

Supplementary Materials: Field-Induced Slow Relaxation in a Dinuclear Dysprosium(III) Complex Based on 3-Methoxycinnamic Acid

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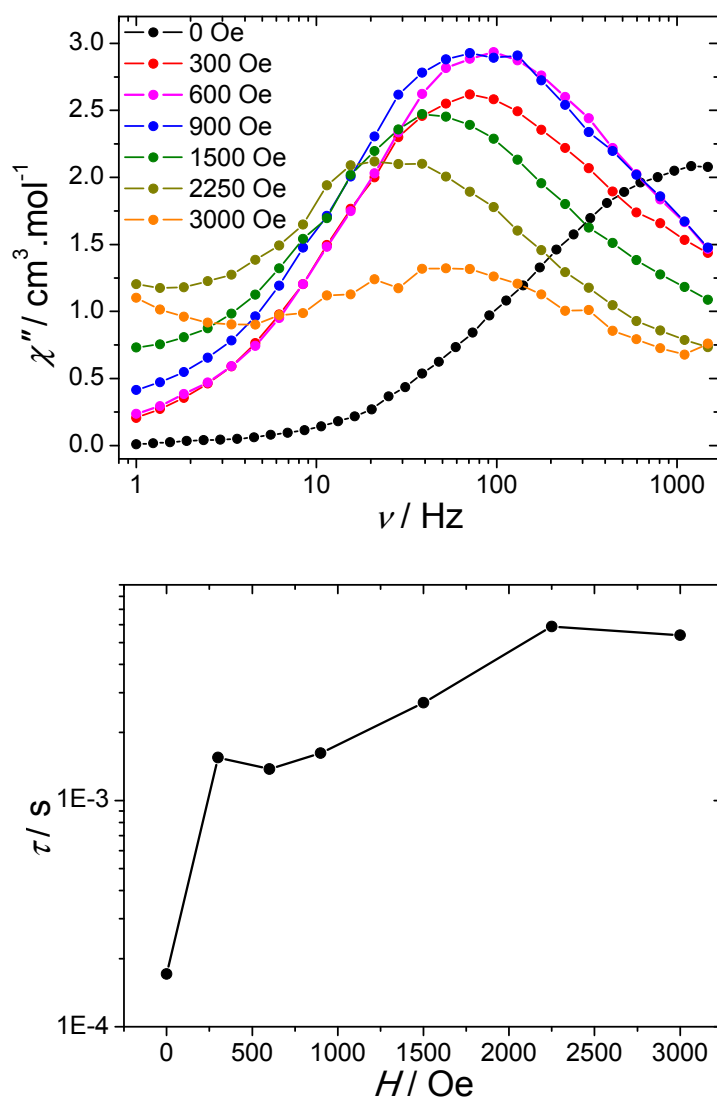


Figure S1. Top: Field dependence of the out-of-phase susceptibility, χ'' , at 1.8 K for **1**. Bottom: Field dependence of the relaxation time. The red solid line represents the fit using equation (1).

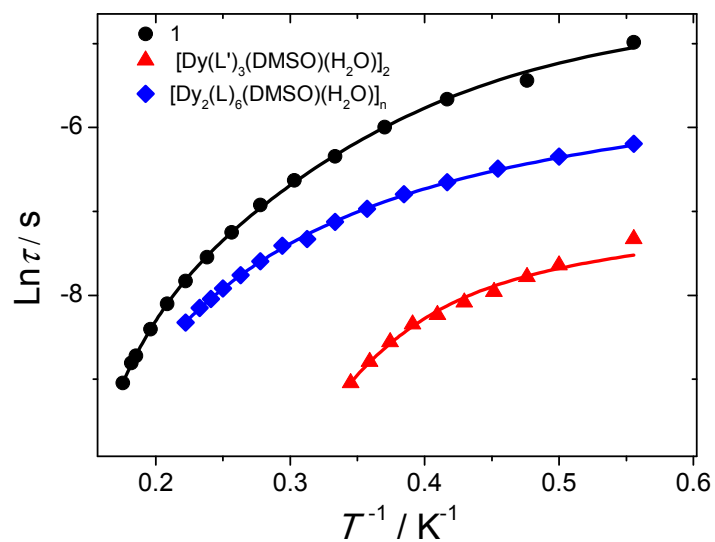


Figure S2. Temperature dependence of the relaxation time for the three different dysprosium compounds. The solid line represent the fit.

