

Determining the Zero-Field Cooling/ Field Cooling Blocking Temperature from AC-Susceptibility data for Single-Molecule Magnets

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1. Experimental Section

1.1. Synthetic procedures

All reactions were conducted in aerobic conditions and the analytical reagents were purchased from commercial sources and used without further purification. The di(1-adamantyl)benzylphosphine was purchased from Sigma-Aldrich. The anhydrous compounds (the DyBr₃ salt and the tetrahydrofuran solvent) were always kept under inert atmosphere conditions.

Oxidation of the di(1-adamantyl)benzylphosphine

In a round-bottom flask, the di(1-adamantyl)benzylphosphine (0.5 g, 1.274 mmol) was dissolved in the minimum amount of methylene chloride and reacted with an excess of 30 % hydrogen peroxide in water (10 mL/g of di(1-adamantyl)benzylphosphine) and allowed to stir under ambient conditions for 12 hours, during which time the solution changed from clear to light yellow in colour. Upon completion, the reaction mixture was washed three times with water, then three times with brine solution, dried with sodium sulphate and filtered. Finally, the solvent was removed under reduced pressure. Yield: 85%. IR (cm⁻¹): IR (cm⁻¹): 3000-2800, ν (C-H, alkyl and aromatic); 1601, ν (C-C, aromatic); 1500-1300, bending(C-H, alkyl and aromatic); 1200-1100, ν (P=O); 698, ω (C-H, aromatic) and ν (P-C); 590, (in-plane benzene ring def.).

¹H NMR (360 MHz, CDCl₃): δ 7.47-7.18 (m, 5H), 3.15 (d, 2H), 2.17-1.70 (m, 30H).

³¹P NMR (203 MHz, CDCl₃): δ 48.45 (s).

Synthesis of [Dy(OPAd₂Bz)₂(H₂O)₄Br]Br₂·4THF (1)

A solution of the anhydrous DyBr₃ solid (48.27 mg, 0.12 mmol) in THF (7 mL) was heated at 80 °C in aerobic conditions until DyBr₃ was dissolved. The colour of the solution changed from clear to yellow. Additional THF was added when necessary while heating. After that, the ligand di(1-adamantyl)benzylphosphine oxide (100 mg, 0.24 mmol) was added, and THF was also added until reaching a final volume of 10 ml. The resulting mixture was sealed in a 15 ml teflon-lined stainless container and kept at 100 °C for three days. The solution obtained was transferred to a beaker and left to stand for 10 minutes, so that the little precipitate obtained remains at the bottom. Then, the solution is taken from the upper part. Crystallisation from slow evaporation produces air/humidity stable and large colourless prismatic single-crystals with a yield of 79%. Anal. Calc. for C₇₀H₁₁₄Br₃DyO₁₀P₂ (1581.82): C, 53.22; H, 7.27; N, 0; Found C, 52.89; H, 6.92; N, 0. IR (cm⁻¹): 3000-2800, ν (C-H, alkyl and aromatic); 1601, ν (C-C, aromatic); 1500-1300, bending(C-H, alkyl and aromatic); 1100-1000, ν (P=O) and ν (C-O, THF); 698, ω (C-H, aromatic) and ν (P-C); 590, in-plane benzene ring def. The amount of THF molecules was determined by TG analysis (see next section).

1.2. Thermogravimetric Analysis (TGA)

TGA measurements of **1** were performed on a METTLER-TOLEDO instrument, mod. TGA/DSC1.

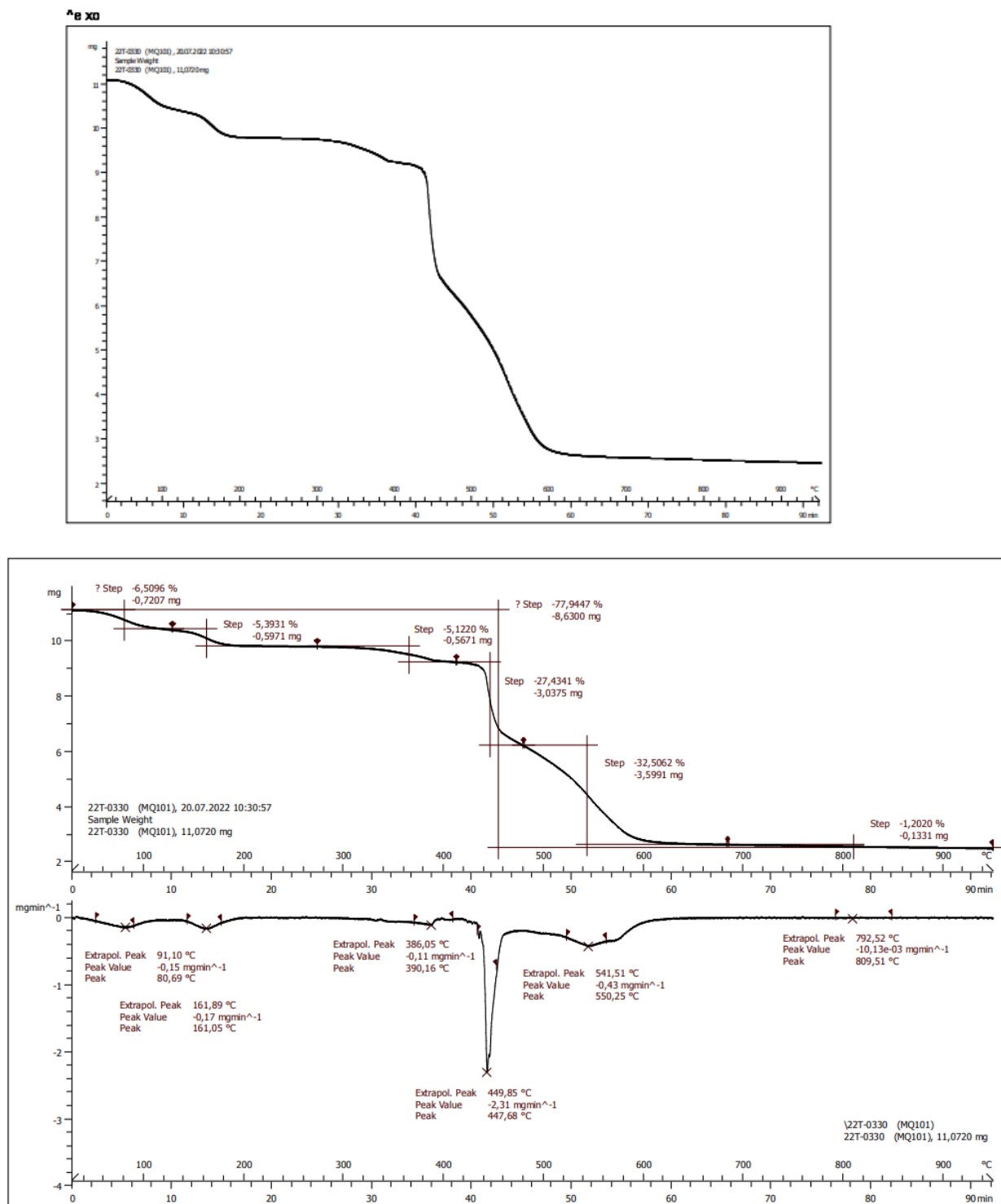


Figure S1. Thermogravimetric analysis (TGA) of **1** at a heating rate of 10 °C/min from 25 to 100 °C under nitrogen purging.

1.3. Physical measurements details

Elemental analysis was performed on a THERMO SCIENTIFIC Model Flash 2000 and ^1H NMR and ^{31}P $\{^1\text{H}\}$ RMN spectra on a 400 Hz “VARIAN DIRECT DRIVE” spectrometer at the “Centro de Instrumentación Científica” (University of Granada). IR spectra were recorded on a Bruker Tensor 27 spectrophotometer by using ATR detection. The X-ray powder diffraction (XRPD) spectrum was registered on a Bruker D8 DISCOVER using $\text{CuK}\alpha$ ($\lambda = 1.5406 \text{ \AA}$) radiation and DECTRIS PILATUS3R 100K-A detector, from 5 to 70° (2θ) at a scanning rate of $0.02^\circ 2\theta/\text{min}$.

1.4. Single-Crystal Structure Determinations

Suitable crystals of **1** were mounted on a glass fibre and used for data collection. X-ray diffraction data were collected at 100 K using a Bruker D8 Venture diffractometer ($\text{MoK}\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$) outfitted with a PHOTON III detector. Unit-cell parameters were determined and refined on all observed reflections using APEX2 software.^{1a} Correction for Lorentz polarization and absorption were applied by SAINT^{1b} and SADABS² programs, respectively.

The structures were solved using SHELXT³ by the intrinsic phasing method and refined by the full-matrix least-squares method on F2 using SHELXL-2014⁴ and the OLEX2 program.⁵ All non-hydrogen atoms were anisotropically refined. Hydrogen atom positions were calculated and isotropically refined as riding models to their parent atoms. One of the THF solvent molecules in structure **1** is disordered (oxygen 5 and carbon atoms C33, C34 and C35), and the disorder model was satisfactory. This model was not satisfactory when C32 was included in it; for this reason, C32 has not been split. The unit cell contains solvent-accessible VOIDS of $182 \text{ \AA}^3$. This is due to the evaporation of a THF molecule, and fortunately, it kept the crystal intact.

A summary of selected data collection and refinement parameters can be found in Table S2 and CCDC 2372498.

Table S1. Continuous Shape Measures for **1**.

Comple x	JETPY-7	JPBPY-7	CTPR-7	COC-7	PBPY-7	HPY-7	HP-7
1	23.027	2.731	6.488	8.128	0.948	25.781	33.952

JETPY-7: Johnson elongated triangular pyramid J7 (C_{3v}); JPBPY-7: Johnson pentagonal bipyramid J13 (D_{5h}); CTPR-7: Capped trigonal prism (C_{2v}); COC-7: Capped octahedron (C_{3v}); PBPY-7: Pentagonal bipyramid (D_{5h}); HPY-7: Hexagonal pyramid (C_{6v}); HP-7: Heptagon (D_{7h}).

Table S2. Crystallographic data for complex 1.

Compound	1
Formula	C ₇₀ H ₁₁₄ Br ₃ DyO ₁₀ P ₂
M_r	1579.78
Crystal System	tetragonal
Space Group	I4 ₁
a (Å)	24.7229(5)
b (Å)	24.7229(5)
c (Å)	12.1090(3)
α (°)	90
β (°)	90
γ (°)	90
V (Å³)	7401.3(4)
Z	4
D_c (g cm⁻³)	1.418
μ(MoK_α) (mm⁻¹)	2.725
T (K)	100
Observed reflections^a	11235 (10398)
R_{int}^a	0.0387 (0.0369)
Parameters	419
GOF	1.057
R₁^{b,a}	0.0341 (0.0300)
wR₂^{c,a}	0.0849 (0.0806)
^a Values in parentheses for reflections with I > 2σ(I)	
^b R ₁ = Σ F _o - F _c /Σ F _o	
^c wR ₂ = {Σ [w(F _o ² - F _c ²) ²] / Σ [w(F _o ²) ²]} ^{1/2}	

Table S3. Selected bond distances (Å) and angles (°) for complex 1.

