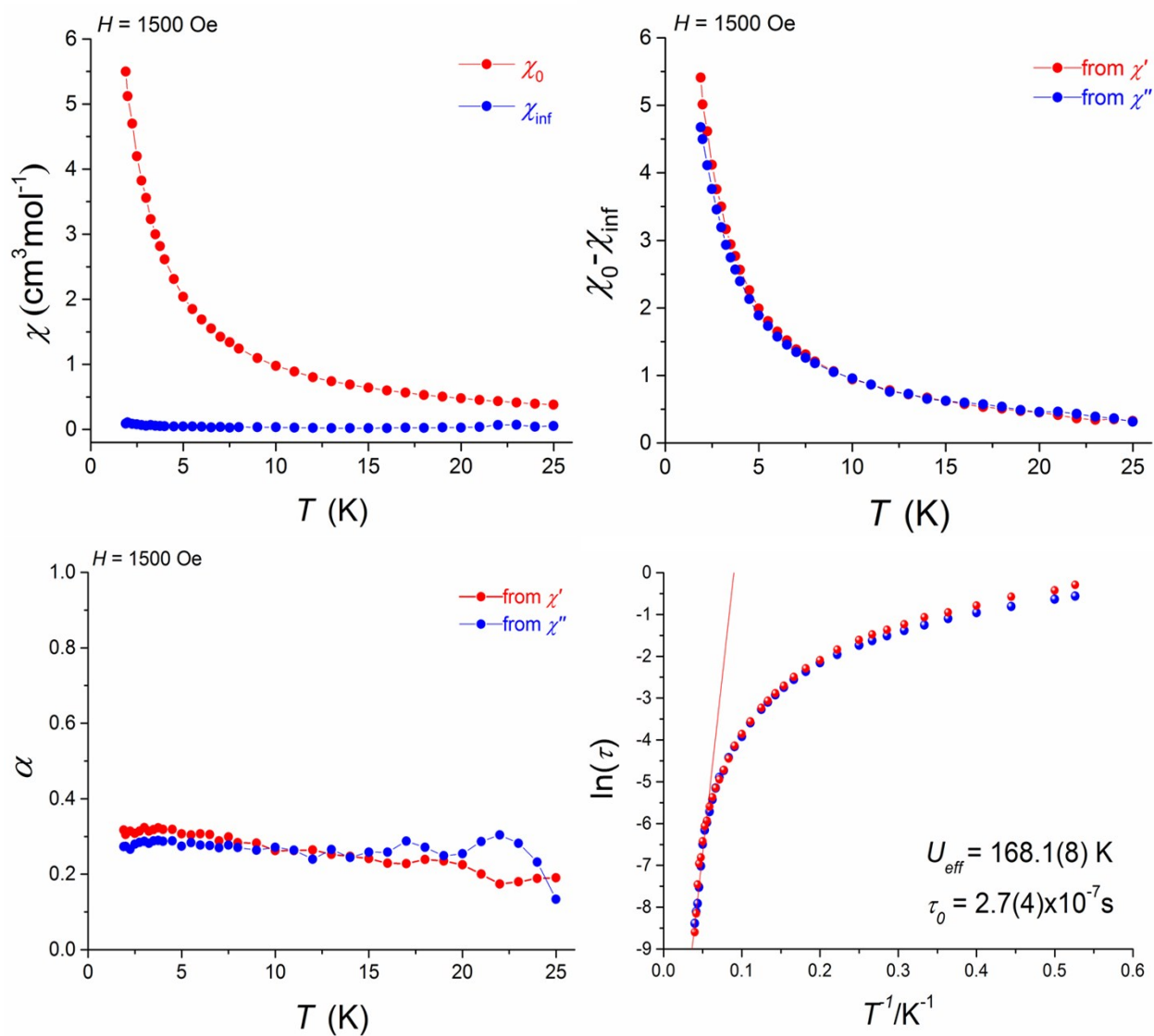


Fig. S16. Data obtained from generalized Debye fits of χ' and χ'' frequency dependent ac data under 1500 Oe applied dc field for **3**. Temperature dependence of χ_0 and χ_{inf} (top left), $\chi_0 - \chi_{\text{inf}}$ (top right), and α (bottom left). Relaxation times of the magnetization $\ln(\tau)$ vs. T^{-1} for **3** (Arrhenius plot using χ' (red) and χ'' (blue) ac data) under 1500 Oe applied dc field (bottom right). The solid red line corresponds to the fit of the data.

