A Dy^{III} complex of a pentadentate Schiff base with field-induced single-ion magnet behavior

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Table S1. Main bond distances (Å) and angles (º) for **1.**

Dy1-O1	2.3390(14)
Dy1-O2	2.2394(14)
Dy1-N2	2.4983(17)
Dy1-N1	2.4915(18)
Dy1-N3	2.5299(17)
Dy-O1W	2.3954(15)
Dy-O2W	2.3816(16)
Dy1-Cl	2.7768(6)
O2-Dy1-N1	163.51(5)
N12-Dy1-N13	63.69(6)

Table S2. SHAPE v2.1. Continuous Shape Measures Calculation (c) 2013 Electronic Structure Group, Universitat de Barcelona.

Geometries with coordination number 8

ETBPY-8	13 D3h	Elongated trigonal bipyramid
TT-8	12Td	Triakistetrahedron
JSD-8	11 D2d	Snubdiphenoid J84
BTPR-8	10 C2v	Biaugmented trigonal prism
JBTPR-8	9 C2v	Biaugment trigonal prism J50
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JGBF-8	7 D2d	Johnson gyrobifastigium J26
TDD-8	6 D2d	Triangular dodecahedron
SAPR-8	5 D4d	Square antiprism
CU-8	4 Oh	Cube
HBPY-8	3 D6h	Hexagonal bipyramid
HPY-8	2 C7v	Heptagonal pyramid
OP-8	1 D8h	Octagon

1

Structure [ML8]	ETBPY-8	TT-8	JSD-8	**BTPR-8**	JBTPR-8	JETBPY8
	21.133,	13.835,	3.985,	**2.511**,	3.351,	25.134,
JGBF-8	**TDD-8**	SARP-8	CU-8	HBPY-8	HPY-8	OP-8
11.063,	**2.138,**	4.482,	13.274,	14.271,	23.383,	31.8

Table S3. Generalised Debye model fitting parameters for **1·**

T/K	χ_S/(cm^{3}mol^{-1})	χ_T/(cm^{3}mol^{-1})	τ/(10^{-4}s)	α
4.5	0.639	3.15	12.63	0.22
5.0	0.514	2.89	6.58	0.24
5.5	0.480	2.60	3.66	0.17
6.0	0.120	2.38	2.13	0.12
6.5	0.440	2.22	1.25	0.09
7.0	0.410	2.09	0.69	0.08
7.5	0.371	1.97	0.38	0.09
8.0	0.297	1.87	0.19	0.12

Table S4. Comparison of some structural and magnetic parameters for Dy^{III} complexes magneto-structurally characterised with the ligand H_2L.

Compound*	d(Dy-O) (Å)[a]	d(Dy-N) (Å)[a]	c.n./ geometry[b]	U_{eff} K/ H_{dc} (Oe)	Ref
[Dy(HL)(NO$_3$)$_2$]	2.2391(16), 2.3663(16)	2.4713(19)-2.4971(19)	9 / TCTPR	No SIM	14
[Dy(L)(NO$_3$)(EtOH)(H$_2$O)]	2.2689(17), 2.2869(17)	2.503(2)-2.538(2)	9 / CSAPR	46.1/1500	14
[Dy(HL')$_2$)][Dy(L)(Cl$_2$)]	2.286(9)	2.480(15)-2.506(10)	7 / PBPY	31/ 3000	14
(Et$_3$NH)[Dy$_{0.09}$Y$_{0.91}$(L)(NO$_3$)$_2$]	2.226(13), 2.322(13)	2.418(13)-2.554(13)	9 / TCTPR	49.1/0	14
[Dy(L)Cl(H$_2$O)$_2$]	2.3390(14), 2.3394(14)	2.4915(18)-2.5299(17)	8 / TDD	113.5/1500	This work

* solvates are omitted; H_2L': (6-(2-hydroxyphenyliminomethyl)-2-methoxyhydroxymethyl)pyridine); [a] distances with the N and O atoms of the N_2O_3 ligand; [b] TCTPR: spherical tricapped trigonal prism; CSAPR: spherical capped square antiprism; PBPY: pentagonal bipyramid; TDD: triangular dodecahedron

Table S5. Crystal data and structure refinement for **1**.

