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Supporting Information

An alkoxyborate-bridging Dy₂ single-molecule magnet with ferromagnetic coupling

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1. Experimental Section

General procedures

All reactions and operations described below were performed under aerobic conditions. The ligands H₂dapp and H^tBu-DDTP were synthesized as previous literature described.^{1,2} Metal salts and other reagents were commercially available and used as received without further purification. The C, H, N, and S elemental analyses were carried out with an Elementar Vario-EL CHNS elemental analyzer. The FT-IR spectra were recorded from KBr pellets in the range of 4000-400 cm⁻¹ on a Thermo NICOLET 6700 spectrometer. Thermogravimetric analysis (TGA) were carried out on a NETZSCH TG209F3 thermogravimetric analyzer. X-ray powder diffraction intensities for polycrystalline samples were measured at room temperature on a RIGAKU D-MAX 2200 VPC diffractometer. The ICP-AES analyses were performed with a TJA IRIS (HR) spectrometer. Single-crystal X-ray measurements were performed with a Bruker D8 QUEST diffractometer (Mo-K α radiation, λ = 0.71073 Å) at 120 K for **1** and **1@Y**. The single-crystal structures were solved using intrinsic phasing methods (SHELXT) and refined by SHELXL-2018 in Olex2 1.5 program.^{3,4} The crystal data for all complexes have been deposited in the Cambridge Structural Database (CCDC 2303420, 2303421 for **1** and **1@Y**, respectively). Magnetic susceptibility measurements were all collected using a Quantum Design MPMS3 SQUID VSM magnetometer. Polycrystalline samples were embedded in Vaseline to prevent torquing.

Synthesis

 $[Dy_2(Hdapp)_2(^tBu-DDTP)_2(B(OMe)_4)](BPh_4)\cdot 3MeOH$ (1). Method 1: A mixture of H₂dapp (0.02 mmol, 6.9 mg), Dy(CF₃SO₃)₃ (0.02 mmol, 12.1 mg), H^tBu-DDTP (0.02 mmol, 14.2 mg), NaBPh₄ (0.02 mmol, 6.8 mg) was dissolved in 6 mL MeOH. The mixture was added with 30 µL triethylamine, then transferred to a Teflon-lined stainless steel autoclave and heated at 75 °C for 48 hours. After cooling to room temperature, red crystals were obtained and collected. Yield: 8.11 mg, 35.6 % based on Dy. Anal. calcd (%) for C₁₀₁H₁₂₂B₂Dy₂N₁₄O₉S₈ (1): C, 53.22; H, 5.40; N, 8.60; S, 11.25. Found (%): C, 53.25; H, 5.24; N, 8.63; S, 11.38. IR (KBr, cm⁻¹): 3434 (br), 2958 (br), 1614 (s), 1452 (vs), 1288 (vs), 1079 (s), 991 (s), 856 (m), 707 (m), 615 (w), 536 (w).

Method 2: The method is similar to method 1, except for adding an additional 0.01 mmol of $Na[(BOMe)_4]$ (0.01 mmol, 1.58mg) and reducing the amount of triethylamine to 10 µL. The mixture was transferred to a Teflon-lined stainless steel autoclave and heated at 75 °C for 48 hours. After cooling to room temperature, red crystals were obtained. Yield: 16.49 mg, 72.4 % based on Dy.

[Y_{1.92}Dy_{0.08}(Hdapp)₂(^tBu-DDTP)₂(B(OMe)₄)](BPh₄)·3MeOH (1@Y). Dy(CF₃SO₃)₃ and Y(CF₃SO₃)₃ were added in a ratio of 1:19 to synthesize **1@Y**. Yield: 6.3 mg, 28% based on Y. Anal. calcd (%) for C₁₀₁H₁₂₂B₂Y_{1.92}Dy_{0.08}N₁₄O₉S₈ **(1@Y)**: C, 56.74; H, 5.75; N, 9.17; S, 12.00. Found (%): C, 56.58; H, 5.54; N, 9.17; S, 12.14. The Dy/Y ratio was determined by ICP-AES (96%:4%), and the phase purity was confirmed by powder XRD. IR (KBr, cm⁻¹): 3421 (br), 2948 (br), 1614 (s), 1454 (vs), 1290 (vs), 1081 (s), 993(s), 854 (m), 705 (m), 628 (w), 534 (w).