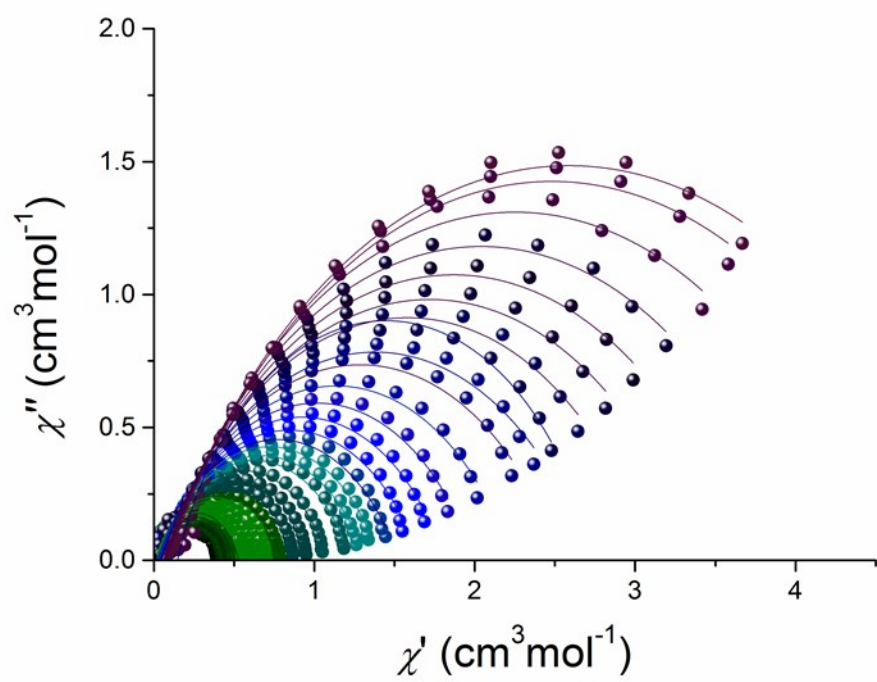


Fig. S17 Cole-Cole plot for ac susceptibility data of **3** under 1500 Oe applied dc field. Solid lines are the best fit to the generalized Debye model.

Table S3. Fitting values from Cole-Cole plot for **3** under 1500 Oe applied dc field.

T (K)	τ (s)	α	X_S	X_T
24	0.00022336	0.17021	0.08628	0.37058
23	0.00037396	0.34579	0.07977	0.35778
22	0.00063948	0.3529	0.0771	0.37389
21	0.00078168	0.28857	0.07062	0.40055
20	0.00098928	0.39176	0.08531	0.40494
19	0.00157741	0.32779	0.08585	0.43837
18	0.00186997	0.29986	0.07987	0.46512
17	0.00241734	0.35525	0.09251	0.48363
16	0.00312527	0.33213	0.08962	0.51696
15	0.00376304	0.35591	0.10122	0.546
14	0.00474089	0.33571	0.11171	0.59324
13	0.00575977	0.35716	0.11935	0.62946
12	0.00751069	0.35845	0.1376	0.68235
11	0.00987896	0.37843	0.15329	0.74922
10	0.01361329	0.35164	0.16512	0.83247
9	0.01764974	0.37394	0.19379	0.91831
8	0.02338924	0.40188	0.22747	1.02594
7.5	0.02563866	0.44431	0.25931	1.07915
7	0.03251272	0.41006	0.26672	1.17136
6.5	0.03692582	0.44039	0.29955	1.24709
6	0.04536374	0.44522	0.33533	1.35397
5.5	0.05642189	0.43744	0.36244	1.48751
5	0.06895749	0.43795	0.40057	1.63621
4.5	0.08691612	0.45395	0.45946	1.81694
4	0.10643058	0.47211	0.53551	2.03925
3.75	0.120198	0.48412	0.58727	2.17402
3.5	0.18466038	0.29301	0.46611	2.42944
3.25	0.16490003	0.45149	0.6363	2.52887
3	0.19010407	0.47832	0.72092	2.7187
2.75	0.22116657	0.46288	0.76197	2.97253
2.5	0.27003114	0.4531	0.8173	3.26272
2.25	0.35289635	0.44494	0.88824	3.61437
2	0.41219035	0.45706	1.00871	3.95336
1.9	0.48678291	0.4661	1.06446	4.11315