

Supplementary Materials

Slow relaxation of the magnetisation in a two-dimensional metal–organic framework with a layered square lattice

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Table S1. Main bond lengths (Å) in (H₃O)[Eu(C₆O₄(CN)Cl)₂(H₂O)]·34H₂O (**1**).

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Eu1	O11W	2.402(7)	Eu1	O12	2.423(4)
Eu1	O2 ¹	2.436(5)	Eu1	O12 ¹	2.423(4)
Eu1	O2	2.436(5)	Eu1	O13	2.436(4)
Eu1	O3	2.441(5)	Eu1	O13 ¹	2.436(4)
Eu1	O3 ¹	2.441(5)			

¹ 1/2 - x, +y, 1/2 - z**Table S2.** Main bond angles (°) in (H₃O)[Eu(C₆O₄(CN)Cl)₂(H₂O)]·34H₂O (**1**).

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
O11W	Eu1	O2	125.11(11)	O12 ¹	Eu1	O3	72.21(15)
O11W	Eu1	O2 ¹	125.11(11)	O12 ¹	Eu1	O3 ¹	131.35(15)
O11W	Eu1	O3	71.95(11)	O12	Eu1	O3	131.35(15)
O11W	Eu1	O3 ¹	71.95(11)	O12	Eu1	O3 ¹	72.22(15)
O11W	Eu1	O12	124.97(10)	O12	Eu1	O12 ¹	110.1(2)
O11W	Eu1	O12 ¹	124.97(10)	O12 ¹	Eu1	O13 ¹	65.27(15)
O11W	Eu1	O13	71.11(11)	O12	Eu1	O13 ¹	142.15(16)
O11W	Eu1	O13 ¹	71.11(11)	O12 ¹	Eu1	O13	142.15(16)
O2	Eu1	O2 ¹	109.8(2)	O12	Eu1	O13	65.27(15)
O2	Eu1	O3 ¹	141.85(15)	O13 ¹	Eu1	O2	132.39(15)
O2	Eu1	O3	64.54(15)	O13	Eu1	O2	72.44(16)
O2 ¹	Eu1	O3 ¹	64.54(15)	O13 ¹	Eu1	O2 ¹	72.44(16)
O2 ¹	Eu1	O3	141.85(15)	O13	Eu1	O2 ¹	132.39(15)
O3 ¹	Eu1	O3	143.9(2)	O13 ¹	Eu1	O3 ¹	83.78(15)
O12	Eu1	O2	70.58(16)	O13 ¹	Eu1	O3	84.70(16)
O12 ¹	Eu1	O2	70.93(15)	O13	Eu1	O3 ¹	84.71(16)
O12 ¹	Eu1	O2 ¹	70.58(16)	O13	Eu1	O3	83.78(15)
O12	Eu1	O2 ¹	70.93(15)	O13 ¹	Eu1	O13	142.2(2)

¹ 1/2 - x, +y, 1/2 - z

Table S3. Main bond lengths (Å) in (H₃O)[Dy(C₆O₄(CN)Cl)₂(H₂O)]·44H₂O (**2**).

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Dy1	O2	2.392(4)	Dy1	O12 ¹	2.399(4)
Dy1	O2 ¹	2.392(4)	Dy1	O13 ¹	2.411(4)
Dy1	O3	2.396(4)	Dy1	O13	2.411(4)
Dy1	O3 ¹	2.396(4)	Dy1	O11W	2.433(6)
Dy1	O12	2.399(4)			

¹ 3/2 – x, +y, 3/2 – z.**Table S4.** Main bond angles (°) in (H₃O)[Dy(C₆O₄(CN)Cl)₂(H₂O)]·44H₂O (**2**).

Atom	Atom	Atom	Angle(°)	Atom	Atom	Atom	Angle(°)
O2	Dy1	O2 ¹	109.36(19)	O3 ¹	Dy1	O12	132.75(13)
O2 ¹	Dy1	O3	142.73(13)	O3 ¹	Dy1	O12 ¹	73.34(13)
O2 ¹	Dy1	O3 ¹	65.97(12)	O3 ¹	Dy1	O13 ¹	83.55(13)
O2	Dy1	O3	65.97(12)	O3 ¹	Dy1	O13	83.85(13)
O2	Dy1	O3 ¹	142.73(13)	O3	Dy1	O13 ¹	83.85(13)
O2	Dy1	O12	69.84(13)	O3	Dy1	O13	83.55(13)
O2	Dy1	O12 ¹	70.74(13)	O3	Dy1	O11W	70.36(9)
O2 ¹	Dy1	O12	70.74(13)	O3 ¹	Dy1	O11W	70.36(9)
O2 ¹	Dy1	O12 ¹	69.84(13)	O12	Dy1	O12 ¹	108.62(19)
O2	Dy1	O13	131.83(13)	O12	Dy1	O13	66.01(13)
O2 ¹	Dy1	O13 ¹	131.83(13)	O12	Dy1	O13 ¹	141.94(13)
O2	Dy1	O13 ¹	73.17(13)	O12 ¹	Dy1	O13 ¹	66.01(13)
O2 ¹	Dy1	O13	73.17(13)	O12 ¹	Dy1	O13	141.94(13)
O2 ¹	Dy1	O11W	125.32(10)	O12 ¹	Dy1	O11W	125.69(9)
O2	Dy1	O11W	125.32(10)	O12	Dy1	O11W	125.69(9)
O3	Dy1	O3 ¹	140.72(19)	O13	Dy1	O13 ¹	141.90(18)
O3	Dy1	O12 ¹	132.74(13)	O13 ¹	Dy1	O11W	70.95(9)
O3	Dy1	O12	73.34(13)	O13	Dy1	O11W	70.95(9)

¹ 3/2 – x, +y, 3/2 – z.

