Electronic Supplementary Information.

Modified Boron Subphthalocyanines with Stable Electrochemistry and Tuneable Bandgaps.

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Table of Contents

1.0 Experimental Information

1.1 General Information

Starting materials and solvents were purchased from various companies and used without further purification.

NMR Spectra were collected at 25 °C at a field-strength of 400 MHz. In order to resolve the isomers of compound **2**, NMR spectra at a field strength of 700 MHz was collected. All ^{1}H and ^{13}C spectra are referenced to residual solvent or TMS and chemical shifts are reported in parts per million while coupling constants are reported in Hz. ^{19}F and ^{11}B NMR are referenced to BF_3-OEt_2 which we arbitrarily assigned to 0 ppm for both nuclei. External standards were used with each NMR experiment.

High resolution mass spectroscopy (HRMS) was acquired with either DART or ESI ionization techniques. For those using DART, the spectra were acquired using an AccuTOF mass spectrometer (JEOL USA Inc. Peabody, MA) with a DART-SVP ion source (Ionsense Inc., Saugus, MA) using He Gas.

Electrochemistry was performed in a solution of DCM with 0.1 M tetraammonium perchlorate as a supporting electrolyte. A 1 mm platinum disc was used as a working electrode with a platinum wire counter electrode and Ag/AgCl reference electrode. All cyclic voltammetry experiments were run with an internal standard of decamethylferrocene at a scanning rate of 100 mV/s. All half wave potentials are corrected to the published halfwave potential of decamethylferrocene (-0.012 V vs. Ag/AgCl).[1] All half wave potentials are reported relative to Ag/AgCl.

Density functional theory (DFT) calculations were implemented using Spartan '06 for windows. Structures were geometry optimized using the Becke-Lee-Yang-Parr exchange correlation function[2] with a 6-31G(D) basis set.

[1] Noviandri, I.; Brown, K.N.; Fleming, D.S.; Gulyas, P.T.; Lay, P.A.; Masters, A.F.; Leonidas, P. *J. Phys. Chem. B* **1999**, 103 (32), 6713-6722.
[2] Becke, A.D. *Phys. Rev. A* **1988**, 38 (6), 3098-3100

1.2 Synthetic Details and Compound Characterization

Compound **1**

Compound was synthesized according to a procedure by Kamino et al.[3]

Compound **2**

Tetrachlorophthalonitrile (1.000 g, 3.76 mmol), 3,5-di-t-butylcatechol (1.755 g, 7.90 mmol), potassium carbonate (1.091 g, 7.90 g), and N,N-dimethylformamide (20 mL) were heated to 100 °C for 6 hours under an atmosphere of argon gas. Upon cooling, water (20 mL) was added to the solution to form a fine slurry. The solids were collected by filtration, washing with water (3 x 50 mL) and methanol (3 x 50 mL) resulting in the pure product as a fine white powder (1.927 g, 91% Yield). HRMS (DART) [M+H] cald for $C_{36}H_{41}N_2O_4$ 565.30663, found 565.30659.

See section 2.0 for detailed NMR analysis.

Compound **3a**

Compound **1** (11.690 g, 34.4 mmol) was dissolved in 1,2-dichlorobenzene (300 mL) under an inert atmosphere. Boron trichloride (81 mL of a 1M solution in heptanes, 81 mmol) was added to this solution and the heptanes were distilled off and the mixture was refluxed for 2 hours. Upon cooling, the dichlorobenzene was removed under vacuum and the resulting black solids were continuously extracted with methanol (48 Hrs) then acetonitrile (24 Hrs) using a soxhlet apparatus. The remaining solids were dried under vacuum resulting in a fine green/black powder assumed to be the chloro substituted subphthalocyanine product (8.01 g, 66 % crude yield).

The crude -Cl substituted subphthalocyanine (500 mg, ~0.47 mmol), 4-t-butylphenol (352 mg, 2.34 mmol), and chlorobenzene (5 mL) were heated at reflux for 48 hours. Upon cooling, the chlorobenzene was removed under vacuum and the resulting green solids were loaded onto a plug of alumina (basic, standard activity) and extracted continuously with dichloromethane using a Kaufman apparatus. The extracted, dark green liquor was then concentrated under vacuum resulting in a dark green powder (319 mg, 58 % Yield). HRMS (ESI) [M+] calcd 1180.2506, found 1180.2770. ^{1}H (400 MHz, CD_2Cl_2): δ 7.21 (d, J = 7.8 Hz, 6 H), 6.96-6.79 (m, 20H), 5.47 (d, J = 8.6 Hz, 2H), 1.06 (s, 9H). ^{11}B (CD_2Cl_2): δ -14.8

Compound **3b**

Using the procedure for **3a**: The crude Cl substituted subphthalocyanine (500 mg, ~0.47 mmol), pentafluorophenol (431 mg, 2.34 mmol), and chlorobenzene (5 mL) were heated at reflux for 18 hours. The product was isolated as a dark green powder (207 mg, 36 % yield). MS (ESI) [M+] calcd 1215.1, found 1215.1. MS signal insufficient for high resolution mass spectroscopy. ^{1}H (400 MHz, CD_2Cl_2): δ 7.29 (dd, J_1 = 8.0 Hz, J_2 = 1.4 Hz, 6 H), 7.16-7.00 (m, 20H). ^{19}F (CD_2Cl_2, referenced to BF_3-$O(Et)_2$): δ -5.35 (d, J = 20.6 Hz, 2F), -10.3 (t, J = 20.6 Hz, 2F), -11.7 (t, J = 20.6 Hz, 1F). ^{11}B (CD_2Cl_2, referenced to BF_3-$O(Et)_2$): δ -14.5

[3] Kamino, B.A.; Chang, Y.; Lu, Z.; Bender, T.P. *Org. Electron.* **2012**, 13, 1479-1485.

Compound **4a**

2 (2.258 g, 4.00 mmol), phthalonitrile (256 mg, 2 mmol), 20 mL 1,2-dichlorobenzene were stirred under an inert atmosphere. Boron trichloride (10 mmol, 10 mL of heptanes solution) was added to the mixture and the heptanes were distilled off were reacted for 2 hours under and inert atmosphere. Upon cooling, the solution was dried under vacuum and the blue solids were continuously extracted with methanol for 18 hours. The remaining solids resembled a dark blue powder (1.554 g, 90% crude yield).

The crude above product (1.000 g, ~1.15 mmol), pentafluorophenol (1.000 g, 5.43 mmol), and chlorobenzene (10 mL) were refluxed under an inert atmosphere for 18 hours. After removal of the chlorobenzene under vacuum, the remaining blue solids were purified by column chromatography over silica gel eluting with 3/2 hexanes/toluene. A fraction containing a single blue spot was isolated (258 mg, 22% Yield) and shown to be a single product on low molecular weight GPC. HRMS (DART) [M+H] calcd for $C_{58}H_{48}BF_5N_6O_5$ 1015.3778, found 1015.3718. ^{1}H (400 MHz, $CDCl_3$): δ 8.80 (dm, J_1 = 20.7 Hz, 4H), 7.91 (q, J = 3.1 Hz, 4H), 7.15 (d, J = 2.3 Hz, 1.7H), 7.07-7.05 (m, 2H), 6.95 (d, J = 2.3 Hz, 0.3H), 1.94 (s, 15.1H), 1.46 (s, 2.9), 1.36 (s, 15.1), 1.29 (s, 2.9). ^{11}B ($CDCl_3$, referenced to BF_3-$O(Et)_2$): δ -14.6. ^{19}F ($CDCl_3$, referenced to BF_3-$O(Et)_2$): δ -5.3 (d, J = 21.4 Hz, 2F), -11.1 (t, J = 21.4 Hz, 2F), -12.0 (t, J = 21.4 Hz, 1F).

Compound **4b**

Compound **2** (4.00 mmol, 2.258 g) tetrafluorophthalonitrile (4.00 mmol, 800 mg), 20 mL 1,2-dichlorobenzene, and BCl_3 (10.0 mmol, 10 mL of a 1M solution in heptanes) were mixed together under argon. The heptanes were then distilled off and the reagents heated at reflux for 2 hours. After cooling the solvent was removed under vacuum and the dark green/blue solids were continuously extracted with methanol using a soxhlet apparatus for 16 hours. The extracted solids were dried and the crude, -Cl substituted product collected (1.511 g, 75% crude yield).

The above crude product (800 mg, ~0.790 mmol), pentafluorophenol (800 mg, 4.35 mmol), and chlorobenzene (8 mL) were refluxed under argon for 10 hours. After removal of the solvent, the solids were purified by flash chromatography over silicon eluting with 5/1 hexanes to toluene. Two green fractions with identical retention times by lmw GPC and UV-VIS absorbance spectra were isolated (fraction 1: 113 mg, 12% Yield, fraction 2: 107 mg, 12% yield). Unfortunately, the second fraction quickly degraded upon heating under vacuum and only the first fraction was characterized. HRMS (DART) [M+] calcd for $C_{58}H_{40}BF_{13}N_6O_5$ 1155.3060, found 1158.2968. ^{1}H (400 MHz, $CDCl_3$): δ 7.18 (2.3 Hz, 2H), 7.08 (2,3 Hz, 2H), 1.83 (s, 18H), 1.37 (s, 18H). ^{11}B ($CDCl_3$, referenced to BF_3-$O(Et)_2$): δ -14.8. ^{19}F ($CDCl_3$, referenced to BF_3-$O(Et)_2$): δ 17.6 (t, J = 18.3 Hz, 2F), 14.9 (t, J = 18.3 Hz, 2F), 4.3 (t, 18.3 Hz, 2F), 3.4 (t, J = 18.3 Hz, 2F), -5.5 (2, J = 22.9 Hz, 2F), -9.9 (t, J =20.6 Hz, 2F), -10.3 (t, J = 22.9 Hz, 1F)

Compound **4c**

Compound **2** (4.00 mmol, 2.258 g) tetrachlorophthalonitrile (4.00 mmol, 1.063 g), 20 mL 1,2-dichlorobenzene, and BCl_3 (10 mmol, 10 mL of a 1M solution in heptanes) were mixed together under

argon. The heptanes were then distilled off and the reagents heated at reflux for 2 hours. After cooling, the solvent was removed under vacuum and the dark green/blue solids were continuously extracted with methanol using a soxhlet apparatus for 16 hours. After extraction, the solids were dried and the crude, -Cl substituted product collected (652 g, 29% crude yield).

The above crude product (500 mg, ~0.438 mmol), pentafluorophenol (500 mg, 2.72 mmol), and chlorobenzene (5 mL) were refluxed under argon for 18 hours. After drying, the resulting dark blue/green powder was purified twice successively over silica gel eluting with a gradient from 10/1 to 3/1 Hexanes/Toluene. HRMS (DART) [M+H] calcd for $C_{58}H_{40}BCl_8F_5N_6O_5$ 1287.0660, found 1287.0719. ^{1}H (400 MHz, $CDCl_3$): δ 7.22-7.19 (m, 1.9H), 7.14 (d, J = 2.3 Hz, 0.8H), 7.10 (d, J = 2.3 Hz, 0.8H), 6.95 (d, J = 2.3 Hz, 0.5H), 1.83 (s, 12H), 1.55 (s, 5.0H), 1.40-1.38 (m, 19H). ^{11}B (XX MHz, $CDCl_3$, referenced to BF_3-$O(Et)_2$): δ -14.7. ^{19}F (XX MHz, $CDCl_3$, referenced to BF_3-$O(Et)_2$): δ -5.4 (m, 2F), -9.9 (m, 2F), -10.6 (m, 1F).

2.0 NMR Study of Phthalonitrile 2

Due to the nature of the substitution reaction, the following three isomers are expected:

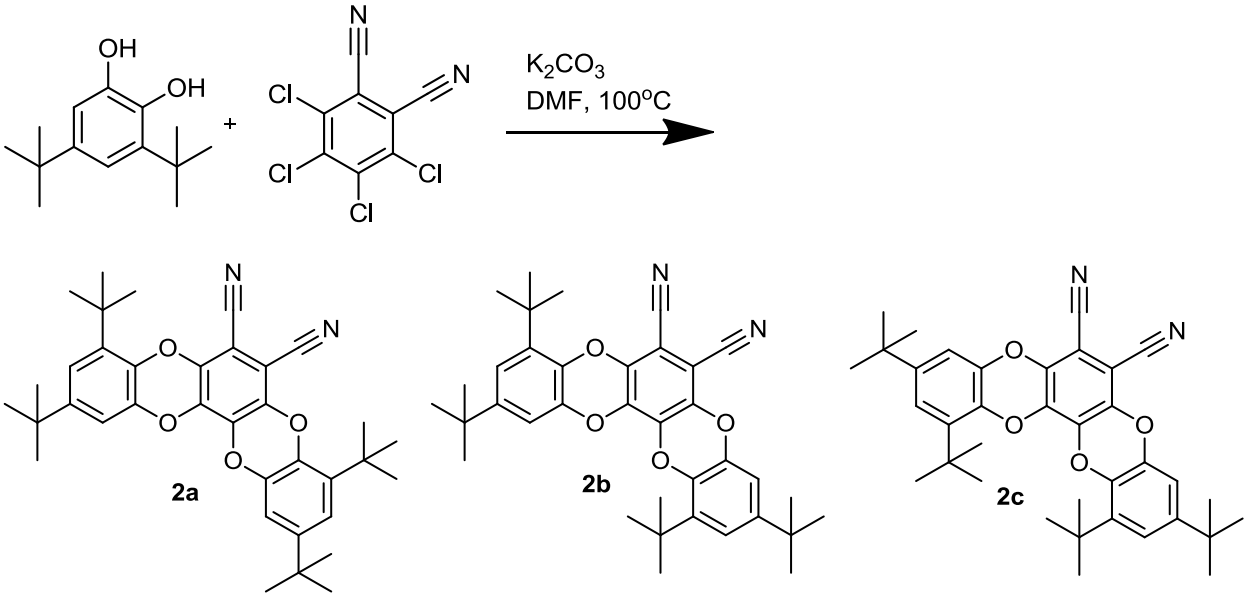

Figure S1: Structures of three expected isomers for compound **2**

HPLC analysis was not able to isolate and quantify the ratios of each isomer. ^{1}H NMR at 400 MHz showed some separation of the aromatic protons for each isomer but the resolution was insufficient. To resolve these peaks, ^{1}H NMR and gCOSY (^{1}H-^{1}H) analysis was performed at 700 MHz (Figures S2-4). The enhanced resolution afforded by the higher field strength allowed enough resolution for accurate integration of a number of peaks. Through ring coupling detected by gCOSY and knowledge of the integration values in the 1D spectrum allowed for quantification of each isomer.

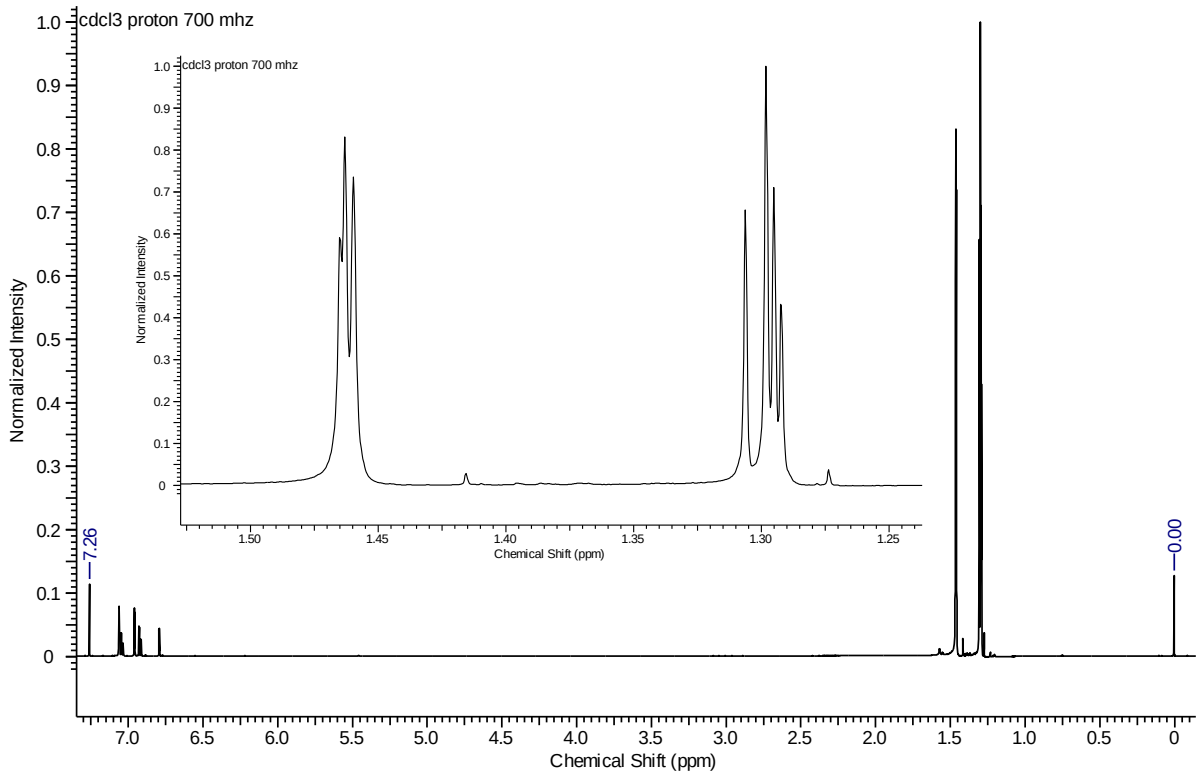

Figure S2: ^{1}H NMR spectrum at 700 MHz in $CDCl_3$ of compound **2**. Inset: Close up of alkyl region of spectrum.

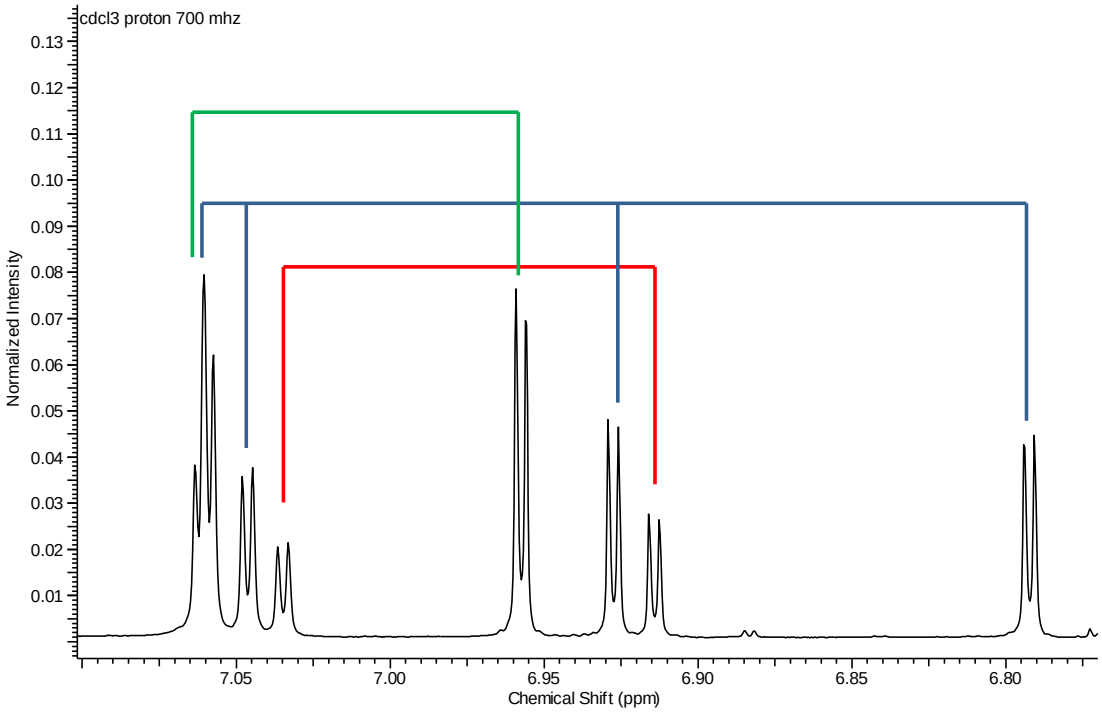

Figure S3: Zoom of aromatic region of ^{1}H NMR spectrum at 700 MHz in $CDCl_3$ of compound **2**. Coloured lines show coupled spin systems from gCOSY experiment.

