Supporting Information

A difunctional Dy(III)-complex exhibiting single-molecule magnet behaviour and fluorescent cellular-imaging

Xuelian Wang,[a#] Zhaopeng Zeng,[b#] Mengyuan Li,[a] Shuman Zhang,[c] Xuhui Qin,[a] Peipei Cen,*[a] Runmei Ding,[c] Danian Tian*[a] and Xiangyu Liu*[b]

[a] *College of Public Health, Key Laboratory of Environmental Factors and Chronic Disease Control, Ningxia Medical University, Yinchuan 750004, China.*

[b] *State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering, College of Chemistry and Chemical Engineering, Xinhua College, Ningxia University, Yinchuan 750021, China.*

[c] *College of Basic Medical Sciences, Ningxia Medical University, Yinchuan 750004, China.*

[#] These authors contributed equally to this work.

***Corresponding author**

Dr. Peipei Cen

E-mail: 13895400691@163.com

***Corresponding author**

Dr. Danian Tian

E-mail: tiandanian@163.com

***Corresponding author**

Prof. Xiangyu Liu

E-mail: xiangyuliu432@126.com

Contents

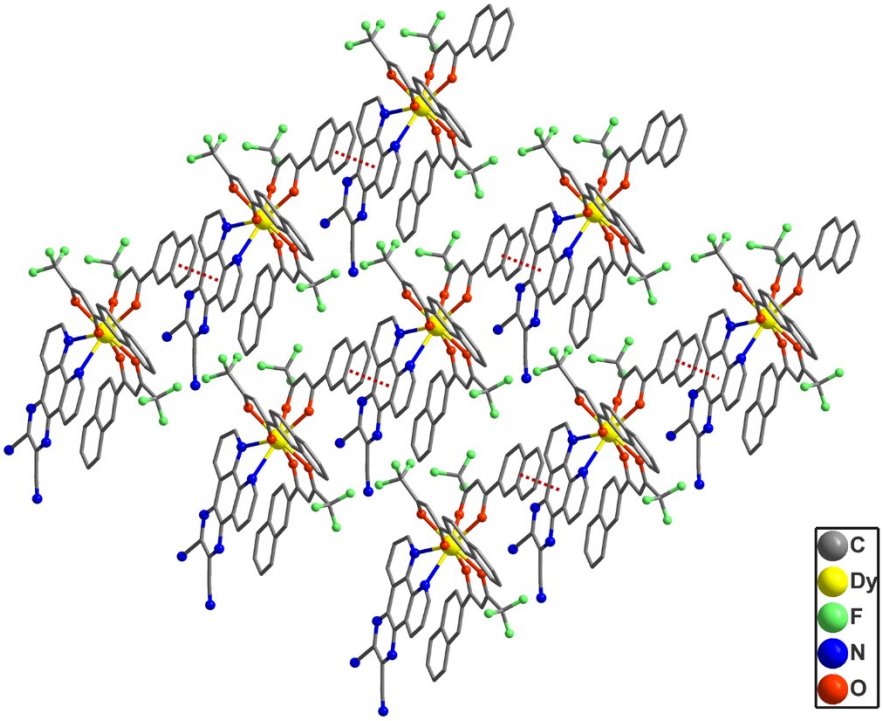

Fig. S1 Crystal packing diagram for complex **1**, the red dashed line represents the π···π interactions.

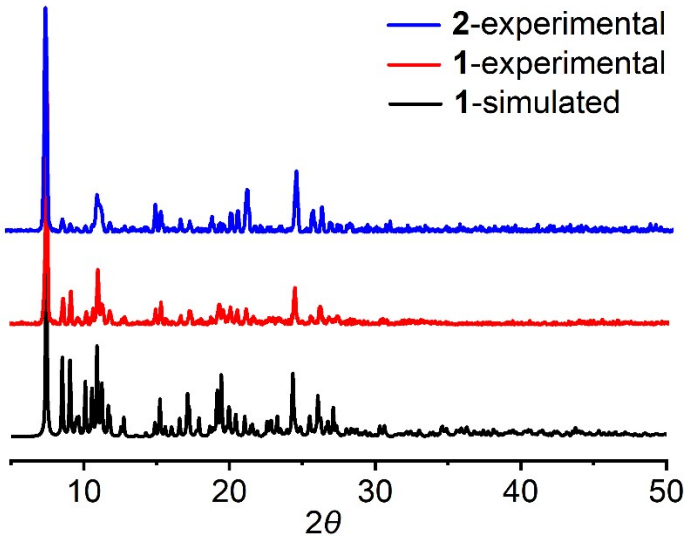

Fig. S2 PXRD curves of **1** and **2**.

