SUPPORTING INFORMATION

Synthesis, structures and magnetic properties of dysprosium(III) complexes based on amino-bis(benzotriazole phenolate) and nitrophenolates: influence over the slow relaxation of the magnetization

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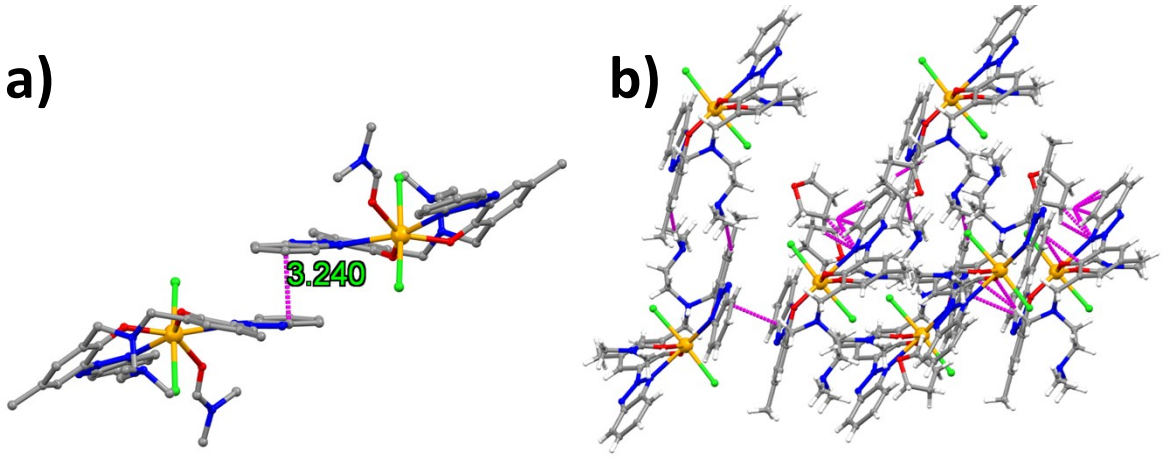

Figure S1: Intermolecular interactions in **1.** The purple dashed lines account for the short contacts intermolecular interactions.

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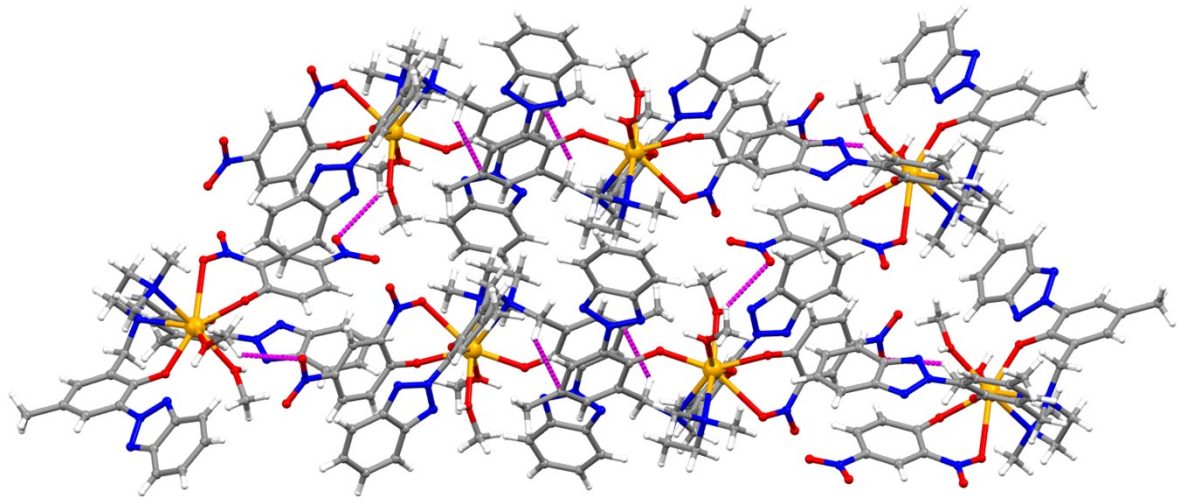