Empirical formula	$C_{19}H_{17}ClDyN_3O_4$
Molecular weight	549.30
Crystal system	Triclinic
Space group	*P*-1
Wavelength (Å)	0.71073
Crystal size (mm^3)	0.119 x 0.088 x 0.036
Colour, shape	Red, plate
T (K)	100
a (Å)	6.6759(11)
b (Å)	11.6406(17)
c (Å)	12.586(2)
α (º)	71.803(5)
β (º)	82.849(6)
γ (º)	81.180(5)
Volume ($Å^3$)	915.1(3)
Z	2
Absorpt. coef. (mm^{-1})	4.621
Reflections collected	41987
Independent reflections	4529 [R_{int}= 0.0344]
Data / restrains / param.	4529 / 0 / 269
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0157; wR_2 = 0.0345
R indices (all data)	R_1 = 0.0176; wR_2 = 0.0353

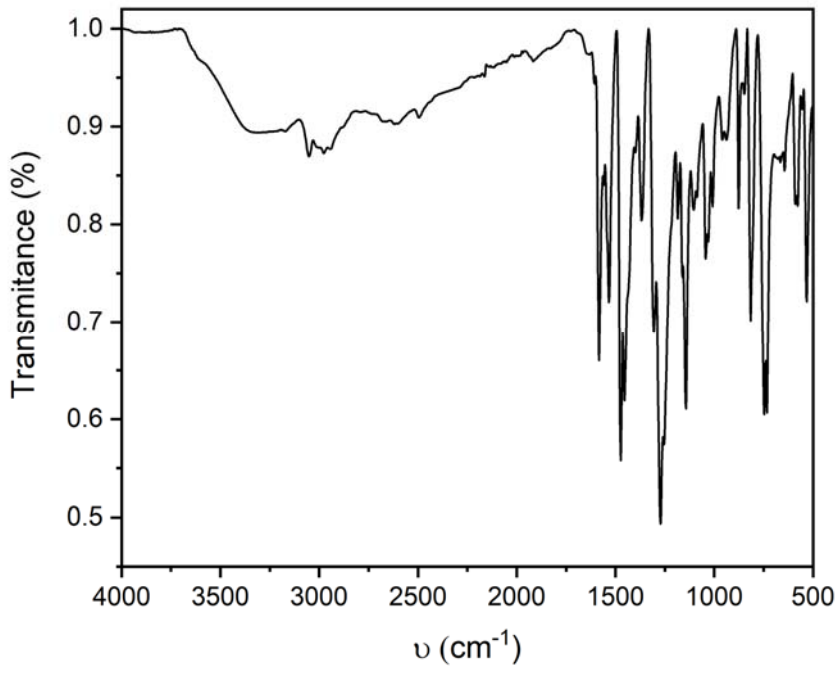

Figure S1. IR spectrum for **1** in the 4000-500 cm^{-1} region.

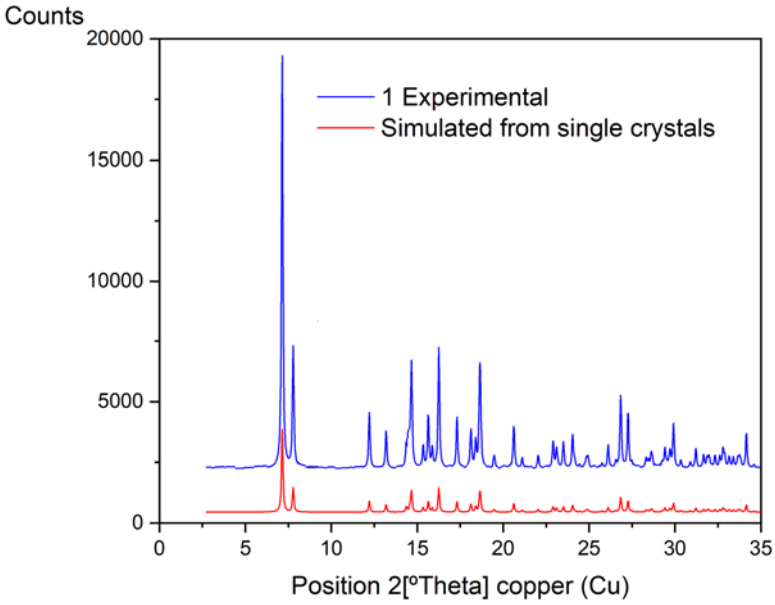

Figure S2. Comparative powder X-ray diffractograms for **1**. Blue: experimental diffractogram for the microcrystalline sample; red: calculated diffractogram using the data obtained from single X ray diffraction studies.