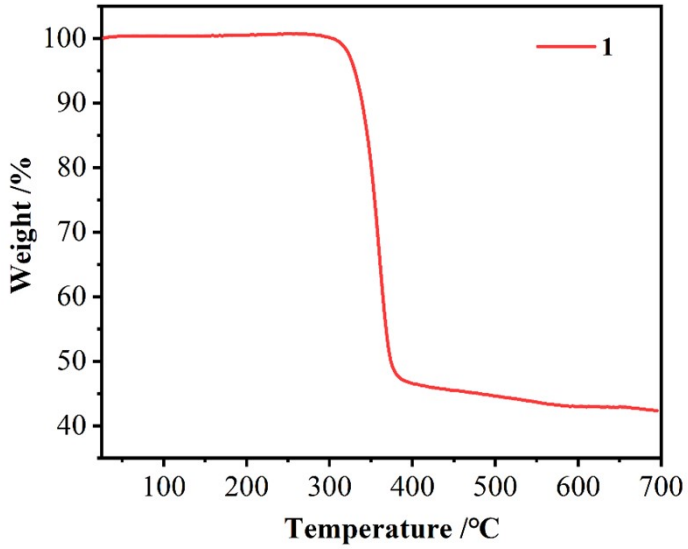

Fig. S3 TGA plot of **1** under N_2 environment.

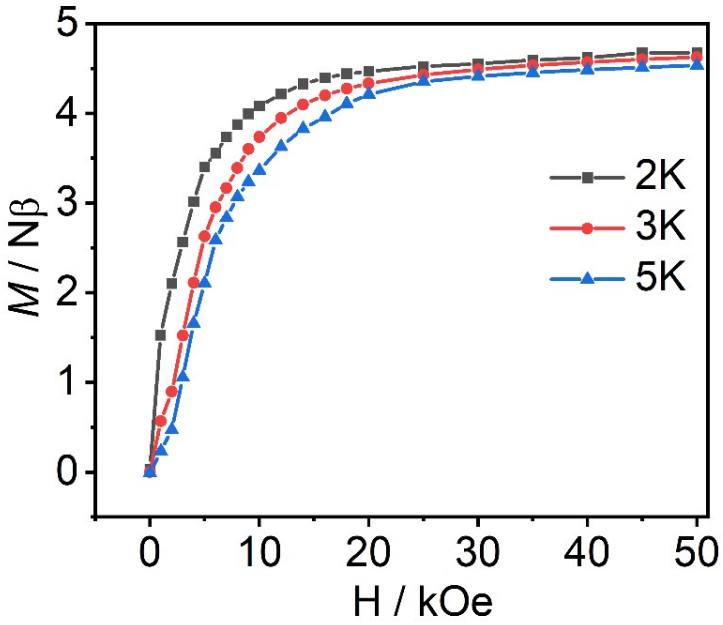

Fig. S4 *M vs H* curves at different temperatures for **1**.

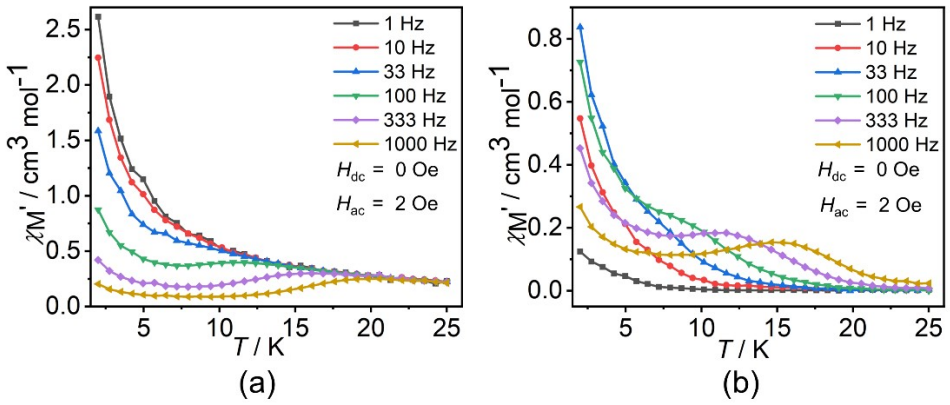

Fig. S5 Temperature dependence of the χ_M' (a) and χ_M'' (b) ac susceptibilities for **1** at different frequencies in an alternating field with an amplitude of 2 Oe (no static field).