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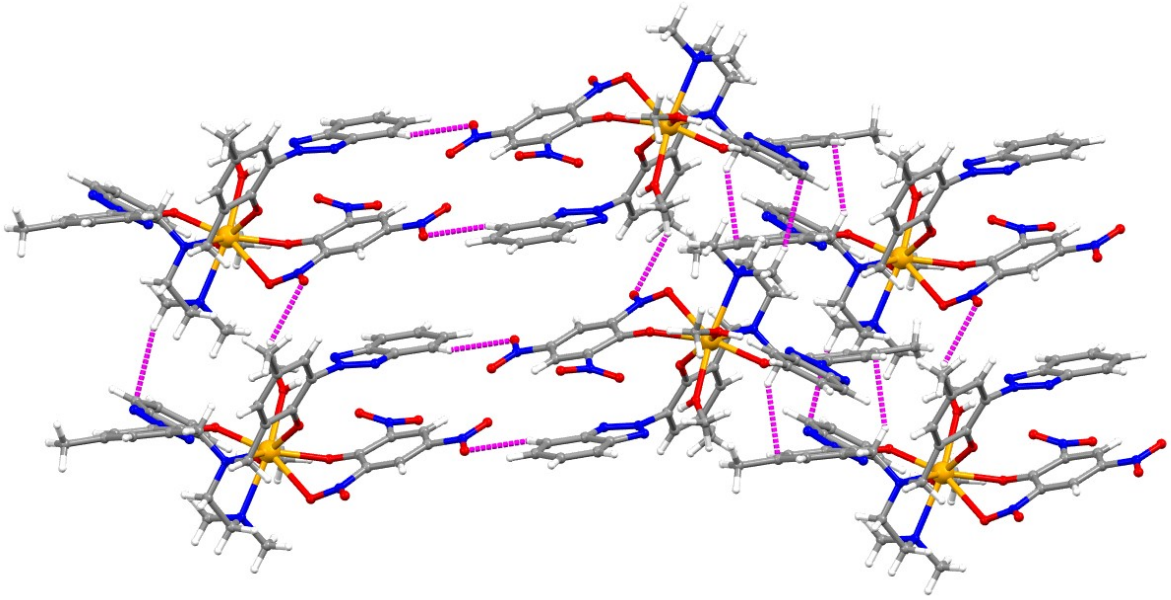

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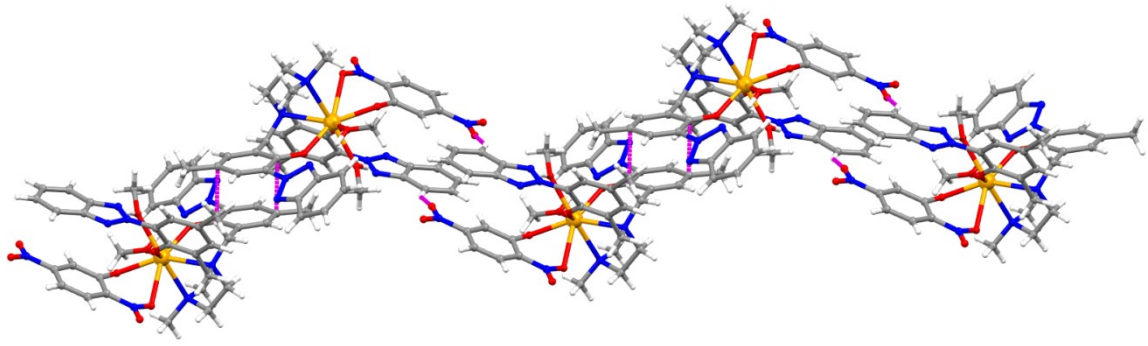

Figure S2: Intermolecular interactions in **2–4.** The purple dashed lines account for the short contacts intermolecular interactions.