Table S5. Crystal data for compounds (H₃O)[Eu(C₆O₄(CN)Cl)₂(H₂O)]·34H₂O (**1**) and (H₃O)[Dy(C₆O₄(CN)Cl)₂(H₂O)]·44H₂O (**2**).

Compound	1	2
CCDC	2401611	2402436
Formula	C ₁₄ H ₂ Cl ₂ EuN ₂ O ₉	C ₁₄ H ₂ Cl ₂ DyN ₂ O ₉
$D_{calc.}/\text{g cm}^{-3}$	0.919	0.933
μ/mm^{-1}	1.689	1.977
Formula Weight	565.04	575.58
Colour	red	pink
Shape	block	plate
Size/mm ³	0.09 × 0.05 × 0.03	0.20 × 0.10 × 0.06
T/K	119.6(8)	120.00(10)
Crystal System	monoclinic	monoclinic
Space Group	$P2_1/n$	$P2_1/n$
$a/\text{\AA}$	11.973(3)	11.9237(4)
$b/\text{\AA}$	13.885(6)	14.0496(8)
$c/\text{\AA}$	12.285(4)	12.2263(5)
$\alpha/^\circ$	90	90
$\beta/^\circ$	90.21(3)	90.254(4)
$\gamma/^\circ$	90	90
$V/\text{\AA}^3$	2042.3(12)	2048.17(16)
Z	2	2
Wavelength/ $\text{\AA}$	0.71073	0.71073
Radiation type	Mo K_α	Mo K_α
$\Theta_{min}/^\circ$	3.317	3.333
$\Theta_{max}/^\circ$	25.437	25.053
Measured Refl's.	10514	14733
Indep't Refl's	3554	3599
Refl's $I \geq 2\sigma(I)$	2486	3259
R_{int}	0.1133	0.0624
Parameters	138	138
Restraints	36	12
Largest Peak	1.413	4.449
Deepest Hole	−1.250	−1.336
GooF	0.959	1.076
wR_2 (all data)	0.1323	0.1455
wR_2	0.1252	0.1432
R_1 (all data)	0.0762	0.0535
R_1	0.0555	0.0506

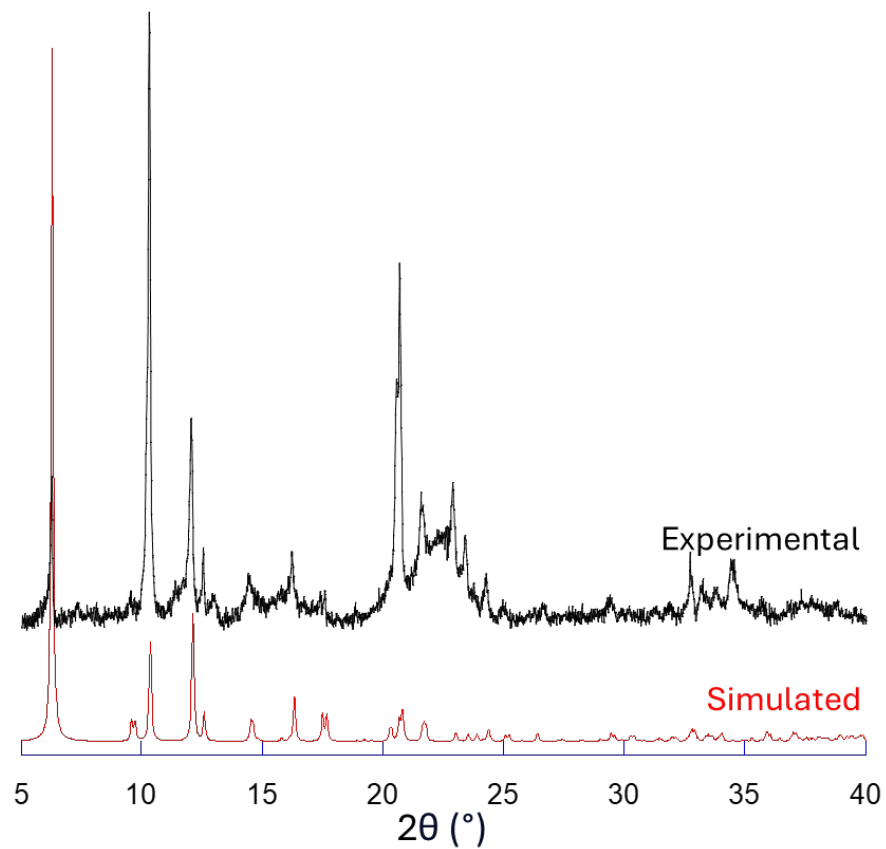


Figure S1. Simulated (red) and experimental (black) X-ray powder diffractograms for compound $(\text{H}_3\text{O})[\text{Dy}(\text{C}_6\text{O}_4(\text{CN})\text{Cl})_2(\text{H}_2\text{O})]\cdot 44\text{H}_2\text{O}$ (**2**).

