Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

for

Cooperative Dinitrogen Capture by a Diboraanthracene/Samarocene Pair

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Experimental Details

All manipulations and syntheses described below were conducted with the rigorous exclusion of air and water using standard Schlenk line and glovebox techniques under an argon or dinitrogen atmosphere. Solvents were sparged with UHP argon and dried by passage through columns containing Q-5 and molecular sieves prior to use. Deuterated NMR solvents were dried over NaK alloy, degassed by three freeze-pump-thaw cycles, and vacuum transferred before use. ^{1}H NMR and ^{11}B NMR spectra were recorded on Bruker GN500, CRYO500, or AVANCE600 MHz spectrometers at 298 K unless otherwise stated and referenced internally to residual protio-solvent resonances. UV-visible spectra were collected at 298 K using a Varian Cary 50 Scan UV-visible spectrophotometer in a 1 mm quartz cuvette. Infrared spectra were recorded as compressed solids on an Agilent Cary 630 ATR-FTIR. Elemental analyses were conducted on a Thermo Scientific FlashSmart CHNS/O Elemental Analyzer at UC Irvine Materials Research Institute's TEMPR facility in Irvine, California. $(C_5Me_5)_2Sm(THF)_2$[1] and 9,10-Me_2-9,10-diboraanthracene[2] were prepared according to literature procedures.

Preparation of $[(C_5Me_5)_2Sm(THF)_2][(C_5Me_5)_2Sm(\eta^2\text{-}N_2B_2C_{14}H_{14})]$, 1. In a nitrogen containing glovebox, $(C_5Me_5)_2Sm(THF)_2$, (40 mg, 0.071 mmol, 2.0 eq) and 9,10-Me_2-9,10-diboraanthracene (7.2 mg, 0.035 mmol, 1.0 eq) were separately placed in two scintillation vials. Both vials were charged with 5 mL of toluene to fully dissolve the powders and were cooled to –78 °C in a cold-well. After cooling for 20 min, the 5 mL solution of boraanthracene was gradually transferred to the $(C_5Me_5)_2Sm(THF)_2$ solution through pipette at –78 °C, leading to an immediate color change from purple to brown. After the mixture was left at –78 °C under a N_2 atmosphere for 12 h, the solution was orange. The solution was concentrated to ca. 5 mL under vacuum, layered with hexanes, and left at –35 °C for 3 days. This produced yellow crystals of **1** suitable

for single crystal X-ray diffraction (10 mg, 23%). IR: 3033w, 2952w, 2900m, 2856m, 2724w, 2322w, 1583w, 1551w, 1493w, 1430m, 1378w, 1291s, 1277s, 1247s, 1184s, 1157m, 1132m, 1107w, 1003s, 959m, 855m, 833m, 737vs, 694m cm^{-1}. Anal. Calcd for **1** $C_{62}H_{90}N_2B_2O_2Sm_2$: C, 61.15; H, 7.45; N, 2.30. Found: C, 60.26; H, 7.30; N, 1.77. C, 60.11; H, 7.27; N, 1.62. C, 60.24; H, 7.28; N, 1.70. The EA data suggests that nitrogen is lost from the compound in the analytical process. This has been consistently observed over many attempts. The C to H to N ratios in the analytical data give formulas of $C_{62}H_{89}N_{1.56}$, $C_{62}H_{89}N_{1.44}$, $C_{62}H_{89}N_{1.50}$, respectively, compared to the calculated value of $C_{62}H_{90}N_2$.