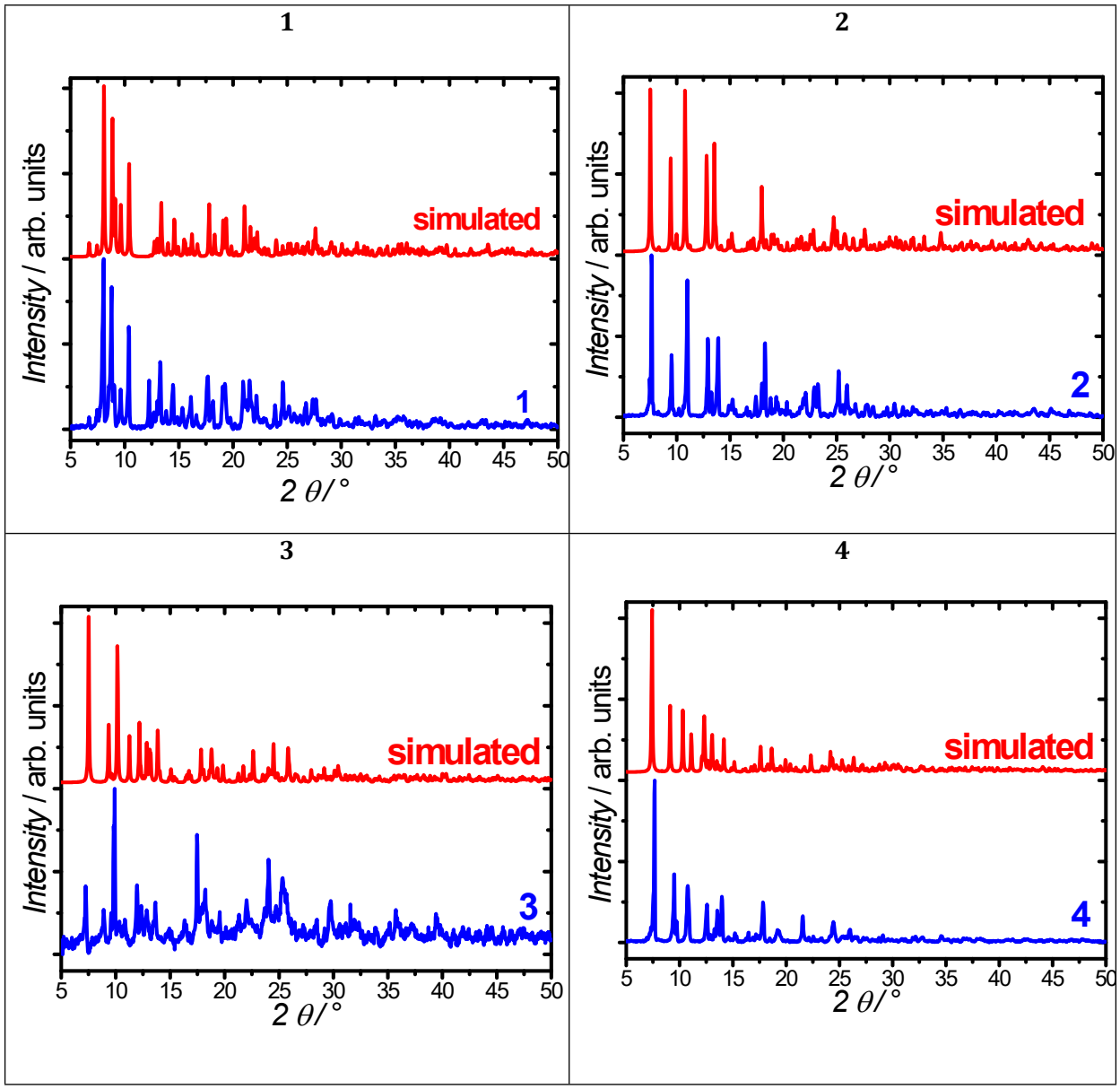

Figure S3: PXRD patterns for **1–4** and comparison with the simulated ones generated from single-crystal data.

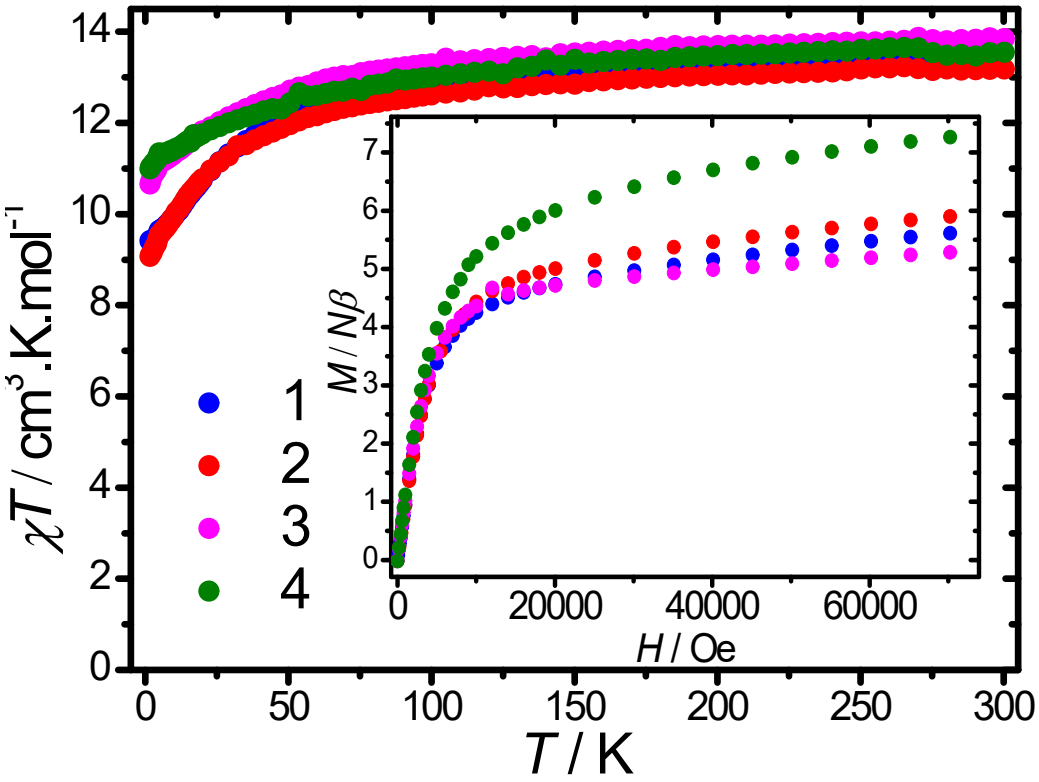

Figure S4: Temperature dependence of χT under an applied magnetic field of 1000 Oe for **1-4**. Inset: field dependence of the magnetization at 1.8 K for **1-4**.