Selected bond distances (Å)	
Dy – O1	2.210(3)
Dy – Br1	2.8860(6)
Dy – O2	2.349(3)
Dy – O3	2.380(3)
O1 – P1	1.516(3)
Selected bond angles (°)	
O1 – Dy – O1	176.73(16)
Br1 – Dy – O2	74.24(9)
O2 – Dy – O3	71.88(13)
O3 – Dy – O3	68.12(17)
O1 – Dy – Br1	91.64(8)
O1 – Dy – O2	88.13(11)
O1 – Dy – O3	90.70(11)
P1 – O1 – Dy	173.67(19)

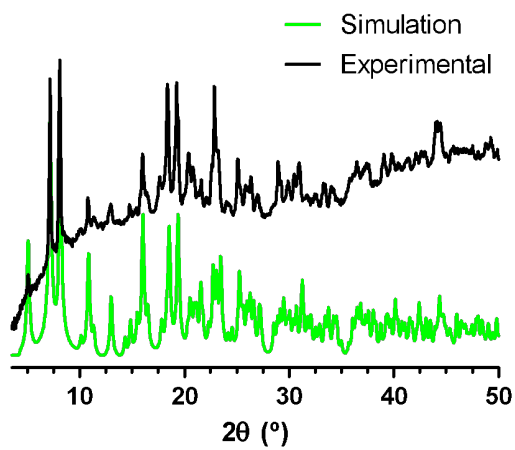


Figure S2. X-ray powder diffractogram for **1** (black) and the calculated from the X-ray crystal structure (green).

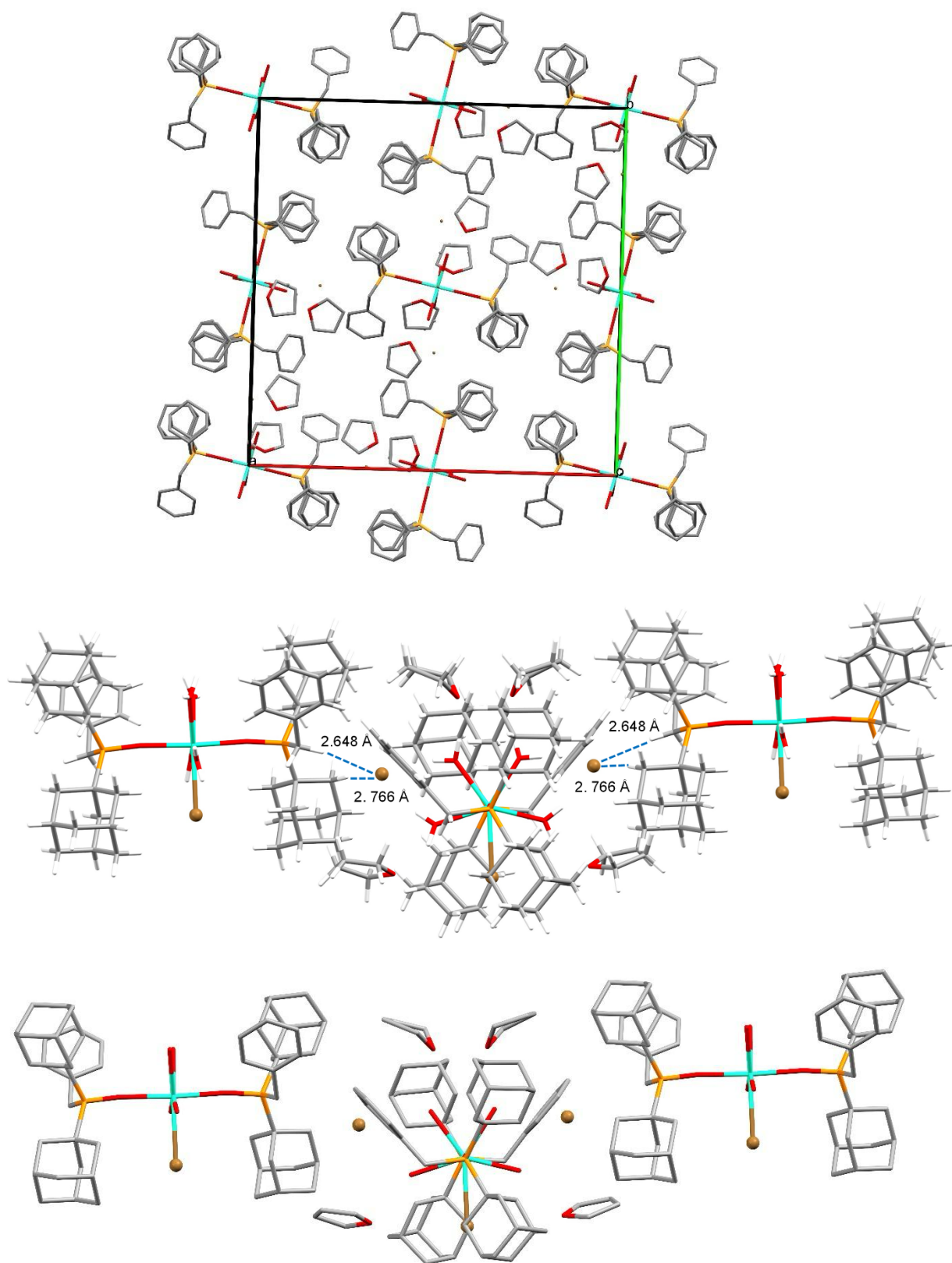


Figure S3. (top) A view of the crystal packing of **1** along the *c* axis. (middle) van der Waals interactions between adjacent units. Bromide atoms are displayed as brown balls. (bottom) The same view as “middle”, with the hydrogen atoms omitted for clarity.

2. Magnetic Studies

The DC magnetic measurements were performed on a polycrystalline sample of **1** using a Quantum Design SQUID MPMS XL-7 device. The temperature dependence of magnetic susceptibility has been measured in the 2-300 K range. The magnetic field dependence of magnetization has been measured under different applied static fields (0-7 T) in the temperature range 2-7 K. The magnetic susceptibility values were corrected for the diamagnetism of the molecular constituents, using the Pascal constants, and the sample holder.

The Zero Field Cool / Field Cool (ZFC/FC) experiment was performed under different conditions by varying the applied field as well as the measurement rate. The sample was initially cooled in absence of an external direct magnetic field. After reaching 2 K, a small magnetic field (50 or 500 Oe) was applied, and the magnetic moment was measured in sweep mode while increasing the temperature to 12 K at a specific rate (from 0.01 to 5 K/min). Then, the sample was cooled again to 2K while applying the field employed for the measurement and the magnetic moment was measured again in the same way. Between measurements at different rates the sample was heated in the absence of a magnetic field. The blocking temperatures for different heating rates and applied DC fields are collected in Table S4.

The in-phase and out-of-phase ac magnetic susceptibility measurements were carried out on a polycrystalline sample of **1**. To allow the study for a larger range of frequencies two equipment were employed. A PPMS-9 physical measurement equipment was employed for 100-10000 Hz frequency range, with an oscillating field $H_{ac} = 10$ Oe and using temperatures in the 2-56 K range. And a SQUID MPMS XL device was employed in the 1-1500 Hz frequency range with an oscillating field of 4 Oe between 15 and 27 K. The Cole-Cole plots were represented between 15 and 27 K and the relaxation time obtained by fitting the curves to the generalized Debye model. Obtained values are summarized in Table S5.

Isothermal magnetisation decay data was collected in the 2–8 K range. Firstly, at the selected temperature the sample was magnetized under an applied magnetic field of 5 T for 5 minutes. The field was set to zero on “No Overshoot” mode and the magnetisation measured for 2500 s. The magnetisation, however, equilibrated to a negative value, indicating a remanent field in the superconducting magnet. The data was fitted using a stretched exponential function, which is commonly employed in the obtention of relaxation times from magnetisation decay.^{6,7} The data was fit by employing Eq. S1 where M_{eq} is the negative equilibrium magnetisation values obtained at each experiment, M_0 is the first datapoint measured, t is the time in seconds since the first measurement, τ is the relaxation time and β is a stretching parameter ($0 < \beta \leq 1$). Obtained values are summarized in Table S6.

$$M = M_{eq} + (M_0 - M_{eq})e^{-\left(\frac{t}{\tau}\right)^\beta} \quad (S1)$$

The DC hysteresis measurements were collected in the 3- 20 K and at a sweep rate of 20mT/s on a Quantum Design instrument, model PPMS-9 (VSM option).

2.1 Susceptibility and magnetisation

The DC magnetic properties of **1** were studied in the 2-300 K temperature range under an applied magnetic field of 0.5 T plotted as $\chi_M T$ vs. T in Fig. S4.a) (χ_M is the molar magnetic susceptibility), with the isothermal magnetisation (M vs. H) shown in Fig. S4.a) (inset).

At 300 K, the $\chi_M T$ value of $14.65 \text{ cm}^3 \text{ K mol}^{-1}$ agrees with that expected for an isolated Dy^{III} ion ($4f^9$, $J = 15/2$, $S = 5/2$, $L = 5$, $g = 4/3$, ${}^6\text{H}_{15/2}$) in the free ion approximation ($14.18 \text{ cm}^3 \text{ K mol}^{-1}$). Upon cooling, the $\chi_M T$ value gradually decreases to $11.76 \text{ cm}^3 \text{ K mol}^{-1}$ at 7 K before rapidly decreasing to the value of $6.21 \text{ cm}^3 \text{ K mol}^{-1}$ at 2 K, which is characteristic of magnetically anisotropic lanthanide systems.

The gradual decrease is consistent with the thermal depopulation of the higher-energy $\pm m_J$ sublevels, which come from the splitting of the spin-orbit ground term ${}^6\text{H}_{15/2}$ by the crystal field effects. This indicates the existence of a large magnetic anisotropy with well-separated low-lying energy levels.

The field dependence of the magnetisation at 2 K (Fig. S4.b)) shows a sinusoidal behaviour at a low field with a saturation value of $6.00 N\mu_B$ at 7 T, which is expected for this kind of SMM. This low saturation value confirms the axial nature ($\pm 15/2$) of the well-isolated ground state.

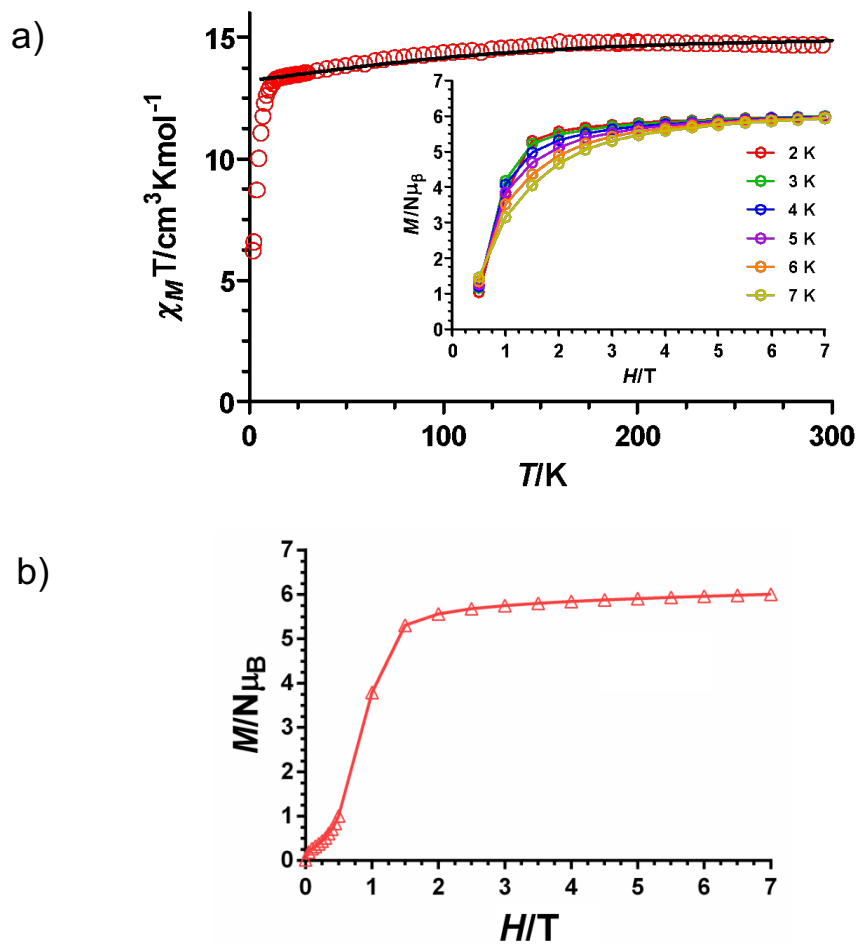


Figure S4. a) Temperature dependence of $\chi_M T$ for **1** (red circles) and that obtained using *ab initio* calculations (solid line, scaled by 1.07). Inset: Magnetisation vs. Field plot at the indicated temperatures; b) Magnetisation vs. Field plot at 2 K.

