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Supporting Information

Modulating the slow magnetic relaxation of a mononuclear Dy(III) single-molecule magnet via magnetic field and dilution effect

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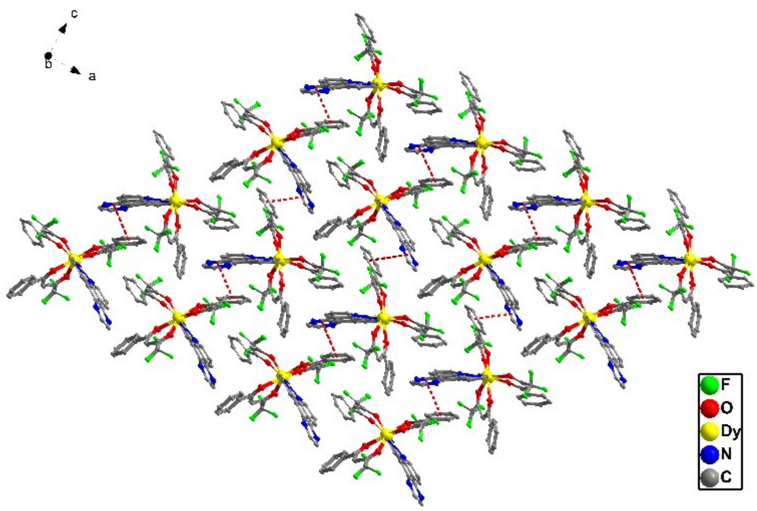

Fig. S1 Molecular stacking chart of complex **1.** H atoms and solvent molecules are omitted for clarity.

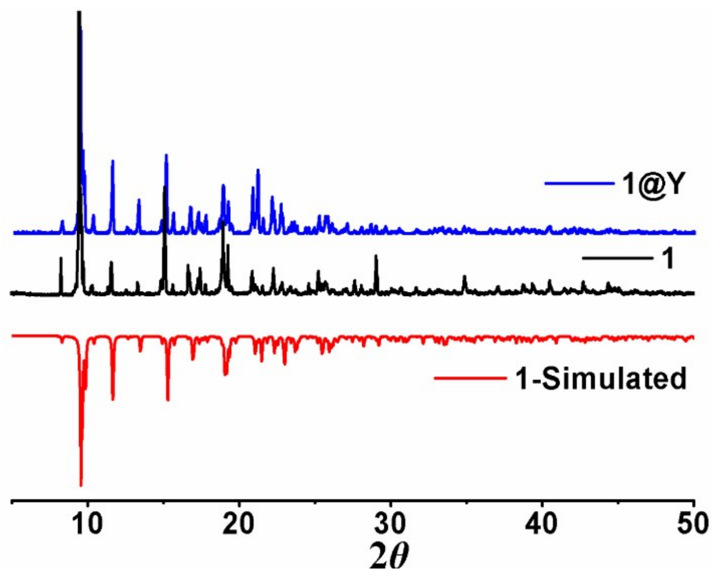

Fig. S2 PXRD curves of **1** and **1@Y**

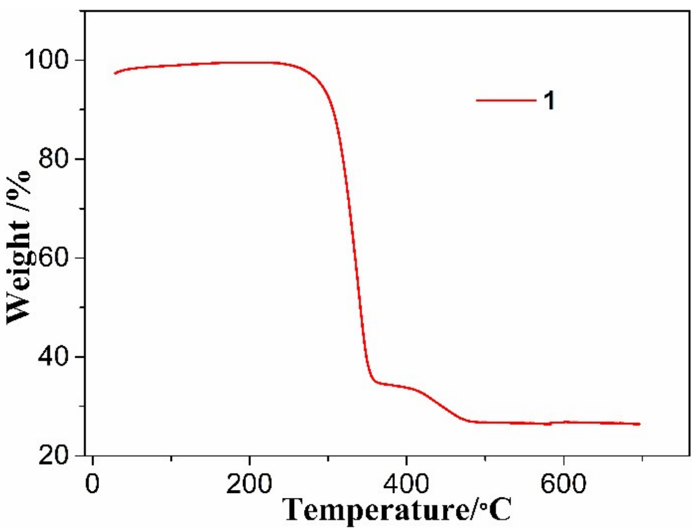

Fig. S3 TGA plots of **1** under N_2 environment.

