Supplementary Materials: Tuning of Hula-Hoop Coordination Geometry in a Dy Dimer

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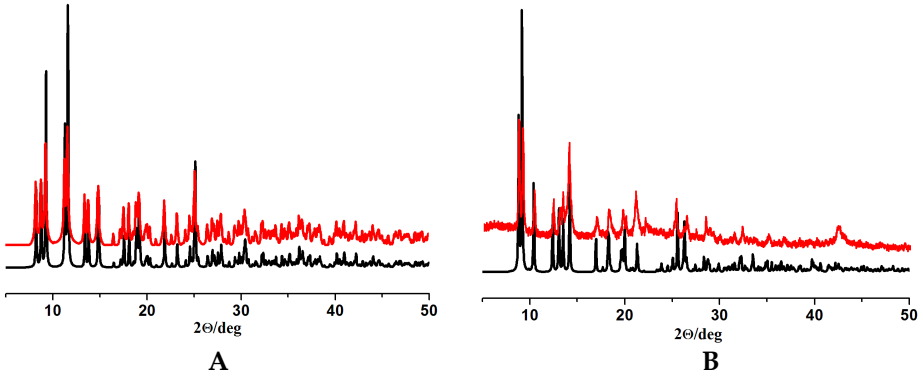

Figure S1. The XRD of compounds **1** (**A**) and **2** (**B**), simulate (black), experimental (red).

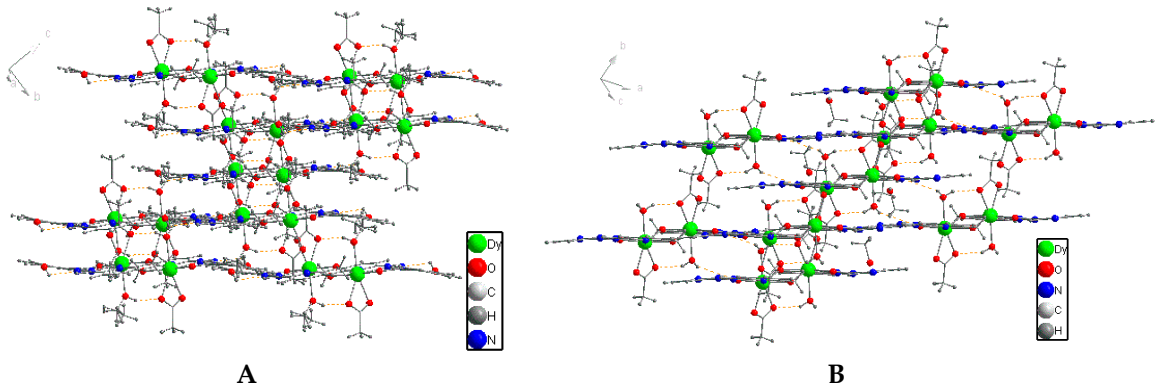

Figure S2. Molecular packing of **1** (**A**) and **2** (**B**); yellow dash: hydrogen bonds.

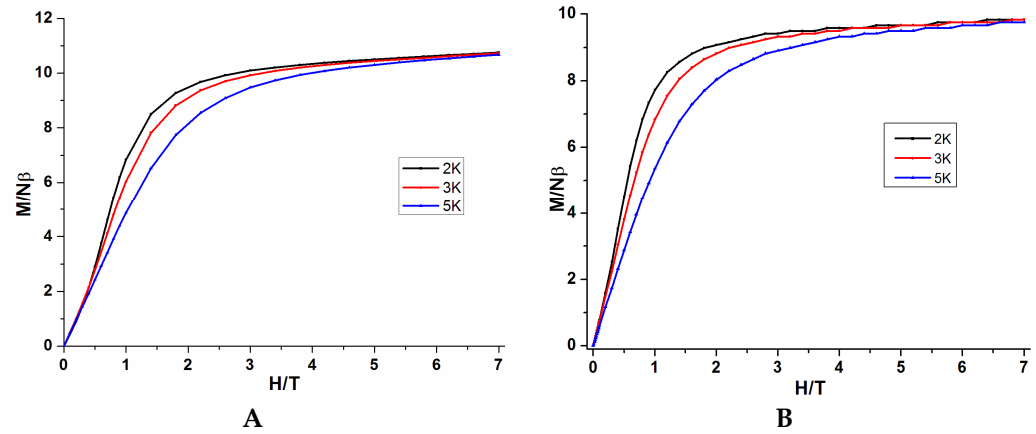

Figure S3. Plots of M *vs.* H for **1** (**A**) and **2** (**B**).