Theoretical calculations.

All *ab initio* calculations are carried out with OpenMOLCAS version 20.1 and are of the CASSCF/RASSI type. The Cholesky decomposition threshold is set to 1×10^{-8} to save disk space. The atomic coordinates are extracted from the experimentally determined single-crystal structures. Solvents and counterion are removed, and the tert-butyl and the disordered 1,3-dithiolanyl groups of the H^tBu-DDTP ligand are replaced with methyl. One of Dy atoms is replaced with a diamagnetic Lu atom. Active space of the CASSCF includes nine electrons in seven 4f orbitals of Dy(III), and 21 sextets for Dy(III) are optimized in state-averaged calculations and then mixed by spin-orbit coupling using RASSI approach⁵. The g-tensors and energies are obtained by the SINGLE_ANISO routine. The ANO-RCC basis sets⁶⁻⁸ were employed for both complexes: Dy. ANO-RCC-VTZP, Lu. ANO-RCC-VDZ, O. ANO-RCC-VDZP, N. ANO-RCC-VDZP, C. ANO-RCC-VDZP, B. ANO-RCC-VDZP, H. ANO-RCC-MB.

The exchange/dipolar interactions between Dy(III)–Dy(III) for **1** have been computed by fitting with the experimental data using POLY_ANISO software.

2. Crystal Data and Structures

Complex 1		1@Y	
Formula	$C_{101}H_{122}B_2Dy_2N_{14}O_9S_8 \qquad C_{101}H_{122}B_2Dy_{0.08}N_{14}O_9S_8 \\$		
Formula weight	2279.22	2137.93	
Temperature / K	120		
Crystal system	monoclinic		
Space group		C2/c	
a / Å	30.434(3)	30.414(3)	
b / Å	16.5429(19)	16.4824(13)	
c / Å	23.330(2)	23.334(3)	
α / °		90	
6 / °	119.182(4)	119.220(4)	
γ/°	90		
Volume / ų	10255.0(19)	10208.9(17)	
Z	Z 4		
$ ho_{calc}$ (g / cm ³)	1.476	1.391	
μ / mm ⁻¹	1.672	1.371	
F (000)	4672.0	4465.0	
Reflections collected	114163	60606	
Independent reflections	10445 [<i>R</i> _{int} = 0.0438]	10401 [<i>R</i> _{int} = 0.0521]	
GOF on <i>F</i> ²	1.061	1.224	
<i>R</i> ₁ , w <i>R</i> ₂ [I ≥ 2σ(<i>I</i>)] ^a	0.0265, 0.0730	0.0563, 0.1418	
R ₁ , wR ₂ (all data)	0.0324, 0.0749	0.0724, 0.1498	
Largest diff. peak/hole / e Å⁻³	1.09/-0.80	1.02/-0.95	
CCDC No.	2303420	2303421	

Table S1. Crystal data and structural refinements for 1 and 1@Y.

 ${}^{a}R_{1} = \overline{\sum ||F_{0}| - |F_{c}|| / \sum |F_{0}|} \cdot wR_{2} = [\sum w(F_{0}^{2} - F_{c}^{2})^{2} / \sum w(F_{0}^{2})^{2}]^{1/2}.$



Figure S1. Thermogravimetric analysis of **1** (left) and **1@Y** (right) under N₂ atmosphere. The red dash lines show the stage due to the escape of solvent molecules. TGA analysis for **1**: calcd(%), 4.22; found (%), 4.01. TGA analysis for **1@Y**: calcd(%), 4.45; found (%), 4.35.



Figure S2. PXRD patterns of 1 and 1@Y compared with the simulated pattern from the single crystal structure.