2.2 Zero Field Cool / Field Cool

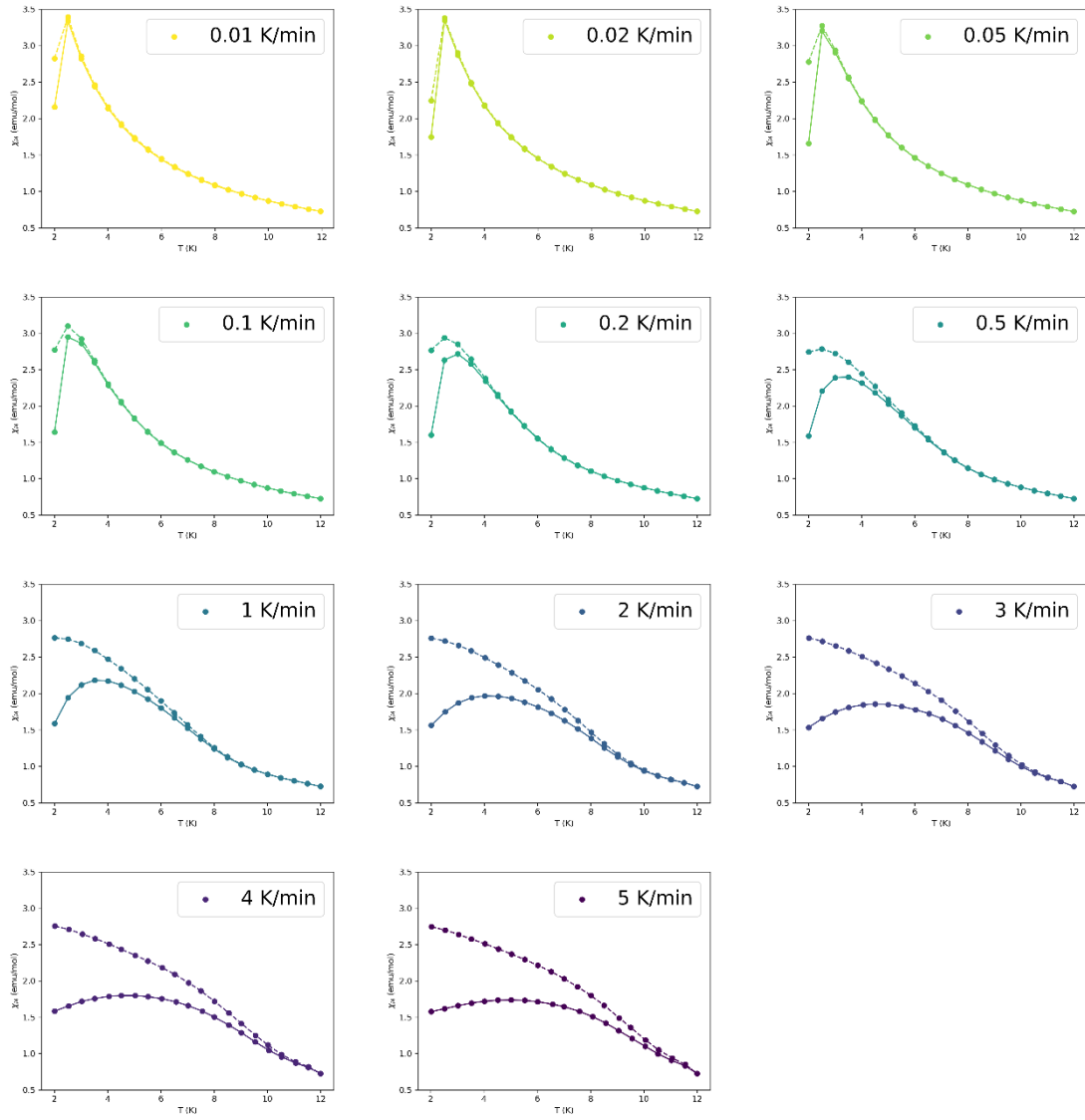


Figure S5. Temperature dependence of χ_M at ZFC and FC conditions with an applied field of 50 Oe and different heating rates.

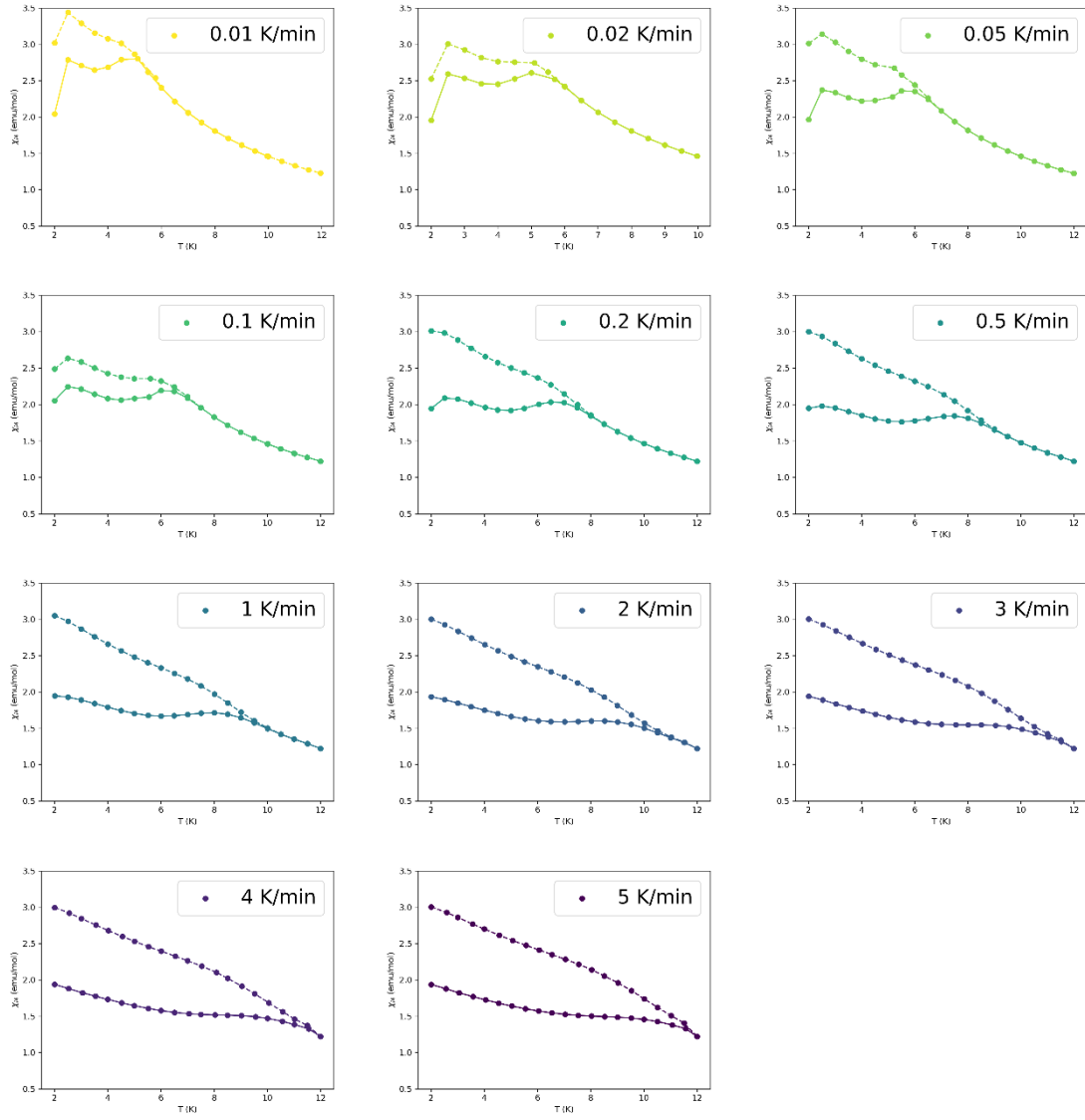


Figure S6. Temperature dependence of χ_M at ZFC and FC conditions with an applied field of 500 Oe and different heating rates. The double peaks at low temperatures, especially at low heating rates, have also been previously reported in magnetically diluted Er^{III} compounds.⁸ Such anomalous behaviour can be attributed to a secondary relaxation process at very low temperature.

Table S4. ZFC/FC blocking temperatures for different heating rates 0.01-5 K/min and applied DC fields of 50 Oe and 500 Oe.

Heating rate (K/min)	T _{B-ZFC/FC} (50 Oe) (K)	T _{B-ZFC/FC} (500 Oe) (K)
0.01	2.5	4.9
0.02	2.5	5.1
0.05	2.6	5.7
0.1	2.7	6.2
0.2	2.8	6.6
0.5	3.3	7.4
1	3.7	7.8
2	4.2	8.3
3	4.5	-
4	4.7	-
5	5.0	-

2.3. In-phase and out-of-phase magnetic susceptibility

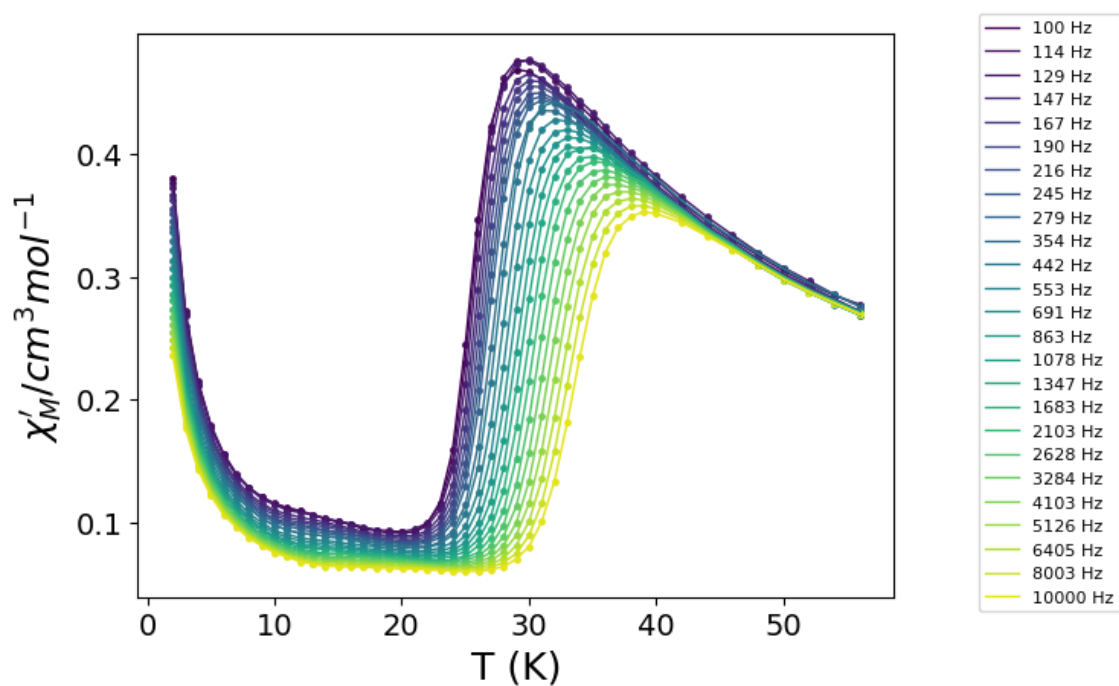


Figure S7. Temperature dependence of the in-phase ac magnetic susceptibility (χ'_M) under zero DC field for compound **1**. The solid lines are a guide for the eye.