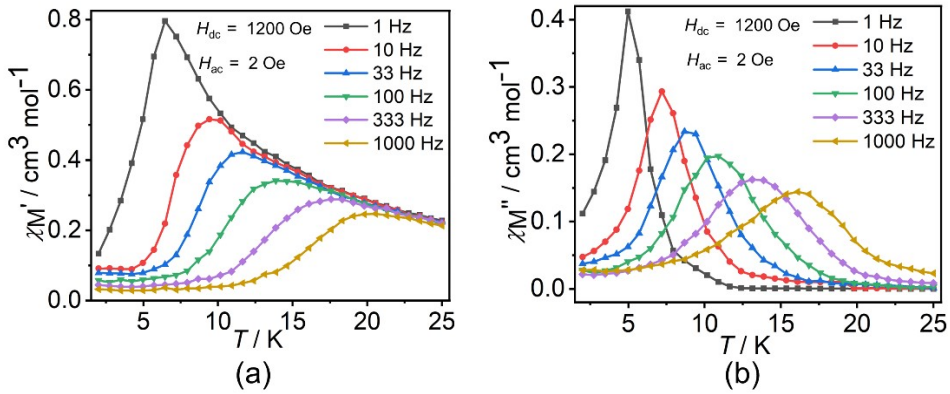

Fig. S6 Temperature dependence of the χ_M' (a) and χ_M'' (b) ac susceptibilities for **1** under a static field of 1200 Oe and an amplitude field of 2 Oe.

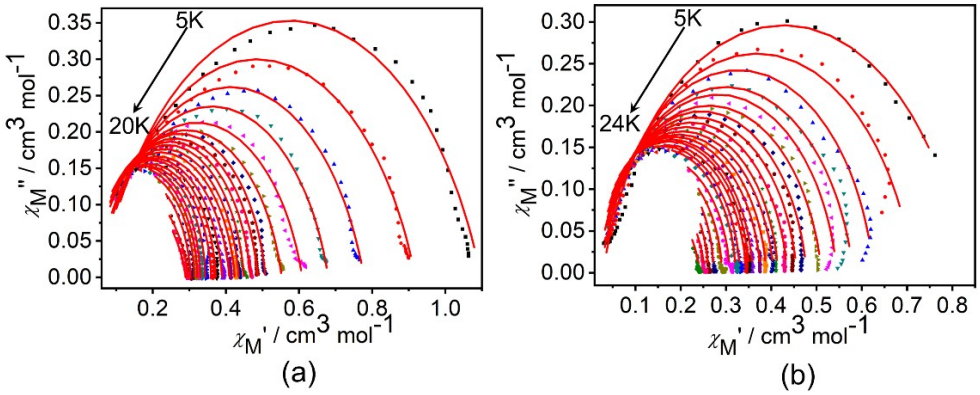

Fig. S7 Cole-Cole plots for complex **1** (a) without a static field and (b) at an applied dc field of 1200 Oe. The solid lines represent the best fit to the measured results.

Table S1. Crystal data and structure refinement details for complex **1**.

complex	**1**
Empirical formula	$C_{58}H_{30}N_6O_6F_9Dy$
Formula weight	1240.38
Crystal system	triclinic
Space group	$P\bar{1}$
Temperature(K)	296
a (Å)	10.4259(16)
b (Å)	11.4821(19)
c (Å)	24.012(4)
α (°)	90.896(5)
β (°)	96.293(5)
γ (°)	115.040(5)
V (Å^3)	2582.5(7)
Z	2
μ (mm^{-1})	1.543
Unique reflections	11832
Observed reflections	105771
R_{int}	0.0454
Final *R* indices [$I > 2\sigma(I)$]	R_1= 0.0349
	wR_2= 0.0872
R indices (all data)	R_1= 0.0436
	wR_2= 0.0925