Figure S3. Infrared spectra for 1 (left) and 1@Y (right).



Figure S4. Molecular structure for **1**. Thermal ellipsoids are at the 50% probability level. Color codes: Dy, green; N, blue; O, red; S, gold; B, pink; C, gray; H, white. The ^tBu-DDTP⁻ ligands are disordered.



Figure S5. Packing of **1** in the crystal structure viewed along the *b* axis. The packing diagram for **1** gives the shortest intermolecular Dy…Dy distance of 10.812 Å. The ^tBu-DDTP⁻ ligands are disordered.



Figure S6. Packing of **1** in the crystal structure viewed along the *b* axis. The dashed lines represent the intermolecular hydrogen bonds. The ^tBu-DDTP⁻ ligands are disordered.

Table S2. Continuous shape measures calculations (CShM) for Dy(III) for 1 and 1@Y.^a

Complex	OP-8 (<i>D</i> _{8h})	НРҮ-8 (С _{7v})	HBPY-8 (D _{6h})	CU-8 (<i>O_h</i>)	SAPR-8 (D _{4d})	TDD-8 (<i>D</i> 2d)	JGBF-8 (D _{2d})	JETBPY-8 (D _{3h})
1	31.946	21.761	14.005	12.179	6.055	3.782	10.418	22.341
1@Y	31.920	21.755	14.047	12.241	6.043	3.736	10.466	22.360

*OP-8 = Octagon; HPY-8 = Heptagonal pyramid; HBPY-8 = Hexagonal bipyramid; CU-8 = Cube; SAPR-8 = Square antiprism; TDD-8 = Triangular dodecahedron; JGBF-8 = Johnson - Gyrobifastigium (J26); JETBPY-8 = Johnson - Elongated triangular bipyramid (J14).

^a (a) S. Alvarez, P. Alemany, D. Casanova, J. Cirera, M. Llunell and D. Avnir, *Coord. Chem. Rev.*, 2005, **249**, 1693–1708; (b) D. Casanova, M. Llunell, P. Alemany and S. Alvarez, *Chem. Eur. J.*, 2005, **11**, 1479–1494.

Table S3. The selected bond lengths (Å) and bond angles (°) for 1 and 1@Y.

1		1@	Y
Dy1-01	2.1326(18)	Dy1-01	2.126(2)
Dy1-021	2.4718(18)	Dy1-02 ¹	2.460(2)
Dy1-03	2.4307(19)	Dy1-03	2.418(2)
Dy1-N1	2.515(2)	Dy1-N1	2.501(3)
Dy1-N3	2.500(2)	Dy1-N3	2.491(3)
Dy1-N4	2.451(2)	Dy1-N4	2.433(3)
Dy1-N5	2.469(2)	Dy1-N5	2.460(3)
Dy1-N7	2.430(2)	Dy1-N7	2.413(3)
01-Dy1-021	150.08(6)	01-Dy1-021	149.89(8)
01-Dy1-03	154.99(7)	01-Dy1-03	154.82(9)
02 ¹ -Dy1-O3	53.46(6)	02 ¹ -Dy1-03	53.69(8)
N1-Dy1-N3	63.28(7)	N1-Dy1-N3	63.37(9)
N3-Dy1-N4	63.72(7)	N3-Dy1-N4	63.88(9)
N4-Dy1-N5	66.26(7)	N4-Dy1-N5	66.43(9)
N5-Dy1-N7	65.21(7)	N5-Dy1-N7	65.25(9)

Symmetry code: 1-x,+y,1/2-z.

1		1@	θY
B1-O2	1.471(3)	B1-O2	1.470(4)
B1-O3	2.462(3)	B1-O3	1.458(4)
O2-B1-O2 ¹	116.2(3)	O2-B1-O2 ¹	115.6(4)
O3-B1-O2 ¹	97.54(10)	O3-B1-O2 ¹	97.59(13)
O3-B1-O2	116.65(11)	O3-B1-O2	116.27(14)
O3 ¹ -B1-O2	97.54(10)	O3 ¹ -B1-O2	97.59(13)
O3 ¹ -B1-O2 ¹	116.65(11)	O3 ¹ -B1-O2 ¹	116.27(14)
O3-B1-O3 ¹	113.5(3)	O3-B1-O3 ¹	114.7(4)

Table S4. The selected bond lengths (Å) and bond angles (°) of $B(OMe_4)^-$ for 1 and 1@Y.