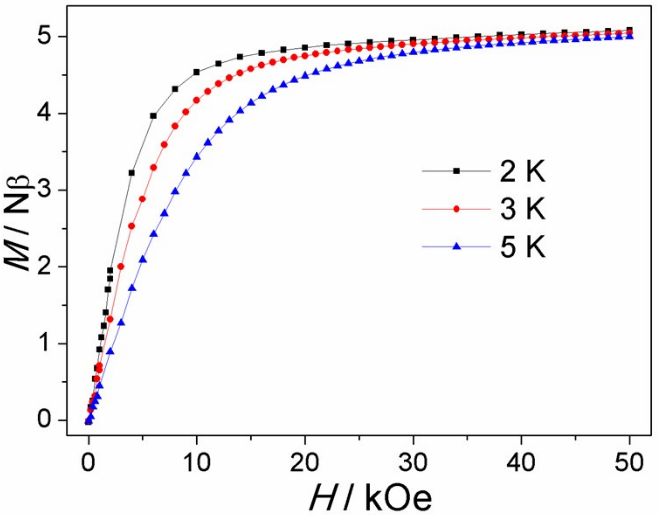

Fig. S4 *M* vs *H* curves for **1**

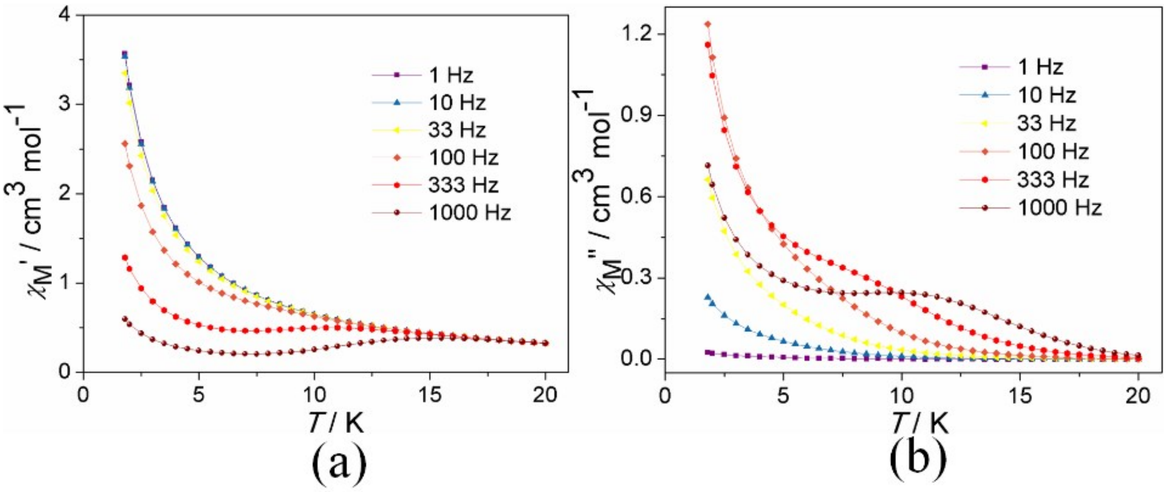

Fig. S5 Temperature dependence of χ' and χ'' susceptibilities for **1** without static field.