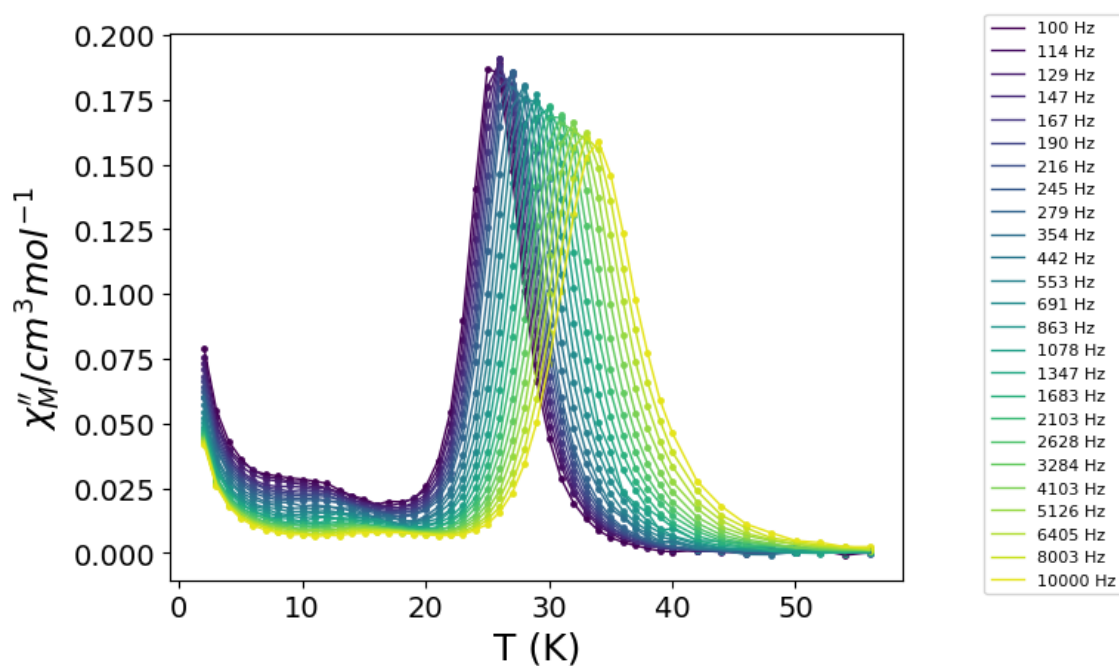


Figure S8. Temperature dependence of the out-of-phase ac magnetic susceptibility (χ''_M) under zero DC field for compound **1**. The solid lines are a guide for the eye.

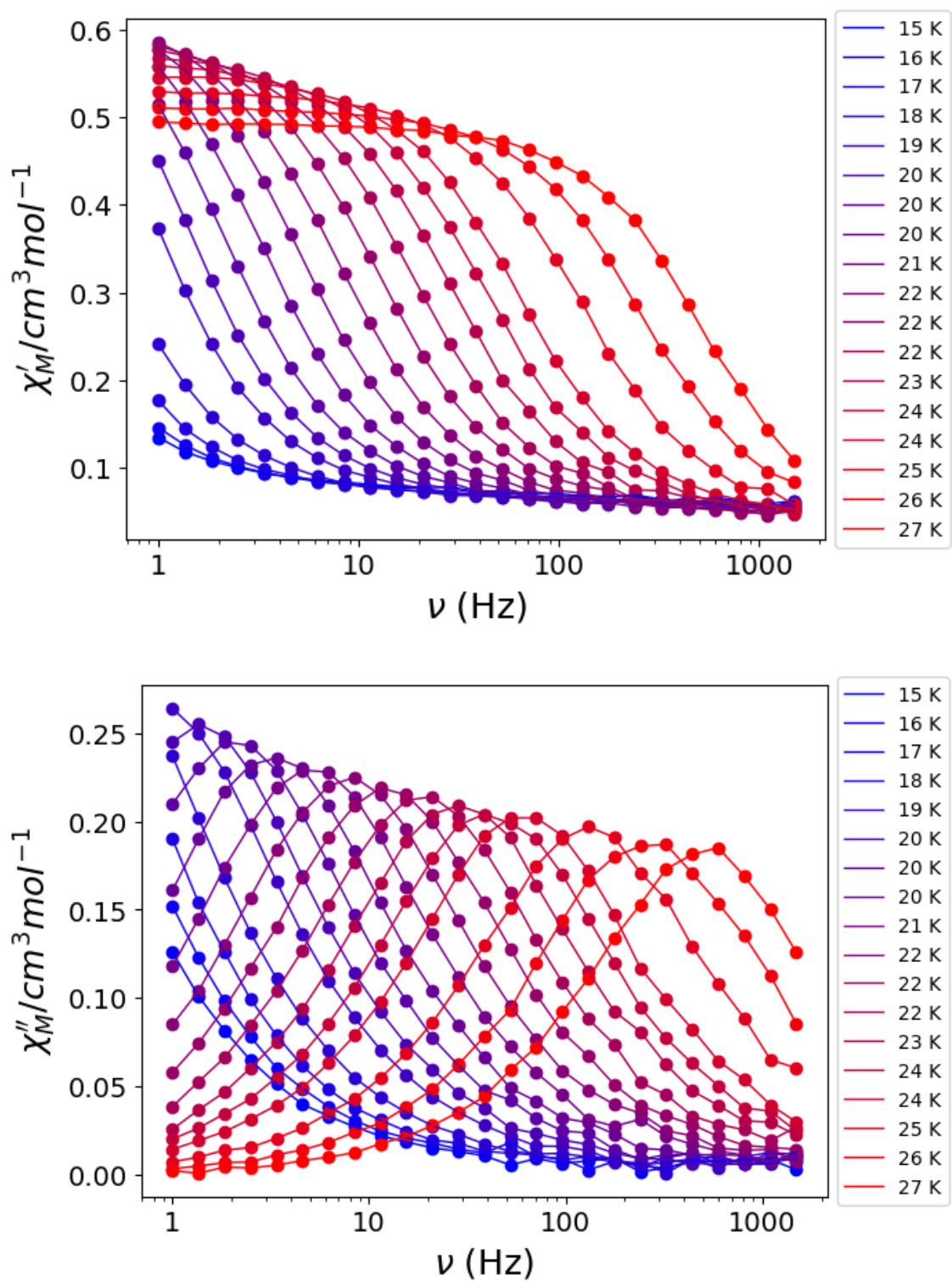


Figure S9. Frequency dependence of the in-phase (top) out-of-phase (bottom) component of the ac susceptibility (χ_M'') under zero DC field for compound **1**. The dots are connected with solid lines to improve visibility.

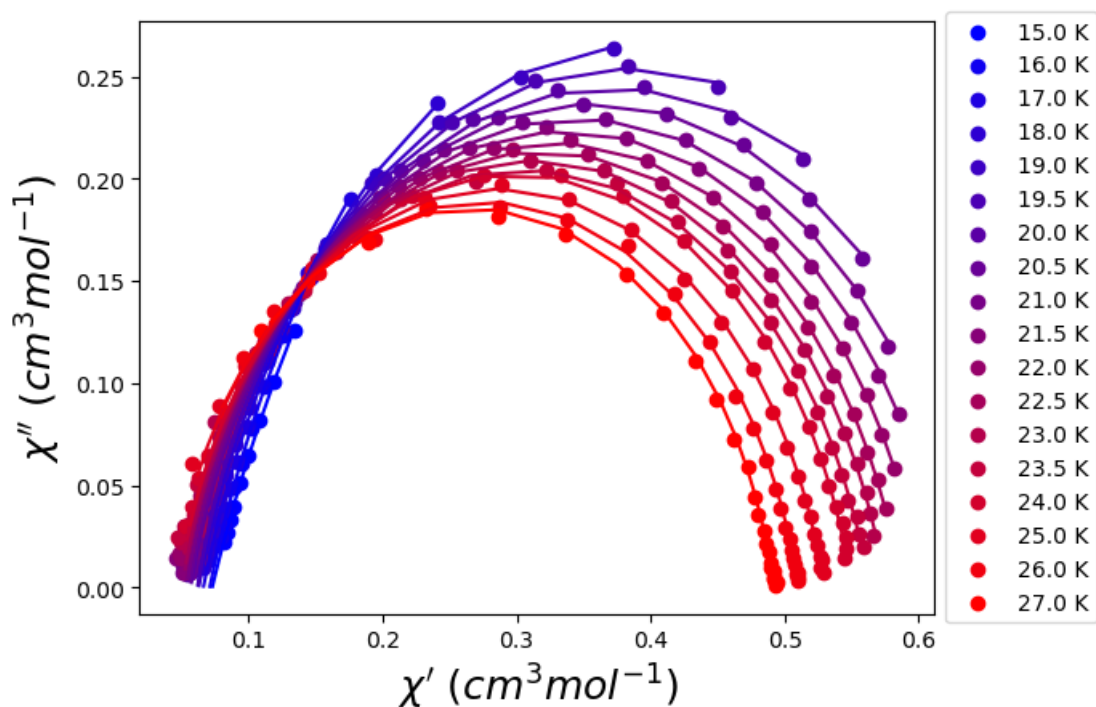


Figure S10. Cole-Cole plot χ'' vs. χ' plot for compound **1** under zero DC field at the indicated temperatures. The solid lines correspond to the best fit to the generalised Debye model

Table S5. Obtained values from the fit of the Cole-Cole plots shown in Figure S10.

T (K)	χ_s	χ_T	$\ln(\tau)$	α
15	0.073	1.328	1.006	0.223
16	0.071	1.060	0.355	0.192
17	0.066	0.944	-0.147	0.188
18	0.063	0.797	-0.850	0.179
19	0.062	0.678	-1.703	0.154
19.5	0.062	0.639	-2.141	0.145
20	0.057	0.629	-2.556	0.159
20.5	0.056	0.601	-3.017	0.151
21	0.054	0.584	-3.464	0.152
21.5	0.051	0.570	-3.903	0.153
22	0.050	0.552	-4.344	0.150
22.5	0.050	0.537	-4.766	0.145
23	0.048	0.527	-5.181	0.147
23.5	0.047	0.515	-5.581	0.146
24	0.048	0.502	-5.966	0.137
25	0.043	0.487	-6.711	0.139
26	0.041	0.468	-7.396	0.136
27	0.042	0.450	-8.039	0.122

2.4 Magnetisation decay

Table S6. Obtained values from the fit of the isothermal magnetisation decay using Eq. S1.