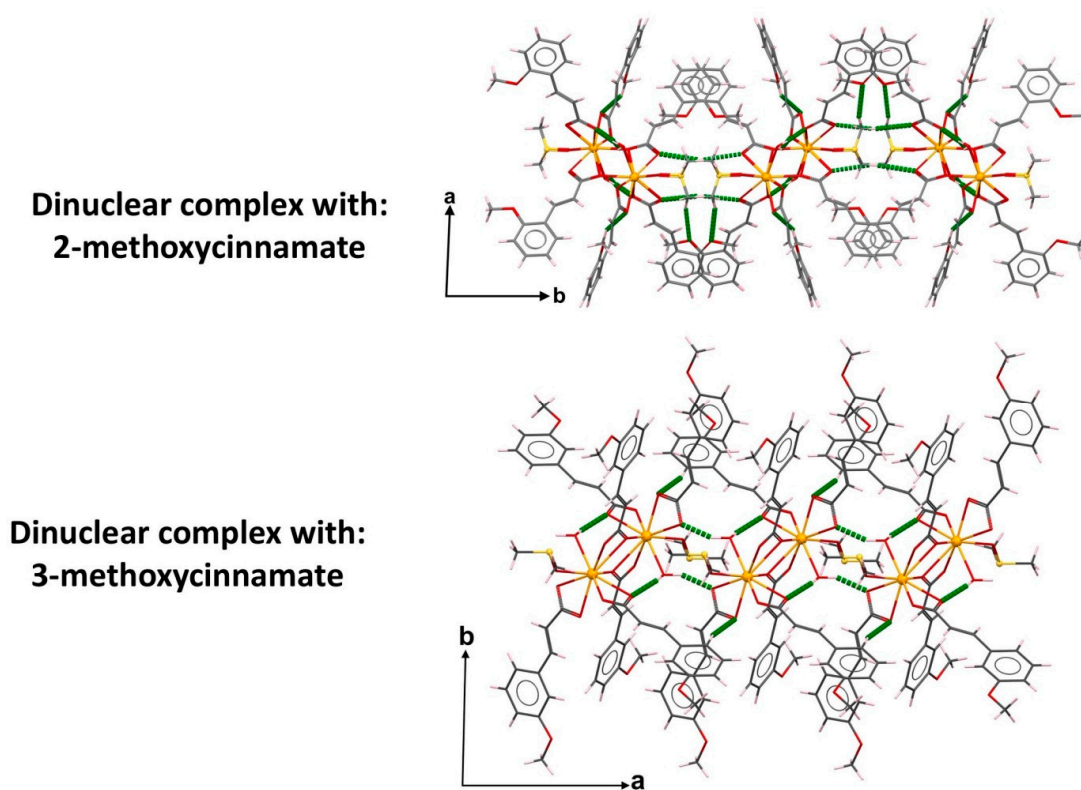


Figure S3. Differences in the packing arrangement between the dinuclear complexes.

Table S1. Crystal data, data collection and refinement details for 1.