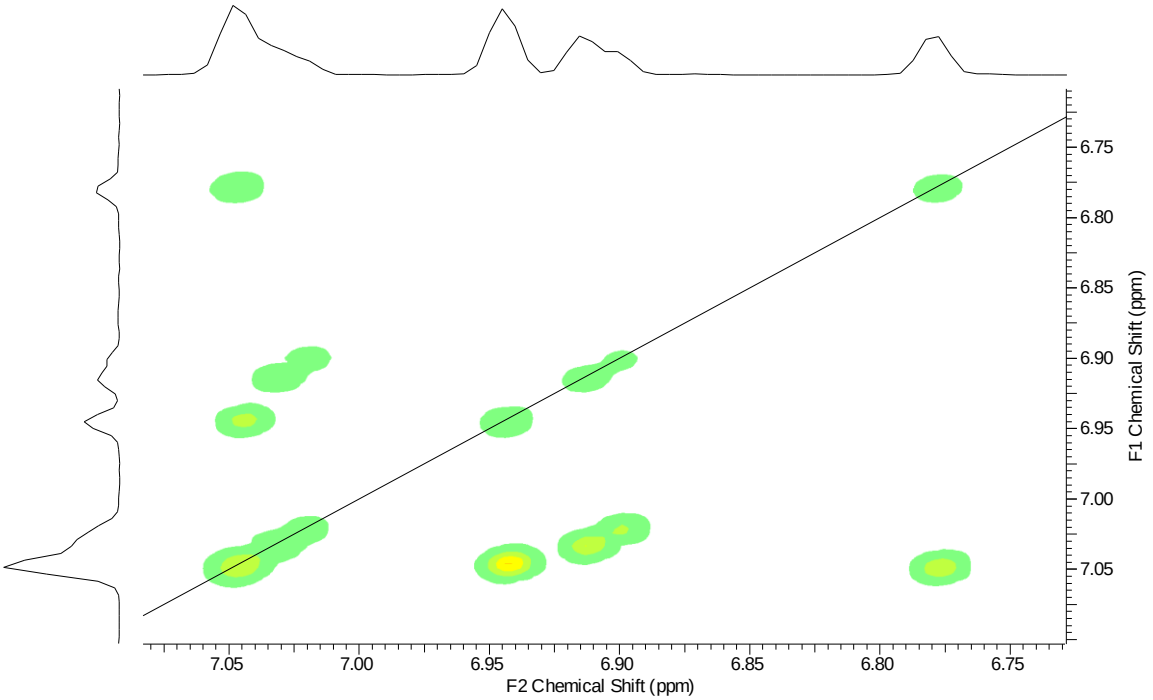

Figure S4: gCOSY (^{1}H, ^{1}H) spectrum at 700 MHz in $CDCl_3$ of compound 2.

^{1}H NMR (700 MHz, $CDCl_3$): δ 7.07-7.05 (m, 4.1 H), 7.05 (d, J = 2.4 Hz, 1.6 H), 7.03 (d, J = 2.4 Hz, 1 H), 6.96 (d, J = 2.4 Hz, 2.6 H), 6.93 (d, J = 2.4 Hz, 1.6 H), 6.91 (d, J = 2.4 Hz, 1 H), 6.79 (d, J = 2.4 Hz, 1.6 H), 1.48-1.45 (m, 61 H), 1.31-1.29 (m, 61 H).

3.0 UV-VIS and PL Plots

3.1 Compound 3a

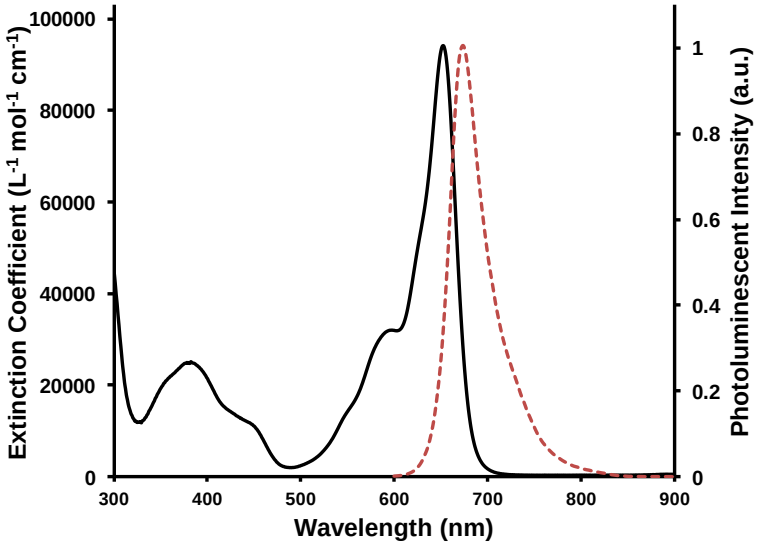

Figure S5: UV-VIS absorbance spectrum of compound **3a** in THF (left axis) and photoluminescence emission spectrum of **3a** in THF at an excitation wavelength of 650 nm.

3.2Compound 3b

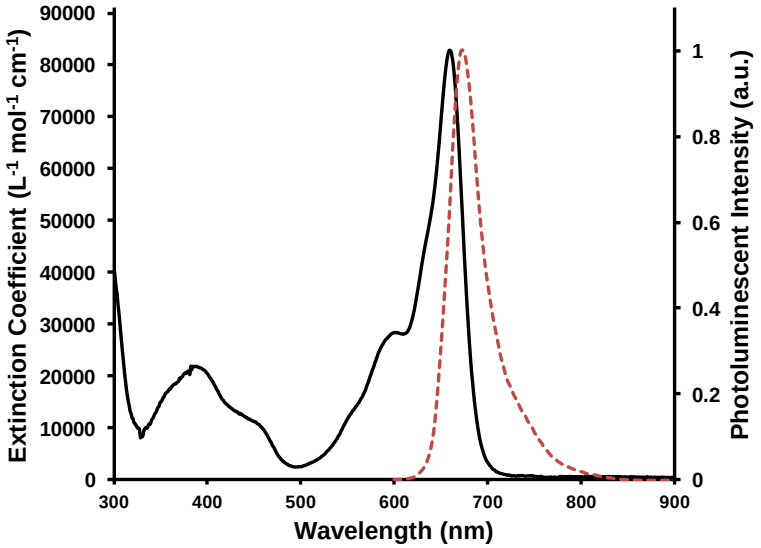

Figure S6: UV-VIS absorbance spectrum of compound **3a** in THF (left axis) and photoluminescence emission spectrum of **3a** in THF at an excitation wavelength of 650 nm.

3.3 Compound 4a

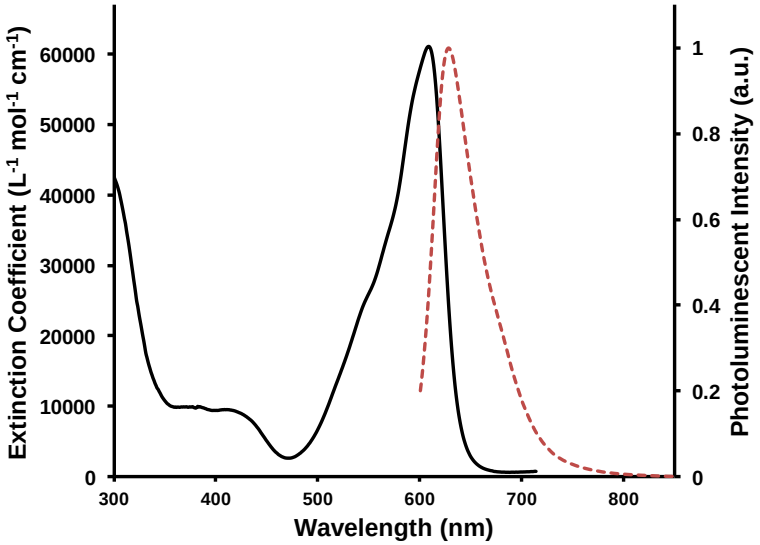

Figure S7: UV-VIS absorbance spectrum of compound **4a** in THF (left axis) and photoluminescence emission spectrum of **4a** in THF at an excitation wavelength of 601 nm.

3.4 Compound 4b

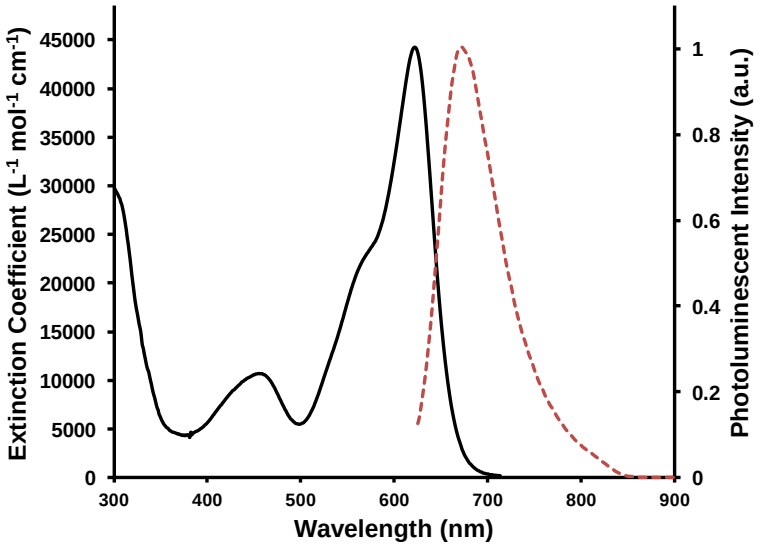

Figure S8: UV-VIS absorbance spectrum of compound **4b** in THF (left axis) and photoluminescence emission spectrum of **4b** in THF at an excitation wavelength of 621 nm.

3.5 Compound 4c

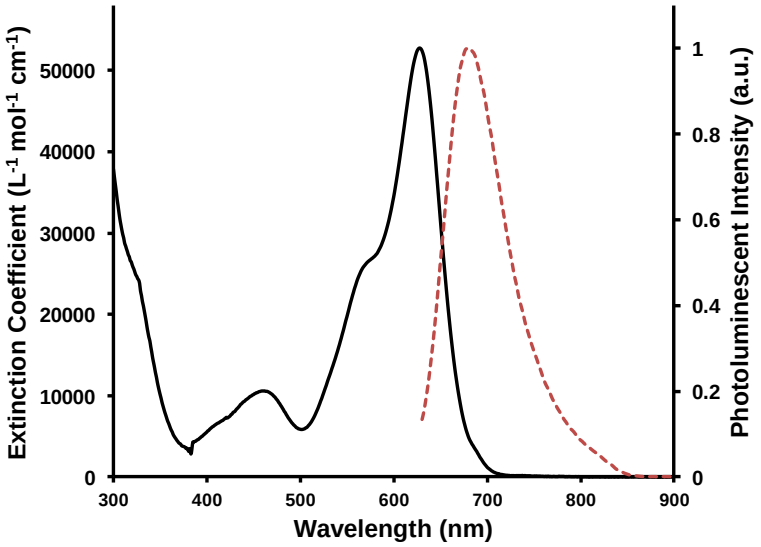

Figure S9: UV-VIS absorbance spectrum of compound **4c** in THF (left axis) and photoluminescence emission spectrum of **4c** in THF at an excitation wavelength of 626 nm.

3.5 (pentfluorophenoxy)boron subphthalocyanine (F_5BsubPc)

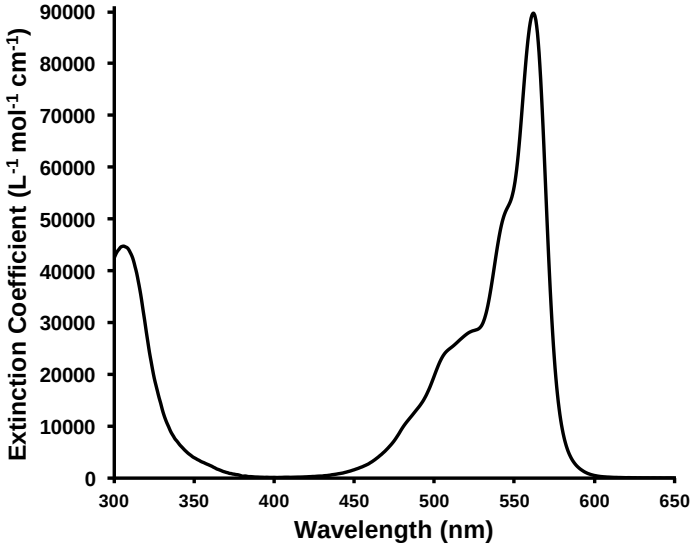

Figure S10: UV-VIS absorbance spectrum of compound **F5-BsubPc** in THF.

4.0 DFT Calculated Molecular Orbitals

4.1 Compound 3a

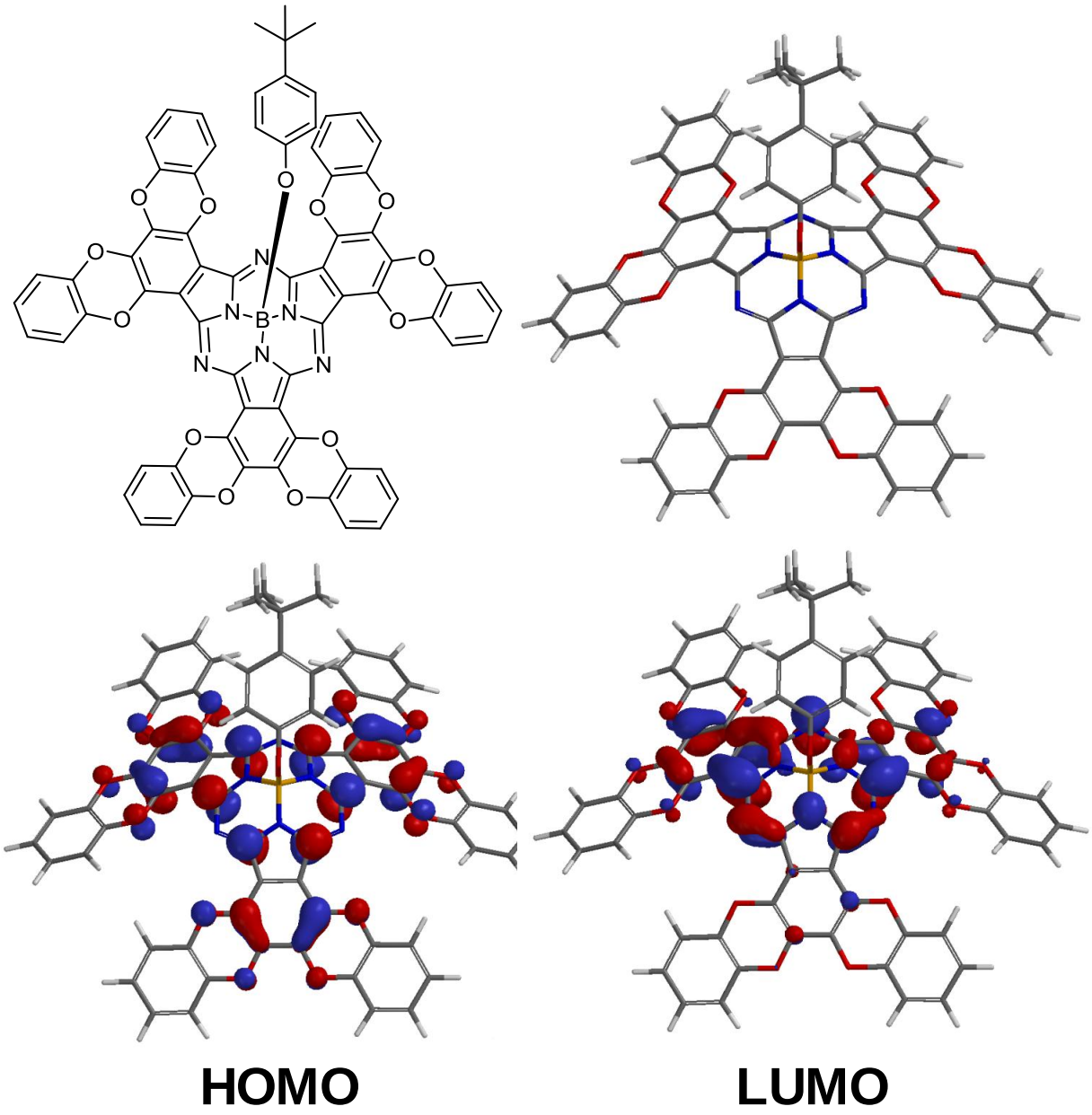

Figure S11: Geometry optimized DFT structures for compound **3a** showing HOMO and LUMO distributions.

4.2 Compound 3b

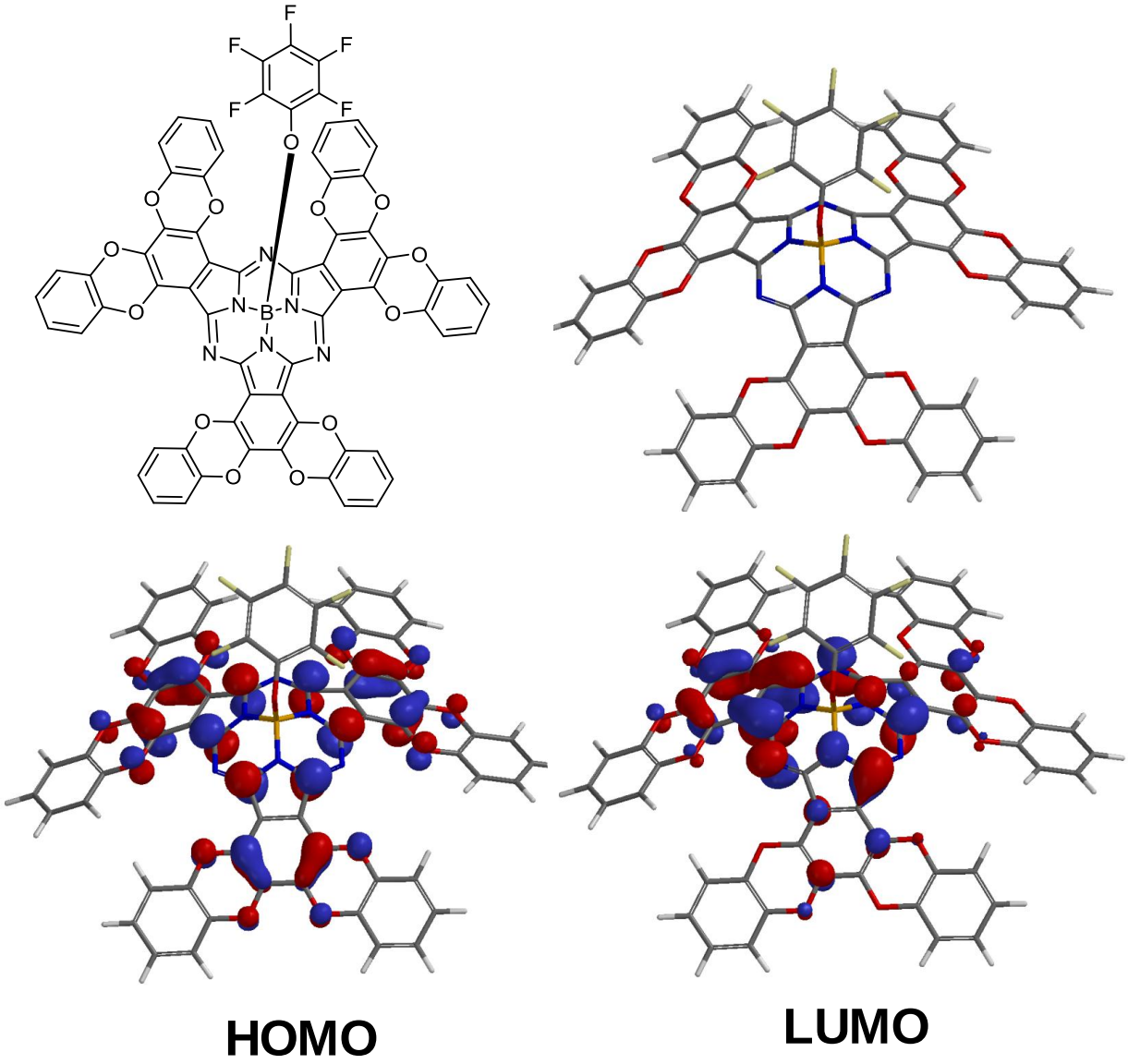

Figure S12: Geometry optimized DFT structures for compound **3b** showing HOMO and LUMO distributions.