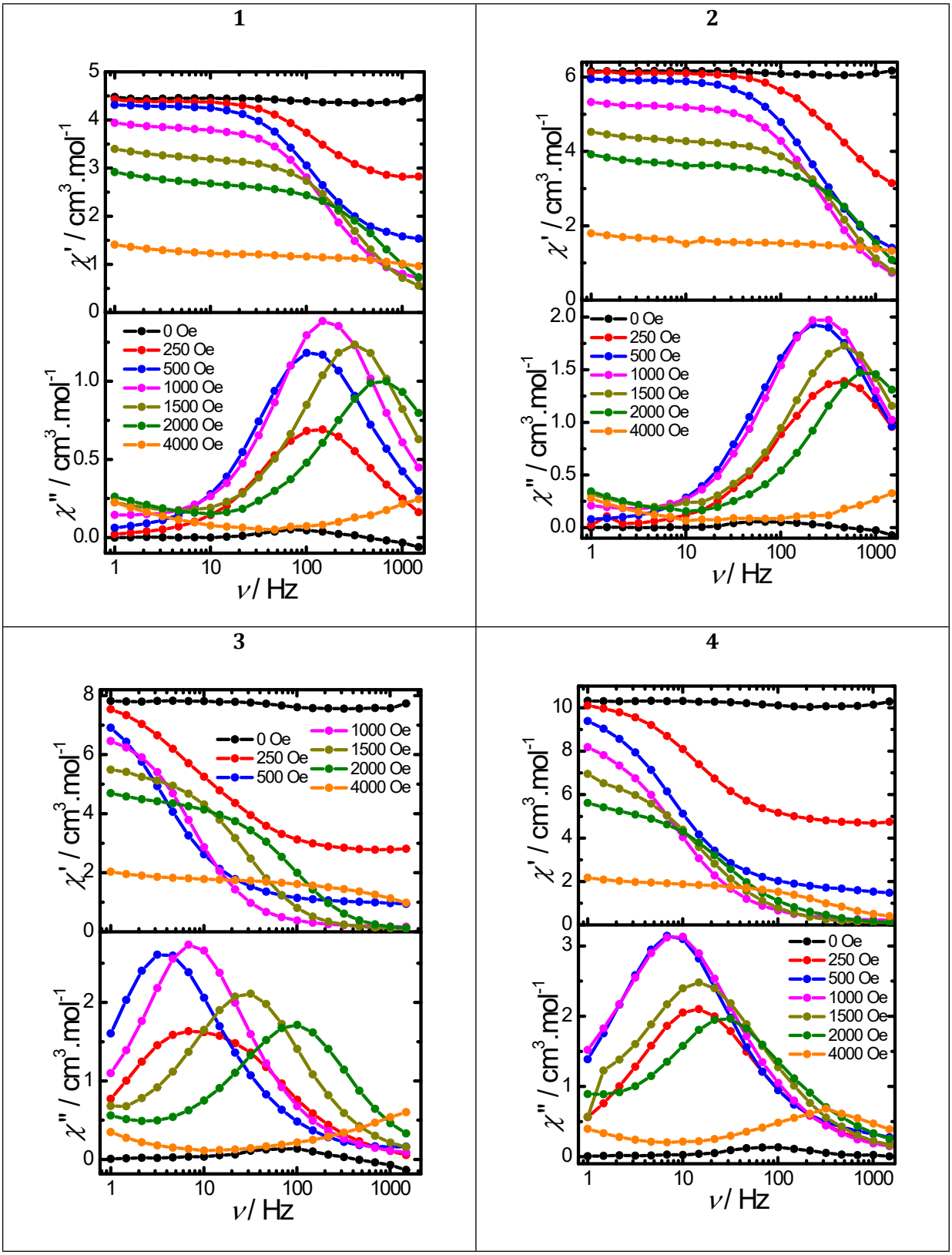

Figure S5: Frequency dependence of χ' and χ'' for **1-4** for various dc fields at 2 K.