NMR Characterization

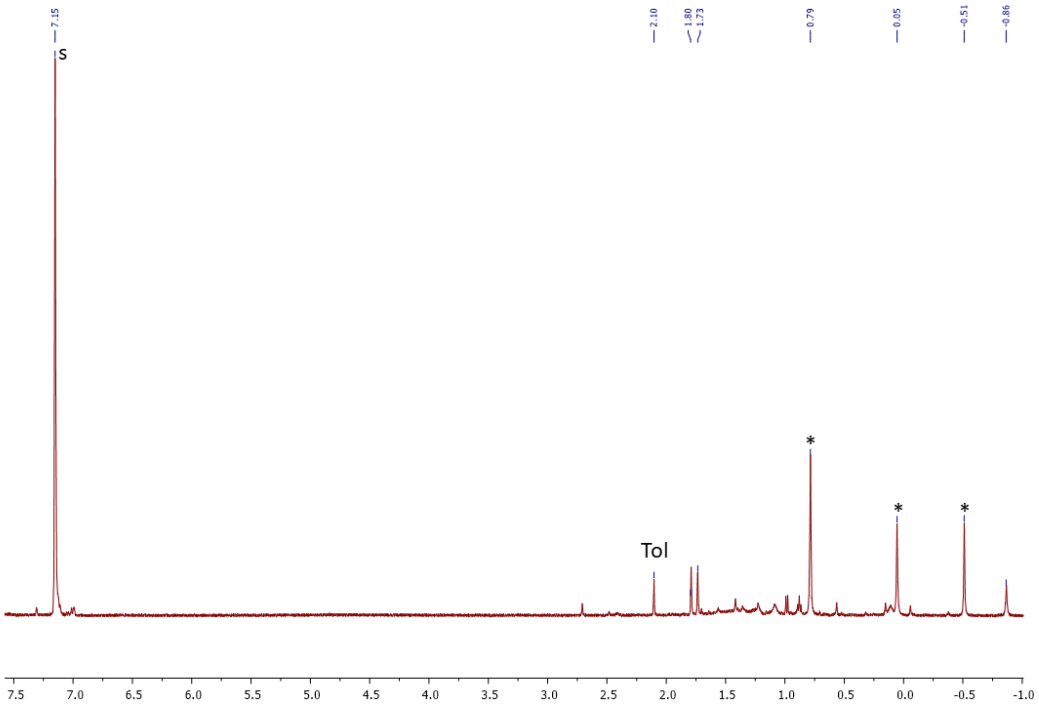

Figure S1. ^1H NMR spectrum taken in C_6D_6 after $(C_5Me_5)_2Sm(THF)_2$ (2 eq) was reacted with 9,10-Me_2-9,10-diboraanthracene (Me_2DBA, 1 eq) in toluene at –78 °C overnight under N_2.

Original peaks of reagents were converted to new peaks as shown above. (Tol: peaks for toluene residue. *: peaks could be assigned to $[(C_5Me_5)_2Sm(THF)_2][(C_5Me_5)_2Sm(\eta_2\text{-}N_2B_2C_{14}H_{14})]$. s: peak for protio impurities of C_6D_6. Other peaks were assigned to synthetic impurities, which have also been observed in the spectrum of $(C_5Me_5)_2Sm(THF)_2$ reagent.

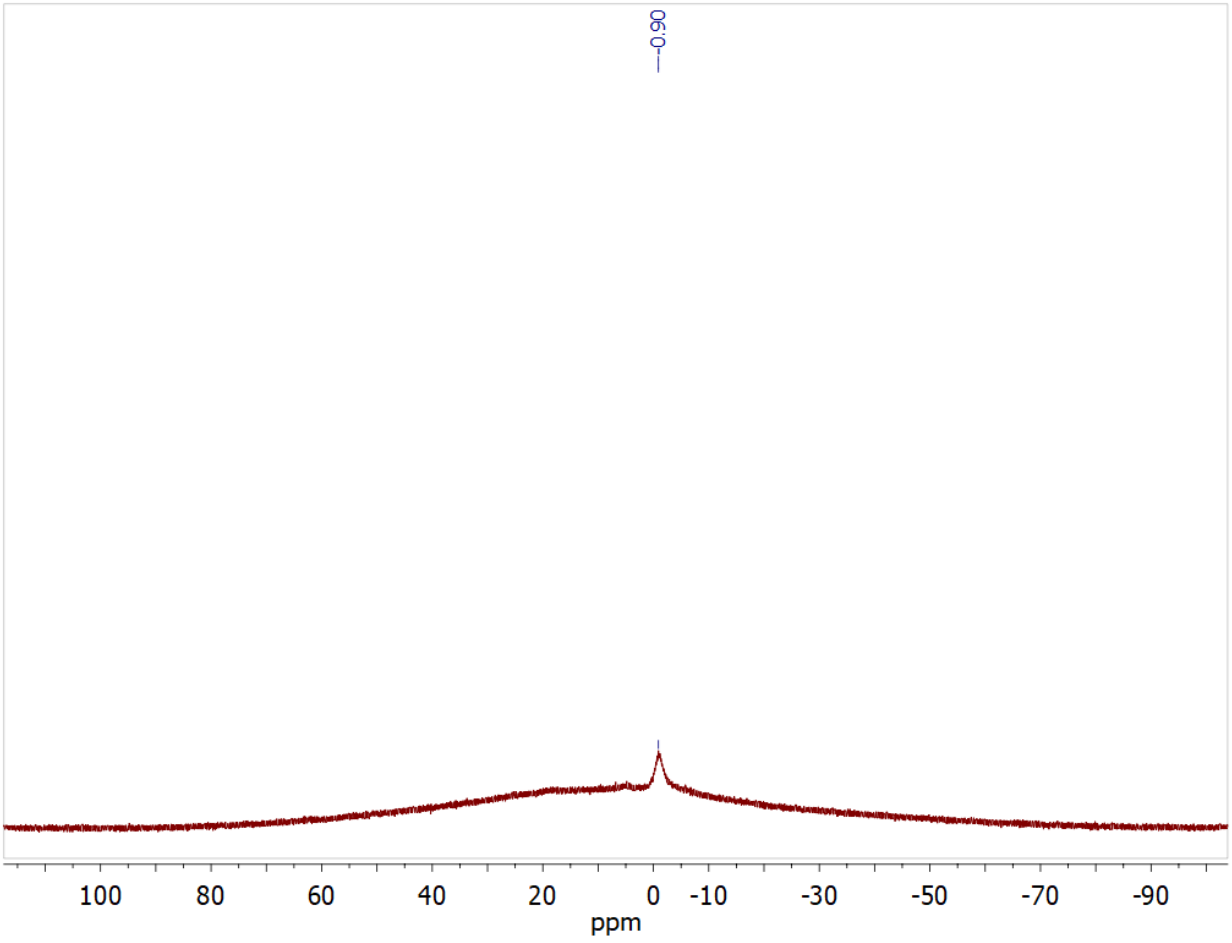

Figure S2. ^{11}B NMR spectrum taken in C_6D_6 after $(C_5Me_5)_2Sm(THF)_2$ (2 eq) was reacted with 9,10-Me_2-9,10-diboraanthracene (B_2Me_2, 1 eq) in toluene at –78 °C under N_2 overnight.