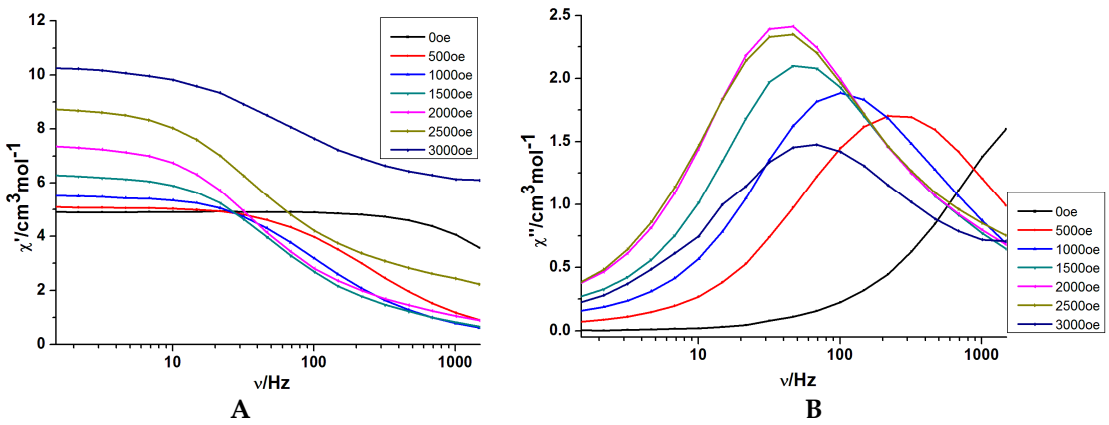

Figure S4. Plots of χ′ (**A**) and χ″ (**B**) *vs.* frequency under different dc magnetic fields for **1** at 2 K.