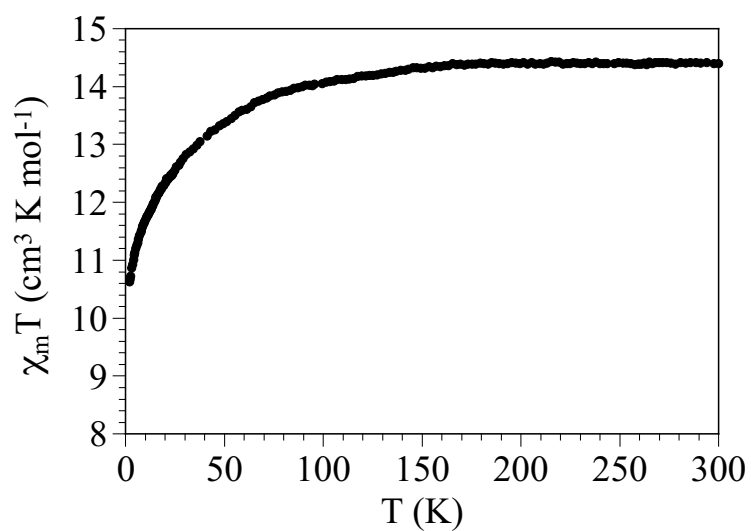


Figure S2. Thermal variation of the $\chi_m T$ product for compound $(\text{H}_3\text{O})[\text{Dy}(\text{C}_6\text{O}_4(\text{CN})\text{Cl})_2(\text{H}_2\text{O})]\cdot 44\text{H}_2\text{O}$ (**2**).

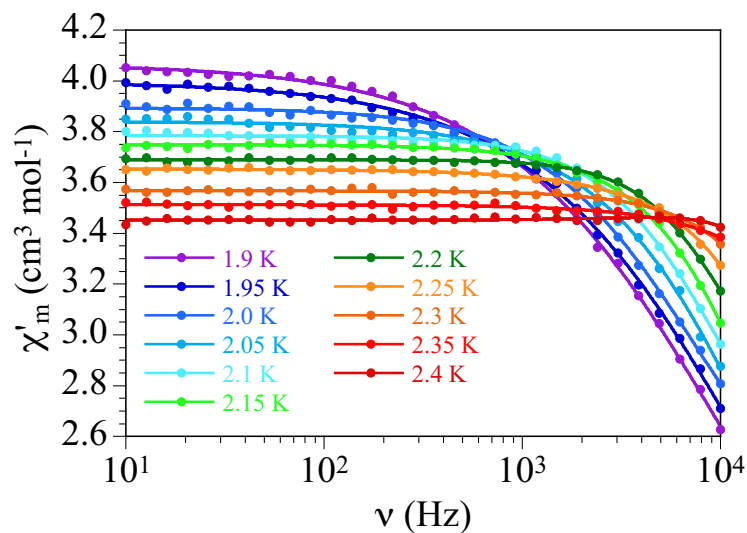


Figure S3. Frequency dependence of χ'_m at different temperatures with an applied DC field of 80 mT for compound 2. Solid lines are the best fit to the Debye model.

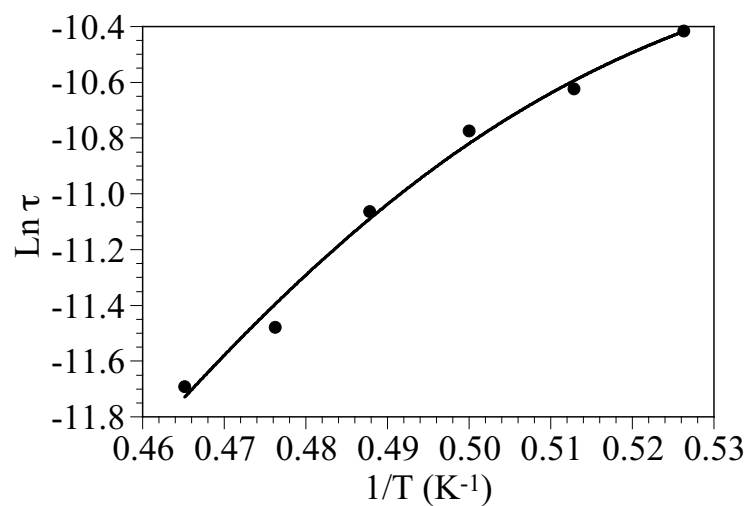


Figure S4. Arrhenius plot of the relaxation times (τ) obtained from the fit of χ'_m , with a DC field of 80 mT. The solid line is the best fit to a model with Orbach and Direct relaxation mechanisms (Equation (2)).