IR Characterization

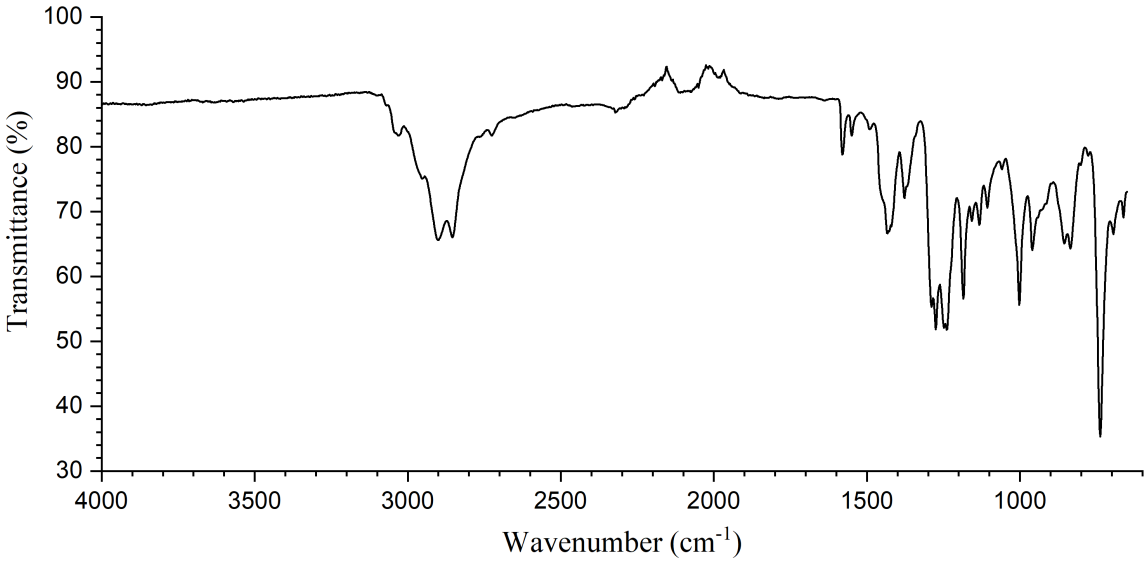

Figure S3. IR spectrum of isolated **1**.

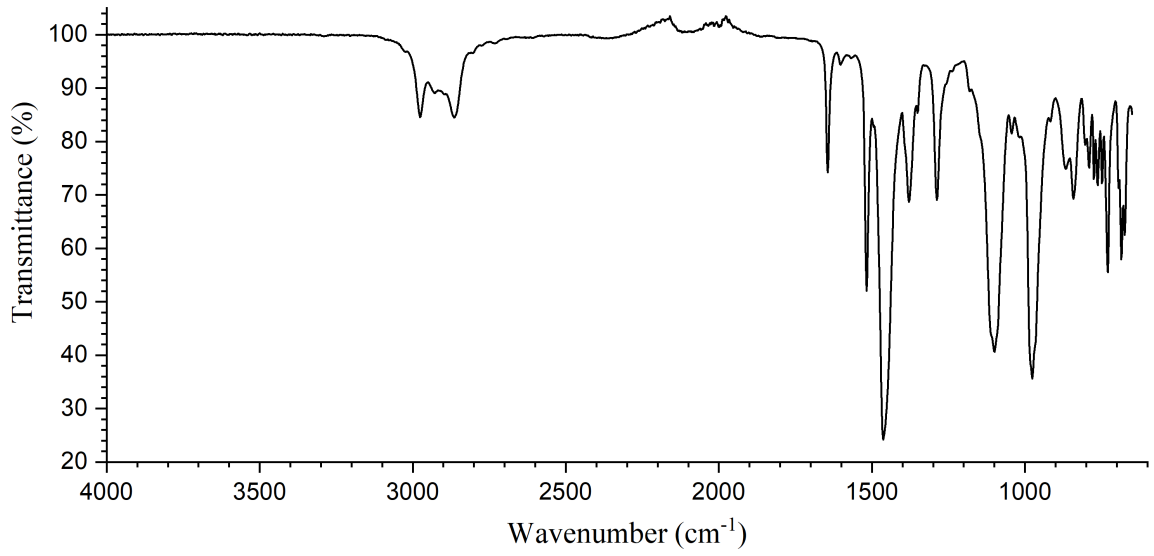

Figure S4. IR spectrum of the reaction mixture between $(C_5Me_5)_2Sm(THF)_2$ and $B(C_6F_5)_3$.