4.3 Compound 4a

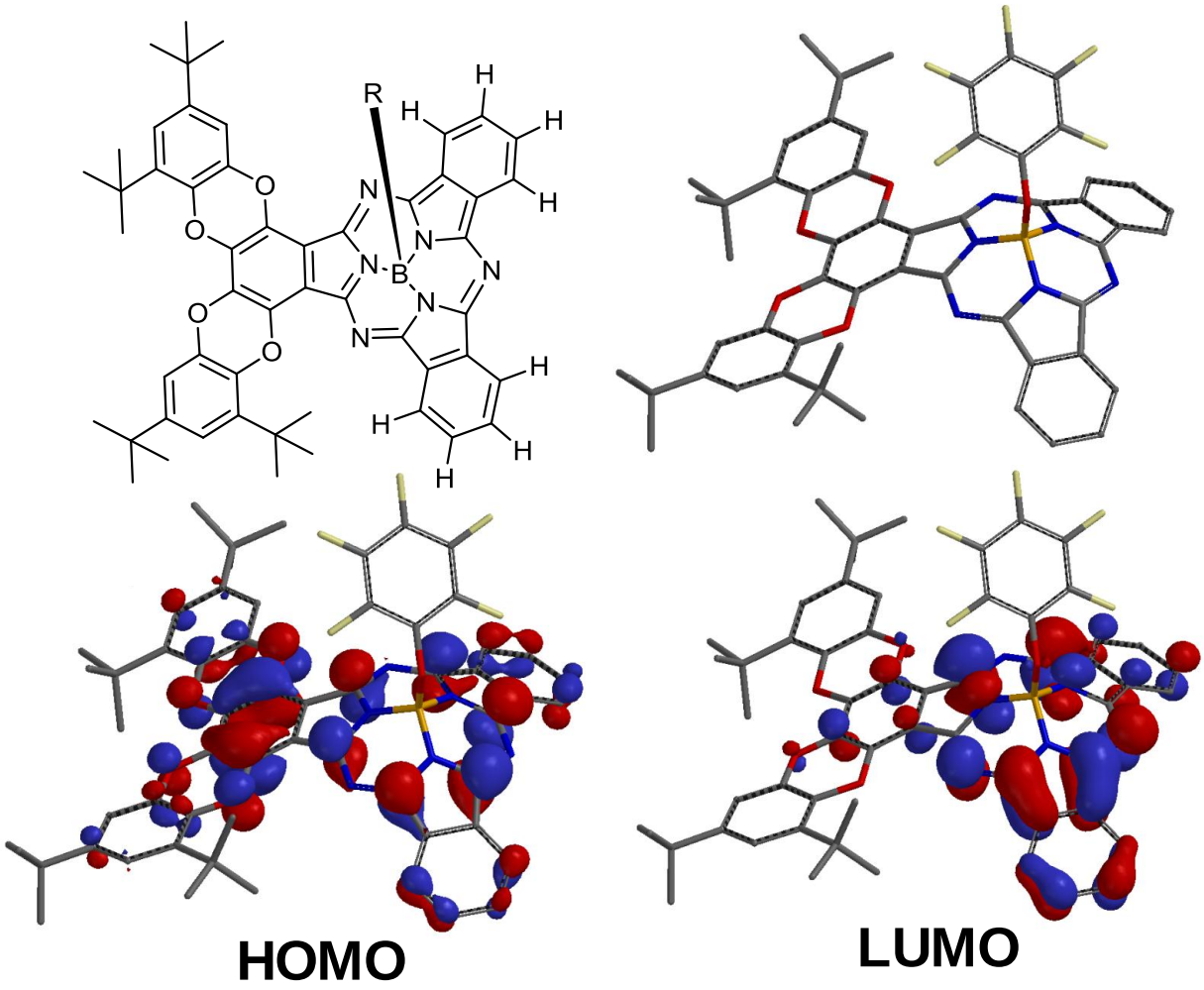

Figure S13: Geometry optimized DFT structures for one isomer of compound **4a** with HOMO and LUMO distributions.

4.4 Compound 4b

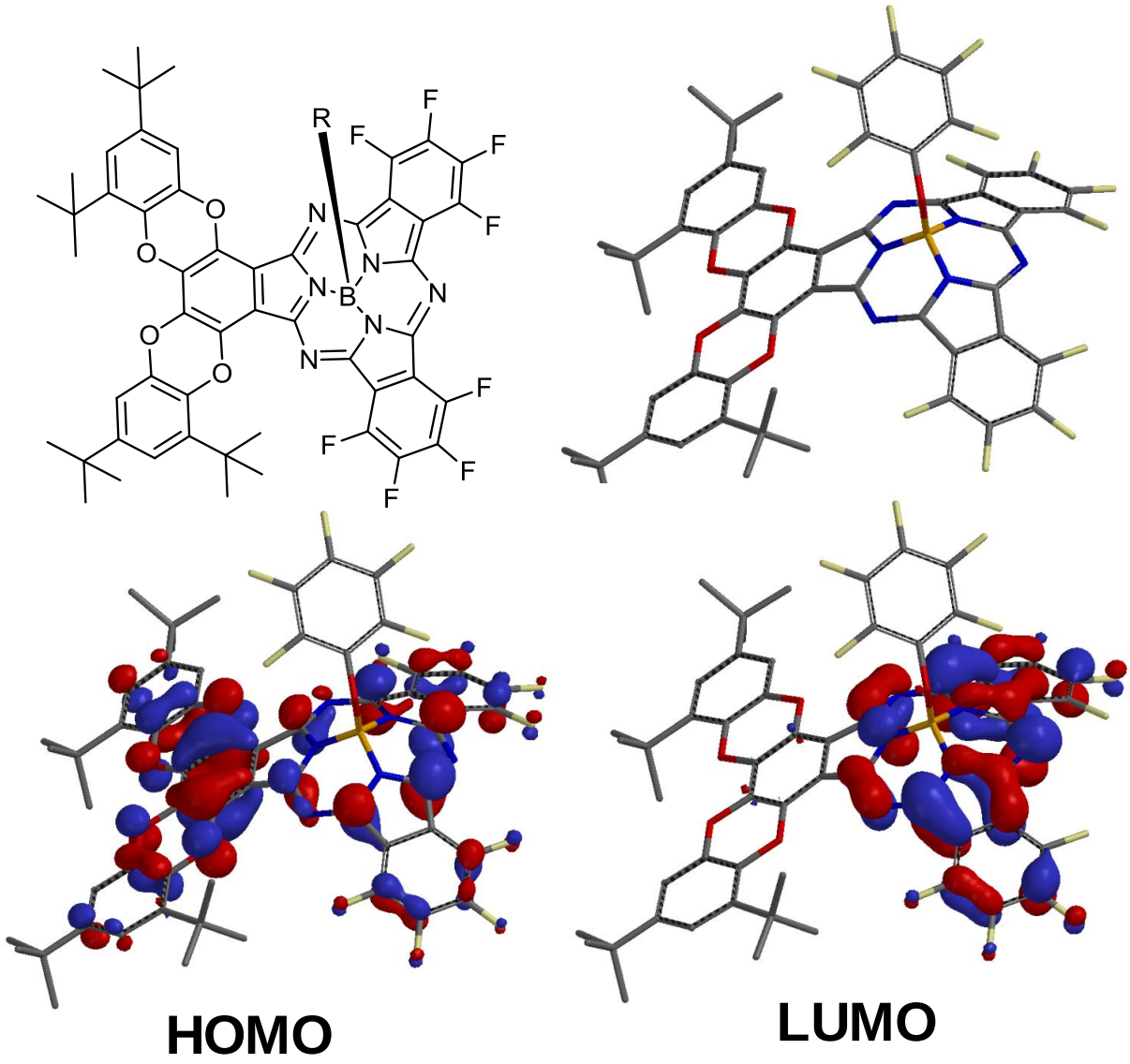

Figure S14: Geometry optimized DFT structures for one isomer of compound **4b** with HOMO and LUMO distributions.

4.5 Compound 4c

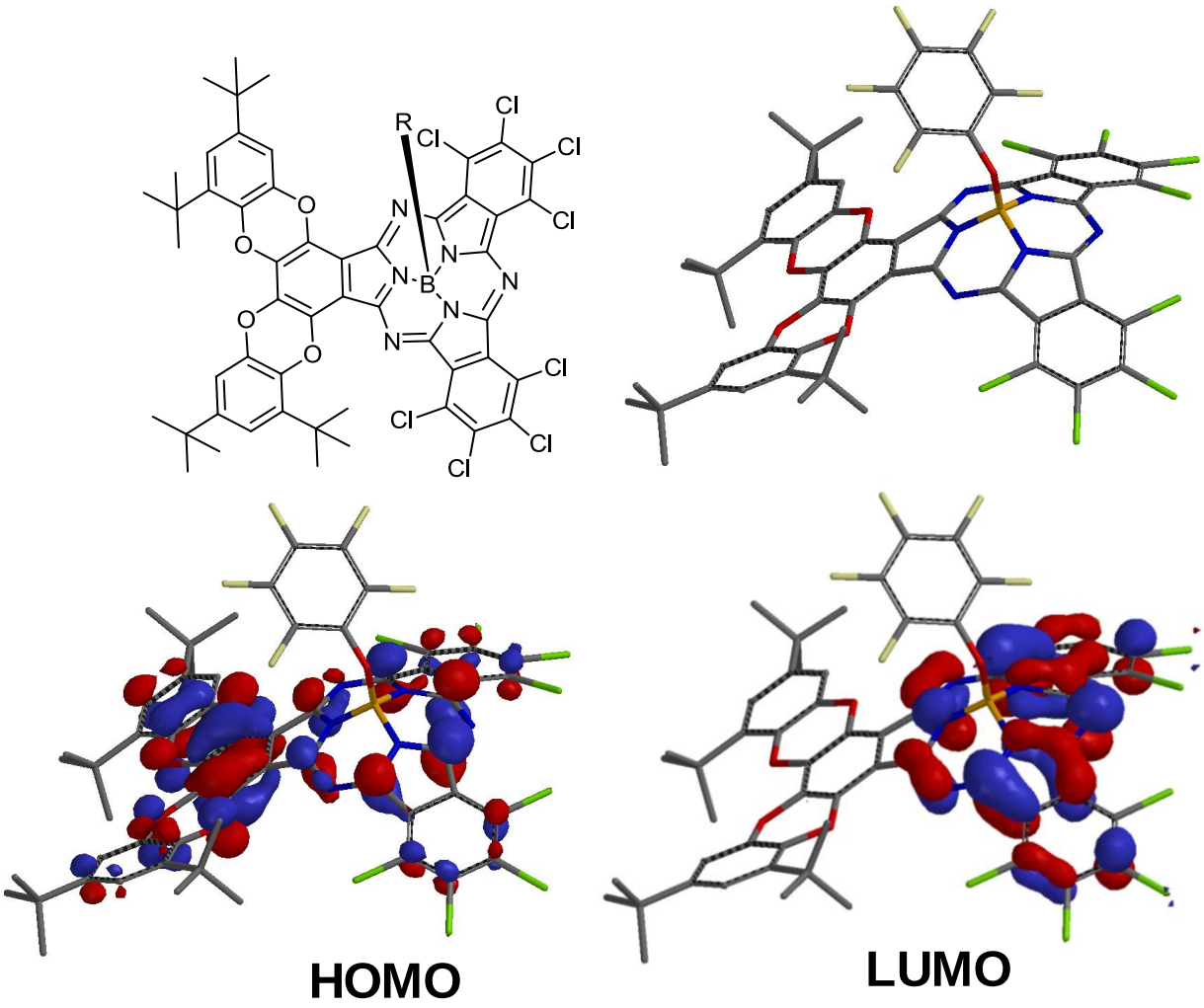

Figure S15: Geometry optimized DFT structures for one isomer of compound **4c** with HOMO and LUMO distributions.

5.0 Cyclic Voltammetry

5.1 Compound 3a

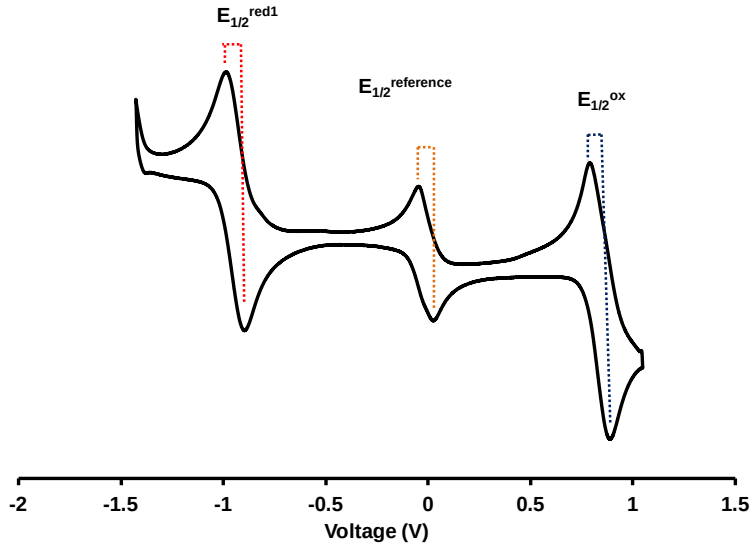

Figure S16: Cyclic voltammogram of compound **3a** in DCM with 0.1M tetrabutylammonium perchlorate and decamethylferrocene as an internal standard.

5.2 Compound 3b

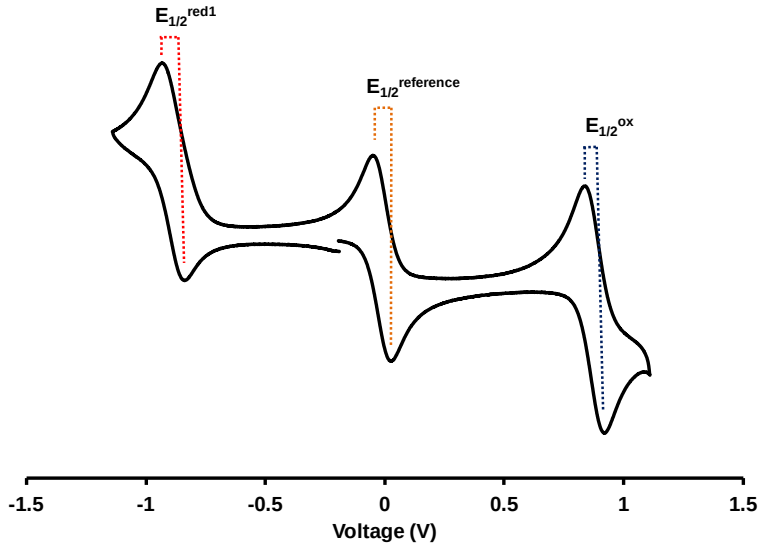

Figure S17: Cyclic voltammogram of compound **3b** in DCM with 0.1M tetrabutylammonium perchlorate and decamethylferrocene as an internal standard.

5.3 Compound 4a

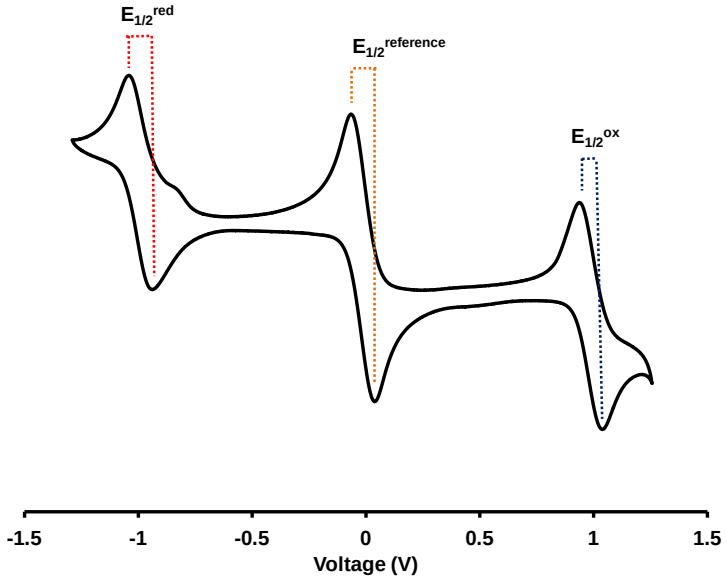

Figure S18: Cyclic voltammogram of compound **4a** in DCM with 0.1M tetrabutylammonium perchlorate and decamethylferrocene as an internal standard.

5.4 Compound 4b

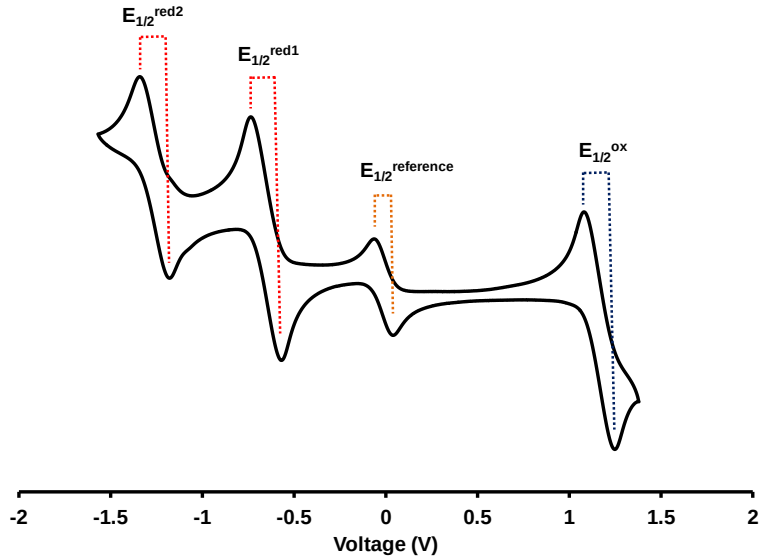

Figure S19: Cyclic voltammogram of compound **4b** in DCM with 0.1M tetrabutylammonium perchlorate and decamethylferrocene as an internal standard.

5.5 Compound 4c

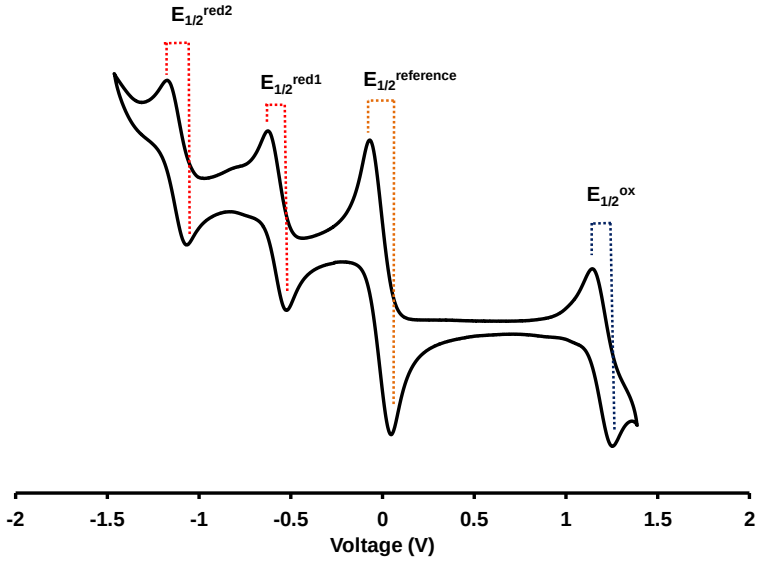

Figure S20: Cyclic voltammogram of compound **4c** in DCM with 0.1M tetrabutylammonium perchlorate and decamethylferrocene as an internal standard.

6.0 X-Ray Crystal Information

6.1 Crystal of 3b·(THF)$_2$ – CCDC Deposition 910746

Crystal grown through slow vapour diffusion of **3b** in THF with hexanes. Crystals isolated as a solvate with two THF molecules per unit cell.

Table S1. Crystal data and structure refinement for **3b·(THF)$_2$** (CCDC deposition 910746).

Identification code	d12296	
Empirical formula	C60 H50 B Cl6 F5 N6 O5	
Formula weight	1253.57	
Temperature	120(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.5648(4) Å	□= 90°.
	b = 17.6316(8) Å	□= 96.526(2)°.
	c = 34.0701(14) Å	□ = 90°.
Volume	5708.4(4) Å^3	
Z	4	
Density (calculated)	1.459 Mg/m^3	
Absorption coefficient	3.360 mm^{-1}	
F(000)	2576	
Crystal size	0.26 x 0.06 x 0.06 mm^3	
Theta range for data collection	2.61 to 65.56°.	
Index ranges	-7<=h<=11, -20<=k<=20, -35<=l<=39	
Reflections collected	36647	
Independent reflections	9635 [R(int) = 0.0504]	
Completeness to theta = 65.56°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6290	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9635 / 6 / 774	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0772, wR2 = 0.2137	
R indices (all data)	R1 = 0.1043, wR2 = 0.2370	
Largest diff. peak and hole	1.042 and -1.491 e.Å^{-3}	

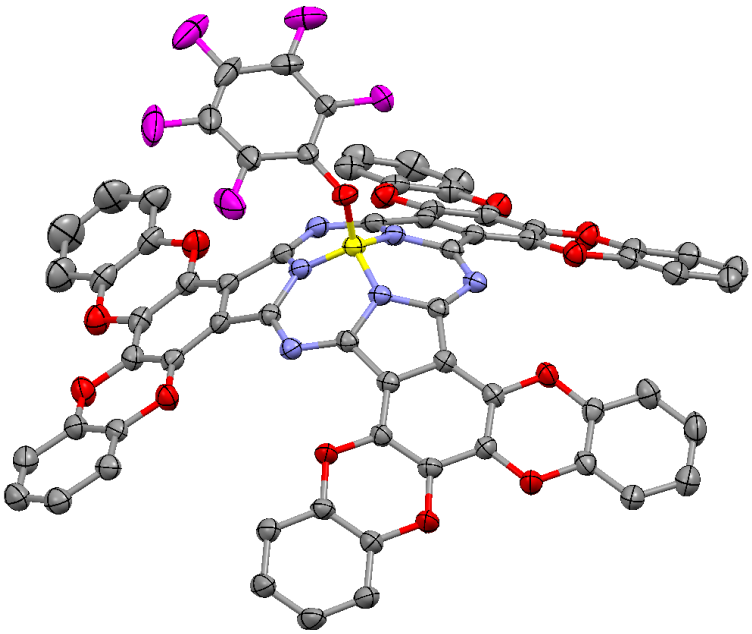

Figure S21. Thermal ellipsoid plot of (a) 3b•$(THF)_2$ (CCDC deposition 910746). Thermal ellipsoids are set at the 50% probability level. Hydrogen atoms and included solvent have been omitted for clarity. Colors: boron – yellow; nitrogen – blue; carbon – grey; oxygen – red; fluorine – magenta.