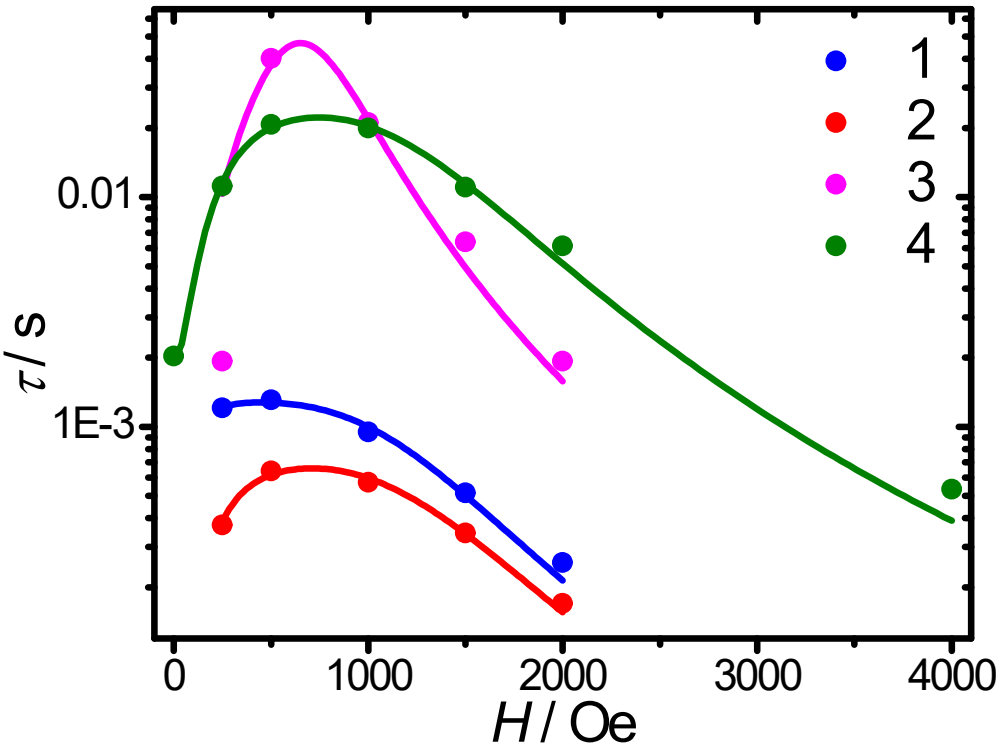

Figure S6: Field dependence of the relaxation time for **1-4** at 2 K. The solid lines represent the fit with Eq. 1.

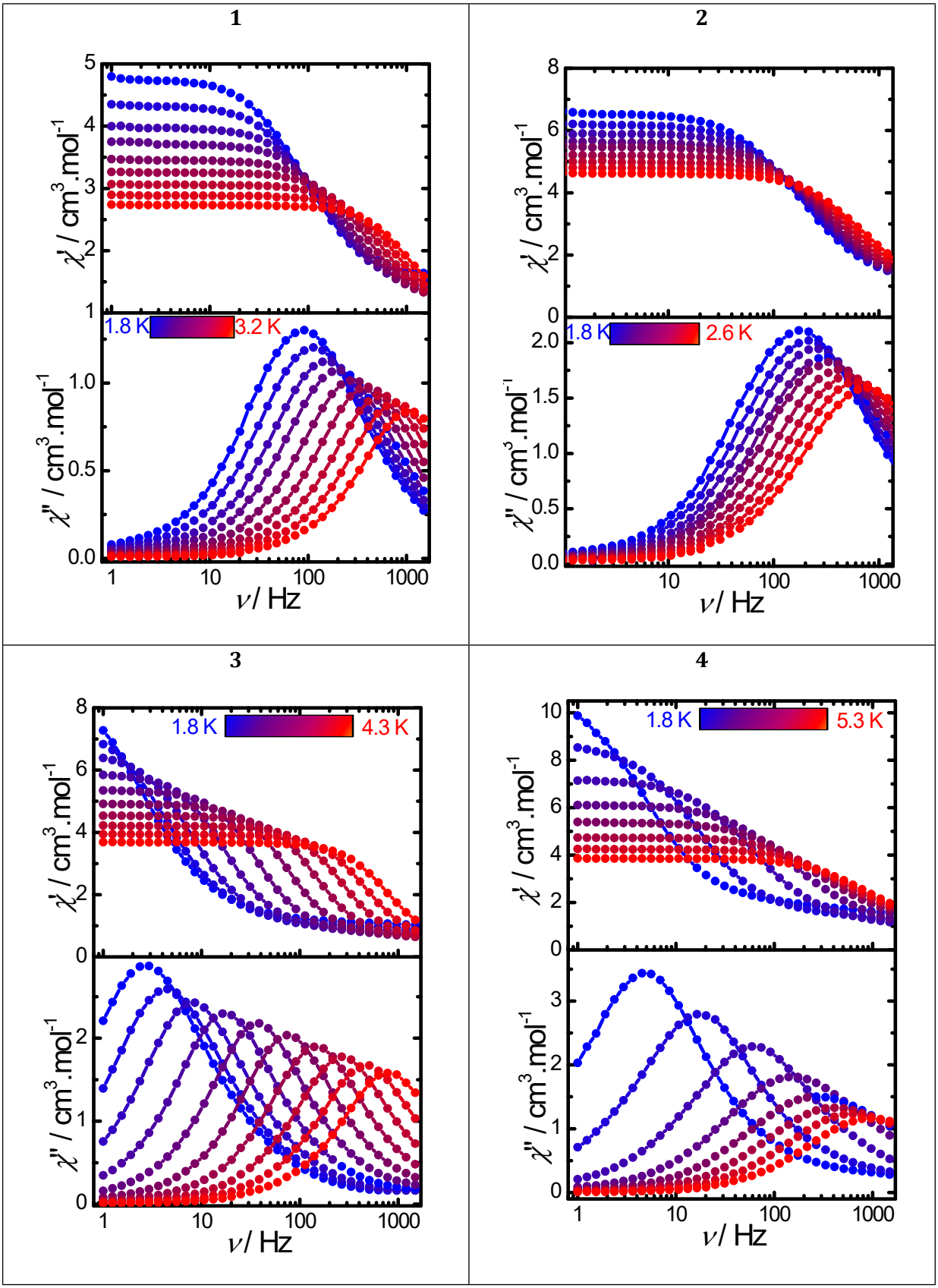

Figure S7: Frequency dependence of χ' and χ'' for **1-4** under a 500 Oe dc field.