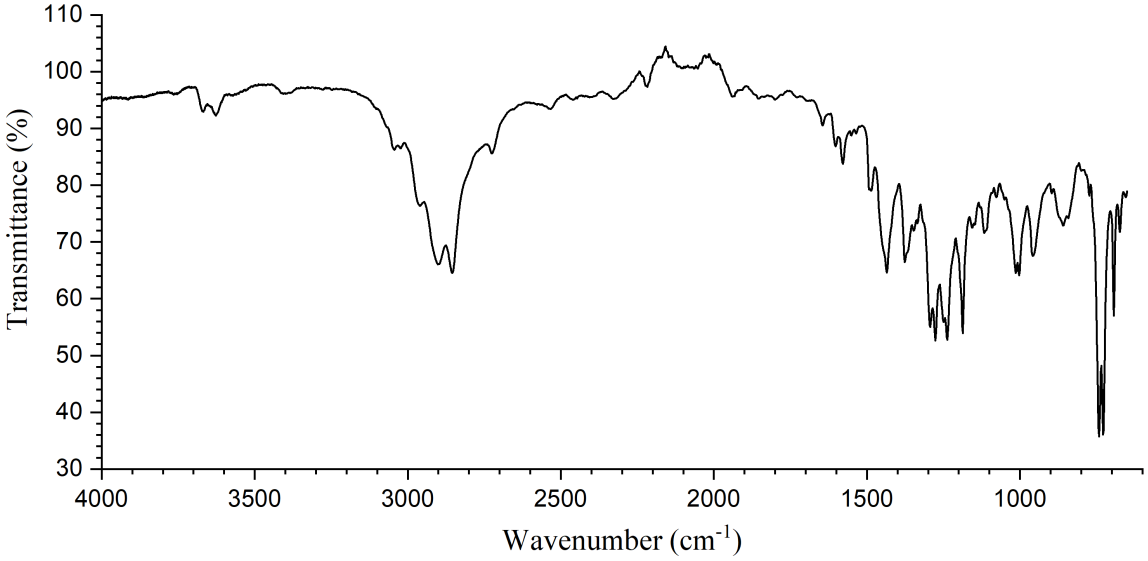

Figure S5. IR spectrum of the reaction mixture between $[(C_5Me_5)_2Sm(THF)_2][(C_5Me_5)_2Sm(\eta_2\text{-}N_2B_2C_{14}H_{14})]$ and MeI.

UV-Visible Characterization

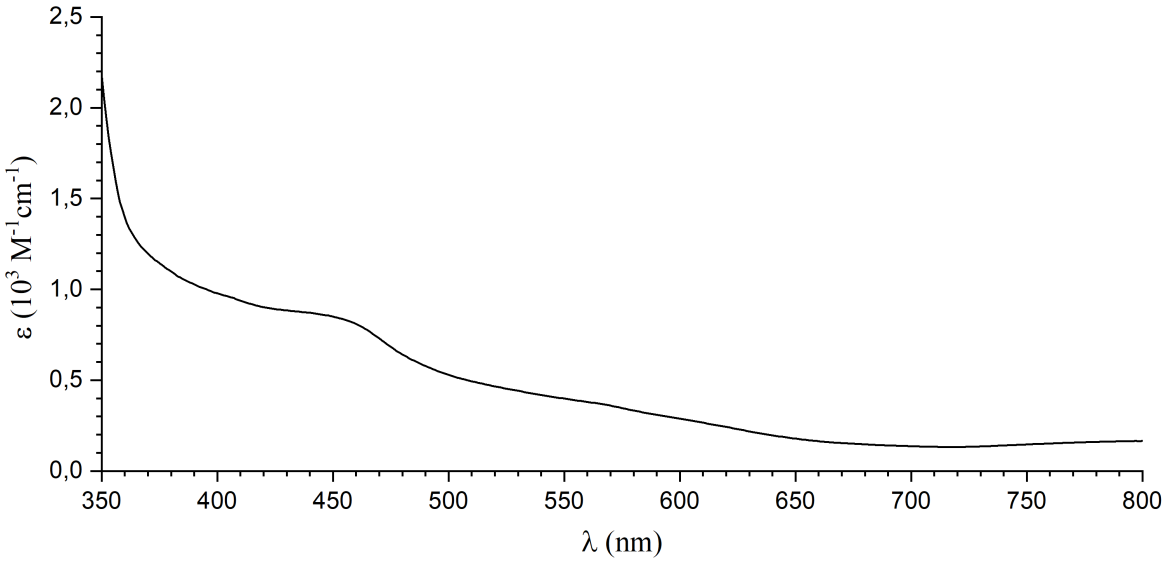

Figure S6. Experimental UV-visible spectrum of a mixture of $Cp^*_2Sm(THF)_2$ (2 eq) and Me_2DBA (1 eq) in toluene after exposure to Ar overnight.

