A Dy_2 Single-Molecule Magnet with the benzoate anions and phenol-O^- bridging groups

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

Compound	**1**
Empirical formula	$C_{62}H_{62}Dy_2N_8O_{22}$
Formula weight	1596.20
Temperature	296(2) K
Crystal system	Monoclinic
space group	$P2_1/c$
a (Å)	13.432(2)
b (Å)	10.503(2)
c (Å)	24.428(4)
α (°)	90
β (°)	98.478(4)
γ (°)	90
V (Å^3)	3408.9(11)
Z	2
F(000)	1596
Goodness-of-fit on F^2	1.577
Final R indices [I>2sigma(I)]	R_1 = 0.1549 wR_2 = 0.2116
R indices (all data)	R_1 = 0.1904 wR_2 = 0.2222
CCDC	1421395

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

Compound **1**			
Dy(1)-O(8)#1	2.322(12)	O(3)-Dy(1)-O(2)	74.4(4)
Dy(1)-O(4)	2.341(12)	O(7)-Dy(1)-O(2)	71.5(4)
Dy(1)-O(3)	2.349(12)	O(4)#1-Dy(1)-O(2)	99.1(4)
Dy(1)-O(7)	2.401(14)	O(8)#1-Dy(1)-O(6)#1	73.8(5)
Dy(1)-O(4)#1	2.421(11)	O(4)-Dy(1)-O(6)#1	133.8(4)
Dy(1)-O(2)	2.439(12)	O(3)-Dy(1)-O(6)#1	71.6(4)
Dy(1)-O(6)#1	2.502(14)	O(7)-Dy(1)-O(6)#1	114.4(5)
Dy(1)-O(1)	2.503(12)	O(4)#1-Dy(1)-O(6)#1	63.5(4)
Dy(1)-N(1)	2.563(15)	O(2)-Dy(1)-O(6)#1	71.3(5)
O(4)-Dy(1)#1	2.421(11)	O(8)#1-Dy(1)-O(1)	139.9(4)
O(6)-Dy(1)#1	2.502(14)	O(4)-Dy(1)-O(1)	105.4(4)
O(8)-Dy(1)#1	2.322(12)	O(3)-Dy(1)-O(1)	74.0(4)
N(5)-C(34)	1.276(19)	O(7)-Dy(1)-O(1)	69.8(4)
O(8)#1-Dy(1)-O(4)	76.3(4)	O(4)#1-Dy(1)-O(1)	137.9(4)
O(8)#1-Dy(1)-O(3)	76.5(4)	O(2)-Dy(1)-O(1)	53.0(4)
O(4)-Dy(1)-O(3)	133.0(4)	O(6)#1-Dy(1)-O(1)	120.2(4)
O(8)#1-Dy(1)-O(7)	143.0(4)	O(8)#1-Dy(1)-N(1)	73.5(4)

O(4)-Dy(1)-O(7)	73.1(4)	O(4)-Dy(1)-N(1)	70.8(4)
O(3)-Dy(1)-O(7)	140.5(4)	O(3)-Dy(1)-N(1)	65.0(4)
O(8)#1-Dy(1)-O(4)#1	82.2(4)	O(7)-Dy(1)-N(1)	114.4(5)
O(4)-Dy(1)-O(4)#1	78.2(4)	O(4)#1-Dy(1)-N(1)	144.2(4)
O(3)-Dy(1)-O(4)#1	134.0(4)	O(2)-Dy(1)-N(1)	116.5(4)
O(7)-Dy(1)-O(4)#1	71.6(4)	O(6)#1-Dy(1)-N(1)	130.2(5)
O(8)#1-Dy(1)-O(2)	139.9(4)	O(1)-Dy(1)-N(1)	69.7(4)
O(4)-Dy(1)-O(2)	143.4(4)		
Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+1			

Table S3. Dy^{III} ion geometry analysis by SHAPE 2.1 software.