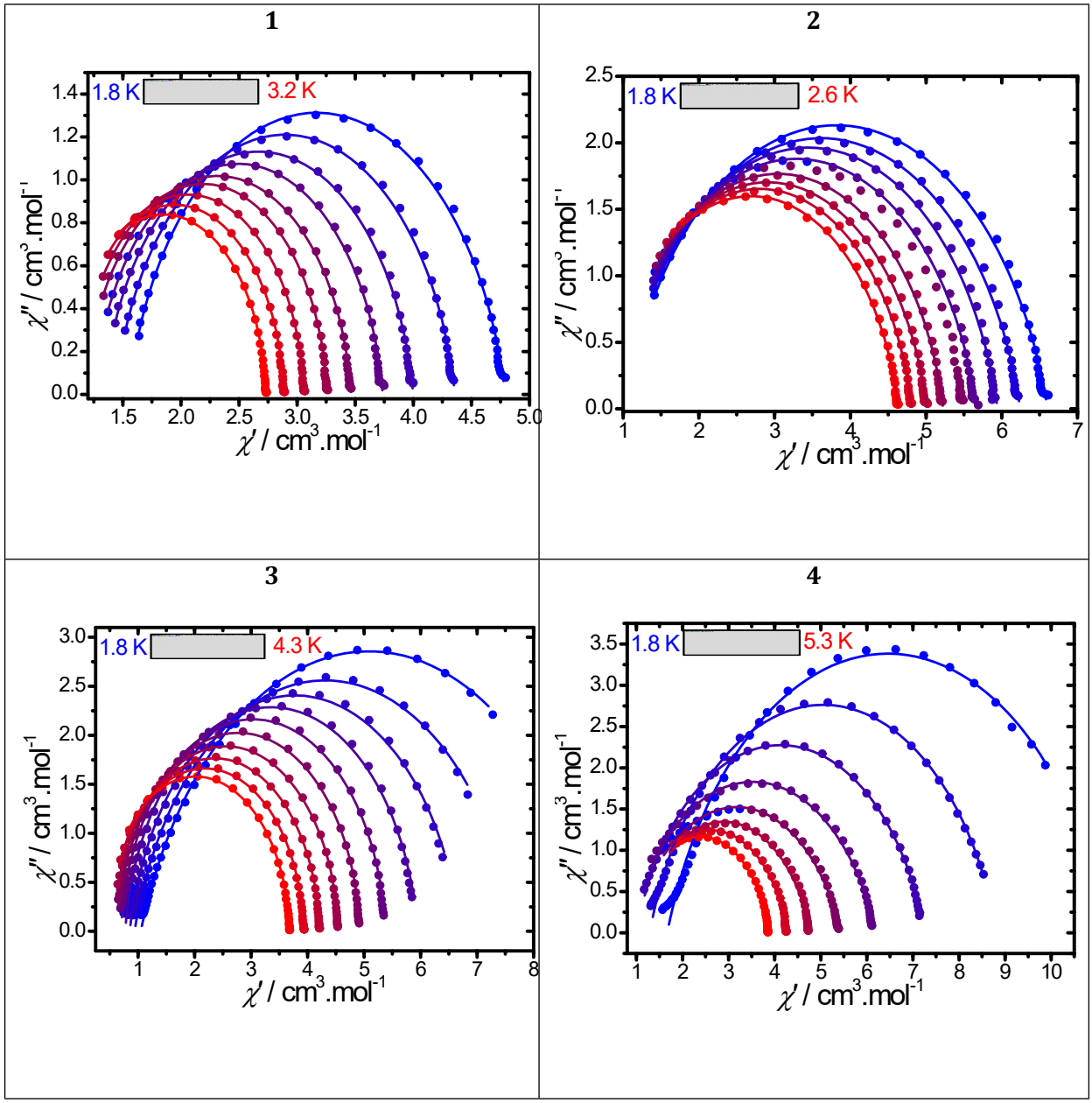

Figure S8: Cole-Cole (Argand) plots obtained using the ac susceptibility data for **1-4** in a 500 Oe dc field. The solid lines correspond to the fit obtained with a generalized Debye model.