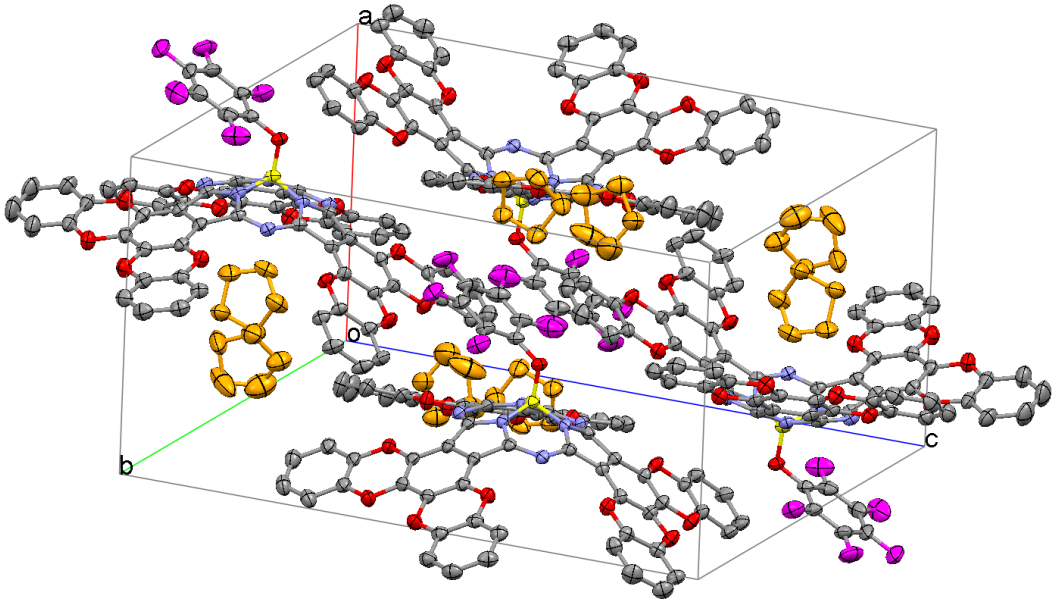

Figure S22. Populated unit cell of (a) 3b•$(THF)_2$ (CCDC deposition 910746). Thermal ellipsoids are set at the 50% probability level. Hydrogen atoms have been omitted for clarity. Colors: boron – yellow; nitrogen – blue; carbon – grey; oxygen – red; fluorine – magenta; THF molecules – orange.

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b·(THF)$_2$** (CCDC deposition 910746). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	10266(1)	8196(1)	1103(1)	69(1)
F(2)	11427(2)	8471(1)	162(1)	83(1)
F(3)	12201(1)	7514(1)	-504(1)	79(1)
F(4)	11780(1)	6284(1)	-220(1)	70(1)
F(5)	10556(1)	6013(1)	699(1)	57(1)
O(1)	7463(2)	7911(1)	-874(1)	45(1)
O(2)	6691(2)	9193(1)	-995(1)	45(1)
O(3)	6435(2)	9917(1)	-82(1)	45(1)
O(4)	6889(1)	9438(1)	1053(1)	37(1)
O(5)	6425(1)	8516(1)	2861(1)	36(1)
O(6)	5193(2)	7915(1)	3743(1)	41(1)
O(7)	5201(2)	6679(1)	3867(1)	41(1)
O(8)	6287(1)	5873(1)	3067(1)	36(1)
O(9)	6649(1)	4591(1)	1495(1)	36(1)
O(10)	5726(1)	3997(1)	481(1)	40(1)
O(11)	5917(1)	4521(1)	-534(1)	41(1)
O(12)	7005(1)	5720(1)	-663(1)	38(1)
O(13)	9747(1)	6979(1)	1385(1)	35(1)
N(1)	8113(2)	7511(1)	917(1)	29(1)
N(2)	7494(2)	8149(1)	1690(1)	29(1)
N(3)	7947(2)	7050(1)	1839(1)	28(1)
N(4)	7425(2)	5956(1)	1888(1)	30(1)
N(5)	8075(2)	6395(1)	1014(1)	29(1)
N(6)	7837(2)	6865(1)	85(1)	32(1)
C(1)	7917(2)	7441(1)	341(1)	31(1)
C(2)	7561(2)	8065(1)	137(1)	31(1)
C(3)	7296(2)	8296(1)	-409(1)	34(1)
C(4)	7324(2)	8199(1)	-1410(1)	41(1)
C(5)	7558(2)	7845(1)	-1886(1)	53(1)
C(6)	7372(3)	8102(2)	-2427(1)	69(1)
C(7)	6971(4)	8708(2)	-2486(2)	81(1)
C(8)	6751(3)	9075(2)	-2002(1)	62(1)
C(9)	6929(2)	8817(1)	-1466(1)	44(1)
C(10)	6916(2)	8919(1)	-464(1)	36(1)
C(11)	6789(2)	9301(1)	19(1)	35(1)
C(12)	6350(2)	10299(1)	405(1)	37(1)
C(13)	6042(2)	10928(1)	327(1)	46(1)
C(14)	5932(2)	11319(1)	802(1)	47(1)
C(15)	6123(2)	11085(1)	1347(1)	44(1)
C(16)	6442(2)	10454(1)	1429(1)	38(1)
C(17)	6558(2)	10066(1)	956(1)	35(1)
C(18)	7028(2)	9076(1)	570(1)	31(1)
C(19)	7431(2)	8457(1)	632(1)	30(1)
C(20)	7725(2)	8075(1)	1136(1)	29(1)
C(21)	7531(2)	7624(1)	2022(1)	28(1)
C(22)	6949(2)	7486(1)	2545(1)	29(1)
C(23)	6382(2)	7866(1)	2922(1)	29(1)

C(24)	5793(2)	8863(1)	3240(1)	32(1)
C(25)	5781(2)	9518(1)	3182(1)	37(1)
C(26)	5136(2)	9877(1)	3541(1)	44(1)
C(27)	4512(2)	9585(1)	3950(1)	46(1)
C(28)	4526(2)	8930(1)	4012(1)	40(1)
C(29)	5178(2)	8572(1)	3657(1)	34(1)
C(30)	5792(2)	7577(1)	3354(1)	32(1)
C(31)	5773(2)	6914(1)	3413(1)	32(1)
C(32)	5140(2)	6020(1)	3898(1)	34(1)
C(33)	4536(2)	5759(1)	4332(1)	39(1)
C(34)	4421(2)	5105(1)	4366(1)	51(1)
C(35)	4945(3)	4718(1)	3979(1)	53(1)
C(36)	5568(2)	4979(1)	3551(1)	43(1)
C(37)	5665(2)	5630(1)	3508(1)	33(1)
C(38)	6318(2)	6527(1)	3034(1)	30(1)
C(39)	6927(2)	6807(1)	2600(1)	28(1)
C(40)	7496(2)	6541(1)	2120(1)	28(1)
C(41)	7643(2)	5905(1)	1327(1)	30(1)
C(42)	7246(2)	5444(1)	902(1)	29(1)
C(43)	6719(2)	4858(1)	958(1)	31(1)
C(44)	6104(2)	4005(1)	1515(1)	35(1)
C(45)	6004(2)	3722(1)	2044(1)	39(1)
C(46)	5449(2)	3146(1)	2086(1)	45(1)
C(47)	5003(2)	2860(1)	1593(1)	47(1)
C(48)	5100(2)	3150(1)	1062(1)	45(1)
C(49)	5658(2)	3720(1)	1024(1)	36(1)
C(50)	6285(2)	4570(1)	468(1)	33(1)
C(51)	6381(2)	4850(1)	-73(1)	33(1)
C(52)	6037(2)	4804(1)	-1071(1)	37(1)
C(53)	5590(2)	4496(1)	-1547(1)	46(1)
C(54)	5714(2)	4759(1)	-2086(1)	52(1)
C(55)	6276(2)	5324(1)	-2152(1)	49(1)
C(56)	6710(2)	5639(1)	-1672(1)	41(1)
C(57)	6587(2)	5380(1)	-1134(1)	34(1)
C(58)	6911(2)	5430(1)	-138(1)	31(1)
C(59)	7353(2)	5727(1)	349(1)	31(1)
C(60)	7833(2)	6358(1)	437(1)	31(1)
C(61)	10362(2)	7099(1)	919(1)	33(1)
C(62)	10623(2)	7714(1)	765(1)	45(1)
C(63)	11207(2)	7864(1)	299(2)	52(1)
C(64)	11589(2)	7387(2)	-45(1)	53(1)
C(65)	11387(2)	6753(1)	97(1)	46(1)
C(66)	10765(2)	6621(1)	577(1)	36(1)
B(1)	8537(2)	6984(1)	1294(1)	30(1)
O(1S)	5577(2)	6961(1)	1230(1)	62(1)
C(1S)	5296(3)	7041(2)	636(2)	67(1)
C(2S)	4103(2)	7214(2)	576(1)	57(1)
C(3S)	3687(3)	7184(2)	1182(1)	64(1)
C(4S)	4735(3)	7255(2)	1547(2)	67(1)
O(2S)	2839(3)	8676(2)	1863(2)	111(1)
C(5S)	2939(4)	9047(2)	1364(2)	126(2)
C(6S)	4166(3)	9064(2)	1258(2)	96(1)
C(7S)	4643(3)	9101(2)	1849(2)	72(1)

C(8S)	3779(3)	8797(2)	2211(2)	74(1)

Table S3. Bond lengths [Å] and angles [°] for **3b·(THF)$_2$** (CCDC deposition 910746).

F(1)-C(62)	1.356(3)
F(2)-C(63)	1.340(3)
F(3)-C(64)	1.341(3)
F(4)-C(65)	1.324(3)
F(5)-C(66)	1.331(3)
O(1)-C(3)	1.367(3)
O(1)-C(4)	1.388(3)
O(2)-C(10)	1.379(3)
O(2)-C(9)	1.384(3)
O(3)-C(11)	1.377(3)
O(3)-C(12)	1.390(3)
O(4)-C(18)	1.368(3)
O(4)-C(17)	1.394(3)
O(5)-C(23)	1.372(3)
O(5)-C(24)	1.388(3)
O(6)-C(30)	1.370(3)
O(6)-C(29)	1.391(3)
O(7)-C(31)	1.368(3)
O(7)-C(32)	1.386(3)
O(8)-C(38)	1.374(3)
O(8)-C(37)	1.383(3)
O(9)-C(43)	1.368(3)
O(9)-C(44)	1.396(3)
O(10)-C(50)	1.379(3)
O(10)-C(49)	1.390(3)
O(11)-C(51)	1.378(3)
O(11)-C(52)	1.391(3)
O(12)-C(58)	1.369(3)
O(12)-C(57)	1.386(3)
O(13)-C(61)	1.353(3)
O(13)-B(1)	1.470(3)
N(1)-C(1)	1.357(3)
N(1)-C(20)	1.374(3)
N(1)-B(1)	1.489(3)
N(2)-C(20)	1.331(3)
N(2)-C(21)	1.344(3)
N(3)-C(40)	1.370(3)
N(3)-C(21)	1.376(3)
N(3)-B(1)	1.477(3)
N(4)-C(41)	1.340(3)
N(4)-C(40)	1.341(3)
N(5)-C(60)	1.364(3)
N(5)-C(41)	1.369(3)
N(5)-B(1)	1.495(3)
N(6)-C(60)	1.340(3)
N(6)-C(1)	1.349(3)
C(1)-C(2)	1.452(3)
C(2)-C(3)	1.382(3)
C(2)-C(19)	1.425(3)
C(3)-C(10)	1.390(3)
C(4)-C(5)	1.365(4)

C(4)-C(9)	1.384(4)
C(5)-C(6)	1.378(4)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.365(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.394(5)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.367(4)
C(8)-H(8A)	0.9500
C(10)-C(11)	1.387(4)
C(11)-C(18)	1.384(3)
C(12)-C(13)	1.380(3)
C(12)-C(17)	1.384(4)
C(13)-C(14)	1.381(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.369(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.391(3)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.373(3)
C(16)-H(16A)	0.9500
C(18)-C(19)	1.392(3)
C(19)-C(20)	1.453(3)
C(21)-C(22)	1.449(3)
C(22)-C(23)	1.379(3)
C(22)-C(39)	1.430(3)
C(23)-C(30)	1.386(3)
C(24)-C(29)	1.379(3)
C(24)-C(25)	1.379(3)
C(25)-C(26)	1.381(3)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.373(4)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.382(3)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.378(3)
C(28)-H(28A)	0.9500
C(30)-C(31)	1.398(3)
C(31)-C(38)	1.379(3)
C(32)-C(33)	1.375(3)
C(32)-C(37)	1.387(3)
C(33)-C(34)	1.380(3)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.379(4)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.379(4)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.374(3)
C(36)-H(36A)	0.9500
C(38)-C(39)	1.392(3)
C(39)-C(40)	1.439(3)
C(41)-C(42)	1.451(3)
C(42)-C(43)	1.393(3)

C(42)-C(59)	1.423(3)
C(43)-C(50)	1.377(3)
C(44)-C(45)	1.370(4)
C(44)-C(49)	1.380(3)
C(45)-C(46)	1.387(3)
C(45)-H(45A)	0.9500
C(46)-C(47)	1.384(4)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.382(4)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.377(3)
C(48)-H(48A)	0.9500
C(50)-C(51)	1.392(3)
C(51)-C(58)	1.385(3)
C(52)-C(53)	1.375(4)
C(52)-C(57)	1.389(3)
C(53)-C(54)	1.378(4)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.375(4)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.385(4)
C(55)-H(55A)	0.9500
C(56)-C(57)	1.372(3)
C(56)-H(56A)	0.9500
C(58)-C(59)	1.381(3)
C(59)-C(60)	1.457(3)
C(61)-C(66)	1.377(3)
C(61)-C(62)	1.377(3)
C(62)-C(63)	1.345(4)
C(63)-C(64)	1.368(4)
C(64)-C(65)	1.393(4)
C(65)-C(66)	1.389(4)
O(1S)-C(4S)	1.413(4)
O(1S)-C(1S)	1.419(4)
C(1S)-C(2S)	1.488(4)
C(1S)-H(1SA)	0.9900
C(1S)-H(1SB)	0.9900
C(2S)-C(3S)	1.507(4)
C(2S)-H(2SA)	0.9900
C(2S)-H(2SB)	0.9900
C(3S)-C(4S)	1.509(4)
C(3S)-H(3SA)	0.9900
C(3S)-H(3SB)	0.9900
C(4S)-H(4SA)	0.9900
C(4S)-H(4SB)	0.9900
O(2S)-C(8S)	1.397(4)
O(2S)-C(5S)	1.402(5)
C(5S)-C(6S)	1.511(6)
C(5S)-H(5SA)	0.9900
C(5S)-H(5SB)	0.9900
C(6S)-C(7S)	1.472(5)
C(6S)-H(6SA)	0.9900
C(6S)-H(6SB)	0.9900

C(7S)-C(8S)	1.501(5)
C(7S)-H(7SA)	0.9900
C(7S)-H(7SB)	0.9900
C(8S)-H(8SA)	0.9900
C(8S)-H(8SB)	0.9900

C(3)-O(1)-C(4)	115.71(19)
C(10)-O(2)-C(9)	115.27(19)
C(11)-O(3)-C(12)	115.71(19)
C(18)-O(4)-C(17)	115.77(19)
C(23)-O(5)-C(24)	115.64(18)
C(30)-O(6)-C(29)	115.00(18)
C(31)-O(7)-C(32)	115.27(18)
C(38)-O(8)-C(37)	115.22(18)
C(43)-O(9)-C(44)	115.63(18)
C(50)-O(10)-C(49)	115.30(19)
C(51)-O(11)-C(52)	115.43(18)
C(58)-O(12)-C(57)	115.72(18)
C(61)-O(13)-B(1)	116.78(19)
C(1)-N(1)-C(20)	113.88(19)
C(1)-N(1)-B(1)	122.95(18)
C(20)-N(1)-B(1)	122.4(2)
C(20)-N(2)-C(21)	116.86(18)
C(40)-N(3)-C(21)	112.39(18)
C(40)-N(3)-B(1)	122.82(18)
C(21)-N(3)-B(1)	122.38(19)
C(41)-N(4)-C(40)	116.66(19)
C(60)-N(5)-C(41)	113.78(18)
C(60)-N(5)-B(1)	122.57(19)
C(41)-N(5)-B(1)	122.2(2)
C(60)-N(6)-C(1)	116.4(2)
N(6)-C(1)-N(1)	122.5(2)
N(6)-C(1)-C(2)	130.4(2)
N(1)-C(1)-C(2)	105.36(18)
C(3)-C(2)-C(19)	120.4(2)
C(3)-C(2)-C(1)	132.2(2)
C(19)-C(2)-C(1)	107.2(2)
O(1)-C(3)-C(2)	118.7(2)
O(1)-C(3)-C(10)	122.6(2)
C(2)-C(3)-C(10)	118.7(2)
C(5)-C(4)-C(9)	120.8(3)
C(5)-C(4)-O(1)	117.7(2)
C(9)-C(4)-O(1)	121.5(2)
C(4)-C(5)-C(6)	119.4(3)
C(4)-C(5)-H(5A)	120.3
C(6)-C(5)-H(5A)	120.3
C(7)-C(6)-C(5)	120.1(3)
C(7)-C(6)-H(6A)	119.9
C(5)-C(6)-H(6A)	119.9
C(6)-C(7)-C(8)	120.6(3)
C(6)-C(7)-H(7A)	119.7
C(8)-C(7)-H(7A)	119.7
C(9)-C(8)-C(7)	119.0(3)

C(9)-C(8)-H(8A)	120.5
C(7)-C(8)-H(8A)	120.5
C(8)-C(9)-O(2)	117.4(2)
C(8)-C(9)-C(4)	120.0(3)
O(2)-C(9)-C(4)	122.6(2)
O(2)-C(10)-C(11)	117.1(2)
O(2)-C(10)-C(3)	121.9(2)
C(11)-C(10)-C(3)	120.9(2)
O(3)-C(11)-C(18)	122.1(2)
O(3)-C(11)-C(10)	116.5(2)
C(18)-C(11)-C(10)	121.4(2)
C(13)-C(12)-C(17)	119.9(2)
C(13)-C(12)-O(3)	118.1(2)
C(17)-C(12)-O(3)	122.0(2)
C(12)-C(13)-C(14)	119.6(3)
C(12)-C(13)-H(13A)	120.2
C(14)-C(13)-H(13A)	120.2
C(15)-C(14)-C(13)	120.4(2)
C(15)-C(14)-H(14A)	119.8
C(13)-C(14)-H(14A)	119.8
C(14)-C(15)-C(16)	120.3(3)
C(14)-C(15)-H(15A)	119.9
C(16)-C(15)-H(15A)	119.9
C(17)-C(16)-C(15)	119.3(3)
C(17)-C(16)-H(16A)	120.4
C(15)-C(16)-H(16A)	120.4
C(16)-C(17)-C(12)	120.5(2)
C(16)-C(17)-O(4)	117.8(2)
C(12)-C(17)-O(4)	121.7(2)
O(4)-C(18)-C(11)	122.6(2)
O(4)-C(18)-C(19)	118.9(2)
C(11)-C(18)-C(19)	118.5(2)
C(18)-C(19)-C(2)	120.1(2)
C(18)-C(19)-C(20)	132.4(2)
C(2)-C(19)-C(20)	107.41(19)
N(2)-C(20)-N(1)	122.8(2)
N(2)-C(20)-C(19)	131.1(2)
N(1)-C(20)-C(19)	104.80(19)
N(2)-C(21)-N(3)	123.1(2)
N(2)-C(21)-C(22)	129.4(2)
N(3)-C(21)-C(22)	105.85(18)
C(23)-C(22)-C(39)	120.5(2)
C(23)-C(22)-C(21)	132.6(2)
C(39)-C(22)-C(21)	106.56(19)
O(5)-C(23)-C(22)	119.2(2)
O(5)-C(23)-C(30)	122.0(2)
C(22)-C(23)-C(30)	118.8(2)
C(29)-C(24)-C(25)	120.4(2)
C(29)-C(24)-O(5)	122.01(19)
C(25)-C(24)-O(5)	117.6(2)
C(24)-C(25)-C(26)	119.1(2)
C(24)-C(25)-H(25A)	120.4
C(26)-C(25)-H(25A)	120.4