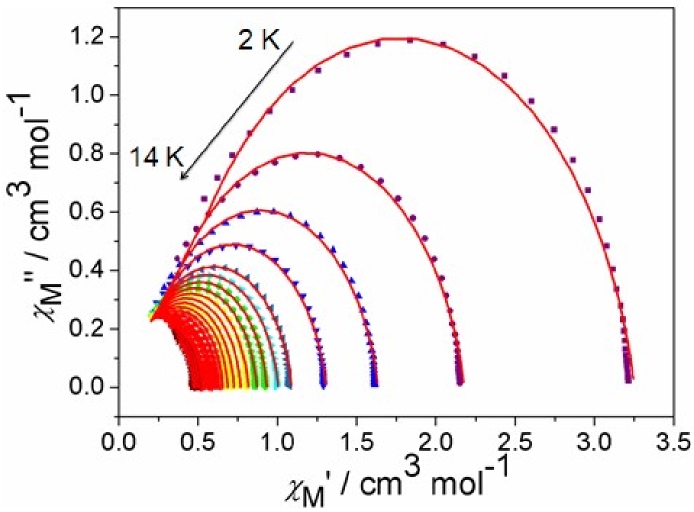

Fig. S6 Cole-Cole plots for **1** without static field. The solid lines represent the best fit to the measured results.

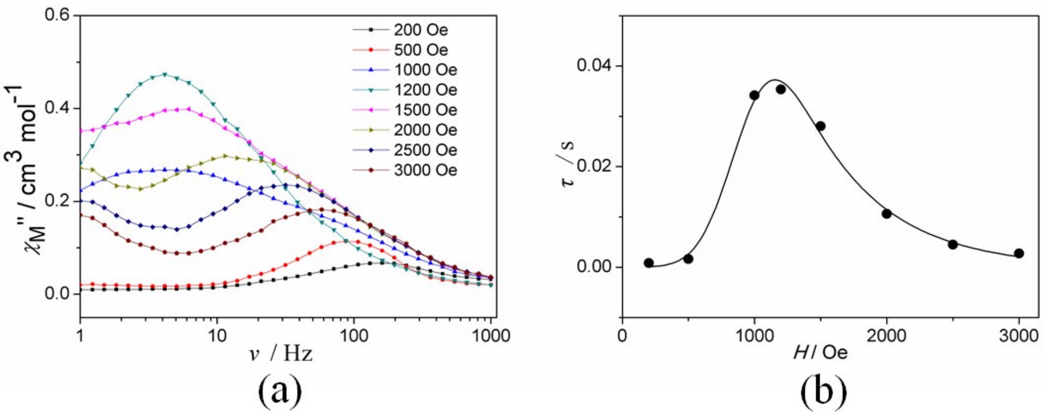

Fig. S7 Plot of the frequency dependence of the χ'' ac susceptibility component under indicated dc field for complex **1** (a). Plot of τ vs. H for **1** under different dc fields K (b), the solid line is guide for eyes.

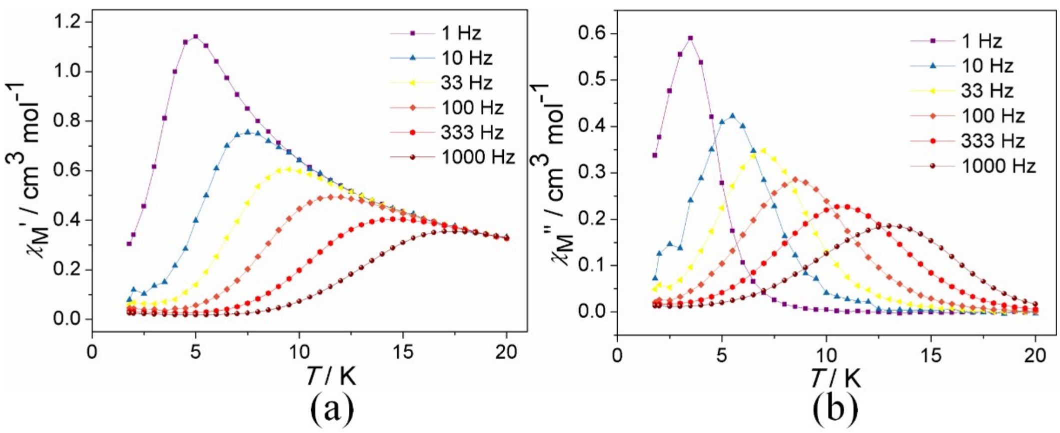

Fig. S8 Temperature dependence of χ' and χ'' susceptibilities for **1** at applied dc fields of 1200 Oe.