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

Complex **1**			
Dy(1)-O(1)	2.310(2)	O(3)-Dy(1)-O(2)	86.96(9)
Dy(1)-O(2)	2.323(2)	O(3)-Dy(1)-O(4)	72.15(8)
Dy(1)-O(3)	2.309(2)	O(3)-Dy(1)-O(5)	79.10(8)
Dy(1)-O(4)	2.313(2)	O(3)-Dy(1)-N(1)	147.65(8)
Dy(1)-O(5)	2.340(2)	O(3)-Dy(1)-N(2)	148.17(8)
Dy(1)-O(6)	2.306(2)	O(4)-Dy(1)-O(2)	77.17(9)
Dy(1)-N(1)	2.551(3)	O(4)-Dy(1)-O(5)	125.55(10)
Dy(1)-N(2)	2.581(3)	O(4)-Dy(1)-N(1)	140.16(8)
O(1)-Dy(1)-O(2)	71.84(8)	O(4)-Dy(1)-N(2)	78.17(9)
O(1)-Dy(1)-O(4)	136.26(8)	O(5)-Dy(1)-N(1)	77.54(9)
O(1)-Dy(1)-O(5)	75.21(9)	O(5)-Dy(1)-N(2)	129.10(8)
O(1)-Dy(1)-N(1)	76.55(8)	O(6)-Dy(1)-O(1)	142.07(8)
O(1)-Dy(1)-N(2)	121.10(9)	O(6)-Dy(1)-O(2)	141.83(8)
O(2)-Dy(1)-O(5)	146.45(8)	O(6)-Dy(1)-O(3)	113.78(9)
O(2)-Dy(1)-N(1)	100.53(9)	O(6)-Dy(1)-N(1)	79.20(8)
O(2)-Dy(1)-N(2)	75.33(8)	O(6)-Dy(1)-N(2)	70.64(9)

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

Configuration	ABOXIY, **1(Dy)**
Hexagonal bipyramid (D_{6h})	16.213
Cube (O_h)	9.557
Square antiprism (D_{4d})	**1.044**
Triangular dodecahedron (D_{2d})	1.102
Johnson gyrobifastigium J26 (D_{2d})	15.073
Johnson elongated triangular bipyramid J14 (D_{3h})	27.951
Biaugmented trigonal prism J50 (C_{2v})	2.213
Biaugmented trigonal prism (C_{2v})	1.658
Snub siphenoid J84 (D_{2d})	3.710
Triakis tetrahedron(T_d)	10.238
Elongated trigonal bipyramid(D_{3h})	23.233

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

T(K)	χ_S	χ_T	α
5.0	0.056	1.097	0.241
6.0	0.052	0.917	0.228
7.0	0.050	0.777	0.206
8.0	0.046	0.680	0.187
9.0	0.032	0.609	0.190
10.0	0.031	0.553	0.159
10.5	0.040	0.508	0.107
11.0	0.034	0.487	0.107
11.5	0.031	0.468	0.099
12.0	0.031	0.449	0.087
12.5	0.029	0.435	0.089
13.0	0.023	0.424	0.098
13.5	0.017	0.410	0.104
14.0	0.019	0.390	0.080
14.5	0.023	0.372	0.052
15.0	0.023	0.360	0.048
15.5	0.029	0.343	0.017
16.0	0.013	0.330	0.022
16.5	0.000	0.322	0.039
17.0	0.000	0.314	0.043
18.0	0.000	0.303	0.050
19.0	0.000	0.297	0.135
20.0	0.000	0.290	0.171

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

T(K)	χ_S	χ_T	α
5.0	0.038	1.642	0.321
6.0	0.042	0.991	0.200
7.0	0.036	0.826	0.181
8.0	0.030	0.715	0.171
9.0	0.034	0.627	0.134
10.0	0.024	0.581	0.153
10.5	0.027	0.546	0.136
11.0	0.023	0.512	0.141
11.5	0.020	0.479	0.124
12.0	0.017	0.457	0.124
12.5	0.015	0.437	0.120
13.0	0.014	0.417	0.112
13.5	0.008	0.406	0.125
14.0	0.008	0.391	0.116
14.5	0.004	0.378	0.112
15.0	0.007	0.361	0.091
15.5	0.004	0.353	0.092
16.0	0.005	0.346	0.098
16.5	0.000	0.333	0.089
17.0	0.000	0.324	0.087
18.0	0.000	0.310	0.103
19.0	0.000	0.293	0.093
20.0	0.000	0.275	0.059
21.0	0.000	0.263	0.087
22.0	0.000	0.254	0.159
23.0	0.000	0.242	0.212
24.0	0.000	0.231	0.138