Supplementary Materials: Slow Magnetic Relaxation in Chiral Helicene-Based Coordination Complex of Dysprosium

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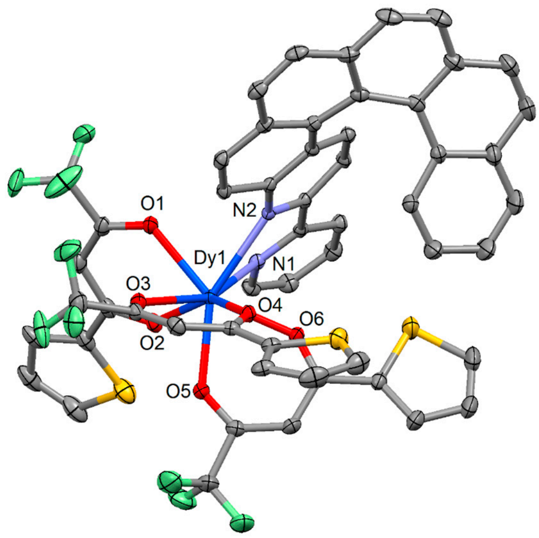

Figure S1. ORTEP view of **1**. Thermal ellipsoids are drawn at 30% probability. Hydrogen atoms and solvent molecules of crystallization are omitted for clarity.

Table S1. X-ray crystallographic data of **1**.

Compounds	1
Formula	$C_{62}H_{40}Cl_2Dy_1F_9N_2O_6S_3$
M/g·mol^{-1}	1409.5
Crystal system	Triclinic
Space group	P-1 (N°2)
Cell parameters	a = 13.3796(6) Å b = 14.6843(7) Å c = 17.4466(9) Å α = 112.428(2)° β = 107.113(2)° γ = 98.907(2)°
Volume/Å^3	2886.5(2)
Z	2
T/K	150(2)
2θ range/°	$2.74 \leq 2\theta \leq 55.04$
ρ_{calc}/g·cm^{-3}	1.622
μ/mm^{-1}	1.579
Independent reflections	13202
$Fo^2 > 2\sigma(Fo)^2$	11,888
Number of variables	716
R_1, wR_2	0.0456, 0.1301

Table S2. SHAPE analysis for **1**.

	$CShM_{SAPR-8}$ (Square Antiprism)	$CShM_{BTPR-8}$ (Biaugmented Trigonal Prism)	$CShM_{TDD-8}$ (Triangular Dodecahedron)
	D_{4d}	C_{2v}	D_{2d}
1	1.212	2.593	1.565

Extended Debye Model

$$\chi_M{}' = \chi_S + (\chi_T - \chi_S)\frac{1+(\omega\tau)^{1-\alpha}\sin\left(\alpha\frac{\pi}{2}\right)}{1+2(\omega\tau)^{1-\alpha}\sin\left(\alpha\frac{\pi}{2}\right)+(\omega\tau)^{2-2\alpha}}$$

$$\chi_M{}'' = (\chi_T - \chi_S)\frac{(\omega\tau)^{1-\alpha}\cos\left(\alpha\frac{\pi}{2}\right)}{1+2(\omega\tau)^{1-\alpha}\sin\left(\alpha\frac{\pi}{2}\right)+(\omega\tau)^{2-2\alpha}}$$

With χ_T the isothermal susceptibility, χ_S the adiabatic susceptibility, τ the relaxation time and α an empiric parameter which describe the distribution of the relaxation time. For SMM with only one relaxing object α is close to zero. The extended Debye model was applied to fit simultaneously the experimental variations of χ_M' and χ_M'' with the frequency f of the oscillating field ($\omega = 2\pi\nu$). Typically, only the temperatures for which a maximum on the χ_M'' vs. ν curves, have been considered. The best fitted parameters τ, α, χ_T, χ_S are listed in Table S4 with the coefficient of determination R^2.