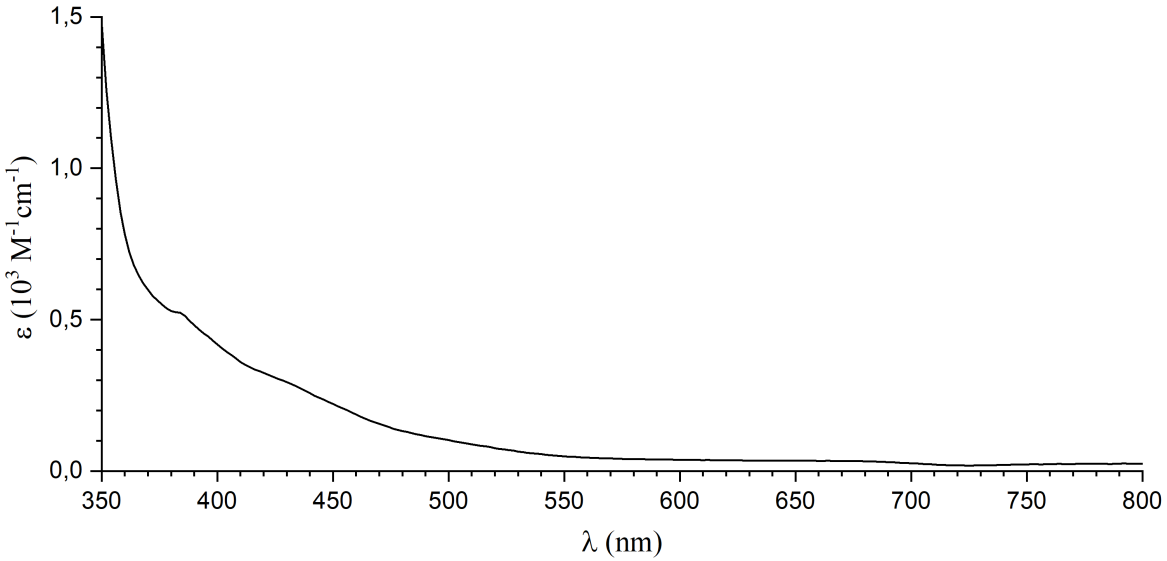

Figure S7. Experimental UV-visible spectrum of a mixture of $Cp^*_2Sm(THF)_2$ (2 eq) and Me_2DBA (1 eq) in toluene after exposure to N_2 overnight.

X-ray Data Collection, Structure, Solution, and Refinement

A yellow crystal of approximate dimensions 0.247 x 0.205 x 0.164 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[4] program package was used to determine the unit-cell parameters and for data collection (30 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[5] and SADABS[6] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[7] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space groups *Cc* and *C*2/*c*. It was later determined that space group *C*2/*c* was correct.

The structure was solved by dual space methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[8] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There were two different independent molecules present and one molecule of *n*-hexane solvent. Both molecules and the solvent were located on two-fold rotation axes.

Least-squares analysis yielded wR2 = 0.0645 and Goof = 1.021 for 356 variables refined against 8043 data (0.74 Å), R1 = 0.0268 for those 6387 data with $I > 2.0\sigma(I)$.

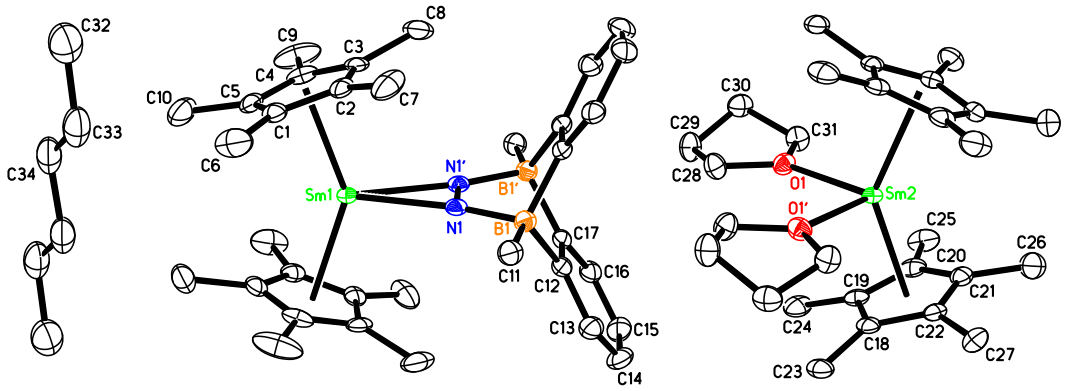

Figure S8. ORTEP representation of **1**. Thermal ellipsoids drawn at the 50% probability level. H atoms excluded for clarity.

Definitions:

$wR2 = [\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

Goof = $S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

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

Identification code	sx3 (Song Xu)	
Empirical formula	$C_{68}H_{104}B_2N_2O_2Sm_2$	
Formula weight	1303.85	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 17.853(2) Å	α = 90°.
	b = 21.946(3) Å	β = 112.1061(15)°.
	c = 17.947(2) Å	γ= 90°.
Volume	6514.7(14) $Å^3$	
Z	4	
Density (calculated)	1.329 Mg/m^3	
Absorption coefficient	1.828 mm^{-1}	
F(000)	2704	
Crystal color	yellow	
Crystal size	0.247 x 0.205 x 0.164 mm^3	
Theta range for data collection	1.542 to 28.831°	
Index ranges	$-24 \le h \le 24$, $-29 \le k \le 29$, $-24 \le l \le 24$	
Reflections collected	39023	
Independent reflections	8043 [R(int) = 0.0374]	
Completeness to theta = 25.242°	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7458 and 0.6593
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8043 / 0 / 356
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I) = 6387 data]	R1 = 0.0268, wR2 = 0.0588
R indices (all data, 0.74 Å)	R1 = 0.0398, wR2 = 0.0645
Largest diff. peak and hole	1.227 and -0.457 e.$Å^{-3}$

Table S2. Bond lengths [Å] and angles [°] for **1**.

Sm(1)-Cnt1	2.416
Sm(1)-N(1)	2.3560(19)
Sm(1)-N(1)#1	2.3560(19)
Sm(1)-C(2)	2.675(2)
Sm(1)-C(2)#1	2.675(2)
Sm(1)-C(1)	2.679(2)
Sm(1)-C(1)#1	2.679(2)
Sm(1)-C(3)#1	2.706(2)
Sm(1)-C(3)	2.706(2)
Sm(1)-C(4)	2.712(2)
Sm(1)-C(4)#1	2.712(2)
Sm(1)-C(5)#1	2.722(2)
Sm(1)-C(5)	2.722(2)
N(1)-N(1)#1	1.252(4)
N(1)-B(1)	1.598(3)
C(1)-C(5)	1.416(3)
C(1)-C(2)	1.416(3)
C(1)-C(6)	1.502(3)
C(2)-C(3)	1.414(4)
C(2)-C(7)	1.502(3)
C(3)-C(4)	1.410(4)