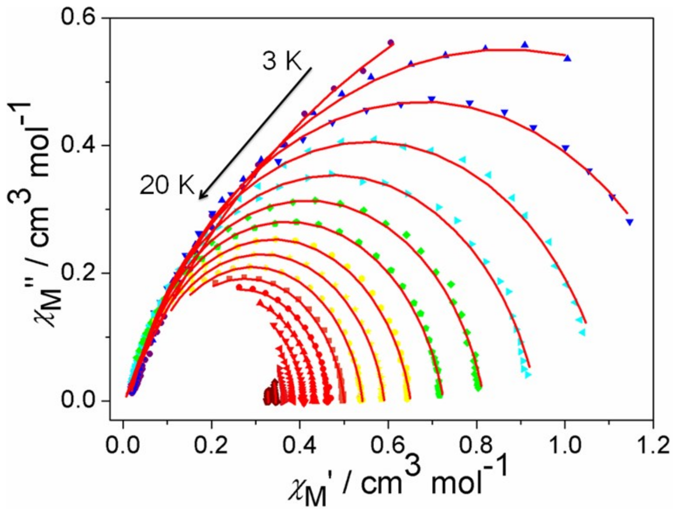

Fig. S9 Cole-Cole plots for **1** at applied dc fields of 1200 Oe. The solid lines represent the best fit to the measured results.

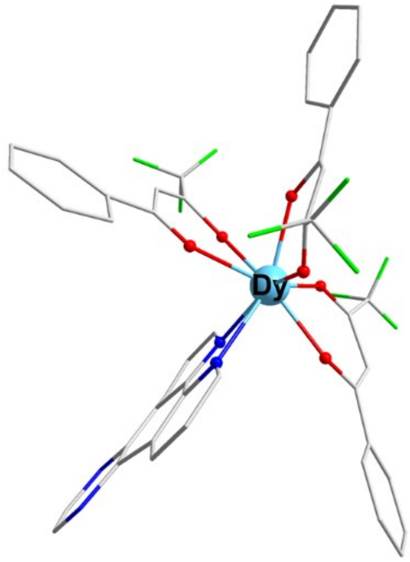

Fig. S10 Calculated model structures of Dy(III) fragment of **1**. H atoms are omitted.

Table S1. Crystal Data and Structure Refinement Details for complexes **1** and **2**.

	1	**2**
Empirical formula	$C_{44}H_{26}DyF_9N_4O_6$	$C_{44}H_{26}YF_9N_4O_6$
Formula weight	1040.19	966.60
Crystal system	orthorhombic	orthorhombic
Space group	*P*na2$_1$	*P*na2$_1$
a (Å)	21.3258(11)	21.53 (2)
b (Å)	10.8147(3)	10.926(10)
c (Å)	17.9497(8)	18.350(16)
α (°)	90	90
β (°)	90	90
γ (°)	90	90
V (Å3)	4139.8(3)	4317(7)
Z	4	4
μ (mm-1)	10.500	1.442
Unique reflections	5776	9327
Observed reflections	10287	22036
Rint	0.0398	0.0990
Final R indices [I >2σ(I)]	R_1 = 0.0725	R_1 = 0.0717
	wR_2 = 0.1713	wR_2 = 0.1495
R indices (all data)	R_1 = 0.0817	R_1 = 0.1948
	wR_2 = 0.1808	wR_2 = 0.1953

Table S2. Selected bond lengths (Å) and bond angles (°) for **1** and **2**.

