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Supplementary Information

Dinuclear dysprosium Schiff base complex showing slow magnetic relaxation in the absence of an external magnetic field

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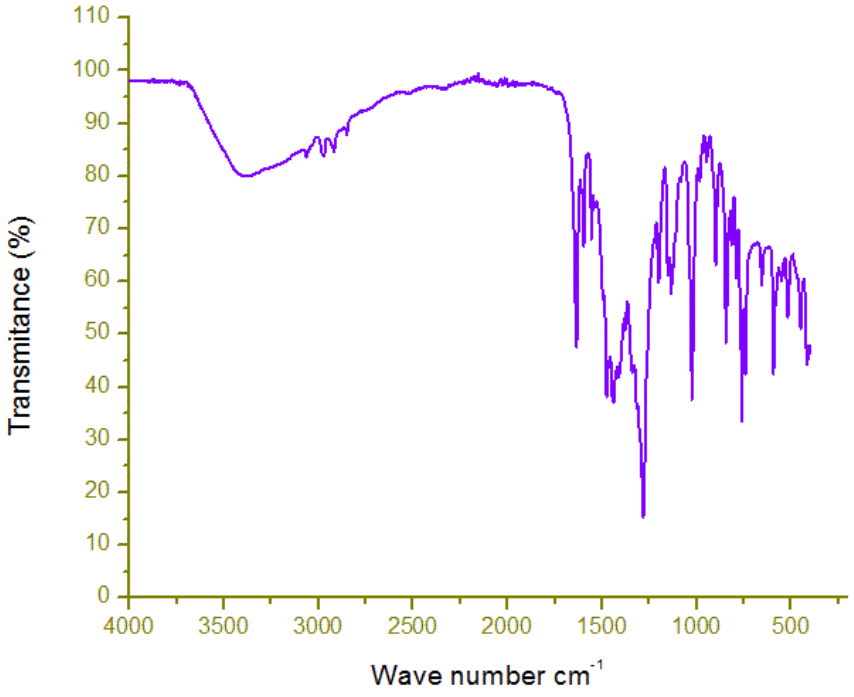

Fig. S1 IR spectrum of complex **1.**

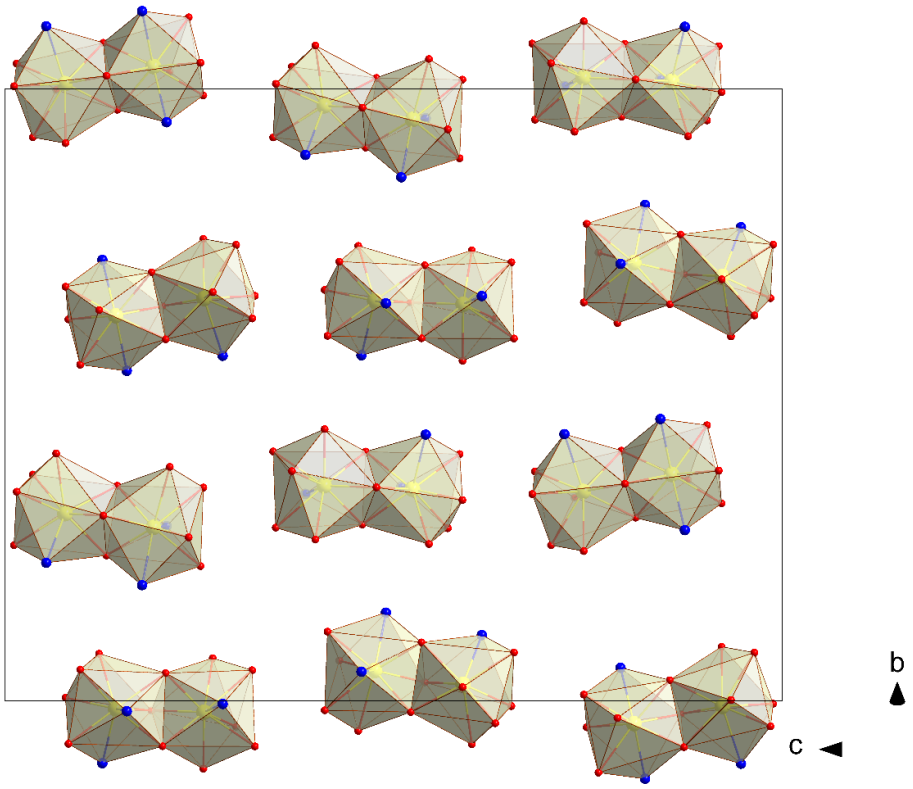

Fig. S2 View of the packing of the structure of **1** along *a* axis. Only the shared polyhedra around the Dy(III) central atoms are shown for clarity.