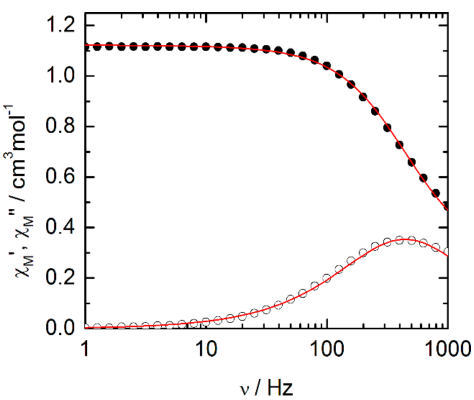

Figure S2. Frequency dependence of the ac susceptibility components χ_M' (full circles) and χ_M'' (empty circles) at 10 K and in zero external dc field for compound **1** with the best fitted curves (red lines) with the extended Debye model.

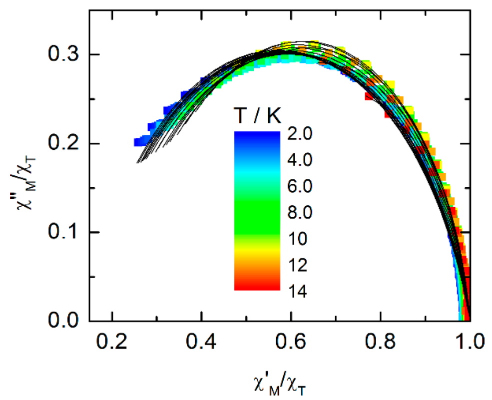

Figure S3. Cole–Cole plots using the ac data performed under zero magnetic field. The black lines correspond to the fits with the extended Debye model.

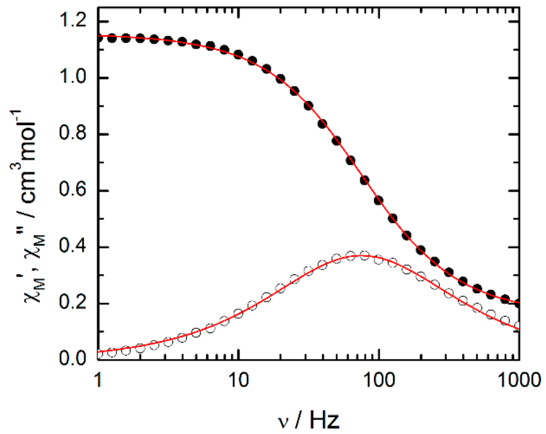

Figure S4. Frequency dependence of the ac susceptibility components χ_M' (full circles) and χ_M'' (empty circles) at 10 K and in 1000 Oe external dc field for compound **1** with the best fitted curves (red lines) with the extended Debye model.

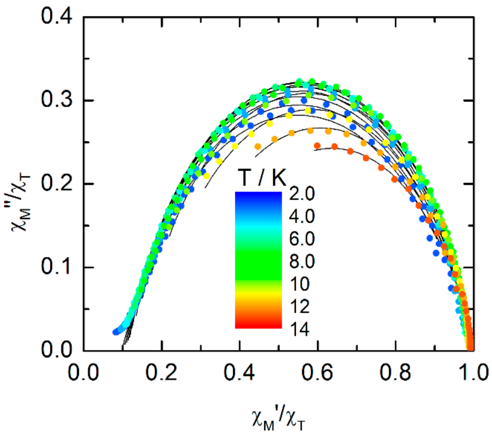

Figure S5. Cole–Cole plots using the ac data performed under 1000 Oe magnetic field. The black lines correspond to the fits with the extended Debye model.

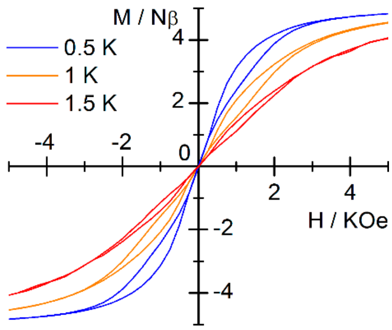

Figure S6. Magnetic hysteresis loops of **1** measured at 0.5, 1.0 and 1.5 K.

Table S3. Best fitted parameters (χ_T, χ_S, τ and α) with the extended Debye model **1** at zero field in the temperature range 2.0–14 K.