C(3)-C(8)	1.507(4)
C(4)-C(5)	1.409(4)
C(4)-C(9)	1.510(4)
C(5)-C(10)	1.507(4)
C(11)-B(1)	1.620(3)
C(12)-C(13)	1.400(3)
C(12)-C(17)	1.413(3)
C(12)-B(1)	1.631(3)
C(13)-C(14)	1.387(4)
C(14)-C(15)	1.381(4)
C(15)-C(16)	1.391(4)
C(16)-C(17)	1.394(3)
C(17)-B(1)#1	1.628(3)
B(1)-C(17)#1	1.628(3)
Sm(2)-Cnt2	2.429
Sm(2)-O(1)	2.4145(16)
Sm(2)-O(1)#1	2.4145(16)
Sm(2)-C(18)	2.708(2)
Sm(2)-C(18)#1	2.708(2)
Sm(2)-C(22)#1	2.711(2)
Sm(2)-C(22)	2.711(2)
Sm(2)-C(20)	2.712(2)
Sm(2)-C(20)#1	2.712(2)

Sm(2)-C(19)#1	2.714(2)
Sm(2)-C(19)	2.714(2)
Sm(2)-C(21)#1	2.718(2)
Sm(2)-C(21)	2.718(2)
O(1)-C(31)	1.460(3)
O(1)-C(28)	1.469(3)
C(18)-C(19)	1.417(3)
C(18)-C(22)	1.422(3)
C(18)-C(23)	1.502(3)
C(19)-C(20)	1.425(3)
C(19)-C(24)	1.501(3)
C(20)-C(21)	1.416(3)
C(20)-C(25)	1.508(3)
C(21)-C(22)	1.420(3)
C(21)-C(26)	1.504(3)
C(22)-C(27)	1.504(3)
C(28)-C(29)	1.510(3)
C(29)-C(30)	1.520(3)
C(30)-C(31)	1.509(3)
C(32)-C(33)	1.530(5)
C(33)-C(34)	1.509(4)
C(34)-C(34)#2	1.530(6)

Cnt1-Sm(1)-Cnt1'	142.1
Cnt1-Sm(1)-N(1)	107.2
Cnt1-Sm(1)-N(1')	109.3
N(1)-Sm(1)-N(1)#1	30.83(9)
N(1)-Sm(1)-C(2)	85.51(7)
N(1)#1-Sm(1)-C(2)	93.22(7)
N(1)-Sm(1)-C(2)#1	93.22(7)
N(1)#1-Sm(1)-C(2)#1	85.51(7)
C(2)-Sm(1)-C(2)#1	178.69(10)
N(1)-Sm(1)-C(1)	111.93(7)
N(1)#1-Sm(1)-C(1)	123.91(7)
C(2)-Sm(1)-C(1)	30.68(7)
C(2)#1-Sm(1)-C(1)	150.59(7)
N(1)-Sm(1)-C(1)#1	123.91(7)
N(1)#1-Sm(1)-C(1)#1	111.93(7)
C(2)-Sm(1)-C(1)#1	150.59(7)
C(2)#1-Sm(1)-C(1)#1	30.68(7)
C(1)-Sm(1)-C(1)#1	122.23(10)
N(1)-Sm(1)-C(3)#1	81.29(7)
N(1)#1-Sm(1)-C(3)#1	89.46(7)
C(2)-Sm(1)-C(3)#1	149.32(8)
C(2)#1-Sm(1)-C(3)#1	30.46(8)
C(1)-Sm(1)-C(3)#1	136.01(8)

C(1)#1-Sm(1)-C(3)#1	50.29(7)
N(1)-Sm(1)-C(3)	89.46(7)
N(1)#1-Sm(1)-C(3)	81.29(7)
C(2)-Sm(1)-C(3)	30.46(8)
C(2)#1-Sm(1)-C(3)	149.32(8)
C(1)-Sm(1)-C(3)	50.29(7)
C(1)#1-Sm(1)-C(3)	136.01(8)
C(3)#1-Sm(1)-C(3)	170.42(11)
N(1)-Sm(1)-C(4)	118.31(7)
N(1)#1-Sm(1)-C(4)	102.32(7)
C(2)-Sm(1)-C(4)	50.16(8)
C(2)#1-Sm(1)-C(4)	130.45(8)
C(1)-Sm(1)-C(4)	50.12(7)
C(1)#1-Sm(1)-C(4)	107.26(8)
C(3)#1-Sm(1)-C(4)	157.53(8)
C(3)-Sm(1)-C(4)	30.17(8)
N(1)-Sm(1)-C(4)#1	102.32(7)
N(1)#1-Sm(1)-C(4)#1	118.31(7)
C(2)-Sm(1)-C(4)#1	130.45(8)
C(2)#1-Sm(1)-C(4)#1	50.16(8)
C(1)-Sm(1)-C(4)#1	107.26(7)
C(1)#1-Sm(1)-C(4)#1	50.12(7)
C(3)#1-Sm(1)-C(4)#1	30.17(8)