Table S1 Crystal data and structure refinement for complex **1**.

Empirical formula	$C_{30}H_{36}$ $Dy_2N_6O_{15}$·$(CH_3OH)_{1.2}$
Formula weight	1082.86
Temperature/K	299.15
Crystal system	trigonal
Space group	R-3
a/Å	27.0452(8)
b/Å	27.0452(8)
c/Å	29.7710(7)
α/°	90
β/°	90

γ/°	120
Volume/Å^3	18858.4(12)
Z	18
ρ_{calc} g/cm^3	1.716
μ/mm^{-1}	3.611
F(000)	9546.0
Crystal size/mm^3	0.356 × 0.196 × 0.171
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.8 to 51.99
Index ranges	-32 ≤ h ≤ 12, -24 ≤ k ≤ 33, -29 ≤ l ≤ 36
Reflections collected	15170
Independent reflections	8246 [R_{int} = 0.0237, R_{sigma} = 0.0390]
Data/restraints/parameters	8246/4/530
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0276, wR_2 = 0.0618
Final R indexes [all data]	R_1 = 0.0372, wR_2 = 0.0662
Largest diff. peak/hole / e Å^{-3}	0.70/-0.47

Table S2 Selected bond distances and bond angles in angstrom (Å) and degree (°), respectively.

O21…Dy2	2.334(3) Å
O32…Dy2	2.436(3) Å
O5…Dy2	2.447(3) Å
O4…Dy2	2.553(4) Å
O8…Dy2	2.456(3) Å
O7…Dy2	2.570(3) Å
O11…Dy2	2.330(3) Å
O31…Dy2	2.293(2) Å
N31…Dy2	2.480(5) Å
O11…Dy1	2.333(3) Å
O12…Dy1	2.404(3) Å
O22…Dy1	2.436(4) Å
O21…Dy1	2.329(3) Å
O2…Dy1	2.477(4) Å
N21…Dy1	2.488(3) Å

O1… Dy1	2.634(4) Å
N11…Dy1	2.537(5) Å
O31…Dy1	2.366(2) Å
Dy2…Dy1	3.4552(8)Å
O11...O21	2.697(5) Å
O21…O31	2.625(3) Å
O11…O31	2.799(4) Å
Dy1---O31---Dy2	95.74(1)°
Dy1---O21---Dy2	95.63(1)°
Dy1---O11---Dy2	95.64(1)°

Table S3 Results of the Continuous Shape Measures calculations using the Program *SHAPE* [54]

S H A P E v2.1

EP-9	1 D_9h	Enneagon
OPY-9	2 C_8v	Octagonal pyramid
HBPY-9	3 D_7h	Heptagonal bipyramid
JTC-9	4 C_3v	Johnson triangular cupola J3
JCCU-9	5 C_4v	Capped cube J8
CCU-9	6 C_4v	Spherical-relaxed capped cube
JCSAPR-9	7 C_4v	Capped square antiprism J10
CSAPR-9	8 C_4v	Spherical capped square antiprism
JTCTPR-9	9 D_3h	Tricapped trigonal prism J51
TCTPR-9	10 D_3h	Spherical tricapped trigonal prism
JTDIC-9	11 C_3v	Tridiminished icosahedron J63
HH-9	12 C_2v	Hula-hoop
MFF-9	13 Cs	Muffin

Structure [ML9] EP-9 OPY-9 HBPY-9 JTC-9 JCCU-9 CCU-9 JCSAPR-9 CSAPR-9 JTCTPR-9 TCTPR-9 JTDIC-9 HH-9 MFF-9

Dy1 36.890, 20.900, 19.377, 14.692, 10.430, 9.157, 2.307, 1.760, 2.610, 1.206, 11.087, 10.850, 1.640

Dy2 36.192, 21.362, 19.416, 14.324, 10.569, 9.227, 3.045, 2.293, 3.102, 1.520, 10.542, 12.052, 2.580

Table S4 Possible hydrogen bonds in **1** [Å,°]

D–H···A	d(D–H)	d(D···A)	d(H···A)	D–H···A
O41–H41···O8	0.82	2.7662(1)	2.02	150
O22–H221···O6^{i}	0.81	2.8751(1)	2.06	178
O12–H121···O41^{i}	0.82	2.7526(1)	1.94	176
O32–H321···O3^{ii}	0.81	2.9614(1)	2.17	165