C(27)-C(26)-C(25)	120.4(2)
C(27)-C(26)-H(26A)	119.8
C(25)-C(26)-H(26A)	119.8
C(26)-C(27)-C(28)	120.6(2)
C(26)-C(27)-H(27A)	119.7
C(28)-C(27)-H(27A)	119.7
C(29)-C(28)-C(27)	119.1(2)
C(29)-C(28)-H(28A)	120.5
C(27)-C(28)-H(28A)	120.5
C(28)-C(29)-C(24)	120.4(2)
C(28)-C(29)-O(6)	117.3(2)
C(24)-C(29)-O(6)	122.3(2)
O(6)-C(30)-C(23)	122.9(2)
O(6)-C(30)-C(31)	116.1(2)
C(23)-C(30)-C(31)	121.0(2)
O(7)-C(31)-C(38)	122.7(2)
O(7)-C(31)-C(30)	116.3(2)
C(38)-C(31)-C(30)	120.9(2)
C(33)-C(32)-O(7)	117.7(2)
C(33)-C(32)-C(37)	120.4(2)
O(7)-C(32)-C(37)	121.9(2)
C(32)-C(33)-C(34)	119.6(3)
C(32)-C(33)-H(33A)	120.2
C(34)-C(33)-H(33A)	120.2
C(35)-C(34)-C(33)	119.9(3)
C(35)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
C(36)-C(35)-C(34)	120.4(2)
C(36)-C(35)-H(35A)	119.8
C(34)-C(35)-H(35A)	119.8
C(37)-C(36)-C(35)	119.8(3)
C(37)-C(36)-H(36A)	120.1
C(35)-C(36)-H(36A)	120.1
C(36)-C(37)-O(8)	117.9(2)
C(36)-C(37)-C(32)	119.8(2)
O(8)-C(37)-C(32)	122.2(2)
O(8)-C(38)-C(31)	122.5(2)
O(8)-C(38)-C(39)	118.5(2)
C(31)-C(38)-C(39)	119.0(2)
C(38)-C(39)-C(22)	119.7(2)
C(38)-C(39)-C(40)	132.2(2)
C(22)-C(39)-C(40)	107.76(19)
N(4)-C(40)-N(3)	123.0(2)
N(4)-C(40)-C(39)	129.5(2)
N(3)-C(40)-C(39)	105.81(17)
N(4)-C(41)-N(5)	122.94(19)
N(4)-C(41)-C(42)	129.9(2)
N(5)-C(41)-C(42)	105.3(2)
C(43)-C(42)-C(59)	120.4(2)
C(43)-C(42)-C(41)	131.9(2)
C(59)-C(42)-C(41)	107.32(19)
O(9)-C(43)-C(50)	122.6(2)
O(9)-C(43)-C(42)	119.1(2)

C(50)-C(43)-C(42)	118.2(2)
C(45)-C(44)-C(49)	120.5(2)
C(45)-C(44)-O(9)	117.8(2)
C(49)-C(44)-O(9)	121.7(2)
C(44)-C(45)-C(46)	119.8(3)
C(44)-C(45)-H(45A)	120.1
C(46)-C(45)-H(45A)	120.1
C(47)-C(46)-C(45)	119.7(3)
C(47)-C(46)-H(46A)	120.1
C(45)-C(46)-H(46A)	120.1
C(48)-C(47)-C(46)	120.2(2)
C(48)-C(47)-H(47A)	119.9
C(46)-C(47)-H(47A)	119.9
C(49)-C(48)-C(47)	119.6(3)
C(49)-C(48)-H(48A)	120.2
C(47)-C(48)-H(48A)	120.2
C(48)-C(49)-C(44)	120.2(2)
C(48)-C(49)-O(10)	117.6(2)
C(44)-C(49)-O(10)	122.2(2)
C(43)-C(50)-O(10)	122.5(2)
C(43)-C(50)-C(51)	121.3(2)
O(10)-C(50)-C(51)	116.2(2)
O(11)-C(51)-C(58)	122.3(2)
O(11)-C(51)-C(50)	116.4(2)
C(58)-C(51)-C(50)	121.3(2)
C(53)-C(52)-C(57)	120.1(2)
C(53)-C(52)-O(11)	117.9(2)
C(57)-C(52)-O(11)	121.9(2)
C(52)-C(53)-C(54)	119.3(3)
C(52)-C(53)-H(53A)	120.4
C(54)-C(53)-H(53A)	120.4
C(55)-C(54)-C(53)	120.8(3)
C(55)-C(54)-H(54A)	119.6
C(53)-C(54)-H(54A)	119.6
C(54)-C(55)-C(56)	119.9(3)
C(54)-C(55)-H(55A)	120.1
C(56)-C(55)-H(55A)	120.1
C(57)-C(56)-C(55)	119.5(3)
C(57)-C(56)-H(56A)	120.2
C(55)-C(56)-H(56A)	120.2
C(56)-C(57)-O(12)	117.8(2)
C(56)-C(57)-C(52)	120.3(2)
O(12)-C(57)-C(52)	121.9(2)
O(12)-C(58)-C(59)	119.1(2)
O(12)-C(58)-C(51)	122.6(2)
C(59)-C(58)-C(51)	118.4(2)
C(58)-C(59)-C(42)	120.4(2)
C(58)-C(59)-C(60)	131.8(2)
C(42)-C(59)-C(60)	107.3(2)
N(6)-C(60)-N(5)	123.2(2)
N(6)-C(60)-C(59)	130.1(2)
N(5)-C(60)-C(59)	105.21(19)
O(13)-C(61)-C(66)	122.4(2)

O(13)-C(61)-C(62)	121.2(2)
C(66)-C(61)-C(62)	116.4(2)
C(63)-C(62)-F(1)	118.3(2)
C(63)-C(62)-C(61)	123.8(3)
F(1)-C(62)-C(61)	117.8(2)
F(2)-C(63)-C(62)	121.6(3)
F(2)-C(63)-C(64)	118.9(3)
C(62)-C(63)-C(64)	119.5(2)
F(3)-C(64)-C(63)	121.4(3)
F(3)-C(64)-C(65)	118.8(3)
C(63)-C(64)-C(65)	119.7(3)
F(4)-C(65)-C(66)	120.6(2)
F(4)-C(65)-C(64)	120.5(3)
C(66)-C(65)-C(64)	118.9(3)
F(5)-C(66)-C(61)	120.2(2)
F(5)-C(66)-C(65)	118.1(2)
C(61)-C(66)-C(65)	121.7(2)
O(13)-B(1)-N(3)	112.3(2)
O(13)-B(1)-N(1)	114.39(19)
N(3)-B(1)-N(1)	105.48(18)
O(13)-B(1)-N(5)	114.38(19)
N(3)-B(1)-N(5)	105.36(19)
N(1)-B(1)-N(5)	104.0(2)
C(4S)-O(1S)-C(1S)	107.4(2)
O(1S)-C(1S)-C(2S)	108.7(3)
O(1S)-C(1S)-H(1SA)	109.9
C(2S)-C(1S)-H(1SA)	109.9
O(1S)-C(1S)-H(1SB)	109.9
C(2S)-C(1S)-H(1SB)	109.9
H(1SA)-C(1S)-H(1SB)	108.3
C(1S)-C(2S)-C(3S)	104.6(3)
C(1S)-C(2S)-H(2SA)	110.8
C(3S)-C(2S)-H(2SA)	110.8
C(1S)-C(2S)-H(2SB)	110.8
C(3S)-C(2S)-H(2SB)	110.8
H(2SA)-C(2S)-H(2SB)	108.9
C(2S)-C(3S)-C(4S)	102.8(3)
C(2S)-C(3S)-H(3SA)	111.2
C(4S)-C(3S)-H(3SA)	111.2
C(2S)-C(3S)-H(3SB)	111.2
C(4S)-C(3S)-H(3SB)	111.2
H(3SA)-C(3S)-H(3SB)	109.1
O(1S)-C(4S)-C(3S)	105.7(3)
O(1S)-C(4S)-H(4SA)	110.6
C(3S)-C(4S)-H(4SA)	110.6
O(1S)-C(4S)-H(4SB)	110.6
C(3S)-C(4S)-H(4SB)	110.6
H(4SA)-C(4S)-H(4SB)	108.7
C(8S)-O(2S)-C(5S)	106.6(3)
O(2S)-C(5S)-C(6S)	105.0(3)
O(2S)-C(5S)-H(5SA)	110.8
C(6S)-C(5S)-H(5SA)	110.8
O(2S)-C(5S)-H(5SB)	110.8

C(6S)-C(5S)-H(5SB)	110.8
H(5SA)-C(5S)-H(5SB)	108.8
C(7S)-C(6S)-C(5S)	102.0(4)
C(7S)-C(6S)-H(6SA)	111.4
C(5S)-C(6S)-H(6SA)	111.4
C(7S)-C(6S)-H(6SB)	111.4
C(5S)-C(6S)-H(6SB)	111.4
H(6SA)-C(6S)-H(6SB)	109.2
C(6S)-C(7S)-C(8S)	103.9(3)
C(6S)-C(7S)-H(7SA)	111.0
C(8S)-C(7S)-H(7SA)	111.0
C(6S)-C(7S)-H(7SB)	111.0
C(8S)-C(7S)-H(7SB)	111.0
H(7SA)-C(7S)-H(7SB)	109.0
O(2S)-C(8S)-C(7S)	108.7(3)
O(2S)-C(8S)-H(8SA)	109.9
C(7S)-C(8S)-H(8SA)	109.9
O(2S)-C(8S)-H(8SB)	109.9
C(7S)-C(8S)-H(8SB)	109.9
H(8SA)-C(8S)-H(8SB)	108.3

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3b·(THF)$_2$** (CCDC deposition 910746). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	56(1)	30(1)	123(2)	-15(1)	8(1)	-5(1)
F(2)	64(1)	57(1)	127(2)	47(1)	0(1)	-19(1)
F(3)	45(1)	130(2)	62(1)	39(1)	13(1)	-12(1)
F(4)	51(1)	89(1)	70(1)	-19(1)	21(1)	14(1)
F(5)	57(1)	26(1)	88(1)	5(1)	25(1)	5(1)
O(1)	62(1)	43(1)	30(1)	-4(1)	7(1)	-2(1)
O(2)	57(1)	43(1)	34(1)	3(1)	3(1)	-1(1)
O(3)	60(1)	34(1)	40(1)	5(1)	3(1)	4(1)
O(4)	48(1)	27(1)	36(1)	-1(1)	4(1)	2(1)
O(5)	43(1)	26(1)	39(1)	-2(1)	17(1)	3(1)
O(6)	52(1)	28(1)	44(1)	2(1)	22(1)	9(1)
O(7)	51(1)	29(1)	42(1)	4(1)	18(1)	4(1)
O(8)	46(1)	24(1)	38(1)	0(1)	6(1)	2(1)
O(9)	40(1)	31(1)	37(1)	-2(1)	3(1)	-3(1)
O(10)	45(1)	34(1)	41(1)	-6(1)	4(1)	-11(1)
O(11)	47(1)	41(1)	36(1)	-7(1)	2(1)	-8(1)
O(12)	40(1)	40(1)	34(1)	-6(1)	7(1)	-4(1)
O(13)	24(1)	41(1)	41(1)	-1(1)	5(1)	-1(1)
N(1)	27(1)	29(1)	32(1)	-4(1)	7(1)	-1(1)
N(2)	29(1)	28(1)	31(1)	-4(1)	4(1)	-2(1)
N(3)	25(1)	28(1)	31(1)	-4(1)	3(1)	2(1)
N(4)	29(1)	29(1)	34(1)	-3(1)	2(1)	4(1)
N(5)	27(1)	29(1)	31(1)	-5(1)	6(1)	2(1)
N(6)	30(1)	32(1)	34(1)	-4(1)	9(1)	-1(1)
C(1)	27(1)	34(1)	33(1)	-4(1)	9(1)	-2(1)
C(2)	29(1)	32(1)	33(1)	-4(1)	8(1)	-6(1)
C(3)	36(1)	34(1)	34(2)	-3(1)	8(1)	-8(1)
C(4)	42(2)	50(2)	32(2)	1(1)	9(1)	-10(1)
C(5)	57(2)	63(2)	39(2)	-6(1)	13(1)	-4(1)
C(6)	92(3)	81(2)	36(2)	-7(2)	17(2)	7(2)
C(7)	107(3)	99(3)	36(2)	10(2)	10(2)	9(2)
C(8)	77(2)	68(2)	41(2)	9(2)	8(2)	1(2)
C(9)	44(2)	54(2)	33(2)	2(1)	7(1)	-11(1)
C(10)	35(1)	40(1)	33(1)	6(1)	2(1)	-7(1)
C(11)	34(1)	30(1)	41(2)	3(1)	3(1)	-3(1)
C(12)	38(1)	31(1)	43(2)	-2(1)	7(1)	-2(1)
C(13)	47(2)	39(1)	52(2)	9(1)	4(1)	-1(1)
C(14)	47(2)	33(1)	63(2)	-2(1)	7(1)	1(1)
C(15)	41(2)	38(1)	54(2)	-7(1)	6(1)	-2(1)
C(16)	35(1)	34(1)	45(2)	-5(1)	3(1)	-2(1)
C(17)	30(1)	29(1)	46(2)	1(1)	5(1)	-2(1)
C(18)	30(1)	32(1)	32(1)	-3(1)	6(1)	-6(1)
C(19)	28(1)	29(1)	34(1)	0(1)	7(1)	-5(1)
C(20)	25(1)	26(1)	35(1)	-4(1)	4(1)	-3(1)
C(21)	27(1)	25(1)	34(1)	-5(1)	1(1)	-1(1)
C(22)	26(1)	29(1)	32(1)	-3(1)	1(1)	1(1)
C(23)	34(1)	25(1)	30(1)	-2(1)	3(1)	2(1)
C(24)	31(1)	30(1)	36(1)	-7(1)	7(1)	3(1)

C(25)	35(1)	30(1)	47(2)	-4(1)	10(1)	-4(1)
C(26)	40(2)	26(1)	66(2)	-10(1)	17(1)	-3(1)
C(27)	40(2)	34(1)	65(2)	-16(1)	21(1)	-2(1)
C(28)	36(1)	37(1)	49(2)	-3(1)	16(1)	0(1)
C(29)	36(1)	28(1)	39(2)	-2(1)	7(1)	1(1)
C(30)	33(1)	32(1)	33(1)	-2(1)	7(1)	5(1)
C(31)	32(1)	31(1)	31(1)	3(1)	6(1)	3(1)
C(32)	34(1)	29(1)	39(2)	4(1)	-3(1)	3(1)
C(33)	36(1)	37(1)	45(2)	8(1)	6(1)	2(1)
C(34)	52(2)	43(2)	57(2)	11(1)	9(1)	-5(1)
C(35)	65(2)	33(1)	62(2)	11(1)	5(2)	-8(1)
C(36)	52(2)	31(1)	47(2)	-3(1)	-1(1)	-1(1)
C(37)	35(1)	35(1)	31(1)	6(1)	-2(1)	-2(1)
C(38)	33(1)	26(1)	30(1)	0(1)	-1(1)	2(1)
C(39)	29(1)	28(1)	28(1)	-1(1)	-1(1)	2(1)
C(40)	25(1)	28(1)	32(1)	0(1)	0(1)	3(1)
C(41)	23(1)	30(1)	36(1)	-1(1)	2(1)	5(1)
C(42)	26(1)	29(1)	33(1)	-5(1)	5(1)	4(1)
C(43)	28(1)	29(1)	36(2)	-3(1)	6(1)	4(1)
C(44)	28(1)	28(1)	49(2)	-2(1)	6(1)	3(1)
C(45)	36(1)	37(1)	45(2)	1(1)	2(1)	5(1)
C(46)	38(2)	42(1)	56(2)	11(1)	3(1)	1(1)
C(47)	42(2)	36(1)	63(2)	4(1)	5(1)	-6(1)
C(48)	39(2)	38(1)	57(2)	-6(1)	4(1)	-6(1)
C(49)	33(1)	32(1)	43(2)	-1(1)	6(1)	3(1)
C(50)	31(1)	28(1)	40(2)	-6(1)	5(1)	0(1)
C(51)	30(1)	33(1)	36(2)	-11(1)	4(1)	0(1)
C(52)	34(1)	40(1)	36(2)	-6(1)	4(1)	5(1)
C(53)	46(2)	45(1)	46(2)	-9(1)	-8(1)	5(1)
C(54)	58(2)	56(2)	40(2)	-12(1)	-9(1)	7(1)
C(55)	52(2)	58(2)	38(2)	-3(1)	-1(1)	9(1)
C(56)	38(1)	46(1)	39(2)	-5(1)	3(1)	5(1)
C(57)	30(1)	41(1)	33(1)	-8(1)	4(1)	6(1)
C(58)	28(1)	33(1)	32(1)	-3(1)	8(1)	4(1)
C(59)	27(1)	30(1)	35(1)	-8(1)	8(1)	4(1)
C(60)	26(1)	34(1)	35(1)	-5(1)	9(1)	3(1)
C(61)	23(1)	28(1)	47(2)	1(1)	4(1)	0(1)
C(62)	30(1)	33(1)	73(2)	7(1)	3(1)	-2(1)
C(63)	37(2)	41(2)	79(2)	22(2)	1(2)	-2(1)
C(64)	31(2)	79(2)	49(2)	30(2)	5(1)	-11(1)
C(65)	30(1)	59(2)	49(2)	-5(1)	8(1)	10(1)
C(66)	30(1)	27(1)	52(2)	6(1)	9(1)	3(1)
B(1)	25(1)	29(1)	36(2)	-2(1)	4(1)	1(1)
O(1S)	43(1)	60(1)	83(2)	-8(1)	-17(1)	10(1)
C(1S)	39(2)	85(2)	79(3)	6(2)	5(2)	-2(2)
C(2S)	44(2)	68(2)	58(2)	-4(2)	1(2)	13(1)
C(3S)	46(2)	89(2)	56(2)	1(2)	-1(2)	19(2)
C(4S)	61(2)	71(2)	67(2)	-14(2)	-15(2)	20(2)
O(2S)	90(2)	117(2)	129(3)	-28(2)	22(2)	-23(2)
C(5S)	84(3)	124(4)	166(5)	73(4)	-60(3)	-30(3)
C(6S)	67(3)	150(4)	70(3)	51(3)	-18(2)	-14(2)
C(7S)	58(2)	68(2)	91(3)	21(2)	6(2)	0(2)
C(8S)	57(2)	83(2)	81(3)	-17(2)	11(2)	-11(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3b·(THF)$_2$** (CCDC deposition 910746).

	x	y	z	U(eq)
H(5A)	7846	7426	-1844	63
H(6A)	7523	7856	-2761	83
H(7A)	6841	8881	-2861	97
H(8A)	6480	9498	-2044	74
H(13A)	5906	11091	-51	55
H(14A)	5724	11752	749	57
H(15A)	6037	11356	1671	53
H(16A)	6578	10292	1807	46
H(25A)	6212	9719	2897	45
H(26A)	5123	10328	3504	52
H(27A)	4067	9836	4194	55
H(28A)	4092	8729	4294	48
H(33A)	4199	6027	4607	47
H(34A)	3981	4923	4656	61
H(35A)	4876	4267	4008	64
H(36A)	5930	4710	3286	52
H(45A)	6315	3920	2380	47
H(46A)	5374	2948	2451	54
H(47A)	4629	2463	1621	57
H(48A)	4783	2957	725	53
H(53A)	5200	4106	-1505	55
H(54A)	5408	4547	-2417	62
H(55A)	6365	5497	-2527	59
H(56A)	7091	6032	-1715	49
H(1SA)	5436	6641	424	81
H(1SB)	5756	7382	470	81
H(2SA)	3699	6909	322	68
H(2SB)	4013	7649	415	68
H(3SA)	3319	6772	1256	76
H(3SB)	3163	7536	1255	76
H(4SA)	4908	7711	1615	80
H(4SB)	4658	7041	1925	80
H(5SA)	2649	9482	1425	151
H(5SB)	2529	8850	1034	151
H(6SA)	4411	8674	1058	115
H(6SB)	4367	9443	1028	115
H(7SA)	4774	9550	1965	87
H(7SB)	5352	8864	1881	87
H(8SA)	4067	8394	2379	88
H(8SB)	3589	9086	2531	88

Table S6. Torsion angles [°] for **3b·(THF)$_2$** (CCDC deposition 910746).