T (K)	M_{eq} (μ_B)	M_0 (μ_B)	$\ln(\tau)$	β
2	-0.005622	0.227250	4.946	0.744
2.5	-0.005858	0.223989	4.963	0.745
3	-0.005829	0.204357	4.982	0.753
4	-0.003196	0.194385	4.888	0.759
5	-0.004583	0.148303	4.806	0.798
6	-0.003978	0.113889	4.547	0.849
7	-0.003241	0.055059	4.219	0.929
8	-0.003026	0.019242	3.763	0.973

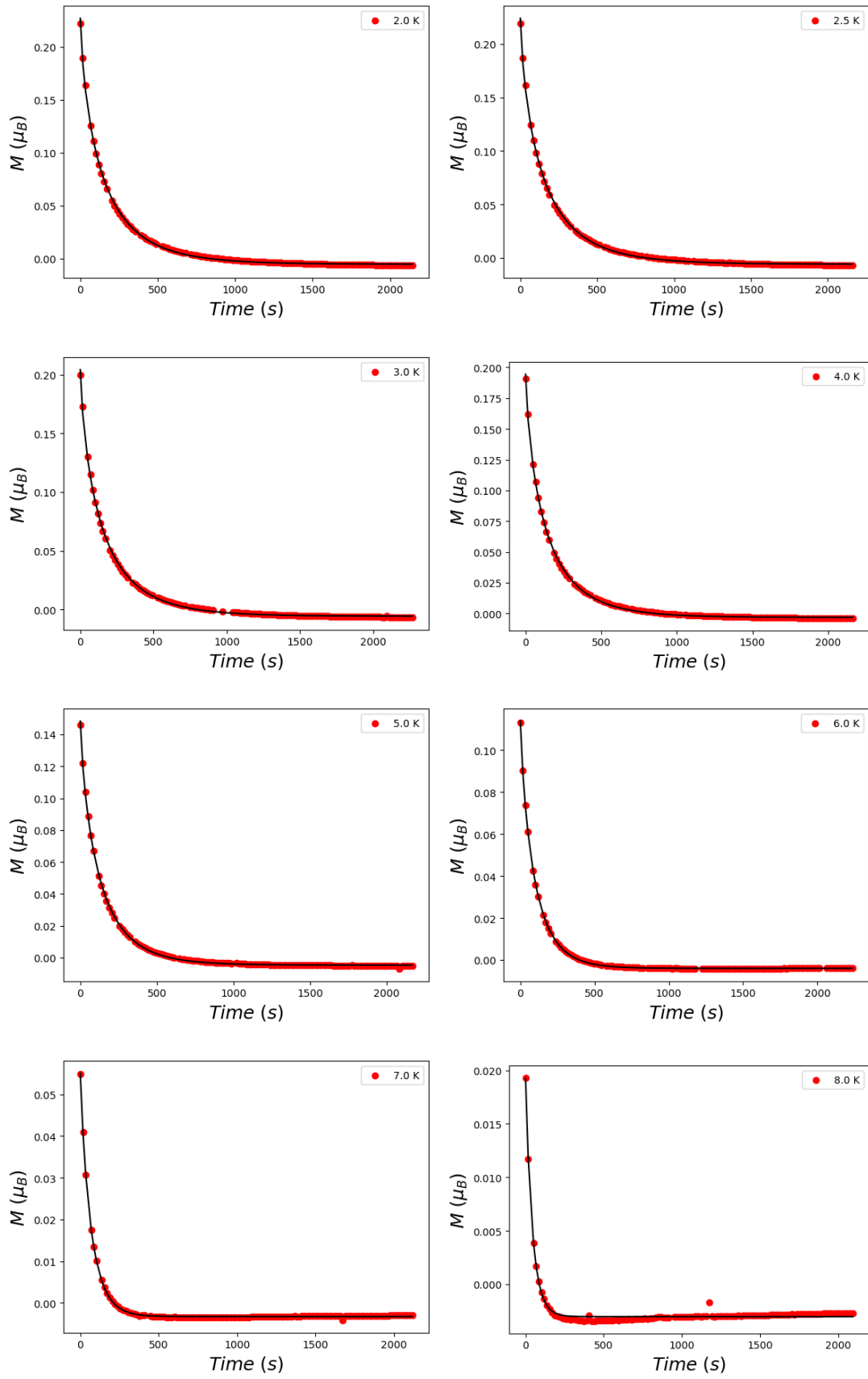


Figure S11. Isothermal magnetisation decay plots between 2 and 8 K. The black line is the fit using Eq. S1.

4. *Ab initio* calculations

Post–Hartree–Fock *ab initio* calculations were carried out on the crystal structure of **1**. For the calculations, two quantum chemistry program packages have been employed, Orca 5.0.3⁹⁻¹¹ and OpenMolcas 18.09.¹²⁻¹⁴ The electronic structure and magnetic properties have been computed using state-averaged complete active space self-consistent field calculations (SA-CASSCF (9,7)).¹⁵ The employed active space includes nine electrons in seven 4f orbitals of Dy^{III} CAS (9,7). Within this active space, we have computed 21 sextets states, 128 quadruplets and 98 doublets. For Orca quantum chemistry package, the spin-orbit effects were included using the quasi-degenerate perturbation theory (QDPT).¹⁶ Scalar relativistic effects were considered by second-order Douglas–Kroll–Hess (DKH) procedure.^{17, 18} In these calculations, all the atoms are described by the def2-TZVPP basis set,^{19, 20} including the corresponding auxiliary basis sets for correlation and Coulomb fitting for all the atoms apart from Dysprosium, for which the SARC2-DKH-QZVP basis set²¹ was used to take into account the relativistic effect. For OpenMolcas quantum chemistry package, the effect of spin–orbit coupling was considered perturbatively in a second step by using the restricted active space state interaction method (RASSI). Dynamic correlation contributions are not essential due to the relatively large ionic character of the Ln–O bonds. The MOLCAS ANO-RCC basis set²²⁻²⁴ was used for all the atoms. The following contractions were used: Dy [9s8p6d4f3g2h]; Br [5s4p2d]; P [5s4p3d2f]; O [4s3p2d1f]; C [3s2p] and H [2s]. In both program packages, the Single Aniso²⁵ approach was also used, which enables calculations of anisotropic magnetic properties and g tensors for the ground and first excited Kramers doublets (KD) and the matrix elements of the transition magnetic moments, which gives an estimation of the probability of transition between two different states of the molecules.²⁶

Table S7. CASSCF (ORCA) and CASSCF+RASSI (OpenMOLCAS) computed relative energies (in cm^{-1}) of the eight low-lying Kramers' doublets, g tensors and tilting angle (θ) of the main anisotropy axes (g_z component) of the corresponding excited (ES1, ES2, etc.) KD with respect to the ground state (GS) KD for **1**. ORCA and OpenMOLCAS results are given.

a) ORCA

Energy (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ ($^\circ$)
0.0	0.0008	0.0008	19.859	
275.2	0.129	0.274	16.920	6.4
336.6	0.419	1.634	17.732	90.0
406.7	2.673	8.120	8.263	77.5
445.6	1.163	2.993	13.167	32.3
467.1	0.067	1.183	7.623	0.9
526.5	2.224	2.326	11.701	39.1
674.4	0.004	0.022	18.945	58.4

b) OpenMOLCAS

Energy (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ ($^\circ$)
0.0	0.0008	0.0008	19.870	
277.5	0.116	0.227	16.967	6.4
345.6	0.484	1.820	17.620	90.0
412.3	8.263	7.766	2.674	12.5
449.8	1.085	2.807	13.199	31.6
473.6	0.432	1.578	7.767	4.1
531.2	2.419	2.680	11.415	37.4
674.9	0.002	0.028	18.921	58.3

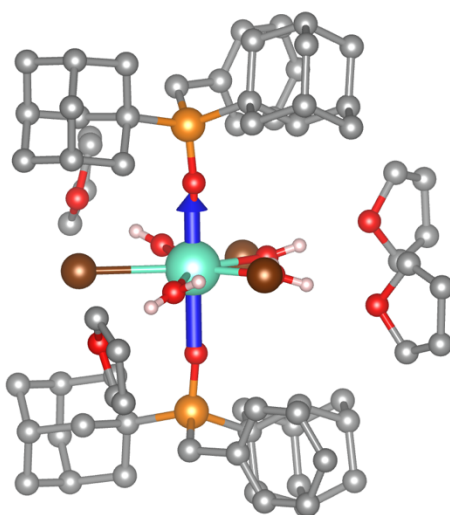


Figure S12. CASSCF+RASSI calculated anisotropy axis for the ground Kramers' doublet of complex **1** using OpenMOLCAS. Code colours: dysprosium (cyan), oxygen (red), bromide (brown), phosphorus (orange), and carbon (grey).

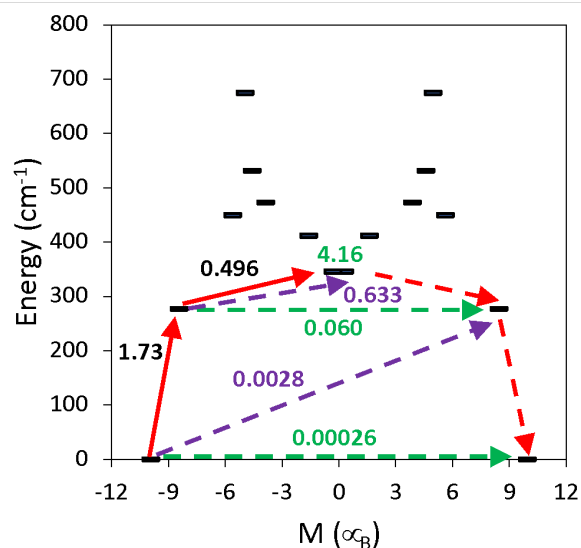


Figure S13. State energies as a function of their average magnetic moment, M , along the main anisotropy axis for **1** obtained with Single Aniso module from CASSCF+RASSI (OpenMOLCAS) calculations. The dashed green arrows correspond to the quantum tunnelling mechanism of ground or excited states, dashed purple arrow shows the hypothetical Orbach relaxation process. The solid red arrow indicates the transition between the ground and excited Kramers' doublets, and the dashed red arrow indicates the excitation pathway to the ground state with the reversed spin. The values close to the arrows indicate the matrix elements of the transition magnetic moments (above 0.1, an efficient spin relaxation mechanism is expected).

4. Theoretical Model

Comparison between Eqs. 7 and 13

The effect of the Curie law approximation inherent to Eq. 13 and the best choice for C_1' are evaluated by comparing the blocking temperatures predicted by Eqs. 13 and 7 for selected experimental cases. Four systems were chosen among the literature data presented in Table S9, as they have shown significant deviations from the Curie law in the χT plot, even at temperatures as high as 50K. The selected molecules were number 2 (refcode: LIRQUB), 4 (BAWL0D), 38 (VAGMOJ) and 43 (EHEHOR).

Eq. 7 from the main text is presented as:

$$\chi_{ZFC} = \chi_T \left[-C_1' \exp \left(-R_H^{-1} \int \tau^{-1} dT \right) + 1 \right] = \lambda \chi_T$$

Where χ_T is the temperature-dependent susceptibility, digitalised from the reported χ^*T plots. Eq. 13 corresponds to:

$$T_B = \frac{R_H \left[1 - C_1' \exp \left(-R_H^{-1} \int_0^{T_B} \tau^{-1} dT \right) \right]}{C_1' \exp \left(-R_H^{-1} \int_0^{T_B} \tau^{-1} dT \right) \tau^{-1}(T_B)}$$

Thus, we calculated the blocking temperature for the four selected cases using Eqs. 13 and 7 for C_1' values ranging from 1 to 0.1 (See Table S8). For the results derived from Eq. 7, the experimental χT plot was digitized from published data to interpolate the χ_T function avoiding the Curie Law approximation.

Table S8. Experimental and calculated ZFC/FC blocking temperatures using Eqs. 7 and 13. Missing values for $T_{B-ZFC/FC}$ correspond to ZFC curves without a discernible maximum.