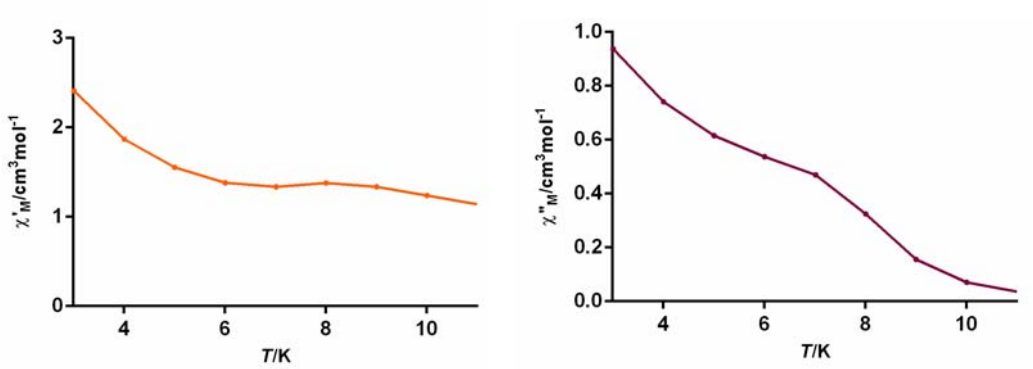

Figure S3. Left) Dependence of χ'_M on temperature for **1** at a frequency of 8000 Hz at H_{dc} = 0. Right) Dependence of χ''_M on temperature for **1** at a frequency of 8000 Hz at H_{dc} = 0.

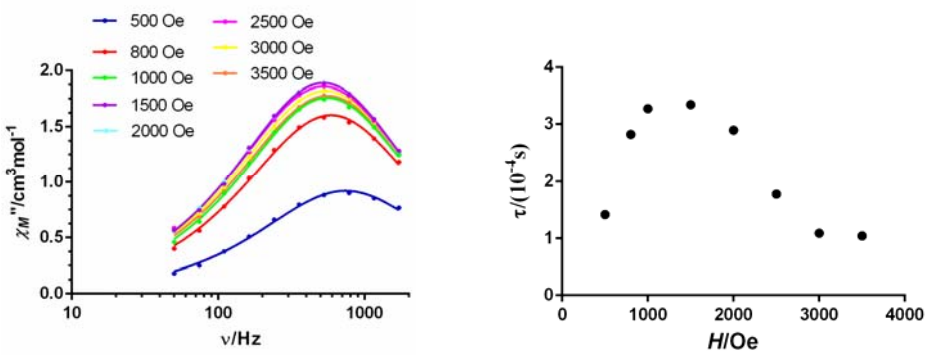

Figure S4. Left) Dependence of χ''_M on frequency for **1** at 5 K under various external applied fields. Right) Dependence of the magnetic relaxation time on field at 5 K for **1**.

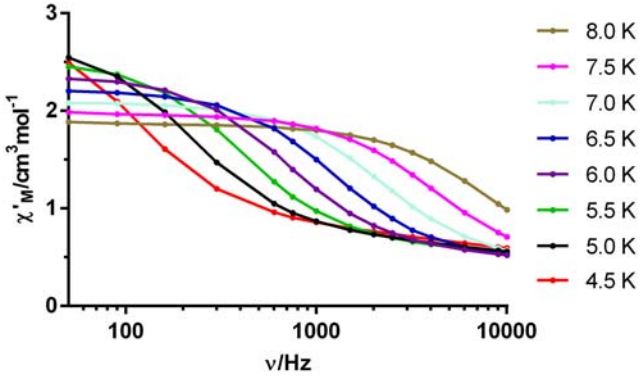

Figure S5. Dependence of χ'_M on frequency for **1** under H_{dc} = 1500 Oe between 4.5 and 8 K.

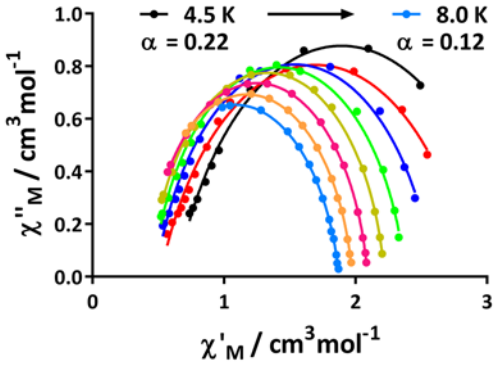

Figure S6. Cole-Cole plot for complex **1** under an external field H_{dc} = 1500 Oe.