C(60)-N(6)-C(1)-N(1)	7.5(3)
C(60)-N(6)-C(1)-C(2)	-155.0(2)
C(20)-N(1)-C(1)-N(6)	-154.3(2)
B(1)-N(1)-C(1)-N(6)	16.0(3)
C(20)-N(1)-C(1)-C(2)	12.0(2)
B(1)-N(1)-C(1)-C(2)	-177.71(19)
N(6)-C(1)-C(2)-C(3)	-18.5(4)
N(1)-C(1)-C(2)-C(3)	176.7(2)
N(6)-C(1)-C(2)-C(19)	157.4(2)
N(1)-C(1)-C(2)-C(19)	-7.4(2)
C(4)-O(1)-C(3)-C(2)	-171.6(2)
C(4)-O(1)-C(3)-C(10)	5.5(3)
C(19)-C(2)-C(3)-O(1)	178.1(2)
C(1)-C(2)-C(3)-O(1)	-6.4(4)
C(19)-C(2)-C(3)-C(10)	0.9(3)
C(1)-C(2)-C(3)-C(10)	176.3(2)
C(3)-O(1)-C(4)-C(5)	175.5(2)
C(3)-O(1)-C(4)-C(9)	-6.4(3)
C(9)-C(4)-C(5)-C(6)	-1.6(4)
O(1)-C(4)-C(5)-C(6)	176.4(3)
C(4)-C(5)-C(6)-C(7)	0.8(5)
C(5)-C(6)-C(7)-C(8)	0.3(6)
C(6)-C(7)-C(8)-C(9)	-0.8(6)
C(7)-C(8)-C(9)-O(2)	-179.3(3)
C(7)-C(8)-C(9)-C(4)	0.0(5)
C(10)-O(2)-C(9)-C(8)	-178.1(2)
C(10)-O(2)-C(9)-C(4)	2.6(3)
C(5)-C(4)-C(9)-C(8)	1.2(4)
O(1)-C(4)-C(9)-C(8)	-176.8(3)
C(5)-C(4)-C(9)-O(2)	-179.5(2)
O(1)-C(4)-C(9)-O(2)	2.5(4)
C(9)-O(2)-C(10)-C(11)	174.0(2)
C(9)-O(2)-C(10)-C(3)	-3.5(3)
O(1)-C(3)-C(10)-O(2)	-0.6(4)
C(2)-C(3)-C(10)-O(2)	176.6(2)
O(1)-C(3)-C(10)-C(11)	-178.0(2)
C(2)-C(3)-C(10)-C(11)	-0.9(4)
C(12)-O(3)-C(11)-C(18)	1.0(3)
C(12)-O(3)-C(11)-C(10)	-177.9(2)
O(2)-C(10)-C(11)-O(3)	0.8(3)
C(3)-C(10)-C(11)-O(3)	178.4(2)
O(2)-C(10)-C(11)-C(18)	-178.0(2)
C(3)-C(10)-C(11)-C(18)	-0.4(4)
C(11)-O(3)-C(12)-C(13)	177.4(2)
C(11)-O(3)-C(12)-C(17)	-2.9(3)
C(17)-C(12)-C(13)-C(14)	-0.7(4)
O(3)-C(12)-C(13)-C(14)	179.0(2)
C(12)-C(13)-C(14)-C(15)	-0.3(4)
C(13)-C(14)-C(15)-C(16)	0.8(4)
C(14)-C(15)-C(16)-C(17)	-0.3(4)
C(15)-C(16)-C(17)-C(12)	-0.6(4)

C(15)-C(16)-C(17)-O(4)	179.4(2)
C(13)-C(12)-C(17)-C(16)	1.1(4)
O(3)-C(12)-C(17)-C(16)	-178.5(2)
C(13)-C(12)-C(17)-O(4)	-178.9(2)
O(3)-C(12)-C(17)-O(4)	1.4(4)
C(18)-O(4)-C(17)-C(16)	-177.9(2)
C(18)-O(4)-C(17)-C(12)	2.1(3)
C(17)-O(4)-C(18)-C(11)	-4.1(3)
C(17)-O(4)-C(18)-C(19)	175.6(2)
O(3)-C(11)-C(18)-O(4)	2.7(4)
C(10)-C(11)-C(18)-O(4)	-178.6(2)
O(3)-C(11)-C(18)-C(19)	-177.0(2)
C(10)-C(11)-C(18)-C(19)	1.7(3)
O(4)-C(18)-C(19)-C(2)	178.59(19)
C(11)-C(18)-C(19)-C(2)	-1.7(3)
O(4)-C(18)-C(19)-C(20)	2.5(4)
C(11)-C(18)-C(19)-C(20)	-177.8(2)
C(3)-C(2)-C(19)-C(18)	0.4(3)
C(1)-C(2)-C(19)-C(18)	-176.1(2)
C(3)-C(2)-C(19)-C(20)	177.4(2)
C(1)-C(2)-C(19)-C(20)	0.9(2)
C(21)-N(2)-C(20)-N(1)	-7.6(3)
C(21)-N(2)-C(20)-C(19)	157.2(2)
C(1)-N(1)-C(20)-N(2)	156.9(2)
B(1)-N(1)-C(20)-N(2)	-13.5(3)
C(1)-N(1)-C(20)-C(19)	-11.4(2)
B(1)-N(1)-C(20)-C(19)	178.24(19)
C(18)-C(19)-C(20)-N(2)	15.4(4)
C(2)-C(19)-C(20)-N(2)	-161.0(2)
C(18)-C(19)-C(20)-N(1)	-177.7(2)
C(2)-C(19)-C(20)-N(1)	5.9(2)
C(20)-N(2)-C(21)-N(3)	9.9(3)
C(20)-N(2)-C(21)-C(22)	-153.6(2)
C(40)-N(3)-C(21)-N(2)	-153.7(2)
B(1)-N(3)-C(21)-N(2)	9.1(3)
C(40)-N(3)-C(21)-C(22)	13.0(2)
B(1)-N(3)-C(21)-C(22)	175.9(2)
N(2)-C(21)-C(22)-C(23)	-15.3(4)
N(3)-C(21)-C(22)-C(23)	179.1(2)
N(2)-C(21)-C(22)-C(39)	157.8(2)
N(3)-C(21)-C(22)-C(39)	-7.8(2)
C(24)-O(5)-C(23)-C(22)	177.2(2)
C(24)-O(5)-C(23)-C(30)	-3.3(3)
C(39)-C(22)-C(23)-O(5)	179.52(19)
C(21)-C(22)-C(23)-O(5)	-8.1(4)
C(39)-C(22)-C(23)-C(30)	0.0(3)
C(21)-C(22)-C(23)-C(30)	172.3(2)
C(23)-O(5)-C(24)-C(29)	1.0(3)
C(23)-O(5)-C(24)-C(25)	-177.8(2)
C(29)-C(24)-C(25)-C(26)	-0.7(4)
O(5)-C(24)-C(25)-C(26)	178.1(2)
C(24)-C(25)-C(26)-C(27)	-0.1(4)
C(25)-C(26)-C(27)-C(28)	0.4(4)

C(26)-C(27)-C(28)-C(29)	0.2(4)
C(27)-C(28)-C(29)-C(24)	-1.1(4)
C(27)-C(28)-C(29)-O(6)	178.2(2)
C(25)-C(24)-C(29)-C(28)	1.4(4)
O(5)-C(24)-C(29)-C(28)	-177.5(2)
C(25)-C(24)-C(29)-O(6)	-177.9(2)
O(5)-C(24)-C(29)-O(6)	3.3(4)
C(30)-O(6)-C(29)-C(28)	175.6(2)
C(30)-O(6)-C(29)-C(24)	-5.1(3)
C(29)-O(6)-C(30)-C(23)	2.9(3)
C(29)-O(6)-C(30)-C(31)	-176.8(2)
O(5)-C(23)-C(30)-O(6)	1.3(4)
C(22)-C(23)-C(30)-O(6)	-179.2(2)
O(5)-C(23)-C(30)-C(31)	-179.1(2)
C(22)-C(23)-C(30)-C(31)	0.5(4)
C(32)-O(7)-C(31)-C(38)	-4.3(3)
C(32)-O(7)-C(31)-C(30)	176.5(2)
O(6)-C(30)-C(31)-O(7)	-2.8(3)
C(23)-C(30)-C(31)-O(7)	177.6(2)
O(6)-C(30)-C(31)-C(38)	178.0(2)
C(23)-C(30)-C(31)-C(38)	-1.7(4)
C(31)-O(7)-C(32)-C(33)	-177.4(2)
C(31)-O(7)-C(32)-C(37)	2.6(3)
O(7)-C(32)-C(33)-C(34)	177.7(2)
C(37)-C(32)-C(33)-C(34)	-2.3(4)
C(32)-C(33)-C(34)-C(35)	2.4(4)
C(33)-C(34)-C(35)-C(36)	-1.2(4)
C(34)-C(35)-C(36)-C(37)	-0.2(4)
C(35)-C(36)-C(37)-O(8)	-179.2(2)
C(35)-C(36)-C(37)-C(32)	0.3(4)
C(38)-O(8)-C(37)-C(36)	177.7(2)
C(38)-O(8)-C(37)-C(32)	-1.9(3)
C(33)-C(32)-C(37)-C(36)	0.9(4)
O(7)-C(32)-C(37)-C(36)	-179.1(2)
C(33)-C(32)-C(37)-O(8)	-179.5(2)
O(7)-C(32)-C(37)-O(8)	0.4(4)
C(37)-O(8)-C(38)-C(31)	0.2(3)
C(37)-O(8)-C(38)-C(39)	-179.9(2)
O(7)-C(31)-C(38)-O(8)	3.0(4)
C(30)-C(31)-C(38)-O(8)	-177.8(2)
O(7)-C(31)-C(38)-C(39)	-176.8(2)
C(30)-C(31)-C(38)-C(39)	2.4(3)
O(8)-C(38)-C(39)-C(22)	178.25(19)
C(31)-C(38)-C(39)-C(22)	-1.9(3)
O(8)-C(38)-C(39)-C(40)	6.2(4)
C(31)-C(38)-C(39)-C(40)	-174.0(2)
C(23)-C(22)-C(39)-C(38)	0.7(3)
C(21)-C(22)-C(39)-C(38)	-173.4(2)
C(23)-C(22)-C(39)-C(40)	174.6(2)
C(21)-C(22)-C(39)-C(40)	0.5(2)
C(41)-N(4)-C(40)-N(3)	-11.0(3)
C(41)-N(4)-C(40)-C(39)	152.3(2)
C(21)-N(3)-C(40)-N(4)	153.9(2)

B(1)-N(3)-C(40)-N(4)	-8.8(3)
C(21)-N(3)-C(40)-C(39)	-12.7(2)
B(1)-N(3)-C(40)-C(39)	-175.5(2)
C(38)-C(39)-C(40)-N(4)	14.4(4)
C(22)-C(39)-C(40)-N(4)	-158.4(2)
C(38)-C(39)-C(40)-N(3)	179.9(2)
C(22)-C(39)-C(40)-N(3)	7.1(2)
C(40)-N(4)-C(41)-N(5)	9.4(3)
C(40)-N(4)-C(41)-C(42)	-152.7(2)
C(60)-N(5)-C(41)-N(4)	-155.0(2)
B(1)-N(5)-C(41)-N(4)	11.8(3)
C(60)-N(5)-C(41)-C(42)	10.8(2)
B(1)-N(5)-C(41)-C(42)	177.61(19)
N(4)-C(41)-C(42)-C(43)	-14.7(4)
N(5)-C(41)-C(42)-C(43)	-179.1(2)
N(4)-C(41)-C(42)-C(59)	157.7(2)
N(5)-C(41)-C(42)-C(59)	-6.7(2)
C(44)-O(9)-C(43)-C(50)	-0.2(3)
C(44)-O(9)-C(43)-C(42)	179.67(19)
C(59)-C(42)-C(43)-O(9)	178.61(19)
C(41)-C(42)-C(43)-O(9)	-9.8(4)
C(59)-C(42)-C(43)-C(50)	-1.5(3)
C(41)-C(42)-C(43)-C(50)	170.1(2)
C(43)-O(9)-C(44)-C(45)	-179.4(2)
C(43)-O(9)-C(44)-C(49)	-0.5(3)
C(49)-C(44)-C(45)-C(46)	-0.2(4)
O(9)-C(44)-C(45)-C(46)	178.7(2)
C(44)-C(45)-C(46)-C(47)	0.3(4)
C(45)-C(46)-C(47)-C(48)	-0.7(4)
C(46)-C(47)-C(48)-C(49)	1.0(4)
C(47)-C(48)-C(49)-C(44)	-0.9(4)
C(47)-C(48)-C(49)-O(10)	-179.5(2)
C(45)-C(44)-C(49)-C(48)	0.5(4)
O(9)-C(44)-C(49)-C(48)	-178.3(2)
C(45)-C(44)-C(49)-O(10)	179.0(2)
O(9)-C(44)-C(49)-O(10)	0.2(3)
C(50)-O(10)-C(49)-C(48)	179.5(2)
C(50)-O(10)-C(49)-C(44)	0.9(3)
O(9)-C(43)-C(50)-O(10)	1.4(3)
C(42)-C(43)-C(50)-O(10)	-178.5(2)
O(9)-C(43)-C(50)-C(51)	-179.2(2)
C(42)-C(43)-C(50)-C(51)	0.9(3)
C(49)-O(10)-C(50)-C(43)	-1.7(3)
C(49)-O(10)-C(50)-C(51)	178.89(19)
C(52)-O(11)-C(51)-C(58)	1.2(3)
C(52)-O(11)-C(51)-C(50)	-179.07(19)
C(43)-C(50)-C(51)-O(11)	180.0(2)
O(10)-C(50)-C(51)-O(11)	-0.6(3)
C(43)-C(50)-C(51)-C(58)	-0.3(3)
O(10)-C(50)-C(51)-C(58)	179.1(2)
C(51)-O(11)-C(52)-C(53)	180.0(2)
C(51)-O(11)-C(52)-C(57)	0.0(3)
C(57)-C(52)-C(53)-C(54)	1.3(4)

O(11)-C(52)-C(53)-C(54)	-178.7(2)
C(52)-C(53)-C(54)-C(55)	-0.1(4)
C(53)-C(54)-C(55)-C(56)	-0.9(4)
C(54)-C(55)-C(56)-C(57)	0.8(4)
C(55)-C(56)-C(57)-O(12)	-178.1(2)
C(55)-C(56)-C(57)-C(52)	0.4(4)
C(58)-O(12)-C(57)-C(56)	-177.01(19)
C(58)-O(12)-C(57)-C(52)	4.5(3)
C(53)-C(52)-C(57)-C(56)	-1.4(4)
O(11)-C(52)-C(57)-C(56)	178.6(2)
C(53)-C(52)-C(57)-O(12)	177.0(2)
O(11)-C(52)-C(57)-O(12)	-3.0(3)
C(57)-O(12)-C(58)-C(59)	177.18(19)
C(57)-O(12)-C(58)-C(51)	-3.3(3)
O(11)-C(51)-C(58)-O(12)	0.5(3)
C(50)-C(51)-C(58)-O(12)	-179.2(2)
O(11)-C(51)-C(58)-C(59)	-180.0(2)
C(50)-C(51)-C(58)-C(59)	0.3(3)
O(12)-C(58)-C(59)-C(42)	178.58(19)
C(51)-C(58)-C(59)-C(42)	-0.9(3)
O(12)-C(58)-C(59)-C(60)	7.8(4)
C(51)-C(58)-C(59)-C(60)	-171.7(2)
C(43)-C(42)-C(59)-C(58)	1.5(3)
C(41)-C(42)-C(59)-C(58)	-171.9(2)
C(43)-C(42)-C(59)-C(60)	174.4(2)
C(41)-C(42)-C(59)-C(60)	0.9(2)
C(1)-N(6)-C(60)-N(5)	-10.6(3)
C(1)-N(6)-C(60)-C(59)	153.3(2)
C(41)-N(5)-C(60)-N(6)	157.0(2)
B(1)-N(5)-C(60)-N(6)	-9.7(3)
C(41)-N(5)-C(60)-C(59)	-10.3(2)
B(1)-N(5)-C(60)-C(59)	-176.98(19)
C(58)-C(59)-C(60)-N(6)	10.9(4)
C(42)-C(59)-C(60)-N(6)	-160.8(2)
C(58)-C(59)-C(60)-N(5)	177.0(2)
C(42)-C(59)-C(60)-N(5)	5.3(2)
B(1)-O(13)-C(61)-C(66)	-93.7(3)
B(1)-O(13)-C(61)-C(62)	86.7(3)
O(13)-C(61)-C(62)-C(63)	-178.3(2)
C(66)-C(61)-C(62)-C(63)	2.1(4)
O(13)-C(61)-C(62)-F(1)	1.6(4)
C(66)-C(61)-C(62)-F(1)	-178.0(2)
F(1)-C(62)-C(63)-F(2)	-0.9(4)
C(61)-C(62)-C(63)-F(2)	179.0(2)
F(1)-C(62)-C(63)-C(64)	179.1(2)
C(61)-C(62)-C(63)-C(64)	-1.0(4)
F(2)-C(63)-C(64)-F(3)	1.9(4)
C(62)-C(63)-C(64)-F(3)	-178.1(3)
F(2)-C(63)-C(64)-C(65)	178.8(2)
C(62)-C(63)-C(64)-C(65)	-1.2(4)
F(3)-C(64)-C(65)-F(4)	-0.8(4)
C(63)-C(64)-C(65)-F(4)	-177.8(3)
F(3)-C(64)-C(65)-C(66)	179.2(2)

C(63)-C(64)-C(65)-C(66)	2.2(4)
O(13)-C(61)-C(66)-F(5)	0.0(4)
C(62)-C(61)-C(66)-F(5)	179.6(2)
O(13)-C(61)-C(66)-C(65)	179.4(2)
C(62)-C(61)-C(66)-C(65)	-1.0(4)
F(4)-C(65)-C(66)-F(5)	-1.7(4)
C(64)-C(65)-C(66)-F(5)	178.4(2)
F(4)-C(65)-C(66)-C(61)	178.9(2)
C(64)-C(65)-C(66)-C(61)	-1.1(4)
C(61)-O(13)-B(1)-N(3)	-162.09(18)
C(61)-O(13)-B(1)-N(1)	-41.9(3)
C(61)-O(13)-B(1)-N(5)	77.9(3)
C(40)-N(3)-B(1)-O(13)	-99.4(2)
C(21)-N(3)-B(1)-O(13)	99.5(2)
C(40)-N(3)-B(1)-N(1)	135.32(19)
C(21)-N(3)-B(1)-N(1)	-25.7(3)
C(40)-N(3)-B(1)-N(5)	25.7(3)
C(21)-N(3)-B(1)-N(5)	-135.3(2)
C(1)-N(1)-B(1)-O(13)	94.5(2)
C(20)-N(1)-B(1)-O(13)	-96.0(2)
C(1)-N(1)-B(1)-N(3)	-141.6(2)
C(20)-N(1)-B(1)-N(3)	27.9(3)
C(1)-N(1)-B(1)-N(5)	-30.9(3)
C(20)-N(1)-B(1)-N(5)	138.6(2)
C(60)-N(5)-B(1)-O(13)	-97.6(3)
C(41)-N(5)-B(1)-O(13)	96.8(3)
C(60)-N(5)-B(1)-N(3)	138.5(2)
C(41)-N(5)-B(1)-N(3)	-27.1(3)
C(60)-N(5)-B(1)-N(1)	27.8(3)
C(41)-N(5)-B(1)-N(1)	-137.8(2)
C(4S)-O(1S)-C(1S)-C(2S)	-17.1(3)
O(1S)-C(1S)-C(2S)-C(3S)	-3.8(4)
C(1S)-C(2S)-C(3S)-C(4S)	21.6(3)
C(1S)-O(1S)-C(4S)-C(3S)	31.2(3)
C(2S)-C(3S)-C(4S)-O(1S)	-32.6(3)
C(8S)-O(2S)-C(5S)-C(6S)	33.9(5)
O(2S)-C(5S)-C(6S)-C(7S)	-37.4(5)
C(5S)-C(6S)-C(7S)-C(8S)	26.0(4)
C(5S)-O(2S)-C(8S)-C(7S)	-17.0(5)
C(6S)-C(7S)-C(8S)-O(2S)	-7.0(4)

Symmetry transformations used to generate equivalent atoms:

6.2 Crystal of 4a·$(CHCl_3)_2$ CCDC Deposition 910747.

Crystals grown by vapour diffusion of **4a** in $CHCl_3$ with MeOH. Crystals were isolated as a solvate with two chloroform molecules per unit cell.

Table S7. Crystal data and structure refinement for **4a·$(CHCl_3)_2$** (CCDC Deposition 910747).