N°	REFCODE	$T_{B-ZFC/FC}$ (exp,K)	C_1'	$T_{B-ZFC/FC}$ (calc. eq 8, K)	$T_{B-ZFC/FC}$ (calc. eq 13, K)
2	LIRQUB	55	1.0	57.0	55.8
			0.9	56.0	54.6
			0.8	54.9	53.1
			0.7	53.5	51.1
			0.6	51.7	47.7
			0.5	49.2	-
			0.4	45.5	-
			0.3	21.0	-
			0.2	20.9	-
			0.1	20.8	-
4	BAWLOD	45	1.0	51.3	50.5
			0.9	50.5	49.8
			0.8	49.4	49.0
			0.7	48.2	47.9
			0.6	46.8	46.4
			0.5	45.0	43.9
			0.4	42.3	-
			0.3	-	-
			0.2	-	-
			0.1	-	-
38	VAGMOJ	6.4	1.0	6.3	6.3
			0.9	6.3	6.3
			0.8	6.3	6.3
			0.7	6.3	6.2
			0.6	6.3	6.2
			0.5	6.2	6.2
			0.4	6.2	6.2
			0.3	6.2	6.2
			0.2	6.2	6.1
			0.1	6.1	-
43	EHEHOR	5.5	1.0	5.3	4.8
			0.9	5.3	4.7
			0.8	5.3	4.6
			0.7	5.3	4.5
			0.6	5.2	4.3
			0.5	5.2	4.0
			0.4	5.2	-
			0.3	5.2	-
			0.2	5.1	-
			0.1	5.1	-

ZFC/FC curves for Tunneling, Orbach and Raman relaxation

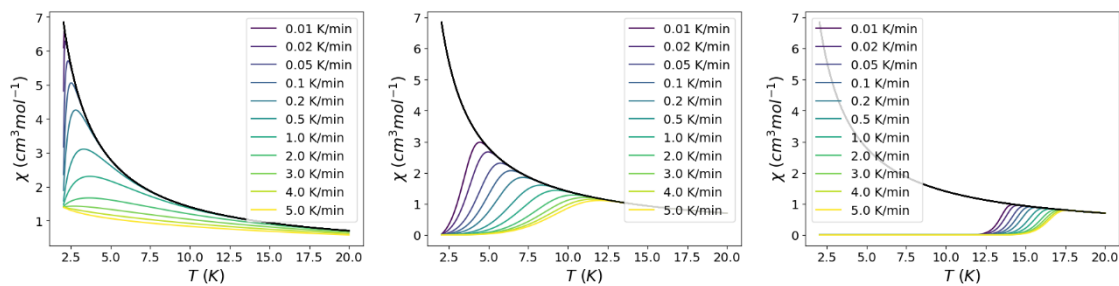


Figure S14. ZFC/FC curves simulated from Eq. 7 for the different demagnetisation mechanisms. (left) Tunnelling, (centre) Raman and (right) Orbach.

5. Model Assessment

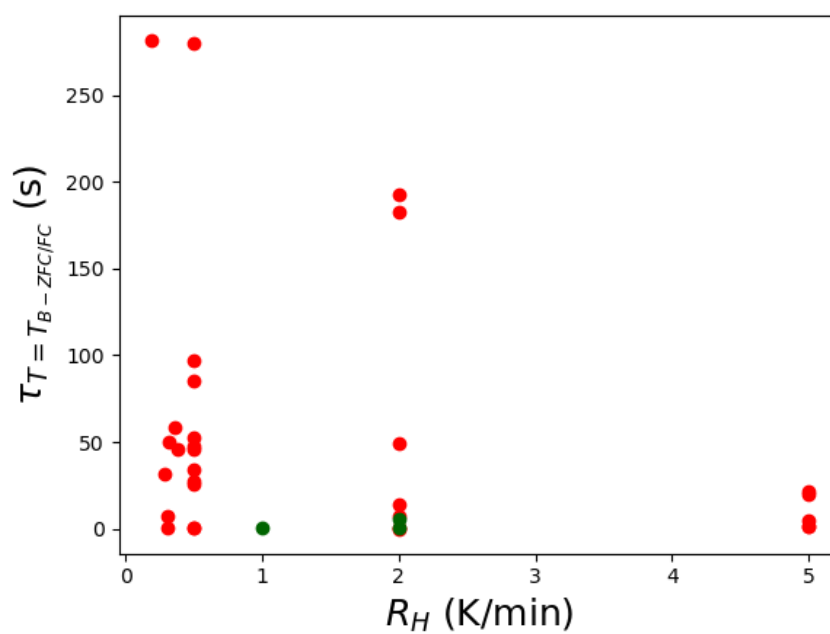


Figure S15. Relaxation time (s) at the ZFC/FC blocking temperature for the systems presented in Table S9 (red and green for lanthanide and transition metal compounds, respectively). Data is presented as a function of the heating rate (K/min).

Table S9. Experimental demagnetisation parameters and ZFC/FC blocking temperatures for literature examples of SMMs. The estimation of T_B based on Eq. 13 is presented employing the experimentally reported heating rate. In the cases where no heating rate is reported, the ZFC/FC blocking temperature was calculated assuming a slow and fast heating rate (0.2 K/min and 5 K/min, respectively). For the ZFC/FC section, R_H corresponds to the heating rate, $\mu_0 H$ is the static magnetic field and τ is the relaxation time at the temperature of $T_{B-ZFC/FC}$. For the demagnetisation parameters, τ_0 and U_{eff} are the Orbach prefactor and effective demagnetisation barrier, respectively, C and n are the usual Raman parameters and τ_{QTM} is the tunnelling relaxation time.

	Compound	REFCODE	Eq.13		ZFC/FC				T_{B-100} (K)	Demagnetisation parameters					Ref.
			R_H (K min ⁻¹)	T_B (K)	R_H (K min ⁻¹)	T_{B-ZFC} (K)	$\mu_0 H$ (T)	τ (s)		τ_0 (s)	U_{eff} (K)	C (s ⁻¹ K ⁻ⁿ)	n	τ_{QTM} (s)	
	Dy^{III} complexes														
1	(Cp ^{iPr5}) ₂ Dy ₂ l ₃	-	0.2 5	71.5 78.7	-	75	0.1	229	72	6.31×10^{-13}	2346.7 6	-	-	-	27
2	[K(2.2.2)][[1-(piperidino)-2,3,4,5-tetraphenylboroly]zDy]	TERGIK	0.2 5	21.2 64.0	-	68*	-	89.7	66	2.01×10^{-13}	2385.61	2.4×10^{-6}	1.93	-	28
3	[(η^5 -Cp*)Dy(η^5 -Cp ^{iPr5})] [B(C ₆ F ₅) ₄]	LIRQUB	2	55.8	2	55 ^a 78*	0.1	192	65	4.2×10^{-12}	2217.27	3.1×10^{-8}	3	2.5×10^4	29
4	[(Cp ^{III}) ₂ Dy][B(C ₆ F ₅) ₄]	MEKDOI	0.2 5	20.0 60.4	-	61*	0.1	152.05	53	1.99×10^{-11}	1759.71	1.66×10^{-6}	2.151	-	30
5	[(Cp ^{III}) ₂ Dy][B(C ₆ F ₅) ₄]	BAWLOD	2	50.5	2	45	0.1	182.68	53	1.09×10^{-11}	1807	1.81×10^{-9}	3.92	-	31
6	[(Cp ^{III}) ₂ Dy _{0.08} Y _{0.92}][B(C ₆ F ₅) ₄]	BAWLOD	0.2 5	18.0 62.7	-	45	0.1	181.18	-	2.06×10^{-11}	1753.95	4.29×10^{-6}	1.88	-	30
7	[Dy(Cp ^{iPr4} Me) ₂][B(C ₆ F ₅) ₄]	WIRHIR	0.2 5	21.7 62.6	-	65*	0.1	219.40	62	4.01×10^{-12}	2121.23	1.57×10^{-6}	2.07	2.45×10^3	32
8	[Dy(Cp ^{iPr5}) ₂][B(C ₆ F ₅) ₄]	WIRGUC	0.2 5	22.2 59.1	-	60*	0.1	162.83	56	1.18×10^{-11}	1919.42	8.04×10^{-7}	2.31	1.19×10^3	

9	[Dy(Cp'Pr ₄ Et) ₂][B(C ₆ F ₅) ₄]	WIRHEN	0.2 5	30.6 69.7	-	60*	0.1	292.64	59	7.79×10 ⁻¹²	1985.61	3.36×10 ⁻⁸	3.02	4.47×10 ²	
10	[Dy(Dtp) ₂][Al{OC(CF ₃) ₃ } ₄]	DUBKET	0.2 5	8.8 40.3	-	25	0.1	289.9	23	1×10 ⁻¹²	1760	1×10 ⁻⁴	1.1	-	33
11	[Dy(L ⁻) ₂ (py) ₅][BPh ₄]	LOWZIJ	2	22.6	2	23	0.2	48.89	-	1.3×10 ⁻¹²	1625.9	1×10 ⁻⁷	3.9	-	34
12	Dy ₂ @C80(CH ₂ Ph)	FAWYOU	5	22.7	5	21.9	0.2	4.78	18.2	3.6×10 ⁻¹²	613	8.2×10 ⁻¹⁰	4.9	3.26×10 ³	35
13	Dy(OSiMe ₃) ₂ (4-MePy) ₃ ⁺	JUQDEH	0.5	10.9	0.5	16	0.2	27.87	11.1	3.02×10 ⁻¹²	1497.84	1.66×10 ⁻⁶	3.6	-	36
14	Dy(OSiMe ₃) ₂ (py) ₃ ⁺	JUQDAD	0.5	12.6	0.5	15	0.2	52.24	12.9	1.55×10 ⁻¹²	1595.68	2.88×10 ⁻⁷	4.1	-	36
15	Dy(OCMe ₃) ₂ (py) ₃ ⁺	RAPDUK01	0.5	11.0	0.5	14	0.2	46.13	10.9	1.38×10 ⁻¹²	1805.75	1.62×10 ⁻⁶	3.6	-	36
16	[Dy(O'Bu) ₂ (py) ₃][BPh ₄]	RAPDUK	0.2 5	9.3 18.3	-	14	0.2	47.76	-	1.17×10 ⁻¹²	1815	1×10 ⁻⁶	3.77	-	37
17	Dy(OPh) ₂ (py) ₃ ⁺ †	JUQGAG	0.5	13.3	0.5	13	0.2	97.47	13.1	1.74×10 ⁻¹²	1197.12	2.14×10 ⁻⁸	5.1		36
18	[Dy(SCS) ₂][K(2,2,2-cryptand)]	EPAHOV	0.36	9.9	0.36	13	0.1	58.23	12	2.04×10 ⁻¹²	1109	4.07×10 ⁻⁶	3.2	446.7	38
19	{[Dy(Cp*) ₂ (μ-Me ₃ AlNEt ₃)] ₂ }[Al{OC(CF ₃) ₃ } ₄] ₂]	HULRAK	0.2 5	9.3 16.6	-	12.5 (22*)	0.1	343.89	-	2.51×10 ⁻¹²	1230	2.51×10 ⁻⁷	4.5	-	39
20	[Dy(SCS) ₂ (K(DME) ₂) ₂]	EPAGOU	0.38	9.6	0.38	12	0.1	46.32	8	1.62×10 ⁻¹²	1160	2.75×10 ⁻⁶	3.5	195	38
21	Dy(OPh) ₂ (THF) ₃ ⁺	JUQFUZ	0.5	10.2	0.5	12	0.2	47.13	10	4.9×10 ⁻¹²	1329.5	1.02×10 ⁻⁶	4	-	36
22	{[L ₂ Dy(H ₂ O) ₃][Br] ₃ ·L ₂ ·H ₂ O}, L: ^t BuPO(NH/Pr) ₂	NAPDOB	2	10.8	2	11.6	-	13,79	-	1.1×10 ⁻¹¹	640	7.2×10 ⁻⁷	4.7	-	40
23	[Dy(Cp ^{III})(Cp*)(PhF-κ-F)][Al{OC(CF ₃) ₃ } ₄]	-	0.2 5	6.1 14.0	-	11	-	38.38	8	2.19×10 ⁻¹²	1582.73	3.16×10 ⁻⁵	2.8	-	41
24	[Dy(Cp ^{III})(Cp*)(PhCl-κ-Cl)][Al{OC(CF ₃) ₃ } ₄]	-	0.2	6.3	-	11	-	45.26	8	2.95×10 ⁻¹²	1618.70	2.95×10 ⁻⁵	2.76		41