Symmetry code: 1-x,+y,1/2-z.

3. Magnetic Characterization



Figure S7. Frequency-dependent ac magnetic susceptibilities (left) and relaxation time τ vs externally applied dc field (right) at 2 K for **1**. The solid lines (left) are the best fit obtained for generalized Debye model.



Figure S8. Cole-Cole plots of **1** under zero (left) and 400 Oe (right) dc applied field from 2–18 K. The solid lines are the best fit for generalized Debye model with α = 0.043–0.187 and 0.044–0.302, respectively.



Figure S9. Normalized magnetic hysteresis loops for **1**. The data were continuously collected with a sweep rate of 200 Oe/s (left) and 700 Oe/s (right) at the indicated temperatures.



Figure S10. Temperature dependence of the molar magnetic susceptibility $\chi_{M}T$ products for **1@Y**. The dc magnetic susceptibilities were collected under a 1 kOe dc field.



Figure S11. ZFC/FC magnetic susceptibility vs temperature for 1@Y.



Figure S12. Frequency-dependent ac magnetic susceptibilities (left) and relaxation time τ vs externally applied dc field (right) at 4 K for **1@Y**. The solid lines (left) are the best fit obtained for generalized Debye model.



Figure S13. Cole-Cole plots of **1@Y** under zero (left) and 400 Oe (right) dc applied field from 2–14 K and 2.5–15 K, respectively. The solid lines are the best fit for the double relaxation time model (left) and generalized Debye model (right) with α = 0.061–0.433 and 0.048–0.299, respectively.



Figure S14. Normalized magnetic hysteresis loops for **1@Y**. The data were continuously collected with a sweep rate of 200 Oe/s (left) and 700 Oe/s (right) at the indicated temperatures.



Figure S15. Field-dependent relaxation times for 1 (2 K) and 1@Y (4 K). The solid lines are guides for the eyes.



Figure S16. Temperature dependence of the relaxation time τ of **1** at zero external field. The red dotted line is the best fit for high temperatures (13–16 K) using the Arrhenius law $\tau^{-1} = \tau_0^{-1} \exp(-U_{\text{eff}}/k_{\text{B}}T)$ with $U_{\text{eff}}/k_{\text{B}} = 52(4)$ K, $\tau_0 = 2.3(8) \times 10^{-6}$ s.



Figure S17. Temperature dependent ratio of relaxation time between **1** and **1@Y** in the temperature range of 2 to 14 K under zero external field.

4. Ab initio calculations

KDs	E/cm⁻¹	g _x	g _y	g z	g₂ Angle/°	Wavefunctions
1	0	0.015	0.021	19.938	4.40	99.4% ±15/2>+0.2% ±11/2>
2	285.4	0.673	1.395	16.117	40.77	52.9% ±13/2>+11.7% ±9/2>+8.1% ±11/2>
3	345.8	1.235	2.924	12.078	51.05	38.3% ±13/2>+15.3% ±7/2>+14.4% ±5/2>
4	433.9	3.075	3.657	12.649	59.00	44.9% ±11/2>+ 19.4% ±9/2>+ 19.3% ±3/2>
5	457.8	0.581	2.779	12.398	76.80	35.1% ±7/2>+30.7% ±1/2>+11.8% ±5/2>
6	487.5	1.767	2.743	11.160	80.99	33.0% ±3/2>+30.9% ±5/2>+14.4% ±9/2>
7	556.3	1.259	2.630	14.816	108.27	31.6% ±9/2>+24.1% ±7/2>+21.9% ±11/2>
8	758.3	0.066	0.113	19.505	84.15	25.4% ±1/2>+23.8% ±3/2>+20.1% ±5/2>

Table S5. Ab initio calculation results for the ${}^{6}H_{15/2}$ multiplet of Dy (III) ion for **1**.