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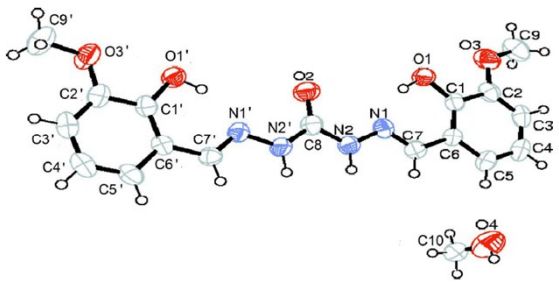
PtL4 structures

JTC-9           4 C3v   Johnson triangular cupola J3
JCCU-9          5 C4v   Capped cube J8
CCU-9           6 C4v   Spherical-relaxed capped cube
JCSAPR-9        7 C4v   Capped square antiprism J10
CSAPR-9         8 C4v   Spherical Capped square antiprism
JTCTPR-9        9 D3h   Tricapped trigonal prism J51
TCTPR-9        10 D3h   Spherical tricapped trigonal prism

Structure [ML9 ]        JTC-9       JCCU-9        CCU-9     JCSAPR-9      CSAPR-9     JTCTPR-9      TCTPR-9
 ABOXIY         ,      16.102,       9.664,       8.554,       2.169,       1.408,       3.318,       1.579
```

Configuration	ABOXIY
Johnson triangular cupola (C_{3v})	16.102
Capped cube (C_{4v})	9.664
Spherical-relaxed capped cube (C_{4v})	8.554
Capped square antiprism (C_{4v})	2.169
Spherical capped square antiprism (C_{4v})	1.408
Tricapped trigonal prism (D_{3h})	3.318
Spherical tricapped trigonal prism (D_{3h})	1.579