Complex **1**			
Dy(1)-O(1)	2.243(4)	O(3)-Dy(1)-O(2)	80.5(7)
Dy(1)-O(2)	2.317(4)	O(3)-Dy(1)-O(4)	73.6(7)
Dy(1)-O(3)	2.231(3)	O(3)-Dy(1)-N(1)	71.5(6)
Dy(1)-O(4)	2.300(1)	O(3)-Dy(1)-N(2)	83.5(7)
Dy(1)-O(5)	2.362(3)	O(4)-Dy(1)-O(2)	125.6(6)
Dy(1)-O(6)	2.378(6)	O(4)-Dy(1)-N(1)	131.2(5)
Dy(1)-N(1)	2.492(1)	O(4)-Dy(1)-N(2)	78.9(7)
Dy(1)-N(2)	2.443(8)	O(5)-Dy(1)-O(2)	76.7(6)
O(1)-Dy(1)-O(2)	75.1(5)	O(5)-Dy(1)-O(3)	138.8(7)
O(1)-Dy(1)-O(3)	128.8(5)	O(5)-Dy(1)-N(1)	71.1(5)
O(1)-Dy(1)-O(4)	85.3(4)	O(5)-Dy(1)-N(2)	95.5(7)
O(1)-Dy(1)-O(5)	77.1(4)	O(6)-Dy(1)-O(1)	69.1(1)
O(1)-Dy(1)-N(1)	143.4(3)	O(6)-Dy(1)-O(2)	136.4(6)
O(1)-Dy(1)-N(2)	137.9(4)	O(6)-Dy(1)-O(3)	142.2(7)
O(2)-Dy(1)-N(1)	80.3(5)	O(6)-Dy(1)-N(1)	115.7(5)
O(2)-Dy(1)-N(2)	144.2(7)	O(6)-Dy(1)-N(2)	69.3(8)

Complex **2**			
Y(1)-O(1)	2.299(7)	O(2)-Y(1)- N(2)	69.0(9)
Y(1)-O(2)	2.300(8)	O(3)-Y(1)- O(5)	136.1(3)
Y(1)-O(3)	2.323(10)	O(3)-Y(1)- N(1)	138.7(7)
Y(1)-O(4)	2.296(8)	O(3)-Y(1)- N(2)	75.2(6)
Y(1)-O(5)	2.325(8)	O(4)-Y(1)- O(1)	78.9(3)
Y(1)-O(6)	2.323(8)	O(4)-Y(1)- O(2)	116.3(3)
Y(1)-N(1)	2.505(15)	O(4)-Y(1)- O(3)	71.8(3)
Y(1)-N(2)	2.522(14)	O(4)-Y(1)- O(5)	75.1(3)
O(1)-Y(1)- O(2)	71.7(3)	O(4)-Y(1)- O(6)	85.8(3)
O(1)-Y(1)- O(3)	121.3(3)	O(4)-Y(1)- N(1)	149.5(7)
O(1)-Y(1)- O(5)	78.5(3)	O(4)-Y(1)- N(2)	143.9(7)
O(1)-Y(1)- O(6)	150.1(3)	O(5)-Y(1)- N(1)	78.5(8)
O(1)-Y(1)- N(1)	81.1(7)	O(5)-Y(1)- N(2)	122.9(8)
O(1)-Y(1)- N(2)	132.1(9)	O(6)-Y(1)- O(3)	76.7(3)
O(2)-Y(1)- O(3)	77.6(3)	O(6)-Y(1)- O(5)	72.8(3)
O(2)-Y(1)- O(5)	144.4(3)	O(6)-Y(1)- N(1)	100.9(9)
O(2)-Y(1)- O(6)	138.2(2)	O(6)-Y(1)- N(2)	72.9(9)
O(2)-Y(1)- N(1)	78.1(10)	N(1)-Y(1)- N(2)	65.1(7)

Table S3. Dy (III) ions geometry analysis of **1** by SHAPE 2.1 software.

