Supporting Information

Efficient Enhancement of Magnetic Anisotropy by Optimizing Ligand-Field in a Typically Tetranuclear Dysprosium Cluster

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Table S1. Summary of the structural data for complexes **1** and **2**

Complex	**1**	**2**
formula	$C_{56}H_{72}Cl_4Dy_4N_{20}O_{14}$	$C_{56}H_{72}Br_4Dy_4N_{20}O_{14}$
M_r	2041.14	2218.94
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a[Å]	11.6810(9)	11.6203(9)
b[Å]	12.2354(9)	12.2946(8)
c[Å]	14.2356(10)	14.2923(10)
α[°]	75.848(2)	75.951(2)
β[°]	69.993(2)	70.984(2)
γ[°]	67.549(2)	68.022(2)
V[Å^3]	1751.6(2)	1773.1(2)
Z	1	1
ρ_{calcd}[mg mm^{-3}]	1.935	2.078
T[K]	150	150
F (000)	992	1064
Goof on F^2	1.052	1.017
$R_1[I>2\sigma(I)]$[a]	0.0571	0.0578
wR_2[all data][b]	0.1458	0.1250

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$, [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2/w(F_o^2)^2]^{1/2}$.

Table S2. Selected Bond Distances (Å) and Bond Angles (°) of complexes **1** and **2**

Complex **1**		Complex **2**	
Dy(1)-O(2)	2.252(4)	Dy(1)-O(2)	2.243(6)
Dy(1)-O(1W)	2.408(5)	Dy(1)-O(1W)	2.393(6)
Dy(1)-O(1)	2.427(4)	Dy(1)- O(1)	2.432(6)
Dy(1)-N(7)	2.428(6)	Dy(1)- N(7)	2.412(7)
Dy(1)-N(2)	2.440(6)	Dy(1)-N(2)	2.432(7)
Dy(1)-N(1)	2.666(5)	Dy(1)-N(1)	2.662(8)
Dy(1)-N(6)	2.690(6)	Dy(1)-N(6)	2.688(8)
Dy(1)-Cl(1)	2.7144(17)	Dy(1)-Br(1)	2.8886(9)
Dy(2)-O(2)	2.242(4)	Dy(2)-O(2)	2.243(6)
Dy(2)-O(2W)	2.357(5)	Dy(2)-O(2W)	2.338(6)
Dy(2)-O(1a)	2.341(4)	Dy(2)-O(1a)	2.346(6)
Dy(2)-O(1)	2.408(4)	Dy(2)-O(1)	2.390(5)
Dy(2)-N(8)	2.432(6)	Dy(2)-N(8)	2.415(8)
Dy(2)-N(3)	2.459(6)	Dy(2)-N(3)	2.464(8)
Dy(2)-N(10)	2.662(6)	Dy(2)-N(10)	2.648(7)
Dy(2)-N(5)	2.674(6)	Dy(2)-N(5)	2.651(7)
Dy(2a)-Dy(1)-Dy(2)	55.862(9)	Dy(2a)-Dy(1)-Dy(2)	55.804(12)
Dy(1a)-Dy(2)-Dy(2a)	69.698(10)	Dy(1a)-Dy(2)-Dy(2a)	69.765(14)
Dy(1a)-Dy(2)-Dy(1)	124.138(9)	Dy(1a)-Dy(2)-Dy(1)	124.196(12)
Dy(2a)-Dy(2)-Dy(1)	54.440(9)	Dy(2a)-Dy(2)-Dy(1)	54.431(12)
Dy(2a)-O(1)-Dy(2)	106.52(17)	Dy(2a)-O(1)-Dy(2)	106.7(2)
Dy(2a)-O(1)-Dy(1)	103.35(17)	Dy(2a)-O(1)-Dy(1)	102.9(2)
Dy(2)-O(1)-Dy(1)	126.23(16)	Dy(2)-O(1)-Dy(1)	126.7(3)
Dy(2a)-O(2)-Dy(1)	112.68(19)	Dy(2a)-O(2)-Dy(1)	112.8(2)