Scheme S1. An *ORTEP* view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 50% probability level. Only one position of the disordered solvent methanol molecule is shown for clarity. (Copied from the Ref. M. M. Sow, Ou. Diouf, M. Seck, A. H. Barry, M. Gaye. Acta Cryst. (2014). E70, o423.)

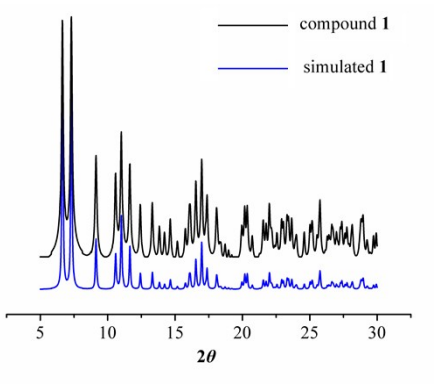


Figure S1. XRPD curve of **1.**

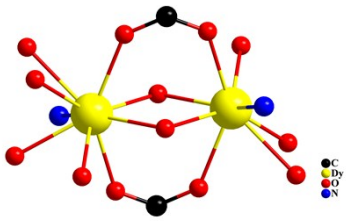


Figure S2. The Dy_2 unit bridged by two oxygen atoms with μ_1:η^2 coordination mode and the two carboxylic groups in the form of μ_2:η^1,η^2.

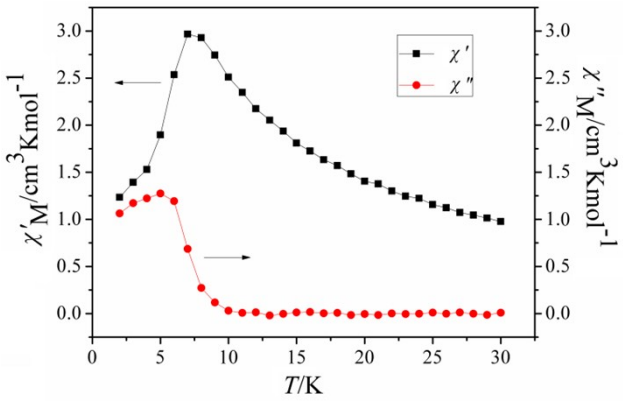
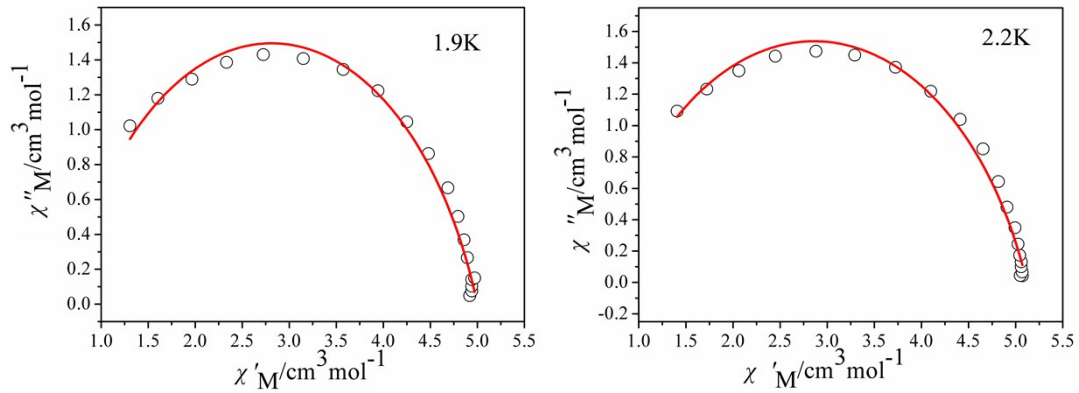
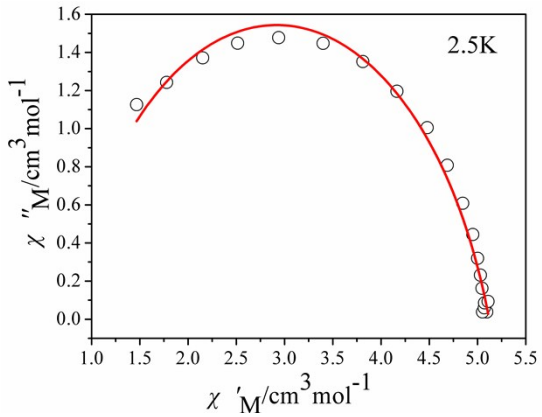
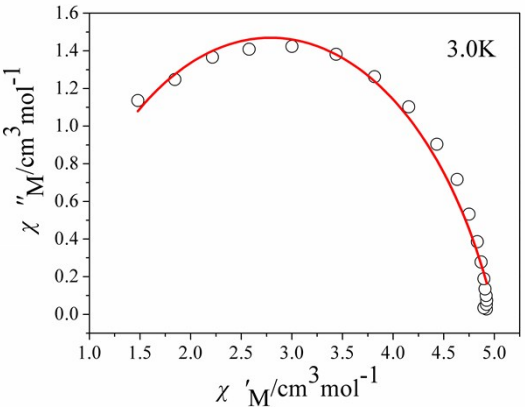
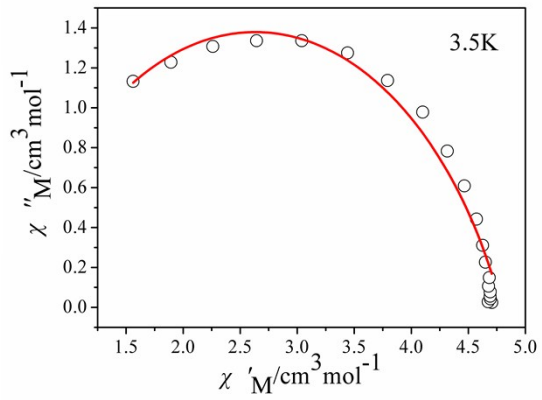


Figure S3. Temperature dependences of χ'_M (top) and χ''_M (bottom) of **1** measured at 1000 Hz without external applied dc field.




2.5K
χ ''M/cm3mol-1
χ 'M/cm3mol-1


3.0K
χ ''M/cm3mol-1
χ 'M/cm3mol-1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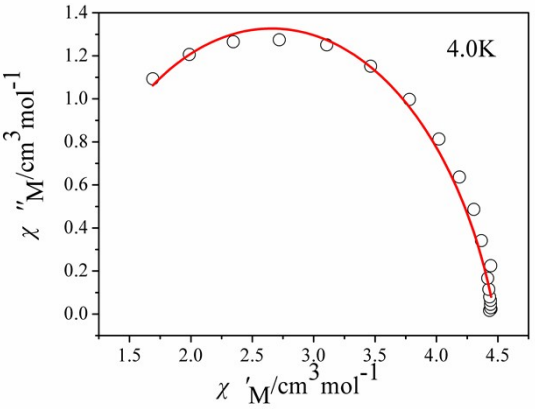
χ 'M/cm3mol-1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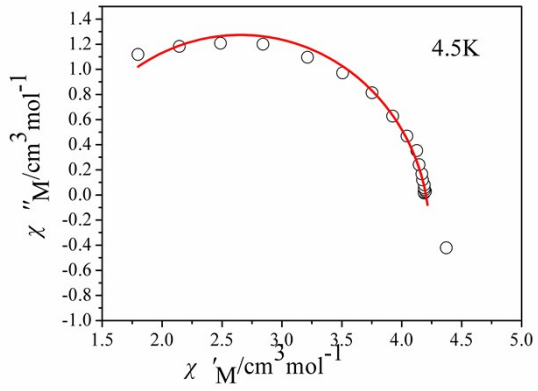