Configuration	ABOXIY, **1(Dy)**
Hexagonal bipyramid (D_{6h})	15.990
Cube (O_h)	9.842
Square antiprism (D_{4d})	**1.094**
Triangular dodecahedron (D_{2d})	1.153
Johnson gyrobifastigium J26 (D_{2d})	14.601
Johnson elongated triangular bipyramid J14 (D_{3h})	28.725
Biaugmented trigonal prism J50 (C_{2v})	1.675
Biaugmented trigonal prism (C_{2v})	1.167
Snub siphenoid J84 (D_{2d})	3.497
Triakis tetrahedron(T_d)	10.494
Elongated trigonal bipyramid(D_{3h})	23.720

Table S4. Relaxation fitting parameters from least-squares fitting of $\chi(f)$ data under zero dc field of **1**.

T(K)	χ_T	χ_S	α
2	3.245	0.283	0.134
3	2.172	0.193	0.131
4	1.629	0.148	0.126
5	1.302	0.121	0.117
6	1.083	0.103	0.106
6.5	0.999	0.096	0.098
7	0.927	0.091	0.092
7.5	0.865	0.085	0.085
8	0.811	0.081	0.078
8.5	0.763	0.078	0.071
9	0.720	0.075	0.065
9.5	0.682	0.074	0.059
10	0.648	0.073	0.054
10.5	0.617	0.073	0.048
11	0.589	0.073	0.044
11.5	0.563	0.074	0.039
12	0.539	0.075	0.036
12.5	0.518	0.076	0.031
13	0.498	0.075	0.029
13.5	0.480	0.074	0.027
14	0.463	0.072	0.026

Table S5. Relaxation fitting parameters from least-squares fitting of $\chi(f)$ data under 1200 Oe dc field of **1**.

T(K)	χ_T	χ_S	α
3	0.154	0.049	0.611
4	2.422	0.036	0.335
5	1.738	0.016	0.278
6	1.342	0.011	0.215
7	1.100	0.014	0.179
8	0.938	0.014	0.163
9	0.817	0.016	0.149
10	0.725	0.019	0.138
11	0.650	0.025	0.128
12	0.591	0.033	0.115
13	0.541	0.042	0.103
14	0.499	0.051	0.097
15	0.464	0.065	0.075
16	0.433	0.077	0.059
17	0.408	0.081	0.053
18	0. 384	0.059	0.052
19	0.363	0.011	0.043
20	0.344	0.054	0.019

Table S6. Relaxation fitting parameters from least-squares fitting of $\chi(f)$ data under 0 Oe dc field of **1@Y**.

T(K)	χ_T	χ_S	α
2	0.153	0.043	0.474
3	0.156	0.036	0.443
4	0.119	0.028	0.430
5	0.095	0.025	0.391
6	0.078	0.021	0.340
6.5	0.071	0.019	0.312
7	0.065	0.016	0.285
7.5	0.061	0.015	0.259
8	0.057	0.014	0.239
8.5	0.053	0.017	0.213
9	0.050	0.021	0.191
9.5	0.047	0.015	0.168
10	0.045	0.011	0.149
10.5	0.043	0.013	0.128
11	0.041	0.015	0.111

Table S7. In wave functions with definite projection of the total moment | J_M > for the lowest three Kramers doublets (KDs) of the Dy(III) for complex **1**.

E/cm^{-1}	wave functions
0.00	98.7%|±15/2> + 0.7%|±13/2>
143.80	1.8%|±15/2> + 95.4%|±13/2> + 0.2%|±11/2>
242.61	5.4%|±13/2> + 77.8%|±11/2> + 4.0 %|±9/2> + 3.3%|±7/2>
297.44	12.8%|±13/2> + 25.9%|±11/2> + 56.7%|±9/2> + 9.0%|±7/2>