Symmetry codes: *a*) -x+1, -y+1, -z

Table S3. Variations of Dy-X bonds around Dy ions for complexes **1-3**

1		**2**		**3**	
Dy1-O2	2.252	Dy1-O2	2.243	Dy1-O2	2.248
Dy1-O1	2.427	Dy1-O1	2.432	Dy1-O1	2.405
Dy1-O1W	2.408	Dy1-O1W	2.393	Dy1-O6	2.382
Dy1-Cl1	2.714	Dy1-Br1	2.888	Dy1-O9	2.411
Dy1-N1	2.666	Dy1-N1	2.662	Dy1-N5	2.680
Dy1-N2	2.440	Dy1-N2	2.432	Dy1-N2	2.394
Dy1-N6	2.690	Dy1-N6	2.688	Dy1-N10	2.681
Dy1-N7	2.428	Dy1-N7	2.412	Dy1-N7	2.435
averaged	2.503	averaged	2.518	averaged	2.454
Dy2-O2	2.242	Dy2-O2	2.243	Dy2-O2	2.251
Dy2-O1	2.408	Dy2-O1	2.390	Dy2-O1	2.408
Dy2-O1a	2.341	Dy2-O1a	2.346	Dy2-O1a	2.333
Dy2-O2W	2.357	Dy2-O2W	2.338	Dy2-O3	2.409
Dy2-N3	2.459	Dy2-N3	2.464	Dy2-N1	2.417
Dy2-N5	2.674	Dy2-N5	2.651	Dy2-N4	2.674
Dy2-N8	2.432	Dy2-N8	2.415	Dy2-N6	2.420
Dy2-N10	2.662	Dy2-N10	2.648	Dy2-N9	2.647
averaged	2.446	averaged	2.436	Averaged	2.444

Symmetry codes: *a*) -x+1,-y+1,-z

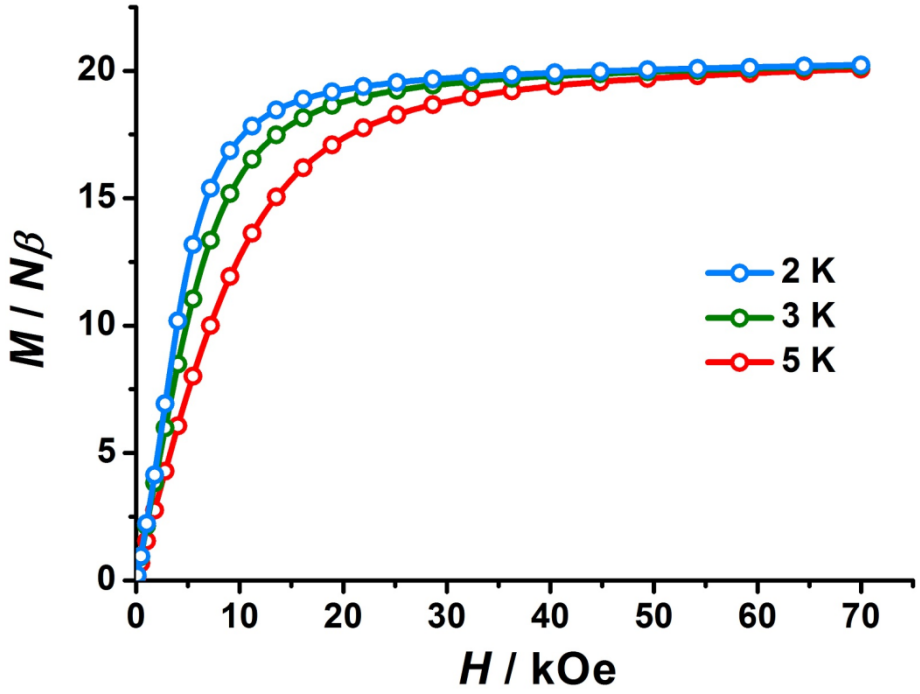

Figure S1. *M* versus *H*/*T* plot for **1** at indicated temperatures.