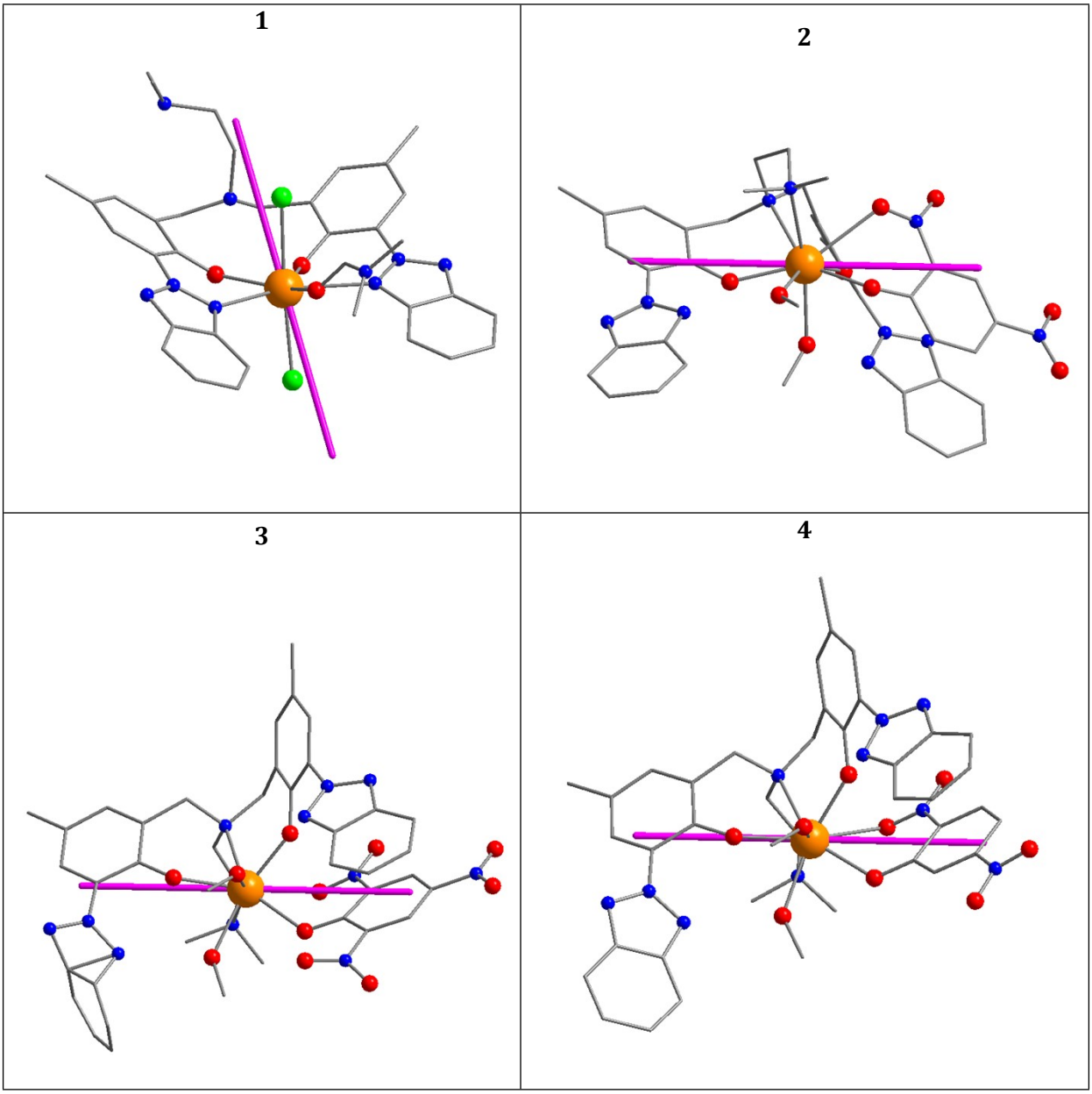

Figure S9: Anisotropic axes (purple) obtained from the MAGELLAN package.[1]

Table S1: Crystal data, data collection and structure refinement details for **1**-**4**.

	1	**2**	**3**	**4**
Formula	$C_{39}H_{48}Cl_2DyN_9O_4$	$C_{40}H_{43}DyN_{10}O_9$	$C_{40}H_{42}DyN_{11}O_{11}$	$C_{40}H_{43}DyN_{10}O_9$
M	1276.25	970.34	1015.35	970.34
T, K	120	293	150	150
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
Z (Z')	2	4	2	2
a, Å	12.7650(7)	11.8504(4)	9.2418(4)	9.1671(5)
b, Å	12.8233(8)	9.1104(3)	11.8854(4)	11.9694(8)
c, Å	14.6204(8)	37.8203(11)	19.2808(7)	19.5627(11)
α, °	76.975(5)	90	81.334(3)	84.620(5)
β, °	64.278(5)	97.811(3)	82.417(3)	84.325(5)
γ, °	68.218(6)	90	88.254(3)	88.419(5)
V, Å^3	1996.2(2)	4045.3(2)	2075.24(14)	2126.2(2)
d_{calcd}, g.cm^{-3}	1.602	1.593	1.625	1.516
μ, mm^{-1}	1.524	1.916	1.875	1.823
F_{000}	954.0	1964.0	1026.0	982.0
wR_2 (all data)	0.0896(9134)	0.0733(9612)	0.0915(9594)	0.1468(9912)
$S(F^2)$	1.025	1.152	1.009	1.027

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

	HP	HPY	PBPY	COC	CTPR	JPBPY	JETPY
1	34.094	23.519	1.127	6.918	5.363	6.395	21.885

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

Table S3: SHAPE analysis for **2-4**.