Formula	C ₃₂ H ₃₅ DyO ₁₁ S
Mass Mw (g/mol)	790.16
Crystal system	Triclinic
Space group	P-1
Temperature (K)	293(2)
a (Å)	8.2231(11)
b (Å)	12.833(2)
c (Å)	17.175(2)
α(°)	80.864(7)
γ(°)	77.901(7)
β(°)	88.862(8)
V(Å ³)	1749.5(4)
Z	2
qcalc. (g.cm ⁻³)	1.5
μ (mm ⁻¹)	2.25
R _i [I > 2σ(I)]	0.0354
wR ₂ [I > 2σ(I)]	0.0763
GOF (F ²)	1.048
Residual electron density, e Å ⁻³ (ρ _{min} /ρ _{max})	1.27/-0.54

$$^a R1 = \sum \|F_o\| - \|F_c\| / \sum \|F_o\|; ^b wR2 = \sqrt{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]}$$

Table S2. Bond lengths and bond angles for 1.

Atom	Atom	Length/Å	Atom	Atom	Atom	Angle/°
Dy1	O1	2.455(3)	O1	Dy1	O8 ⁱ	106.63(9)
Dy1	O2	2.414(3)	O2	Dy1	O5	128.13(10)
Dy1	O4	2.408(3)	O2	Dy1	O7	88.70(10)
Dy1	O5	2.452(3)	O2	Dy1	O8 ⁱ	76.34(9)
Dy1	O7	2.419(3)	O4	Dy1	O1	74.57(10)
Dy1	O8 ⁱ	2.617(3)	O4	Dy1	O2	79.37(10)
Dy1	O8	2.336(3)	O4	Dy1	O7	149.31(10)
Dy1	O10	2.310(3)	O8	Dy1	O8 ⁱ	67.08(10)
Dy1	O11	2.380(2)				

Symmetry code: (i) 1-X, 1-Y, 2-Z

Table S3. Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O11—H11A...O5 ⁱⁱ	0.9700	1.7800	2.692 (4)	154.00
O11—H11B...O2 ⁱ	0.9700	1.8700	2.715 (4)	144.00
C3—H3...O2	0.9300	2.5500	2.868 (6)	100.00
C10—H10A...O9 ⁱⁱⁱ	0.9600	2.5900	3.360 (7)	138.00
C13—H13...O4	0.9300	2.4700	2.821 (5)	102.00
C20—H20A...O4 ^{iv}	0.9600	2.4600	3.409 (7)	168.00
C23—H23...O7	0.9300	2.4600	2.810 (6)	102.00

Symmetry codes : (i) -x+1, -y+1, -z+2 ; (ii) -x, -y+1, -z+2 ; (iii) x+1, y, z-1 ; (iv) -x+1, -y+1, -z+1.

Table S4. SHAPE analysis.

	JJCU	CCU	JCSAPR	CSAPR	JTCTPR	TCTPR
1	10.049	8.522	3.020	2.116	3.093	2.584
JJCU: Capped cube						
CCU: Spherical-relaxed capped cube						
JCSAPR: Capped square antiprism						
CSAPR: Spherical capped square antiprism						
JTCTPR: Tricapped trigonal prism						
TCTPR: Spherical tricapped trigonal prism						

Table S5. Fitting of the Cole-Cole plots with a generalized Debye model for temperature ranging from 1.8 to 5.7 K under a 2250 Oe DC field for **1**.

<i>T</i> (K)	α	χ^s (cm ³ ·mol ⁻¹)	χ^r (cm ³ ·mol ⁻¹)
1.8	4.64744	5.55985	0.89909
2.1	3.94644	4.92406	0.871
2.4	3.77389	4.75026	0.86587
2.7	3.72501	4.51057	0.88919
3	3.34129	4.61308	0.80774
3.3	3.04781	4.66123	0.73563
3.6	2.91137	4.69504	0.6903
3.9	2.54359	4.85934	0.51422
4.2	2.47852	4.8564	0.43933
4.5	2.4661	4.78597	0.37824
4.8	2.4739	4.68053	0.33631
5.1	2.58814	4.6709	0.18245
5.4	2.50496	4.41138	0.29951
5.5	2.36457	4.206	0.41677
5.7	2.73292	4.39344	0.15239