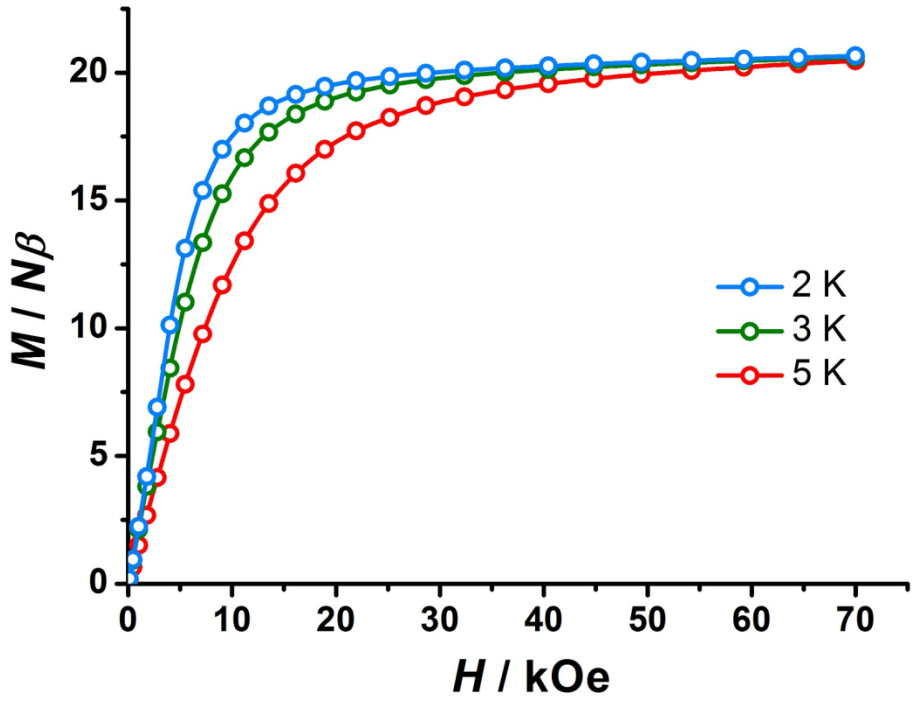

Figure S2. *M* versus *H*/*T* plot for **2** at indicated temperatures.

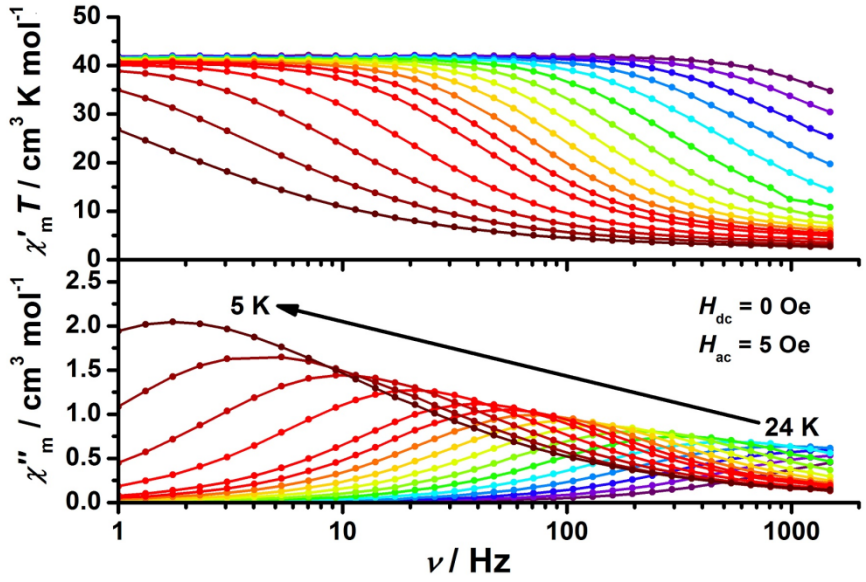

Figure S3. Frequency dependence of the in-phase (χ',) and out-of-phase (χ'') susceptibilities for **1** below 24 K under a zero dc field.

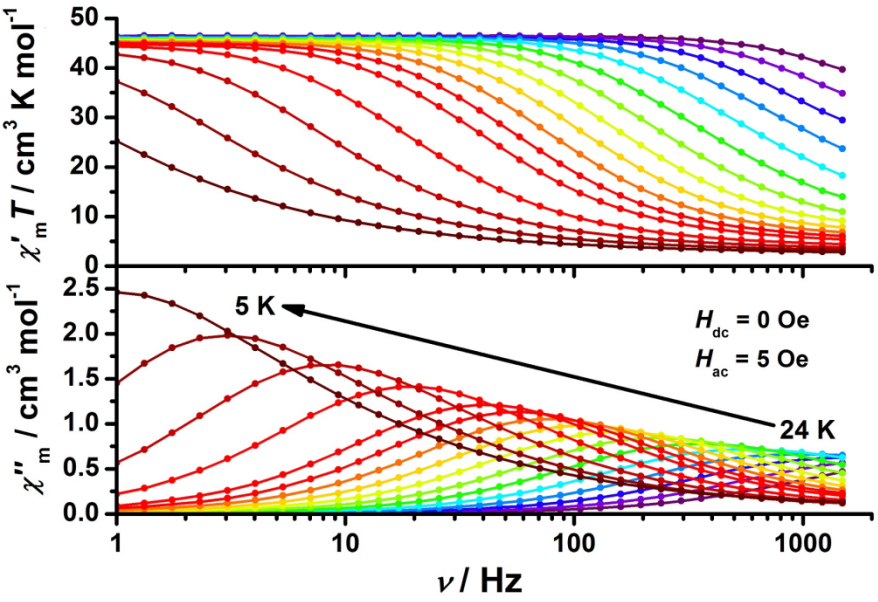

Figure S4. Frequency dependence of the in-phase (χ',) and out-of-phase (χ'') susceptibilities for **2** below 24 K under a zero dc field.