	SAPR	TDD	JGBF	JETBPY	JBTPR	BTPR
2	2.484	1.444	14.766	26.315	3.137	2.916
3	1.608	1.792	15.571	27.634	3.269	2.852
4	2.028	1.474	14.757	26.838	3.636	2.675

SAPR: Square antiprism (D_{4d})
TDD: Triangular dodecahedron (D_{2d})
JGBF: Johnson gyrobifastigium (D_{2d})
JETBPY: Johnson elongated triangular bipyramid (D_{3h})
JBTPR: Johnson biaugmented trigonal prism (C_{2v})
BTPR: Biaugmented trigonal prism (C_{2v})

Table S4: Fit parameters of the field dependence of the relaxation time for **1-4** at 2K.

Compound	$D\ (s^{-1}K^{-1}Oe^{-4})$	$B_1\ (s^{-1})$	$B_2\ (Oe^{-2})$	*K*
1	1.2×10^{-10}	123607.8	0.0288	751.9
2	1.60×10^{-10}	1.11×10^{6}	0.0135	1271.6
3	1.97×10^{-11}	188184.0	0.031	0
4	4.94×10^{-12}	490.1	1.4×10^{-4}	35.7

Table S5: Fitting of the Cole-Cole plots with a generalized Debye model under a 500 Oe dc field for **1**.

T (K)	χ_S ($cm^3.\ mol^{-1}$)	χ_T ($cm^3.\ mol^{-1}$)	α
1.79963	1.54766	4.7907	0.1335
1.97499	1.43207	4.35793	0.11986
2.14985	1.33346	3.99881	0.10349
2.32508	1.24874	3.73669	0.09274
2.4997	1.17245	3.46344	0.07473
2.67457	1.11991	3.25929	0.05494
2.84954	1.06181	3.05999	0.04436
3.02452	1.0106	2.88525	0.0373
3.19959	0.96511	2.73146	0.03261

Table S6: Fitting of the Cole-Cole plots with a generalized Debye model under a 500 Oe dc field for **2**.

T (K)	χ_S (cm^3. mol^{-1})	χ_T (cm^3. mol^{-1})	α
1.79936	1.02569	6.604	0.16905
1.9	0.986	6.24475	0.16139
2.00028	0.95712	5.9439	0.15053
2.10008	0.90831	5.66586	0.14859
2.29982	0.8568	5.22764	0.13435
2.39971	0.80519	5.01057	0.1331
2.49973	0.79261	4.81403	0.12383
2.59967	0.74413	4.63523	0.12429

Table S7: Fitting of the Cole-Cole plots with a generalized Debye model under a 500 Oe dc field for **3**.

T (K)	χ_S (cm^3. mol^{-1})	χ_T (cm^3. mol^{-1})	α
1.79967	1.04904	9.12248	0.21596
2.07792	0.93811	7.68742	0.1736
2.35559	0.85282	6.70032	0.12307
2.63305	0.77302	5.94464	0.07799
2.91074	0.69994	5.3797	0.05
3.18852	0.63192	4.92348	0.03687
3.46641	0.56504	4.5411	0.03304
3.74452	0.50017	4.2131	0.032
4.02173	0.43029	3.93332	0.03348
4.2984	0.35887	3.68131	0.03237

Table S8: Fitting of the Cole-Cole plots with a generalized Debye model under a 500 Oe dc field for **4**.

T (K)	χ_S (cm^3. mol^{-1})	χ_T (cm^3. mol^{-1})	α
1.82498	1.66792	11.2442	0.21667
2.29998	1.28936	8.82139	0.19413
2.79985	0.99367	7.25938	0.20041
3.29974	0.85294	6.19488	0.23544
3.80027	0.91775	5.4362	0.24471
4.29837	1.01706	4.77616	0.20888
4.79944	1.01236	4.27383	0.17187
5.29977	0.92491	3.86989	0.14742

Table S9: Fitting of the Cole-Cole plots with a generalized Debye model under a 500 Oe dc field for **1-3**.

Compound	n	C ($s^{-1}.K^{-n}$)
1	5.1 ± 0.2	17 ± 3
2	4.1 ± 0.2	92 ± 13
3	7.82 ± 0.02	0.056 ± 0.002

References

1 N. F. Chilton, D. Collison, E. J. L. McInnes, R. E. P. Winpenny and A. Soncini, *Nat. Commun.*, 2013, **4**, 2551.