 Table S6. LoProp charge analysis for the coordination sphere of Dy(III) for 1.

		1	
01	-0.9565	N1	-0.3934
02	-0.6257	N2	-0.2129
03	-0.6123	N3	-0.2471
		N4	-0.3929
		N5	-0.1974
		N6	-0.4121
		N7	-0.4918
<axial>_{av}</axial>	-0.7315	<equatorial>av</equatorial>	-0.3354

Table S7. Weight of individual crystal field parameters (CFs) on the crystal field splitting, where the CFs are given in irreducible tensor operators (ITO) for Dy(III) in **1**.⁹

k	q	B_k^q / cm ⁻¹	Weight (in %)
2	-2	-2.1162E+00	14.56
2	-1	5.9276E-02	0.41
2	0	-2.5807E+00	17.76
2	1	7.1789E-01	4.94
2	2	-4.4581E-01	3.07
4	-4	3.2326E-03	4.04
4	-3	-5.8605E-04	0.73
4	-2	4.2759E-04	0.53
4	-1	8.0844E-04	1.01
4	0	-7.4018E-03	9.24
4	1	-1.8089E-03	2.26
4	2	4.7409E-03	5.92
4	3	-4.6677E-04	0.58
4	4	-2.5075E-03	3.13
6	-6	5.0254E-05	5.89
6	-5	-6.2755E-06	0.74
6	-4	7.6831E-06	0.90
6	-3	-1.6843E-05	1.97
6	-2	1.0120E-05	1.19
6	-1	-1.9869E-05	2.33
6	0	-2.4348E-05	2.85
6	1	-9.2072E-06	1.08
6	2	-1.7460E-05	2.04
6	3	-2.7487E-06	0.32
6	4	-5.3574E-06	0.63
6	5	-1.2349E-05	1.45
6	6	6.7239E-05	7.88



Figure S18. Temperature dependence of the molar magnetic susceptibility $\chi_{M}T$ products for **1**. The dc magnetic susceptibilities were collected under a 1 kOe dc field. The solid lines represent simulation results for different exchange interaction J_{exch} within the range of -0.75 to +0.75 cm⁻¹.



Figure S19. Temperature dependence of the difference of molar magnetic susceptibility ($\chi_{cal}T - \chi_{exp}T$) using the exchange interaction J_{exch} varying from -0.75 to +0.75 cm⁻¹.

 Table S8 SMMs with boron-containing-bridging ligands.

Compound	bridging ligand	Ref.
[{Dy(Cp*)(µ-BH ₄)} ₂ (Fv ^{tttt})]		10
[{Dy(η ⁵ -Cp*)(μ-BH ₄)} ₂ (η ⁵ :η ⁵ -Fv ^{tttt})]	BH4_	11
$[{Dy(\eta^{5}-Cp^{*})}_{2}(\mu-BH_{4})(\eta^{5}-Fv^{tttt})][B(C_{6}F_{5})_{4}]$		11
[Dy ₂ Cp* ₄ (µ-BPh ₄)][Al(OC(CF ₃) ₃) ₄]	BPh₄ [−]	12
$[\textit{closo-nido-}(\eta^{5}\text{-}C_2B_9H_{11})(\mu\text{-}H_2)Dy(Im^{Dipp}N)(THF)]_2$	$C_2B_9H_{11}^{2-}$	13
$[\textit{exo-nido-}(\mu\text{-}H_4\text{-}\textit{o-xylylene-}C_2B_9H_9)\text{Dy}(\text{Im}^{\text{Dipp}}\text{N})(\text{THF})]_2$	<i>o</i> -C ₆ H ₄ (CH ₂) ₂ -C ₂ B ₉ H ₉ ²⁻	13

Where $Fv^{tttt} = 1,1',3,3'$ -tetra-*tert*-butylpentafulvalenyl; $Cp^* = 1,2,3,4,5$ -pentamethylcyclopentadiene; $Im^{Dipp}N^- = 1,3$ -bis(2,6-diisopropylphenyl)-imidazolin-2-iminato, xylylene = $C_6H_4(CH_2)_2$.