Identification code	d1245	
Empirical formula	C74 H40 B F5 N6 O15	
Formula weight	1358.93	
Temperature	150(1) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.0798(5) Å	□= 90°.
	b = 20.9681(8) Å	□= 91.723(3)°.
	c = 23.1817(11) Å	□ = 90°.
Volume	5869.0(4) $Å^3$	
Z	4	
Density (calculated)	1.538 Mg/m^3	
Absorption coefficient	1.009 mm^{-1}	
F(000)	2784	
Crystal size	0.13 x 0.12 x 0.04 mm^3	
Theta range for data collection	2.84 to 66.07°.	
Index ranges	-13<=h<=14, -23<=k<=24, -27<=l<=26	
Reflections collected	38252	
Independent reflections	10022 [R(int) = 0.0747]	
Completeness to theta = 66.07°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9607 and 0.8800	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10022 / 0 / 910	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1333	
R indices (all data)	R1 = 0.0696, wR2 = 0.1430	
Largest diff. peak and hole	0.574 and -0.421 $e.Å^{-3}$	

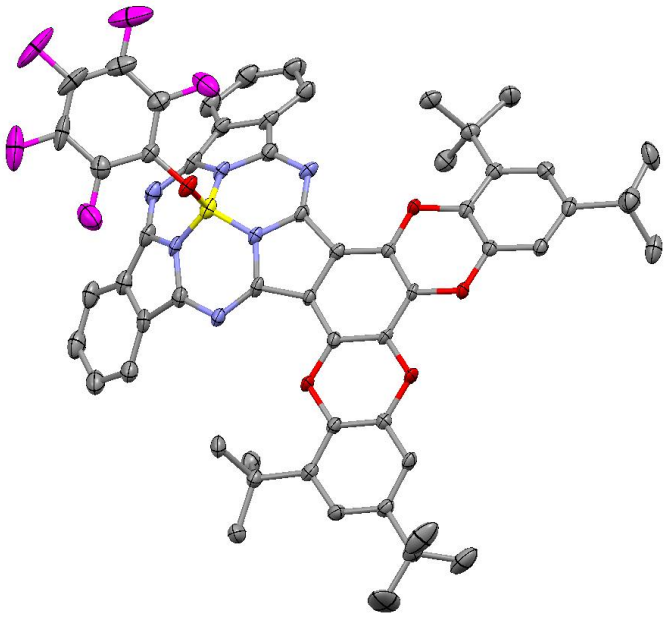

Figure S23. Thermal ellipsoid plot of **4a•$(CHCl_3)_2$** (CCDC deposition 910747). Thermal ellipsoids are set at the 50% probability level. Hydrogen atoms and included solvent have been omitted for clarity. Colors: boron – pink; nitrogen – blue; carbon – grey; oxygen – red; fluorine – magenta.

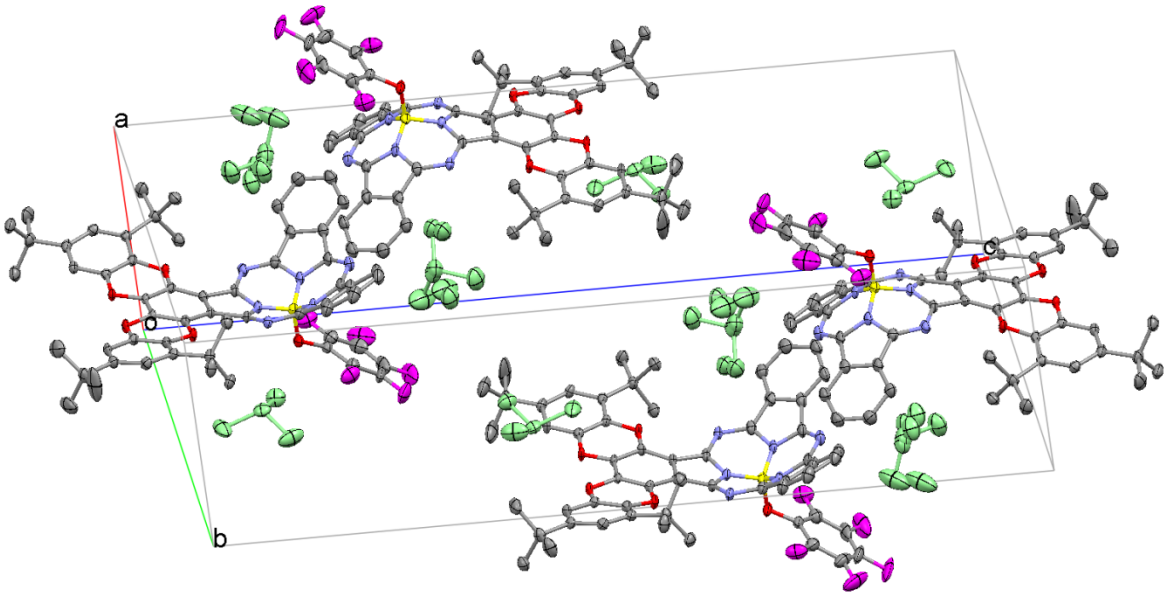

Figure S24. Thermal ellipsoid plot of **4a•$(CHCl_3)_2$** (CCDC deposition 910747). Thermal ellipsoids are set at the 50% probability level. Hydrogen atoms and included solvent have been omitted for clarity. Colors: boron – pink; nitrogen – blue; carbon – grey; oxygen – red; fluorine – magenta; chloroform molecules - green.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4a·$(CHCl_3)_2$** (CCDC Deposition 910747). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	3691(3)	3614(2)	1772(1)	56(1)
F(2)	2316(4)	3311(2)	2399(1)	88(1)
F(3)	1498(4)	4455(3)	2852(1)	93(2)
F(4)	2187(4)	5910(3)	2691(1)	85(1)
F(5)	3617(3)	6218(2)	2070(1)	57(1)
O(1)	6714(3)	3631(2)	191(1)	23(1)
O(2)	6703(3)	4493(2)	-513(1)	21(1)
O(3)	6767(3)	6014(2)	-476(1)	23(1)
O(4)	6846(3)	6765(2)	266(1)	24(1)
O(5)	4278(3)	5080(2)	1573(1)	29(1)
N(1)	6760(3)	6407(2)	1182(1)	23(1)
N(2)	6622(4)	5696(2)	1770(1)	25(1)
N(3)	7664(4)	4950(2)	2305(1)	32(1)
N(4)	6533(4)	4359(2)	1727(1)	25(1)
N(5)	6581(4)	3798(2)	1096(1)	26(1)
N(6)	6126(3)	5107(2)	1150(1)	22(1)
C(1)	6948(4)	6342(2)	1576(1)	26(1)
C(2)	7781(5)	6798(3)	1870(1)	30(1)
C(3)	8350(5)	7523(3)	1851(1)	35(1)
C(4)	9197(5)	7782(3)	2181(1)	42(1)
C(5)	9500(5)	7330(3)	2520(1)	43(1)
C(6)	8947(5)	6611(3)	2538(1)	38(1)
C(7)	8059(5)	6349(3)	2212(1)	33(1)
C(8)	7384(5)	5623(3)	2135(1)	31(1)
C(9)	7314(5)	4326(3)	2090(1)	30(1)
C(10)	7912(5)	3569(3)	2117(1)	31(1)
C(11)	8789(5)	3210(3)	2418(1)	37(1)
C(12)	9291(5)	2507(3)	2342(1)	40(1)
C(13)	8949(5)	2148(3)	1976(1)	40(1)
C(14)	8108(5)	2508(3)	1673(1)	34(1)
C(15)	7577(4)	3211(3)	1746(1)	29(1)
C(16)	6777(4)	3759(2)	1490(1)	26(1)
C(17)	6342(4)	4476(2)	933(1)	22(1)
C(18)	6523(4)	4767(2)	544(1)	20(1)
C(19)	6568(4)	5574(2)	565(1)	18(1)
C(20)	6431(4)	5780(2)	972(1)	23(1)
C(21)	6676(4)	4400(2)	194(1)	18(1)
C(22)	6994(4)	3289(2)	-160(1)	22(1)
C(23)	7352(4)	2530(2)	-156(1)	23(1)
C(24)	7427(4)	2187(2)	-520(1)	25(1)
C(25)	7201(4)	2579(2)	-877(1)	25(1)
C(26)	6970(4)	3356(2)	-866(1)	23(1)
C(27)	6883(4)	3705(2)	-510(1)	20(1)
C(28)	6733(4)	4833(2)	-146(1)	18(1)
C(29)	6763(4)	5621(2)	-126(1)	19(1)
C(30)	6936(4)	6800(2)	-439(1)	21(1)
C(31)	6996(4)	7198(2)	-782(1)	24(1)

C(32)	7197(4)	7977(2)	-771(1)	25(1)
C(33)	7369(4)	8325(2)	-402(1)	24(1)
C(34)	7293(4)	7938(2)	-48(1)	23(1)
C(35)	7036(4)	7164(2)	-76(1)	21(1)
C(36)	6747(4)	5997(2)	234(1)	20(1)
C(37)	7704(4)	2089(2)	236(1)	27(1)
C(38)	6435(5)	2049(3)	472(1)	32(1)
C(39)	8936(5)	2486(3)	483(1)	34(1)
C(40)	8164(6)	1276(3)	161(1)	39(1)
C(41)	7196(5)	2165(2)	-1279(1)	29(1)
C(42)	5755(5)	2275(3)	-1516(1)	36(1)
C(43)	8341(5)	2495(3)	-1502(1)	41(1)
C(44)	7468(6)	1313(3)	-1223(2)	48(1)
C(45)	7178(5)	8435(3)	-1158(1)	33(1)
C(46)	5705(6)	8361(4)	-1384(2)	68(2)
C(47)	7566(12)	9246(4)	-1088(2)	101(3)
C(48)	8209(6)	8090(4)	-1412(2)	56(2)
C(49)	7470(4)	8353(3)	355(1)	26(1)
C(50)	7813(6)	9192(3)	310(1)	38(1)
C(51)	8676(5)	7996(3)	630(1)	33(1)
C(52)	6096(5)	8310(3)	549(1)	31(1)
C(53)	3692(4)	4927(3)	1903(1)	26(1)
C(54)	3349(5)	4190(3)	1999(1)	36(1)
C(55)	2628(5)	4025(3)	2318(2)	48(1)
C(56)	2214(6)	4600(4)	2545(2)	55(2)
C(57)	2559(6)	5345(4)	2464(1)	51(2)
C(58)	3295(5)	5497(3)	2146(1)	36(1)
B(1)	5813(5)	5062(3)	1565(1)	25(1)
C(1S)	10804(5)	4825(3)	1039(2)	42(1)
Cl(1)	10092(1)	4823(1)	540(1)	70(1)
Cl(2)	10407(2)	3960(1)	1259(1)	56(1)
Cl(3)	10143(2)	5575(1)	1296(1)	78(1)
C(2S)	7847(8)	84(4)	1708(2)	64(2)
Cl(4)	6645(2)	-643(1)	1634(1)	70(1)
Cl(5)	7921(2)	606(1)	1267(1)	75(1)
Cl(6)	9536(3)	-188(2)	1898(1)	113(1)
C(2SA)	8044(13)	53(7)	1732(4)	64(2)
Cl(4A)	6411(12)	-259(8)	1533(4)	70(1)
Cl(5A)	8264(14)	1023(6)	1619(4)	75(1)
Cl(6A)	9462(13)	-467(8)	1600(7)	113(1)

Table S9. Bond lengths [Å] and angles [°] for **4a**·$(CHCl_3)_2$ (CCDC Deposition 910747).

F(1)-C(54)	1.338(6)
F(2)-C(55)	1.331(7)
F(3)-C(56)	1.340(6)
F(4)-C(57)	1.333(7)
F(5)-C(58)	1.340(6)
O(1)-C(21)	1.356(5)
O(1)-C(22)	1.392(5)
O(2)-C(28)	1.384(4)
O(2)-C(27)	1.400(5)
O(3)-C(29)	1.379(4)
O(3)-C(30)	1.399(5)
O(4)-C(36)	1.360(5)
O(4)-C(35)	1.390(5)
O(5)-C(53)	1.340(5)
O(5)-B(1)	1.472(5)
N(1)-C(20)	1.335(5)
N(1)-C(1)	1.337(5)
N(2)-C(1)	1.372(6)
N(2)-C(8)	1.373(5)
N(2)-B(1)	1.488(6)
N(3)-C(8)	1.336(6)
N(3)-C(9)	1.343(6)
N(4)-C(16)	1.367(6)
N(4)-C(9)	1.372(5)
N(4)-B(1)	1.492(6)
N(5)-C(17)	1.328(5)
N(5)-C(16)	1.336(5)
N(6)-C(17)	1.365(5)
N(6)-C(20)	1.378(5)
N(6)-B(1)	1.479(6)
C(1)-C(2)	1.450(6)
C(2)-C(3)	1.394(7)
C(2)-C(7)	1.408(6)
C(3)-C(4)	1.387(7)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.406(7)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.378(8)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(6)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.445(7)
C(9)-C(10)	1.450(7)
C(10)-C(11)	1.400(6)
C(10)-C(15)	1.416(6)
C(11)-C(12)	1.365(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.405(7)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.388(6)
C(13)-H(13A)	0.9500

C(14)-C(15)	1.372(7)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.459(6)
C(17)-C(18)	1.450(5)
C(18)-C(21)	1.379(6)
C(18)-C(19)	1.426(6)
C(19)-C(36)	1.378(5)
C(19)-C(20)	1.454(5)
C(21)-C(28)	1.393(5)
C(22)-C(23)	1.382(6)
C(22)-C(27)	1.395(6)
C(23)-C(24)	1.390(6)
C(23)-C(37)	1.549(6)
C(24)-C(25)	1.392(6)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.388(6)
C(25)-C(41)	1.553(6)
C(26)-C(27)	1.371(6)
C(26)-H(26A)	0.9500
C(28)-C(29)	1.393(6)
C(29)-C(36)	1.398(5)
C(30)-C(31)	1.371(6)
C(30)-C(35)	1.386(5)
C(31)-C(32)	1.387(6)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.391(6)
C(32)-C(45)	1.546(6)
C(33)-C(34)	1.394(6)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.388(6)
C(34)-C(49)	1.548(6)
C(37)-C(40)	1.529(6)
C(37)-C(38)	1.532(6)
C(37)-C(39)	1.537(6)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(43)	1.517(7)
C(41)-C(42)	1.529(6)
C(41)-C(44)	1.534(7)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800

C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(47)	1.490(8)
C(45)-C(48)	1.510(7)
C(45)-C(46)	1.532(7)
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-C(50)	1.528(6)
C(49)-C(51)	1.535(6)
C(49)-C(52)	1.540(6)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(58)	1.384(7)
C(53)-C(54)	1.388(7)
C(54)-C(55)	1.383(7)
C(55)-C(56)	1.361(9)
C(56)-C(57)	1.388(9)
C(57)-C(58)	1.384(7)
C(1S)-Cl(3)	1.744(6)
C(1S)-Cl(1)	1.756(6)
C(1S)-Cl(2)	1.760(5)
C(1S)-H(1S)	1.0000
C(2S)-Cl(4)	1.721(7)
C(2S)-Cl(6)	1.738(8)
C(2S)-Cl(5)	1.771(7)
C(2S)-H(2S)	1.0000
C(2SA)-Cl(4A)	1.721(7)
C(2SA)-Cl(6A)	1.738(8)
C(2SA)-Cl(5A)	1.771(7)
C(2SA)-H(2SA)	1.0000

C(21)-O(1)-C(22)	116.6(3)
C(28)-O(2)-C(27)	115.6(3)
C(29)-O(3)-C(30)	115.4(3)
C(36)-O(4)-C(35)	117.0(3)
C(53)-O(5)-B(1)	121.6(3)
C(20)-N(1)-C(1)	117.6(4)
C(1)-N(2)-C(8)	112.8(4)
C(1)-N(2)-B(1)	122.1(3)

C(8)-N(2)-B(1)	123.3(4)
C(8)-N(3)-C(9)	117.7(4)
C(16)-N(4)-C(9)	112.7(4)
C(16)-N(4)-B(1)	121.8(3)
C(9)-N(4)-B(1)	123.4(4)
C(17)-N(5)-C(16)	117.7(4)
C(17)-N(6)-C(20)	114.2(3)
C(17)-N(6)-B(1)	122.2(4)
C(20)-N(6)-B(1)	122.9(3)
N(1)-C(1)-N(2)	122.9(4)
N(1)-C(1)-C(2)	130.3(4)
N(2)-C(1)-C(2)	105.3(4)
C(3)-C(2)-C(7)	121.0(4)
C(3)-C(2)-C(1)	131.5(4)
C(7)-C(2)-C(1)	107.4(4)
C(4)-C(3)-C(2)	117.4(5)
C(4)-C(3)-H(3A)	121.3
C(2)-C(3)-H(3A)	121.3
C(3)-C(4)-C(5)	121.8(5)
C(3)-C(4)-H(4A)	119.1
C(5)-C(4)-H(4A)	119.1
C(6)-C(5)-C(4)	120.9(4)
C(6)-C(5)-H(5A)	119.6
C(4)-C(5)-H(5A)	119.6
C(5)-C(6)-C(7)	118.1(5)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	120.8(5)
C(6)-C(7)-C(8)	131.0(4)
C(2)-C(7)-C(8)	107.9(4)
N(3)-C(8)-N(2)	122.4(4)
N(3)-C(8)-C(7)	130.2(4)
N(2)-C(8)-C(7)	105.2(4)
N(3)-C(9)-N(4)	122.3(4)
N(3)-C(9)-C(10)	130.3(4)
N(4)-C(9)-C(10)	105.5(4)
C(11)-C(10)-C(15)	120.5(4)
C(11)-C(10)-C(9)	131.4(4)
C(15)-C(10)-C(9)	107.9(4)
C(12)-C(11)-C(10)	117.8(4)
C(12)-C(11)-H(11A)	121.1
C(10)-C(11)-H(11A)	121.1
C(11)-C(12)-C(13)	121.8(4)
C(11)-C(12)-H(12A)	119.1
C(13)-C(12)-H(12A)	119.1
C(14)-C(13)-C(12)	120.7(5)
C(14)-C(13)-H(13A)	119.6
C(12)-C(13)-H(13A)	119.6
C(15)-C(14)-C(13)	118.2(4)
C(15)-C(14)-H(14A)	120.9
C(13)-C(14)-H(14A)	120.9
C(14)-C(15)-C(10)	121.0(4)
C(14)-C(15)-C(16)	131.9(4)

C(10)-C(15)-C(16)	106.7(4)
N(5)-C(16)-N(4)	122.6(4)
N(5)-C(16)-C(15)	129.7(4)
N(4)-C(16)-C(15)	105.9(3)
N(5)-C(17)-N(6)	122.4(3)
N(5)-C(17)-C(18)	132.0(4)
N(6)-C(17)-C(18)	104.4(3)
C(21)-C(18)-C(19)	120.5(3)
C(21)-C(18)-C(17)	131.4(4)
C(19)-C(18)-C(17)	108.1(3)
C(36)-C(19)-C(18)	120.2(3)
C(36)-C(19)-C(20)	132.7(4)
C(18)-C(19)-C(20)	107.0(3)
N(1)-C(20)-N(6)	121.7(3)
N(1)-C(20)-C(19)	132.6(4)
N(6)-C(20)-C(19)	104.5(3)
O(1)-C(21)-C(18)	118.7(3)
O(1)-C(21)-C(28)	122.5(3)
C(18)-C(21)-C(28)	118.7(4)
C(23)-C(22)-O(1)	118.9(3)
C(23)-C(22)-C(27)	120.8(4)
O(1)-C(22)-C(27)	120.3(4)
C(22)-C(23)-C(24)	116.9(4)
C(22)-C(23)-C(37)	121.6(4)
C(24)-C(23)-C(37)	121.5(4)
C(23)-C(24)-C(25)	122.9(4)
C(23)-C(24)-H(24A)	118.6
C(25)-C(24)-H(24A)	118.6
C(26)-C(25)-C(24)	118.5(4)
C(26)-C(25)-C(41)	120.1(4)
C(24)-C(25)-C(41)	121.3(4)
C(27)-C(26)-C(25)	119.4(4)
C(27)-C(26)-H(26A)	120.3
C(25)-C(26)-H(26A)	120.3
C(26)-C(27)-C(22)	121.0(4)
C(26)-C(27)-O(2)	117.3(3)
C(22)-C(27)-O(2)	121.7(3)
O(2)-C(28)-C(29)	118.3(3)
O(2)-C(28)-C(21)	121.1(3)
C(29)-C(28)-C(21)	120.6(3)
O(3)-C(29)-C(28)	117.5(3)
O(3)-C(29)-C(36)	121.6(4)
C(28)-C(29)-C(36)	120.9(3)
C(31)-C(30)-C(35)	121.3(4)
C(31)-C(30)-O(3)	116.3(3)
C(35)-C(30)-O(3)	122.4(3)
C(30)-C(31)-C(32)	120.1(4)
C(30)-C(31)-H(31A)	120.0
C(32)-C(31)-H(31A)	120.0
C(31)-C(32)-C(33)	117.7(4)
C(31)-C(32)-C(45)	120.3(4)
C(33)-C(32)-C(45)	122.0(4)
C(32)-C(33)-C(34)	123.5(4)

C(32)-C(33)-H(33A)	118.3
C(34)-C(33)-H(33A)	118.3
C(35)-C(34)-C(33)	116.7(4)
C(35)-C(34)-C(49)	121.7(4)
C(33)-C(34)-C(49)	121.6(4)
C(30)-C(35)-C(34)	120.7(4)
C(30)-C(35)-O(4)	120.7(4)
C(34)-C(35)-O(4)	118.7(3)
O(4)-C(36)-C(19)	119.2(3)
O(4)-C(36)-C(29)	122.1(3)
C(19)-C(36)-C(29)	118.6(4)
C(40)-C(37)-C(38)	107.7(4)
C(40)-C(37)-C(39)	107.5(4)
C(38)-C(37)-C(39)	109.7(4)
C(40)-C(37)-C(23)	111.4(4)
C(38)-C(37)-C(23)	111.6(3)
C(39)-C(37)-C(23)	108.7(3)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(43)-C(41)-C(42)	110.3(4)
C(43)-C(41)-C(44)	108.5(4)
C(42)-C(41)-C(44)	108.6(4)
C(43)-C(41)-C(25)	109.3(4)
C(42)-C(41)-C(25)	108.6(3)
C(44)-C(41)-C(25)	111.6(4)
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5