T/K	χ_T/cm³·mol⁻¹	χ_S/cm³·mol⁻¹	α	τ/s	R^2
2	5.33406	0.75513	0.21293	0.00082	0.99948
2.2	4.92216	0.71559	0.21137	0.00081	0.9995
2.4	4.50091	0.67372	0.21014	0.0008	0.99951
2.6	4.16608	0.63459	0.20901	0.00078	0.99951
2.8	3.87621	0.60214	0.20787	0.00077	0.99952
3	3.62664	0.57655	0.20628	0.00075	0.99953
3.5	3.13078	0.51369	0.20342	0.00071	0.99952
4	2.75152	0.47973	0.19654	0.00068	0.99953
4.5	2.46062	0.43222	0.19482	0.00065	0.99949
5	2.21271	0.41406	0.18855	0.00063	0.99958
5.5	2.01594	0.39104	0.18175	0.00061	0.99961
6	1.85223	0.37052	0.17638	0.00058	0.99963
7	1.59461	0.34004	0.16132	0.00054	0.99967
8	1.39993	0.31156	0.14681	0.00048	0.99973
9	1.24507	0.29276	0.12980	0.00043	0.99979
10	1.12302	0.27477	0.11504	0.00036	0.99985
11	1.02265	0.26158	0.10483	0.00029	0.99991
12	0.93270	0.25978	0.10034	0.00022	0.99995
13	0.86428	0.27474	0.09995	0.00016	0.99994
14	0.80504	0.30597	0.10308	0.00011	0.99998

Table S4. Best fitted parameters (χ_T, χ_S, τ and α) with the extended Debye model **1** at 1 kOe in the temperature range 3.0–14 K.

T/K	χ_T/cm³·mol⁻¹	χ_S/cm³·mol⁻¹	α	τ/s	R^2
3	4.44971	0.32750	0.41308	0.99823	0.99686
3.5	3.43103	0.31081	0.33274	0.34553	0.99781
4	2.91020	0.28559	0.28715	0.16694	0.99861
4.5	2.56236	0.26229	0.26010	0.09240	0.99906
5	2.29025	0.24308	0.23799	0.05507	0.99931
5.5	2.07574	0.22728	0.22285	0.03515	0.99948
6	1.90277	0.21281	0.21079	0.02338	0.99959
7	1.65922	0.18794	0.21108	0.01192	0.99965
8	1.44953	0.17243	0.19795	0.00640	0.99979
9	1.28653	0.16177	0.19118	0.00363	0.99980
10	1.16025	0.15462	0.19213	0.00212	0.99982
11	1.05708	0.15413	0.20342	0.00123	0.99979
12	0.96460	0.16295	0.22570	0.00065	0.99979
13	0.89279	0.19187	0.19187	0.00036	0.99984
14	0.83034	0.22740	0.24939	0.00020	0.99992

Table S5. Computed energies, *g*-tensor and wavefunction composition of the ground state doublet in the effective spin ½ model for **1**.

	Energy (cm⁻¹)	g_x	g_y	g_z	**Wavefunction Composition**
1	0.0	0.03	0.05	19.55	0.94 |±15/2> + 0.06 |±11/2>
2	81.529	0.13	0.26	17.00	0.81 |±13/2> + 0.10 |±11/2>
3	165.017	2.85	3.77	13.49	0.60 |±11/2> + 0.13 |±9/2> + 0.12 |±13/2>
4	210.544	9.73	5.77	0.25	0.51 |±9/2> + 0.24 |±7/2> + 0.10 |±11/2>
5	262.035	7.48	4.30	0.97	0.36 |±7/2> + 0.26 |±5/2> + 0.13 |±3/2> + 0.10 |±1/2>
6	305.348	10.9	7.24	2.57	0.32 |±1/2> + 0.27 |±3/2> + 0.21 |±5/2> + 0.10 |±7/2>
7	418.141	0.17	0.19	19.57	0.24 |±5/2> + 0.22 |±3/2> + 0.18 |±7/2> + 0.16 |±1/2>
8	618.005	0.00	0.01	19.76	0.37 |±1/2> + 0.31 |±3/2> + 0.19 |±5/2>