 Table S9 Dinuclear air-stable Dy(III)-based SMMs with "head-to-tail" arrangements of principle magnetic axes.

Complex	Bridge ligand	Local symmetry	Shortest Dy–X ^a bond / Å	Ref.
[Dy ₂ (L ² _{<i>R/S</i>}) ₂ (4-Me-PhO) ₂ (OH) ₂](BPh ₄) ₂	04-	<i>C</i> _{2v}	O, 2.138(6)	14
$[Ln_2Cu_{10}(quinha)_{10}(sal)_2(OH)(py)_9](CF_3SO_3)_3$	ОП	D _{5h}	O, 2.143(5)	15
$[Dy_2(L^{E}_{S/R})_2(\mu_2-F)_2F_2](BPh_4)_2$	F⁻	<i>C</i> ₂ <i>v</i>	F, 2.102(6)	16
[Dy ₂ (L ^{N6} ₅) ₂ (N ₃) ₂ Cl ₂](BPh ₄) ₂	N -	<i>C</i> _{2v}	N, 2.331(19)	17
[Dy ₂ (L ^{N6} ₅) ₂ (N ₃) ₄]Cl ₂	IN3	<i>C</i> _{2v}	N, 2.317(12)	17
[Dy ₂ (Py ₃ CO) ₂ (CF ₃ SO ₃) ₄ (H ₂ O) ₂]		<i>C</i> _{2v}	0, 2.245(2)	18
[Dy ₂ (Py ₃ CO) ₂ (PhCOO) ₄ (MeOH) ₂]	Py ₃ CU	<i>C</i> _{2v}	O, 2.254(6)	18
[Dy ₂ ovph ₂ Cl ₂ (MeOH) ₃]	Ovph⁻	C _{2v} / D _{5h}	0, 2.125 (45)	19
$[Dy_2(L^{E1}_{S/R})_2L_2O_2](BPh_4)_2$	O ² -	<i>C</i> _{2v}	O, 2.138(18)	20
$[Dy_2(L^{E1}_{S/R})_2Cl_2O_2](BPh_4)_2$	O_2^2	<i>C</i> _{2v}	O, 2.236(7)	22
[Dy ₂ (Hdapp) ₂ (^t Bu-DDTP) ₂ (B(OMe) ₄)](BPh ₄)	B(OMe) ₄ ⁻	D _{2d}	O, 2.1326(18)	This work

^{*a*} X is atom that coordinated to Dy ions.

 $L^{2}_{R/S}$ = a chiral macrocycle derived from 2,6-diformylpyridine and (1R,2R)/(1S,2S)-diaminocyclohexane; H₂bpte = 1,2-bis(3-(pyridin-2-yl)-1H-1,2,4-triazol-5-yl)ethane; H₂quinha = quinaldichydroxamic acid; Hsal = salicylaldehyde; $L^{E}_{R/S}$ = *SSSSS-/RRRR*-(2*E*,6*E*,9*E*,13*E*)-4,5,11,12-tetraphenyl-3,6,10,13-tetraaza-1,8(2,6)-dipyridinacyclotetradecaphane-2,6,9,13-tetraene; L^{N6}_{S} = hexaazamacrocyclic neutral Schiff base ligand derived from 2,6-diformylpyridine and (1R, 2R)/(1S, 2S)-diaminocyclohexane; H₂ovph = pyridine-2-carboxylic acid [(2-hydroxy-3-methoxyphenyl)methylene] hydrazide); $L^{E1}_{S/R}$ is a chiral macrocyclic ligand derived from 2,6-diformylpyridine and (1S,2S)/(1R,2R)-1,2-diphenylethylenediamine); HL = 2,6-diphenylphenol.

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