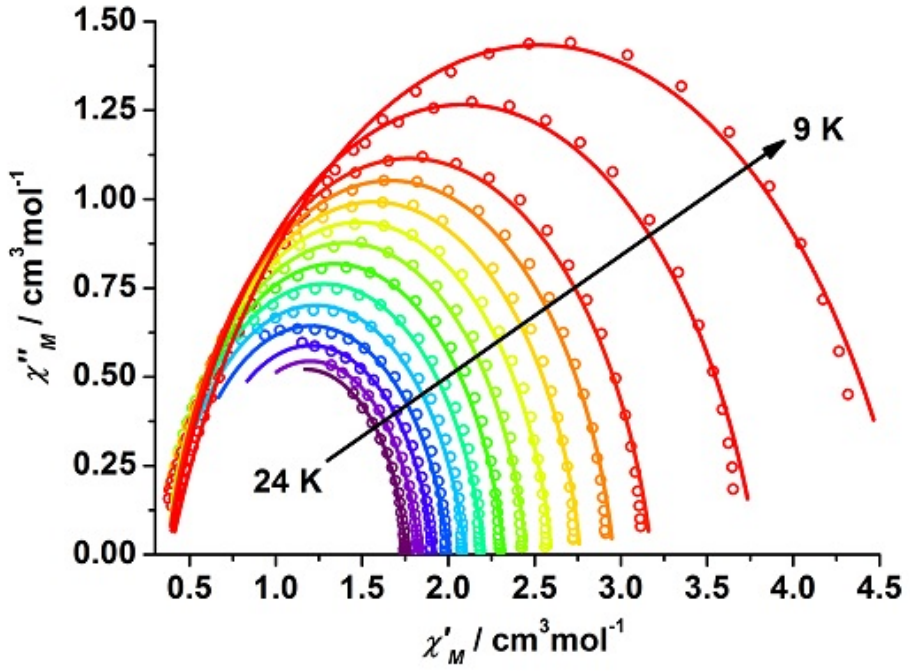

Figure S5. The Cole–Cole plots of **1**. The solid lines correspond to the best fit.

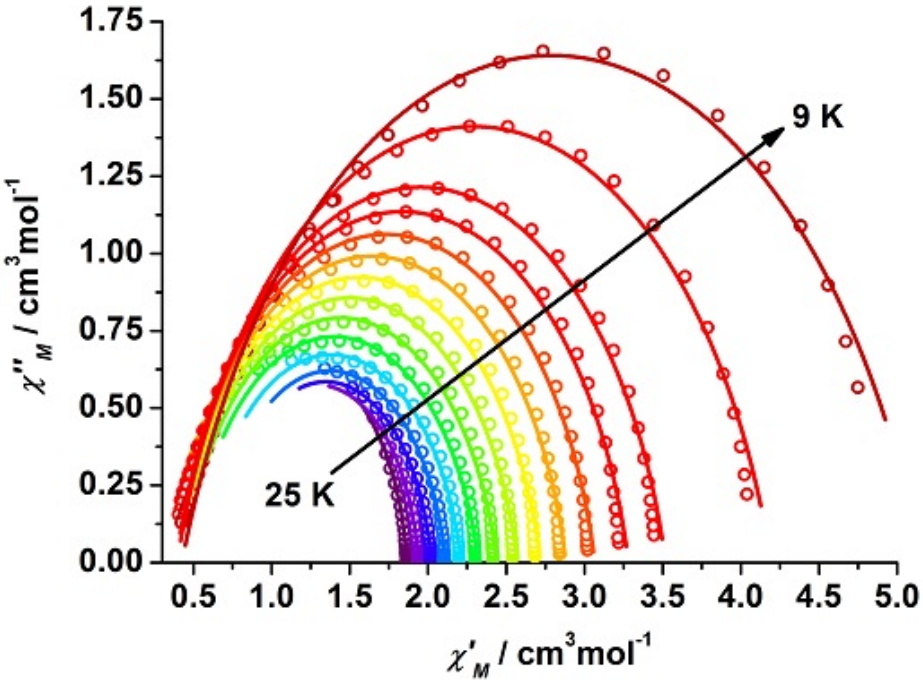

Figure S6. The Cole–Cole plots of **2**. The solid lines correspond to the best fit.