			5	14.6											
25	[Dy(SCS) ₂][Na(DME) ₃]	EPAHAH	0.32	9.0	0.32	11	0.1	50.43	8	1.51×10 ⁻¹²	1015	2.95×10 ⁻⁶	3.54	182	38
26	Dy(CyPh ₂ PO) ₂ (H ₂ O) ₃ ·(PMo ₁₂ O ₄₀)· 3CyPh ₂ PO·H ₂ O	-	0.2 5	6.2 9.9	-	9	0.1	9.5	6	2.6×10 ⁻¹¹	449	3.12×10 ⁻⁷	5.8	-	42
27	[Dy(NCN) ₂][K(DB18C6)(THF)(toluene)]	EPAJAJ	0.28	8.5	0.28	10	0.1	32.06	-	2.95×10 ⁻¹²	757	6.02×10 ⁻⁷	4.49	79.43	38
28	[Dy(BIPM ^{TMS}) ₂][K(18C6)(THF) ₂] †	RUXCUK	0.189	11	0.189	10	0.1	281.69	12	5.65×10 ⁻¹³	813	3.55×10 ⁻⁹	6	-	43
29	Dy(bbpen-CH ₃)Br]	FICBOL	0.2 5	2.8 5.9	-	8.8	0.2	1.98	-	1.02×10 ⁻¹²	1162	5.35×10 ⁻⁴	3.15	-	44
30	(PPh ₄)[Dy ₂ (bbpen) ₂ Co(CN) ₆]]·3.5MeCN	POYJIZ	2	6.1	2	8.5	0.2	0.40	-	5.7×10 ⁻¹³	1065	1.2×10 ⁻⁴	3.46	0.43	45
31	[Dy _{0.05} Y _{0.95} (bbpen)Br]	IMOTUB	0.2 5	4.6 8.5	-	8.3	0.2	7.89	-	2.71×10 ⁻¹³	1191	1.75×10 ⁻⁵	4.2	-	46
32	[Dy(bbpen)Br]	IMOTUB	0.2 5	3.5 7	-	8 (9.5*)	0.2	4.63	-	1.51×10 ⁻¹²	1088	1.49×10 ⁻⁴	3.5	-	46
33	{[L ₂ Dy(H ₂ O) ₅][Cl] ₃ ·L ₂ }, L: 'BuPO(NH/Pr) ₂	NAPDAM	2	7.3	2	8.2	-	7.8	-	4.4×10 ⁻¹²	624	6.5×10 ⁻⁶	4.7	-	40
34	[K(crypt-222)][(Cp ^{Me6H} ₂ Dy) ₂ (μ-N ₂)]	LEPGIZ	0.2 5	6.9 8.6	-	7.5	1	14.69	6.6	1.7×10 ⁻⁸	155.54	2.1×10 ⁻⁶	4.13	6.7×10 ²	47
35	Dy(OCMe ₃)(Cl)(THF) ₅] ⁺	ZIFPIQ01	0.5	7.7	0.5	7	0.2	0.70	-	4.36×10 ⁻¹²	938.13	1.78×10 ⁻⁶	4.5	0.708	36
36	DyScS@C ₃ (6)-C ₈₂	XAJLAZ	5	7.8	5	7.3	0.3	20.12	5.4	5.3	9.78	-	-	-	48
37	DyScS@C ₃ (8)-C ₈₂	XAJLED	5	6.2	5	7.3	0.3	21.17	4.9	11.3	4.60	-	-	-	
38	Dy(OPh)(Cl)(THF) ₅] ⁺	JUQFOT	0.5	5.8	0.5	6.8	0.2	25.51	5.1	4.47×10 ⁻¹¹	736.7	1.51×10 ⁻⁵	4.1	-	36
39	[(Cp* ₂ Dy) ₂ (μ-bpym*)](BPh ₄)	YEZBOW	0.2 5	6.6 7.8	-	6.5	-	28.41	-	1.03×10 ⁻⁷	126.33	-		2385.6	29
40	[(Cp* ₂ Dy) ₄ (tz) ₄ ·3(C ₆ H ₆) †	VAGMOJ	0.3	6.3	0.3	6.4	0.1	7.67	-	1×10 ⁻⁸	130.94	-	-	-	49

41	[Dy _{0.07} Y _{0.93} (DiMeQ) ₂ (H ₂ O)Cl ₃]	TOQDUB	0.3	2.8	0.3	6	0.01	0.96	-	-	-	4×10 ⁻⁴	4	1.9	50
42	[Dy(bbpen)(tpo) ₂][BPh ₄]	VORCUD	0.2 5	2.7 5.4	-	7*	0.2	0.48	-	1.73×10 ⁻¹²	944	3.88×10 ⁻⁴	3.69	0.64	51
43	[Dy(H ₃ L ^{1,2,4}) ₂]	IPULUD	2	4.4	2	6*	0.1	1.28	-	2.2×10 ⁻¹⁰	367.7	4.9×10 ⁻⁵	5.4	-	52
44	[Dy(L ^x)Cl(DMF)] _n	IROYUM	3	6.2	3	5.8*	0.05	6.96	-	2.03×10 ⁻¹¹	399	1.27×10 ⁻⁶	6.62	-	53
45	[Dy(Cy ₃ PO) ₂ (μ-I)(I) ₂ ·4C ₇ H ₈]	EHEHOR	0.5	4.8	0.5	5.5 ^a (12*)	0.2	34.07	-	7.3×10 ⁻¹²	1323	1.04×10 ⁻⁴	3.31	-	54
46	[Dy ^{III} L ^{N6} _π (L ₂) ₂][BPh ₄]	RARNIL	0.2 5	1.3 2.7	-	5.1 (13*)	0.1	0.09	-	3.10×10 ⁻¹²	1454.68	2.29×10 ⁻²	2.51	9.68×10 ⁻²	55
47	[Dy(O ^t Bu) ₂ (L) ₄] ⁺ , L = 4-pyrrolidin-1-ylpyridine	ZUZSEV	0.2 5	2.1 4.4	-	5	0.1	3.9	-	2.13×10 ⁻¹²	1810	1.94×10 ⁻³	3.08	0.17	56
48	[Dy(O ^t Bu)Cl(py) ₃][BPh ₄]	-	0.2 5	5.4 12.1	-	5	0.1	212.68	-	5×10 ⁻¹²	896	4.21×10 ⁻⁵	2.93	-	42
49	Dy(OSiMe ₃)(Cl)(THF) ₅ ⁺	JUQCIK	0.5	6.6	0.5	4.5	0.2	279.58	5.9	2.82×10 ⁻¹¹	801.44	6.46×10 ⁻⁶	4.2	-	36
50	Dy(OSiMe ₃)(Br)(THF) ₅ ⁺	JUQCUW	0.5	6.1	0.5	4.5	0.2	0.81	-	1.07×10 ⁻¹¹	732.37	6.61×10 ⁻⁶	4.5	0.813	36
51	Dy(OCMe ₃)(Br)(THF) ₅ ⁺	JUQCOQ	0.5	5.2	0.5	4.5	0.2	85.73	3.2	1.7×10 ⁻¹¹	818.71	4.47×10 ⁻⁵	3.7	-	36
52	[Dy _{0.05} Y _{0.95} (μ-OH)(DBP) ₂ (THF)] ₂	OWOXAB	0.2 5	2.3 4.5	-	4.5 ^a	0.25	4.34	-	2.1×10 ⁻¹²	755	8.3×10 ⁻⁴	3.74	-	57
53	[Dy(μ-OH)(DBP) ₂ (THF)] ₂	OWOXAB	0.2 5	2.8 5.3	-	2.5 ^a	0.25	14.47	-	3.5×10 ⁻¹²	754	2.7×10 ⁻⁴	4	-	57
54	[(THF) ₃ (μ-H) ₃ Li] ₂ [(η ⁵ -C ₆ H ₄ (CH ₂) ₂ C ₂ B ₉ H ₉)Dy _{0.1} Y _{0.9} (η ² :η ⁵ -C ₆ H ₄ (CH ₂) ₂ C ₂ B ₉ H ₉) ₂ Li]	ZUNHOI	0.2 5	3.0 6.1	-	6.4*	0.2	3.96	-	3.6×10 ⁻¹¹	804	3.4×10 ⁻⁴	3.4	5	58
55	[(THF) ₃ (μ-H) ₃ Li] ₂ [(η ⁵ -C ₆ H ₄ (CH ₂) ₂ C ₂ B ₉ H ₉)Dy(η ² :η ⁵ -C ₆ H ₄ (CH ₂) ₂ C ₂ B ₉ H ₉) ₂ Li]	ZUNHOI	0.2	2.2	-	6.2*	0.2	0.21	-	4×10 ⁻¹¹	804	1.7×10 ⁻³	2.93	0.22	58

			5	4.8											
56	[DyL ^{ON3} /C ₅ H ₁₀ NS ₂) ₂]	PUKFAF	0.2 5	1.4 2.5	-	5*	0.1	0.02	-	2.99×10 ⁻¹²	638	2×10 ⁻²	3.24	0.017	59
57	[Dy(Cp ^{III})(Cp*)(C ₆ H ₄ F ₂ -κ ² -F,F)][Al{OC(CF ₃) ₃ }] ₄]	-	0.2 5	1.2 2.3	-	4	-	0.30	-	7.94×10 ⁻¹²	1223	4.57×10 ⁻²	2.24	0.437	41
58	[Dy(O ^t Bu) ₂ (L) ₄]*, L = 1,4-piperidin-1-ylpyridine	ZUZZIZ	0.2 5	2.3 5.2	-	4	0.1	14.63	-	1.36×10 ⁻¹²	1886	1.49×10 ⁻³	2.76	0.28	56
59	[K(DME) _n][L ^A DyCl ₂]	JIZVIA	0.2 5	1.9 4.1	-	4	0.1	0.02	-	7×10 ⁻¹⁴	1334	3.01×10 ⁻³	3	0.023	60
60	[K(DME) _n][L ^A DyI ₂]	DUXGUB	0.2 5	2.4 4.8	-	4	0.1	0.32	-	3.37×10 ⁻¹⁴	1278	9.89×10 ⁻⁴	3.35	0.33	60
61	[(Cp*) ₂ Dy(NH ₃) ₂](BPh ₄)	KEPREF	0.2 5	1.3 2.6	-	4	0.1	0.86	-	2.6×10 ⁻¹²	785.61	0.022	2.86	2.8 ×10 ⁻³	61
62	[Dy(pz) ₂ (THF) ₃](BPh ₄)	BADKUQ	0.2 5	1.4 2.5	-	4	0.2	0.10	-	9.05×10 ⁻¹²	521	2.1×10 ⁻²	3.01	0.12	60
63	[Dy(pz) ₂ (py) ₃](BPh ₄)·2py	BADLAX	0.2 5	2.6 4.9	-	3.5	0.2	3.55	-	8.5×10 ⁻¹²	470	3.5×10 ⁻⁴	4.13	4.55	
64	[Dy(bbpen)NO ₃]	POYJAR	2	2.2	2	3.3	0.2	0.07	-	1.5×10 ⁻¹⁰	725	0.015	2.94	0.075	45
65	[(Cp*) ₂ Dy(BPh ₄)]	-	0.2 5	1.5 3.0	-	3.2	0.1	2.78	-	2×10 ⁻⁸	448.92	0.009	3.17	0.0142	62
66	[(C ₂ B ₉ H ₁₁) ₂ Dy _{0.09} Y _{0.91} (THF) ₂][Na(THF)]	ZUNGOH	0.2 5	2.8 5.1	-	3.2 ^a	0.2	0.2	-	1.27×10 ⁻⁹	430	1.9×10 ⁻⁴	4.46	0.20	58
67	[Dy(L ₁) ₂ (THF) ₂](BPh ₄)	QILBUL	0.2 5	1.4 2.8	-	3.1	0.2	0.01	-	5×10 ⁻⁸	378.42	1.5×10 ⁻²	3	0.014	63
68	[Dy(pz) ₂ (NS) ₃](BPh ₄)	BADLEB	0.2 5	1.7 3.1	-	3	0.2	0.47	-	8.2×10 ⁻¹²	444	4.9×10 ⁻³	3.77	0.55	62
69	[Dy(Cy ₃ PO) ₂ l ₃ (CH ₃ CN)]	AJICOO	0.2 5	1.4 2.7	-	3 (7.4*)	0.2	2.30	-	5×10 ⁻¹²	1002	1.7×10 ⁻²	2.95	4.7 ×10 ⁻³	62