C(3)-Sm(1)-C(4)#1	157.53(8)
C(4)-Sm(1)-C(4)#1	138.21(12)
N(1)-Sm(1)-C(5)#1	130.35(7)
N(1)#1-Sm(1)-C(5)#1	135.21(7)
C(2)-Sm(1)-C(5)#1	131.00(7)
C(2)#1-Sm(1)-C(5)#1	50.21(7)
C(1)-Sm(1)-C(5)#1	100.52(7)
C(1)#1-Sm(1)-C(5)#1	30.39(7)
C(3)#1-Sm(1)-C(5)#1	49.83(7)
C(3)-Sm(1)-C(5)#1	139.69(8)
C(4)-Sm(1)-C(5)#1	111.31(8)
C(4)#1-Sm(1)-C(5)#1	30.07(7)
N(1)-Sm(1)-C(5)	135.21(7)
N(1)#1-Sm(1)-C(5)	130.35(7)
C(2)-Sm(1)-C(5)	50.21(7)
C(2)#1-Sm(1)-C(5)	131.00(7)
C(1)-Sm(1)-C(5)	30.39(7)
C(1)#1-Sm(1)-C(5)	100.52(7)
C(3)#1-Sm(1)-C(5)	139.69(8)
C(3)-Sm(1)-C(5)	49.83(7)
C(4)-Sm(1)-C(5)	30.07(7)
C(4)#1-Sm(1)-C(5)	111.31(8)
C(5)#1-Sm(1)-C(5)	90.51(10)

N(1)#1-N(1)-B(1)	118.04(11)
N(1)#1-N(1)-Sm(1)	74.59(4)
B(1)-N(1)-Sm(1)	167.37(14)
C(5)-C(1)-C(2)	107.9(2)
C(5)-C(1)-C(6)	126.0(2)
C(2)-C(1)-C(6)	126.0(2)
C(5)-C(1)-Sm(1)	76.50(13)
C(2)-C(1)-Sm(1)	74.52(13)
C(6)-C(1)-Sm(1)	116.72(16)
C(3)-C(2)-C(1)	107.9(2)
C(3)-C(2)-C(7)	126.1(2)
C(1)-C(2)-C(7)	125.9(3)
C(3)-C(2)-Sm(1)	75.97(14)
C(1)-C(2)-Sm(1)	74.80(13)
C(7)-C(2)-Sm(1)	117.19(16)
C(4)-C(3)-C(2)	107.9(2)
C(4)-C(3)-C(8)	126.5(3)
C(2)-C(3)-C(8)	125.3(3)
C(4)-C(3)-Sm(1)	75.14(13)
C(2)-C(3)-Sm(1)	73.56(13)
C(8)-C(3)-Sm(1)	121.28(16)
C(5)-C(4)-C(3)	108.4(2)
C(5)-C(4)-C(9)	125.9(3)

C(3)-C(4)-C(9)	125.5(3)
C(5)-C(4)-Sm(1)	75.38(13)
C(3)-C(4)-Sm(1)	74.69(13)
C(9)-C(4)-Sm(1)	119.94(17)
C(4)-C(5)-C(1)	107.8(2)
C(4)-C(5)-C(10)	125.3(3)
C(1)-C(5)-C(10)	126.3(3)
C(4)-C(5)-Sm(1)	74.56(13)
C(1)-C(5)-Sm(1)	73.11(13)
C(10)-C(5)-Sm(1)	124.96(17)
C(13)-C(12)-C(17)	118.8(2)
C(13)-C(12)-B(1)	126.9(2)
C(17)-C(12)-B(1)	114.3(2)
C(14)-C(13)-C(12)	121.2(2)
C(15)-C(14)-C(13)	119.9(2)
C(14)-C(15)-C(16)	119.9(2)
C(15)-C(16)-C(17)	121.1(2)
C(16)-C(17)-C(12)	119.1(2)
C(16)-C(17)-B(1)#1	126.6(2)
C(12)-C(17)-B(1)#1	114.30(19)
N(1)-B(1)-C(11)	108.45(18)
N(1)-B(1)-C(17)#1	102.12(18)
C(11)-B(1)-C(17)#1	118.6(2)

N(1)-B(1)-C(12)	101.84(18)
C(11)-B(1)-C(12)	119.0(2)
C(17)#1-B(1)-C(12)	104.34(18)
Cnt2-Sm(2)-Cnt2'	139.7
Cnt2-Sm(2)-O(1)	104.1
Cnt2-Sm(2)-O(1')	103.3
O(1)-Sm(2)-O(1)#1	93.15(8)
O(1)-Sm(2)-C(18)	100.91(6)
O(1)#1-Sm(2)-C(18)	77.94(6)
O(1)-Sm(2)-C(18)#1	77.94(6)
O(1)#1-Sm(2)-C(18)#1	100.91(6)
C(18)-Sm(2)-C(18)#1	178.36(9)
O(1)-Sm(2)-C(22)#1	91.28(6)
O(1)#1-Sm(2)-C(22)#1	127.86(7)
C(18)-Sm(2)-C(22)#1	151.11(7)
C(18)#1-Sm(2)-C(22)#1	30.43(7)
O(1)-Sm(2)-C(22)	127.86(7)
O(1)#1-Sm(2)-C(22)	91.28(6)
C(18)-Sm(2)-C(22)	30.43(7)
C(18)#1-Sm(2)-C(22)	151.10(7)
C(22)#1-Sm(2)-C(22)	124.88(10)
O(1)-Sm(2)-C(20)	88.06(7)
O(1)#1-Sm(2)-C(20)	127.09(7)