χ 'M/cm3mol-1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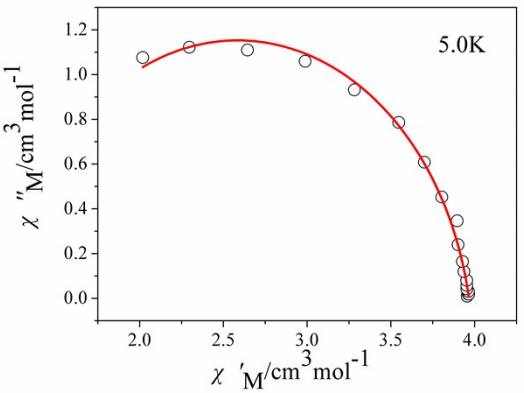
χ 'M/cm3mol-1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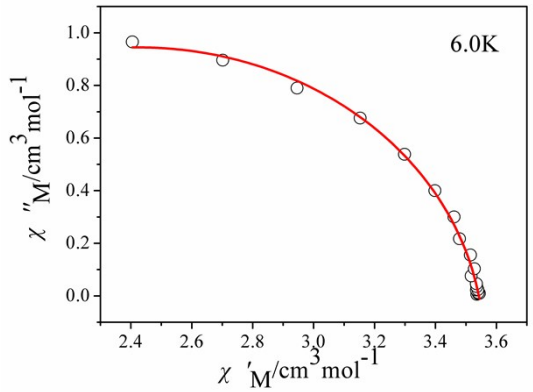
χ 'M/cm3mol-1


6.0K
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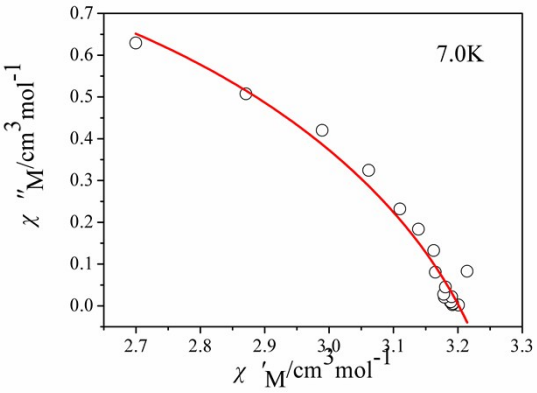
χ 'M/cm3mol-1


7.0K
χ ''M/cm3mol-1
χ 'M/cm3mol-1

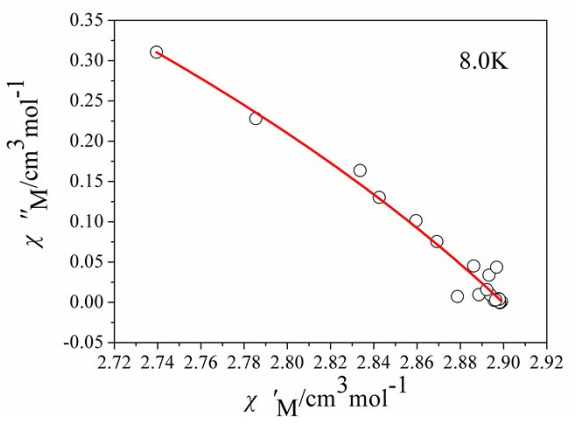


Figure S4. Simulations of dynamical susceptibility $\chi(\omega)$ ranging from 1.9 to 8.0 K in a Cole-Cole diagram. Red lines were performed using the sum of two modified Debye functions with the fitting parameters in Table S3.

Table S4. Relaxation fitting parameters from Least-Squares Fitting of $\chi(\omega)$ data.

T(K)	$\Delta\chi_1$ (cm^3mol^{-1})	$\Delta\chi_2$ (cm^3mol^{-1})	α_1
1.9	4.998	0.628	0.236
2.2	5.119	0.600	0.239
2.5	5.120	0.710	0.220
3.0	5.000	0.578	0.253
3.5	4.790	0.470	0.277
4.0	4.470	0.840	0.196
4.5	4.202	1.108	0.123
5.0	3.960	1.203	0.117
6.0	3.540	1.306	0.107
7.0	3.201	0.782	0.209
8.0	2.900	0.834	0.240