70	$[\text{Dy}_{0.19}\text{Y}_{1.81}(\text{nb})_4(\text{H}_2\text{L})_2]$	VANXOA	0.2 5	2.2 3.6	-	3 (3.9*)	0.1	0.29	-	1.15×10^{-11}	281.5	5.75×10^{-4}	5.23	0.31	64
71	$[\text{Dy}_{0.10}\text{Y}_{1.90}(\text{nb})_4(\text{H}_2\text{L})_2]$	VANXOA	0.2 5	2.3 3.7	-	3 (4.2*)	0.1	0.45	-	1.07×10^{-11}	285	4.06×10^{-4}	5.36	0.48	64
72	$[\text{Dy}(\text{L}_2)_2(\text{py})_2][\text{BPh}_4]$	QILCAS	0.2 5	1.4 2.6	-	3	0.2	0.02	-	1.5×10^{-8}	388.49	2×10^{-2}	3	0.017	63
73	$[\text{Dy}_2(\text{hfac})_6(\text{NITThienPh})_2]_n$	KEVRUA01	0.2 5	2.5 2.8	-	3	0.005	0.076	-	1.73×10^{-9} 7.73×10^{-15}	53 98	-	-	-	65
74	$[\text{Dy}_3(\mu_3\text{CO}_3)(\text{Clbbpen})_3](\text{CF}_3\text{SO}_3) \cdot 6\text{MeCN}$	GUNDIF	2	3.7	2	4.2*	0.2	17.87	-	1.3×10^{-9}	504	4.5×10^{-4}	4.39	-	66
75	$[(\text{Cp}^*_2\text{Dy})_2(\mu\text{-tpz})][\text{BPh}_4]$	HOLJEZ	0.2 5	2.1 2.5	-	2.7	0.1	0.12	-	2.1×10^{-7}	35.9	-	-	-	67
76	$[(\text{C}_2\text{B}_9\text{H}_{11})_2\text{Dy}(\text{THF})_2][\text{Na}(\text{THF})_6]$	ZUNGOH	0.2 5	1.7 3.2	-	4.5*	0.2	0.01	-	1.2×10^{-9}	430	5.5×10^{-3}	3.5	0.015	58
77	$[\text{Dy}(\text{L}^{\text{E}})(4\text{-MeOPhO})_2](\text{BPh}_4) \cdot 3\text{THF}$	QORWAY	0.2 5	1.4 2.7	-	2.5 (6*)	0.2	0.13	-	1.85×10^{-12}	1338	1.95×10^{-2}	2.82	0.131	68
78	$[\text{Dy}(\text{L}^{\text{E}})(\text{naPhO})_2](\text{BPh}_4) \cdot 4\text{THF}$	QORWIG	0.2 5	1.6 3.2	-	2.5 (4*)	0.2	0.08	-	1.15×10^{-12}	1226	7.1×10^{-3}	3.2	0.085	68
79	$[\text{Dy}^{\text{III}}(\text{bpyN}_4)(\text{Ph}_3\text{SiO})_2](\text{BPh}_4)$	DIVBUJ	0.2 5	1.1 1.8	-	8.5*	0.2	1.54	-	3.52×10^{-8}	584	1.18×10^{-1}	2.46	0.0288	69
80	$[\text{Dy}_2(\text{L}^*)_2\text{Cl}_2(\text{CH}_3\text{OH})_3]_n \cdot n\text{CH}_3\text{OH}$	IROYOG	3	3.3	3	2.4*	0.05	15.77	-	1.54×10^{-8}	195	9.08×10^{-4}	4.85	-	53
81	$[(\text{L}^{\text{CO}})\text{Dy}(\text{N}^*)_2]$	PAXRIS	0.2 5	1.1 1.6	-	2.2	0.1	-	-	1.7×10^{-7}	190	0.19	3.46	4.4×10^{-3}	70
82	$\text{Dy}(\text{bbpen-CH}_3)\text{Cl}$	FICBIF	0.2 5	1.8 3.7	-	7*	0.2	0.11	-	2.36×10^{-10}	723	4.6×10^{-3}	2.97	0.11	44
83	$[\text{Dy}(\text{acac})_3\text{bpm}]$	FIKREA	1	2.5	1	3*	0.1	3.28	-	3.2×10^{-11}	309	1.4×10^{-3}	4.9	4.5×10^{-3}	71
84	$[\text{L}^1\text{Co(III)Br}_2\text{Dy(III)-(acac)}_2] \cdot \text{CH}_2\text{Cl}_2$	CIHSUK	0.2	1.9	-	2	0.15	0.16	-	1.03×10^{-10}	312.26	2.16×10^{-3}	4.39	0.16	72

			5	3.3											
85	$[L^2Co(III)Cl_2Dy_{0.05}Y_{0.95}(acac)Cl(H_2O)]$	CIHTEV	0.2 5	2.3 3.9	-	1.9	0.15	0.06	-	9.36×10^{-9}	220.88	3.99×10^{-4}	5.14	0.06	72
86	$[Cr^{III}_2Dy^{III}_2(OMe)_2(O_2CPh)_4(mdea)_2(NO_3)_2]$	--	0.2 5	4.0 4.7	-	3.7	0.1	55.67	-	5.1×10^{-8}	77	-	-	-	73
87	$[Dy_3Cr_3(\mu_3-F)(\mu_3-OH)_3(mdea)_3(piv)_6DMF] \cdot H_2O \cdot CH_3CN$	--	0.2 5	1.4 1.8	-	1.6	0.1	1.23	-	3×10^{-5}	17	1.3×10^{-6}	2	6×10^7	74
	Tb^{III} complexes														
88	$(Cp^{IPr5})_2Tb_2I_3$	--	0.2 5	65.6 72.8	-	70	0.1	17.61	65	7.9×10^{-12}	1989.9	-	-	-	27
89	$Tb_2@C80(CH_2Ph)$	FAWYOU03	5	28.6	5	28.9	0.2	1.69	25.2	1.66×10^{-12}	799	-	-	6.5×10^4	75
90	$Tb_2@C79N$	-	5	27.5	5	28	0.2	1.32	24.1	2.4×10^{-12}	757	5.76×10^{-10}	3.9	1.65×10^4	76
91	$[K(crypt-222)][(Cp^{Me4H_2}Tb)_2(\mu-N_2)]$	LEPGEV	0.2 5	19.9 23.3	-	20	1	54.54	20	1.3×10^{-7}	397.12	-	-	4×10^4	47
92	$[K(crypt-222)(THF)_2][(Cp^{Me4H_2}Tb(THF))_2(\mu-N_2)]$	LEPGUL	0.2 5	11.3 16.6	-	14.5	1	37.22	14	1.4×10^{-9}	348.2	-	-	3.64×10^3	47
93	$[K(18-crown-6)(THF)_2][[(Me_3Si)_2N]_2(THF)Tb)_2(\mu-\eta^2:\eta^2-N_2)]$	CAJRIQ	0.2 5	14.7 16.9	-	14	-	111.79	13.9	8.20×10^{-9}	326.7	-	-	-	77
94	$[Cu_3Tb_2(Htris)_2(Hztris)_2(NO_3)_6]_n \cdot 2nC_2H_5OH$	IJARAP	0.2 5	2.5 3.0	-	2.4	0.03	16.93	-	1.7×10^{-7}	44.2	-	-	-	78
	Er^{III} complexes														
95	$[Er_{0.05}Y_{0.95}(COT)_2][K(18C6)]$	YIWTUV01	0.2 5	10.9 12.7	-	10	0.1	162.97	-	6.9×10^{-8}	215.83	-	-	-	79
96	$([Er-TiPS_2COT]^+)_2 \dagger$	VEBHOD	0.2 5	5.6 8.4	-	5.4	0.01	81.95	-	2.60×10^{-10}	198.56	1.50×10^{-7}	6.7	-	80
	Ho^{III} complexes														
97	$(Cp^{IPr5})_2Ho_2I_3$	-	0.2	28.2	-	28	1	61.46	-	2.40×10^{-11}	800	-	-	-	81

			5	31.4											
	Transition Metal complexes														
98	[K(crypt-222)][Fe'(C(SiMe ₃) ₃) ₂]	-	0.2 5	4.0 7.2	-	4.5	0.1	44.23	-	6.91×10 ⁻¹⁰	342.8	2.27×10 ⁻⁵	4.59	-	⁸²
99	[Fe ₄ (NC)Ph ₂] ₆]	-	1	2.2	-	2.2	0.05	0.63	-	9.1×10 ⁻⁹	39.7	-	-	-	⁸³
100	Mn ₁₂ -BuCl	-	0.2 5	3.1 3.7	-	2.9	0.01	33.84	-	3.5×10 ⁻⁸	60	-	-	-	⁸⁴
101	[Mn ₁₂ O ₁₂ (CH ₃ (CH ₂) ₁₆ CO ₂) ₁₁ (CH ₃ CO ₂) ₅ (H ₂ O) ₄]	-	0.2 5	3.4 4.3	-	3.0	0.1	63.6	-	1.03×10 ⁻⁴	40	-	-	-	⁸⁵
102	[Mn ₁₂ O ₁₂ (CH ₃ (CH ₂) ₁₆ CO ₂) ₁₆]·2CH ₃ COOH·4H ₂ O immobilized (SiIS-Mn12N1)	-	0.2 5	3.2 4.4	-	2.7	0.01	105.27	-	3.3×10 ⁻³	28	-	-	-	⁸⁶
103	[Mn ₁₂ O ₁₂ (CH ₃ COO) ₁₆ (H ₂ O) ₄]·2CH ₃ COOH·4H ₂ O	-	0.2 5	3.1 3.5	-	3.4	0.1	130.15	-	7.76×10 ⁻¹¹	76	-	-	-	⁸⁷
104	[Mn ₁₂ O ₁₂ (CN-o-C ₆ H ₄ CO ₂) ₁₂ (CH ₃ CO ₂) ₄ (H ₂ O) ₄] ·8CH ₂ Cl ₂ †	-	0.2 5	1.7 1.9	-	2.0	1	0.07	-	2×10 ⁻⁹	34.8	-	-	-	⁸⁸
105	Co ₄ L ₄ ·0.5H ₂ O	-	0.2 5	1.9 2.2	-	4.5*	0.001	9×10 ⁻⁵	-	5.4×10 ⁻⁹	38.8	-	-	-	⁸⁹
106	[L ₂ Co](TBA) ₂ †	-	2	2.4	2	3.5	0.5	0.69	-	1.46×10 ⁻¹⁰	325	4.92×10 ⁻³	4.54	-	⁹⁰
107	Mn ₂ ^{II} Mo ^{III}	DOCVY	2	3.3	2	3	0.0005	0.16		2.0 x 10-8	58.5	-	-	-	⁹¹

QTM values in italics were not considered to calculate T_B as they should be quenched by the static magnetic field to allow the observation of T_B in the ZFC/FC experiment.

† One process was used to calculate T_B .

* T_{irrev} .

^a Not explicitly informed in the article but estimated value from ZFC/FC curves.

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