C(18)-Sm(2)-C(20)	50.15(7)
C(18)#1-Sm(2)-C(20)	130.75(7)
C(22)#1-Sm(2)-C(20)	104.96(7)
C(22)-Sm(2)-C(20)	50.12(8)
O(1)-Sm(2)-C(20)#1	127.09(7)
O(1)#1-Sm(2)-C(20)#1	88.06(7)
C(18)-Sm(2)-C(20)#1	130.75(7)
C(18)#1-Sm(2)-C(20)#1	50.14(7)
C(22)#1-Sm(2)-C(20)#1	50.11(8)
C(22)-Sm(2)-C(20)#1	104.96(7)
C(20)-Sm(2)-C(20)#1	131.08(10)
O(1)-Sm(2)-C(19)#1	98.59(6)
O(1)#1-Sm(2)-C(19)#1	77.85(6)
C(18)-Sm(2)-C(19)#1	149.55(7)
C(18)#1-Sm(2)-C(19)#1	30.30(7)
C(22)#1-Sm(2)-C(19)#1	50.15(7)
C(22)-Sm(2)-C(19)#1	132.99(7)
C(20)-Sm(2)-C(19)#1	154.03(8)
C(20)#1-Sm(2)-C(19)#1	30.44(7)
O(1)-Sm(2)-C(19)	77.85(6)
O(1)#1-Sm(2)-C(19)	98.59(6)
C(18)-Sm(2)-C(19)	30.30(7)
C(18)#1-Sm(2)-C(19)	149.55(7)

C(22)#1-Sm(2)-C(19)	133.00(8)
C(22)-Sm(2)-C(19)	50.15(7)
C(20)-Sm(2)-C(19)	30.44(7)
C(20)#1-Sm(2)-C(19)	154.03(8)
C(19)#1-Sm(2)-C(19)	174.90(10)
O(1)-Sm(2)-C(21)#1	121.57(6)
O(1)#1-Sm(2)-C(21)#1	118.24(7)
C(18)-Sm(2)-C(21)#1	131.48(7)
C(18)#1-Sm(2)-C(21)#1	50.09(7)
C(22)#1-Sm(2)-C(21)#1	30.33(7)
C(22)-Sm(2)-C(21)#1	101.08(7)
C(20)-Sm(2)-C(21)#1	105.29(8)
C(20)#1-Sm(2)-C(21)#1	30.23(7)
C(19)#1-Sm(2)-C(21)#1	50.05(7)
C(19)-Sm(2)-C(21)#1	134.96(7)
O(1)-Sm(2)-C(21)	118.24(7)
O(1)#1-Sm(2)-C(21)	121.57(6)
C(18)-Sm(2)-C(21)	50.09(7)
C(18)#1-Sm(2)-C(21)	131.48(7)
C(22)#1-Sm(2)-C(21)	101.08(7)
C(22)-Sm(2)-C(21)	30.33(7)
C(20)-Sm(2)-C(21)	30.23(7)
C(20)#1-Sm(2)-C(21)	105.29(8)

C(19)#1-Sm(2)-C(21)	134.95(7)
C(19)-Sm(2)-C(21)	50.06(7)
C(21)#1-Sm(2)-C(21)	87.06(10)
C(31)-O(1)-C(28)	108.84(17)
C(31)-O(1)-Sm(2)	120.06(13)
C(28)-O(1)-Sm(2)	131.11(13)
C(19)-C(18)-C(22)	108.1(2)
C(19)-C(18)-C(23)	123.6(2)
C(22)-C(18)-C(23)	127.9(2)
C(19)-C(18)-Sm(2)	75.10(13)
C(22)-C(18)-Sm(2)	74.90(13)
C(23)-C(18)-Sm(2)	121.84(15)
C(18)-C(19)-C(20)	107.9(2)
C(18)-C(19)-C(24)	124.2(2)
C(20)-C(19)-C(24)	127.6(2)
C(18)-C(19)-Sm(2)	74.60(13)
C(20)-C(19)-Sm(2)	74.71(14)
C(24)-C(19)-Sm(2)	121.65(15)
C(21)-C(20)-C(19)	108.0(2)
C(21)-C(20)-C(25)	124.7(2)
C(19)-C(20)-C(25)	126.8(2)
C(21)-C(20)-Sm(2)	75.10(14)
C(19)-C(20)-Sm(2)	74.85(13)

C(25)-C(20)-Sm(2)	122.37(17)
C(20)-C(21)-C(22)	108.2(2)
C(20)-C(21)-C(26)	125.0(2)
C(22)-C(21)-C(26)	125.1(2)
C(20)-C(21)-Sm(2)	74.67(13)
C(22)-C(21)-Sm(2)	74.56(13)
C(26)-C(21)-Sm(2)	128.79(17)
C(21)-C(22)-C(18)	107.8(2)
C(21)-C(22)-C(27)	124.4(2)
C(18)-C(22)-C(27)	127.3(2)
C(21)-C(22)-Sm(2)	75.10(13)
C(18)-C(22)-Sm(2)	74.67(13)
C(27)-C(22)-Sm(2)	122.76(17)
O(1)-C(28)-C(29)	105.06(19)
C(28)-C(29)-C(30)	103.3(2)
C(31)-C(30)-C(29)	101.1(2)
O(1)-C(31)-C(30)	105.03(19)
C(34)-C(33)-C(32)	113.2(2)
C(33)-C(34)-C(34)#2	113.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x+1,-y,-z+1

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