Symmetry codes: i: 1/3-x+y, 2/3-x, -1/3+z; ii: 2/3-y, 1/3+x-y, 1/3+z;

Table S5 Additional non-covalent contacts in **1** [Å,°]

D–H···A	d(D–H)	d(D···A)	d(H···A)	D–H···A
C19–H19A···O41^{i}	0.96	3.279(8)	2.69	120
C35–H35···O41^{iii}	0.93	3.574(8)	2.69	160
C28–H28···O5^{i}	0.98	3.209(6)	2.46	133
C36–H36···O3^{iv}	1.01	3.400(8)	2.65	131
C27–H27···O9^{v}	0.81	3.507(7)	2.63	150
C36–H36···O9^{vi}	1.01	3.403(5)	2.70	127
C37–H37B···O9^{vi}	0.97	3.450(6)	2.63	142

Symmetry codes: i: 1/3-x+y, 2/3-x, -1/3+z; ii: 2/3-y, 1/3+x-y, 1/3+z; iii: -1/3+y, 1/3-x+y, 1/3+z; iv: x-y, x, 1-z; v: 1-x, 1-y, 1-z; vi: -1/3+y, 1/3-x+y, 4/3-z.

Table S6 Fitted AC susceptibility data at T = 2.0 K [a]

B/T	χ_S	$\chi_{T(LF)}$	α_{LF}	τ_{LF}/ms	$\chi_{T(HF)}$	α_{HF}	τ_{HF}/μs
0.0	60.0	60.7	0.22	**0.33**	69	0.01	5.4
0.1	10.1	11.3	0.50(12)	**20.9(83)**	68.6(1)	0.25(4)	2.1
0.2	10.0	13.4	0.50(5)	**49.8(77)**	67.2(2)	0.23(7)	1.7
0.3	50.2	56.6	0.46(3)	**48.2(39)**	65.2(2)	0.30(28)	3.3
0.4	40.4	50.3	0.42(2)	**51.0(27)**	61.8(2)	0.60(50)	0.10
0.5	28.8	42.0	0.40(1)	**56.5(20)**	56.5(2)	0.60(37)	0.31

[a]AC susceptibility components in unit of 10^{-6} m^3 mol^{-1} [SI]. Standard deviation is not displayed when its value is greater than the value of the optimized parameter. Note: 20.9(83) means 20.9 ± 8.3.

The Debye equation for AC susceptibility can be extended to the *two-set Debye model*

$$\chi(\omega) = \chi_S + \frac{\chi_{T1} - \chi_S}{1 + (\mathrm{i}\omega\tau_1)^{1-\alpha_1}} + \frac{\chi_{T2} - \chi_{T1}}{1 + (\mathrm{i}\omega\tau_2)^{1-\alpha_2}}$$

which splits into the in-phase component

$$\chi'(\omega) = \chi_S + (\chi_{T1} - \chi_S)\frac{1+(\omega\tau_1)^{1-\alpha_1}\sin(\pi\alpha_1/2)}{1+2(\omega\tau_1)^{1-\alpha_1}\sin(\pi\alpha_1/2)+(\omega\tau_1)^{2-2\alpha_1}}$$
$$+(\chi_{T2} - \chi_{T1})\frac{1+(\omega\tau_2)^{1-\alpha_2}\sin(\pi\alpha_2/2)}{1+2(\omega\tau_2)^{1-\alpha_2}\sin(\pi\alpha_2/2)+(\omega\tau_2)^{2-2\alpha_2}}$$

and the out-of-phase component

$$\chi''(\omega) = (\chi_{T1} - \chi_S)\frac{(\omega\tau_1)^{1-\alpha_1}\cos(\pi\alpha_1/2)}{1+2(\omega\tau_1)^{1-\alpha_1}\sin(\pi\alpha_1/2)+(\omega\tau_1)^{2-2\alpha_1}}$$
$$+(\chi_{T2} - \chi_{T1})\frac{(\omega\tau_2)^{1-\alpha_2}\cos(\pi\alpha_2/2)}{1+2(\omega\tau_2)^{1-\alpha_2}\sin(\pi\alpha_2/2)+(\omega\tau_2)^{2-2\alpha_2}}$$

with the constraint for the isothermal and adiabatic susceptibilities $\chi_S < \chi_{T1} < \chi_{T2}$ in order to get positive contributions from each primitive component.