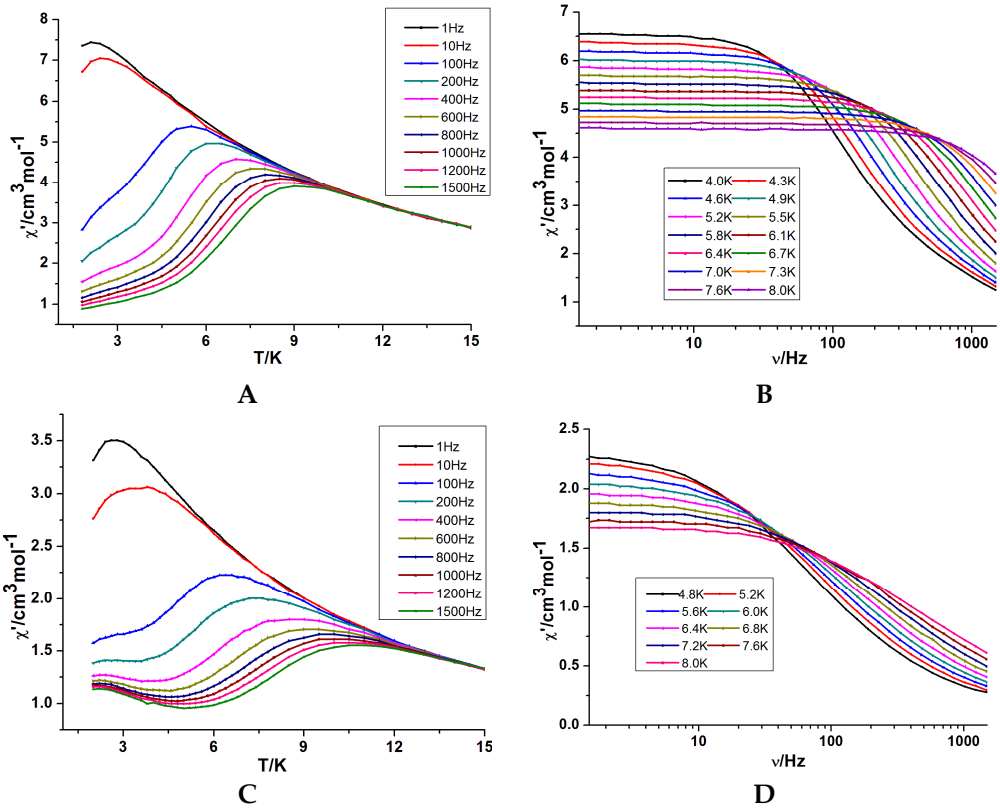

Figure S5. Temperature dependence (**A**) and frequency dependence (**B**) of the in-phase ac susceptibility for **1** (**A,B**) under 2000 Oe dc field and Temperature dependence (**C**) and frequency dependence (**D**) of the in-phase ac susceptibility for **2** under zero dc field.

Table S1. Crystal data and structure refinement for compounds **1** and **2**.

Compound	1	2
Formula	$C_{44}H_{44}Dy_2N_6O_{12}$	$C_{32}H_{38}Dy_2N_8O_{12}$
Mr (g mol^{-1})	1159.82	1051.70
Colour	Pale-yellow	Pale-yellow
Crystal System	triclinic	triclinic
Space Group	$P\bar{1}$	$P\bar{1}$
T (K)	180(2)	150(2)
a (Å)	9.8233(9)	9.8189(12)
b (Å)	10.2588(10)	10.0060(11)
c (Å)	10.9391(11)	10.5795(12)
α (°)	92.521(8)	85.777(9)
β (°)	99.381(8)	65.913(9)
γ (°)	99.221(8)	86.200(9)
V (Å)	1070.81(18)	945.6(2)
Z	1	1
D_x (g·cm^{-3})	1.799	1.847
μ (mm^{-1})	3.533	3.991
F(000)	570	514
Reflns collected	10674	9105
Unique data	3787	4316
Rint	0.115	0.0424
Data with I > 2σ(I)	3362	3987
parameters/restraints	289/1	255/6
S on F^2	1.02	1.058
R_1 [I > 2σ(I)]	0.048	0.0348
wR_2 (all data)	0.125	0.092
Largest diff peak/hole [e·Å^{-3}]	+1.69/−1.23	+1.40/−2.95
CCDC No.	1442826	1442827

Table S2. Analysis of Cole–Cole plots of complexes **1** and **2**.

Complex	T (K)	χ_0 (cm^3/mol)	χ_{inf} (cm^3/mol)	α	R^2
	5.5 K	5.7274(4)	0.9582(3)	0.0938(5)	0.99586
	5.8 K	5.5240(3)	1.0721(1)	0.0564(2)	0.99767
	6.1 K	5.3759(2)	1.0672(1)	0.0534(2)	0.99837
1	6.4 K	5.2296(1)	1.0761(4)	0.0465(8)	0.99806
	6.7 K	5.0843(6)	1.1682(8)	0.0288(6)	0.99758
	7.1 K	4.9576(8)	0.9891(1)	0.0472(2)	0.99782
	7.4 K	4.8305(6)	1.0288(4)	0.0379(2)	0.99588
	4.8 K	2.3653(8)	0.1010(3)	0.3235(5)	0.9943
	5.0 K	2.2811(4)	0.1131(2)	0.3219(9)	0.99542
	5.2 K	2.1750(9)	0.1286(4)	0.3163(5)	0.99589
	5.4 K	2.0769(2)	0.1528(8)	0.3054(9)	0.99438
2	5.6 K	1.9880(1)	0.1638(7)	0.3069(2)	0.99501
	5.8 K	1.9026(8)	0.1825(3)	0.3022(9)	0.99537
	6.0 K	1.8350(7)	0.2073(3)	0.3070(7)	0.993
	6.2 K	1.7586(8)	0.2367(1)	0.3020(6)	0.98917
	6.4 K	1.7008(3)	0.2510(4)	0.3094(8)	0.99265