C(41)-C(44)-H(44A)	109.5
C(41)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(41)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(47)-C(45)-C(48)	108.1(6)
C(47)-C(45)-C(46)	111.1(6)
C(48)-C(45)-C(46)	107.5(4)
C(47)-C(45)-C(32)	112.7(4)
C(48)-C(45)-C(32)	109.5(4)
C(46)-C(45)-C(32)	107.8(4)
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(45)-C(48)-H(48A)	109.5
C(45)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(45)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-C(51)	107.6(4)
C(50)-C(49)-C(52)	107.1(4)
C(51)-C(49)-C(52)	109.6(4)
C(50)-C(49)-C(34)	111.8(3)
C(51)-C(49)-C(34)	110.3(3)
C(52)-C(49)-C(34)	110.2(3)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5

H(52B)-C(52)-H(52C)	109.5
O(5)-C(53)-C(58)	121.8(4)
O(5)-C(53)-C(54)	121.3(4)
C(58)-C(53)-C(54)	116.8(4)
F(1)-C(54)-C(55)	118.0(5)
F(1)-C(54)-C(53)	119.6(4)
C(55)-C(54)-C(53)	122.3(5)
F(2)-C(55)-C(56)	120.0(5)
F(2)-C(55)-C(54)	120.5(6)
C(56)-C(55)-C(54)	119.5(5)
F(3)-C(56)-C(55)	120.6(6)
F(3)-C(56)-C(57)	119.3(6)
C(55)-C(56)-C(57)	120.1(5)
F(4)-C(57)-C(58)	120.0(6)
F(4)-C(57)-C(56)	120.6(5)
C(58)-C(57)-C(56)	119.4(5)
F(5)-C(58)-C(53)	119.2(4)
F(5)-C(58)-C(57)	119.0(5)
C(53)-C(58)-C(57)	121.8(5)
O(5)-B(1)-N(6)	109.1(3)
O(5)-B(1)-N(2)	116.2(4)
N(6)-B(1)-N(2)	104.9(4)
O(5)-B(1)-N(4)	115.5(4)
N(6)-B(1)-N(4)	105.3(3)
N(2)-B(1)-N(4)	104.8(3)
Cl(3)-C(1S)-Cl(1)	111.3(3)
Cl(3)-C(1S)-Cl(2)	109.5(3)
Cl(1)-C(1S)-Cl(2)	109.4(3)
Cl(3)-C(1S)-H(1S)	108.9
Cl(1)-C(1S)-H(1S)	108.9
Cl(2)-C(1S)-H(1S)	108.9
Cl(4)-C(2S)-Cl(6)	115.3(5)
Cl(4)-C(2S)-Cl(5)	110.7(4)
Cl(6)-C(2S)-Cl(5)	109.5(4)
Cl(4)-C(2S)-H(2S)	107.0
Cl(6)-C(2S)-H(2S)	107.0
Cl(5)-C(2S)-H(2S)	107.0
Cl(4A)-C(2SA)-Cl(6A)	115.5(5)
Cl(4A)-C(2SA)-Cl(5A)	110.3(5)
Cl(6A)-C(2SA)-Cl(5A)	109.7(5)
Cl(4A)-C(2SA)-H(2SA)	107.0
Cl(6A)-C(2SA)-H(2SA)	107.0
Cl(5A)-C(2SA)-H(2SA)	107.0

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4a·(CHCl$_3$)$_2$** (CCDC Deposition 910747). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	51(2)	34(2)	83(2)	-13(2)	12(2)	-4(1)
F(2)	60(2)	81(3)	127(4)	58(3)	27(2)	-9(2)
F(3)	58(2)	184(5)	42(2)	45(2)	31(2)	10(2)
F(4)	82(3)	128(4)	49(2)	-41(2)	18(2)	23(2)
F(5)	60(2)	41(2)	72(2)	-15(2)	15(2)	1(1)
O(1)	38(2)	21(2)	12(1)	2(1)	8(1)	2(1)
O(2)	31(1)	21(2)	10(1)	-1(1)	5(1)	1(1)
O(3)	38(2)	23(2)	9(1)	3(1)	6(1)	1(1)
O(4)	41(2)	20(2)	10(1)	1(1)	8(1)	-1(1)
O(5)	28(2)	43(2)	17(1)	7(1)	7(1)	3(1)
N(1)	27(2)	28(2)	15(2)	1(1)	7(1)	3(1)
N(2)	31(2)	35(2)	12(2)	1(2)	9(1)	3(2)
N(3)	39(2)	42(2)	16(2)	2(2)	4(2)	3(2)
N(4)	30(2)	33(2)	13(2)	5(1)	6(1)	0(2)
N(5)	29(2)	32(2)	16(2)	7(2)	5(1)	-1(2)
N(6)	26(2)	28(2)	13(2)	1(1)	4(1)	0(1)
C(1)	30(2)	30(2)	20(2)	-2(2)	6(2)	6(2)
C(2)	33(2)	37(3)	21(2)	-9(2)	9(2)	4(2)
C(3)	40(3)	39(3)	27(2)	-7(2)	11(2)	-3(2)
C(4)	46(3)	47(3)	35(3)	-14(2)	13(2)	-8(2)
C(5)	45(3)	61(4)	23(2)	-11(2)	3(2)	-2(2)
C(6)	41(3)	55(3)	18(2)	-7(2)	1(2)	1(2)
C(7)	36(2)	43(3)	20(2)	-3(2)	6(2)	5(2)
C(8)	35(2)	43(3)	14(2)	0(2)	5(2)	1(2)
C(9)	32(2)	46(3)	14(2)	6(2)	7(2)	2(2)
C(10)	36(2)	37(3)	21(2)	10(2)	8(2)	2(2)
C(11)	39(3)	50(3)	22(2)	9(2)	4(2)	5(2)
C(12)	42(3)	50(3)	30(3)	15(2)	4(2)	8(2)
C(13)	48(3)	38(3)	36(3)	11(2)	11(2)	9(2)
C(14)	41(3)	38(3)	24(2)	8(2)	9(2)	5(2)
C(15)	32(2)	38(3)	19(2)	11(2)	7(2)	0(2)
C(16)	29(2)	30(2)	21(2)	2(2)	7(2)	0(2)
C(17)	26(2)	28(2)	12(2)	1(2)	4(2)	-2(2)
C(18)	21(2)	24(2)	16(2)	4(2)	3(2)	2(2)
C(19)	22(2)	22(2)	12(2)	0(2)	4(1)	1(2)
C(20)	25(2)	32(2)	12(2)	1(2)	5(2)	6(2)
C(21)	21(2)	20(2)	15(2)	1(2)	5(2)	0(2)
C(22)	21(2)	28(2)	17(2)	-1(2)	5(2)	-1(2)
C(23)	23(2)	25(2)	20(2)	2(2)	3(2)	-1(2)
C(24)	26(2)	23(2)	25(2)	0(2)	5(2)	0(2)
C(25)	24(2)	34(2)	19(2)	-4(2)	6(2)	-3(2)
C(26)	26(2)	27(2)	15(2)	-1(2)	5(2)	-2(2)
C(27)	20(2)	23(2)	18(2)	0(2)	4(2)	-1(2)
C(28)	20(2)	25(2)	10(2)	-1(2)	5(1)	1(2)
C(29)	22(2)	25(2)	11(2)	3(2)	5(2)	-1(2)
C(30)	24(2)	20(2)	18(2)	0(2)	4(2)	0(2)
C(31)	31(2)	29(2)	11(2)	3(2)	5(2)	3(2)
C(32)	29(2)	27(2)	19(2)	6(2)	7(2)	3(2)

C(33)	30(2)	22(2)	23(2)	4(2)	8(2)	1(2)
C(34)	23(2)	28(2)	19(2)	3(2)	6(2)	1(2)
C(35)	23(2)	24(2)	16(2)	3(2)	6(2)	2(2)
C(36)	23(2)	23(2)	15(2)	-2(2)	4(2)	0(2)
C(37)	32(2)	26(2)	23(2)	4(2)	2(2)	2(2)
C(38)	36(2)	34(3)	26(2)	10(2)	4(2)	0(2)
C(39)	31(2)	41(3)	28(2)	6(2)	-1(2)	3(2)
C(40)	59(3)	30(3)	30(2)	7(2)	9(2)	9(2)
C(41)	37(2)	26(2)	24(2)	-9(2)	4(2)	2(2)
C(42)	40(3)	44(3)	24(2)	-8(2)	1(2)	-3(2)
C(43)	39(3)	60(3)	26(2)	-13(2)	9(2)	3(2)
C(44)	70(4)	40(3)	33(3)	-17(2)	0(2)	9(3)
C(45)	48(3)	29(2)	21(2)	8(2)	4(2)	2(2)
C(46)	57(3)	105(6)	41(3)	39(3)	6(3)	18(3)
C(47)	224(11)	44(4)	33(3)	19(3)	11(5)	-28(5)
C(48)	62(4)	71(4)	39(3)	25(3)	20(3)	8(3)
C(49)	32(2)	30(2)	18(2)	-2(2)	7(2)	-4(2)
C(50)	60(3)	28(3)	27(2)	-5(2)	12(2)	-10(2)
C(51)	36(2)	39(3)	25(2)	-4(2)	0(2)	-4(2)
C(52)	38(2)	34(3)	23(2)	-9(2)	9(2)	-1(2)
C(53)	24(2)	34(3)	19(2)	3(2)	5(2)	0(2)
C(54)	31(2)	40(3)	37(3)	4(2)	7(2)	-3(2)
C(55)	35(3)	52(4)	57(3)	25(3)	8(2)	-5(2)
C(56)	42(3)	95(5)	30(3)	29(3)	12(2)	-1(3)
C(57)	42(3)	91(5)	22(2)	-17(3)	10(2)	12(3)
C(58)	38(2)	39(3)	31(2)	-3(2)	4(2)	2(2)
B(1)	24(2)	34(3)	18(2)	1(2)	4(2)	3(2)
C(1S)	29(2)	44(3)	55(3)	3(2)	11(2)	-2(2)
Cl(1)	32(1)	126(2)	53(1)	22(1)	1(1)	-5(1)
Cl(2)	56(1)	48(1)	64(1)	5(1)	10(1)	-7(1)
Cl(3)	61(1)	50(1)	125(2)	-29(1)	23(1)	1(1)
C(2S)	72(4)	75(5)	46(3)	0(3)	11(3)	-9(3)
Cl(4)	88(1)	65(1)	55(1)	5(1)	5(1)	-19(1)
Cl(5)	105(2)	58(1)	60(1)	14(1)	2(1)	-1(1)
Cl(6)	71(1)	120(2)	141(3)	67(2)	-18(2)	-5(1)
C(2SA)	72(4)	75(5)	46(3)	0(3)	11(3)	-9(3)
Cl(4A)	88(1)	65(1)	55(1)	5(1)	5(1)	-19(1)
Cl(5A)	105(2)	58(1)	60(1)	14(1)	2(1)	-1(1)
Cl(6A)	71(1)	120(2)	141(3)	67(2)	-18(2)	-5(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4a·$(CHCl_3)_2$** (CCDC Deposition 910747).

	x	y	z	U(eq)
H(3A)	8166	7827	1621	42
H(4A)	9583	8278	2178	50
H(5A)	10094	7523	2740	52
H(6A)	9163	6302	2765	46
H(11A)	9027	3448	2667	44
H(12A)	9888	2254	2542	49
H(13A)	9298	1653	1934	48
H(14A)	7905	2275	1422	41
H(24A)	7643	1661	-527	30
H(26A)	6873	3643	-1104	27
H(31A)	6899	6939	-1029	28
H(33A)	7548	8855	-391	29
H(38A)	5636	1821	308	48
H(38B)	6184	2561	550	48
H(38C)	6674	1738	708	48
H(39A)	9205	2195	724	51
H(39B)	8650	2998	552	51
H(39C)	9740	2519	329	51
H(40A)	7388	1003	9	59
H(40B)	8418	1019	414	59
H(40C)	8979	1285	11	59
H(42A)	5589	2816	-1566	54
H(42B)	5023	2073	-1365	54
H(42C)	5728	2004	-1768	54
H(43A)	8183	3041	-1539	62
H(43B)	8317	2247	-1760	62
H(43C)	9260	2411	-1350	62
H(44A)	7478	1071	-1481	72
H(44B)	6720	1088	-1086	72
H(44C)	8378	1235	-1065	72
H(46A)	5699	8589	-1646	101
H(46B)	5022	8623	-1238	101
H(46C)	5452	7823	-1411	101
H(47A)	8475	9277	-924	151
H(47B)	6844	9497	-953	151
H(47C)	7636	9497	-1342	151
H(48A)	9162	8122	-1273	84
H(48B)	8169	8368	-1662	84
H(48C)	7964	7557	-1465	84
H(50A)	7044	9440	143	57
H(50B)	8688	9242	187	57
H(50C)	7928	9434	571	57
H(51A)	8872	8309	867	50
H(51B)	9521	7967	492	50
H(51C)	8405	7485	705	50
H(52A)	5331	8545	375	47
H(52B)	6218	8579	803	47

H(52C)	5865	7778	594	47
H(1S)	11850	4877	1053	51
H(2S)	7495	437	1904	77
H(2SA)	8071	15	2025	77

Table S12. Torsion angles [°] for **4a·(CHCl$_3$)$_2$** (CCDC Deposition 910747).

C(20)-N(1)-C(1)-N(2)	-9.6(6)
C(20)-N(1)-C(1)-C(2)	153.9(4)
C(8)-N(2)-C(1)-N(1)	155.0(4)
B(1)-N(2)-C(1)-N(1)	-10.5(6)
C(8)-N(2)-C(1)-C(2)	-12.0(5)
B(1)-N(2)-C(1)-C(2)	-177.6(4)
N(1)-C(1)-C(2)-C(3)	17.7(8)
N(2)-C(1)-C(2)-C(3)	-176.6(5)
N(1)-C(1)-C(2)-C(7)	-158.1(4)
N(2)-C(1)-C(2)-C(7)	7.6(5)
C(7)-C(2)-C(3)-C(4)	0.0(7)
C(1)-C(2)-C(3)-C(4)	-175.3(5)
C(2)-C(3)-C(4)-C(5)	1.3(7)
C(3)-C(4)-C(5)-C(6)	-0.8(8)
C(4)-C(5)-C(6)-C(7)	-1.0(7)
C(5)-C(6)-C(7)-C(2)	2.3(7)
C(5)-C(6)-C(7)-C(8)	176.6(5)
C(3)-C(2)-C(7)-C(6)	-1.8(7)
C(1)-C(2)-C(7)-C(6)	174.5(4)
C(3)-C(2)-C(7)-C(8)	-177.3(4)
C(1)-C(2)-C(7)-C(8)	-1.0(5)
C(9)-N(3)-C(8)-N(2)	7.4(6)
C(9)-N(3)-C(8)-C(7)	-153.2(5)
C(1)-N(2)-C(8)-N(3)	-153.4(4)
B(1)-N(2)-C(8)-N(3)	12.0(6)
C(1)-N(2)-C(8)-C(7)	11.4(5)
B(1)-N(2)-C(8)-C(7)	176.8(4)
C(6)-C(7)-C(8)-N(3)	-17.7(8)
C(2)-C(7)-C(8)-N(3)	157.2(5)
C(6)-C(7)-C(8)-N(2)	179.1(5)
C(2)-C(7)-C(8)-N(2)	-6.0(5)
C(8)-N(3)-C(9)-N(4)	-8.4(6)
C(8)-N(3)-C(9)-C(10)	153.2(5)
C(16)-N(4)-C(9)-N(3)	154.0(4)
B(1)-N(4)-C(9)-N(3)	-10.0(6)
C(16)-N(4)-C(9)-C(10)	-11.5(5)
B(1)-N(4)-C(9)-C(10)	-175.5(4)
N(3)-C(9)-C(10)-C(11)	16.4(8)
N(4)-C(9)-C(10)-C(11)	-179.7(5)
N(3)-C(9)-C(10)-C(15)	-157.6(4)
N(4)-C(9)-C(10)-C(15)	6.3(5)
C(15)-C(10)-C(11)-C(12)	-0.6(7)
C(9)-C(10)-C(11)-C(12)	-174.0(5)
C(10)-C(11)-C(12)-C(13)	0.0(7)
C(11)-C(12)-C(13)-C(14)	1.5(8)
C(12)-C(13)-C(14)-C(15)	-2.4(7)
C(13)-C(14)-C(15)-C(10)	1.8(7)
C(13)-C(14)-C(15)-C(16)	174.1(5)
C(11)-C(10)-C(15)-C(14)	-0.3(7)
C(9)-C(10)-C(15)-C(14)	174.5(4)
C(11)-C(10)-C(15)-C(16)	-174.3(4)

C(9)-C(10)-C(15)-C(16)	0.5(5)
C(17)-N(5)-C(16)-N(4)	10.2(6)
C(17)-N(5)-C(16)-C(15)	-152.4(4)
C(9)-N(4)-C(16)-N(5)	-154.3(4)
B(1)-N(4)-C(16)-N(5)	9.9(6)
C(9)-N(4)-C(16)-C(15)	11.8(5)
B(1)-N(4)-C(16)-C(15)	176.1(4)
C(14)-C(15)-C(16)-N(5)	-15.4(8)
C(10)-C(15)-C(16)-N(5)	157.7(4)
C(14)-C(15)-C(16)-N(4)	179.8(5)
C(10)-C(15)-C(16)-N(4)	-7.1(5)
C(16)-N(5)-C(17)-N(6)	-8.1(6)
C(16)-N(5)-C(17)-C(18)	157.5(4)
C(20)-N(6)-C(17)-N(5)	156.2(4)
B(1)-N(6)-C(17)-N(5)	-14.5(6)
C(20)-N(6)-C(17)-C(18)	-12.7(4)
B(1)-N(6)-C(17)-C(18)	176.6(3)
N(5)-C(17)-C(18)-C(21)	17.7(7)
N(6)-C(17)-C(18)-C(21)	-174.9(4)
N(5)-C(17)-C(18)-C(19)	-160.6(4)
N(6)-C(17)-C(18)-C(19)	6.8(4)
C(21)-C(18)-C(19)-C(36)	0.9(5)
C(17)-C(18)-C(19)-C(36)	179.4(3)
C(21)-C(18)-C(19)-C(20)	-177.8(3)
C(17)-C(18)-C(19)-C(20)	0.7(4)
C(1)-N(1)-C(20)-N(6)	7.7(6)
C(1)-N(1)-C(20)-C(19)	-158.1(4)
C(17)-N(6)-C(20)-N(1)	-156.0(4)
B(1)-N(6)-C(20)-N(1)	14.6(6)
C(17)-N(6)-C(20)-C(19)	13.2(4)
B(1)-N(6)-C(20)-C(19)	-176.1(3)
C(36)-C(19)-C(20)-N(1)	-18.8(7)
C(18)-C(19)-C(20)-N(1)	159.7(4)
C(36)-C(19)-C(20)-N(6)	173.6(4)
C(18)-C(19)-C(20)-N(6)	-7.9(4)
C(22)-O(1)-C(21)-C(18)	-174.5(3)
C(22)-O(1)-C(21)-C(28)	8.0(5)
C(19)-C(18)-C(21)-O(1)	176.0(3)
C(17)-C(18)-C(21)-O(1)	-2.2(6)
C(19)-C(18)-C(21)-C(28)	-6.4(5)
C(17)-C(18)-C(21)-C(28)	175.4(4)
C(21)-O(1)-C(22)-C(23)	165.8(3)
C(21)-O(1)-C(22)-C(27)	-15.6(5)
O(1)-C(22)-C(23)-C(24)	171.2(3)
C(27)-C(22)-C(23)-C(24)	-7.4(6)
O(1)-C(22)-C(23)-C(37)	-10.9(5)
C(27)-C(22)-C(23)-C(37)	170.5(4)
C(22)-C(23)-C(24)-C(25)	1.9(6)
C(37)-C(23)-C(24)-C(25)	-176.0(4)
C(23)-C(24)-C(25)-C(26)	3.8(6)
C(23)-C(24)-C(25)-C(41)	-175.9(4)
C(24)-C(25)-C(26)-C(27)	-4.1(6)
C(41)-C(25)-C(26)-C(27)	175.6(4)

C(25)-C(26)-C(27)-C(22)	-1.3(6)
C(25)-C(26)-C(27)-O(2)	177.6(3)
C(23)-C(22)-C(27)-C(26)	7.3(6)
O(1)-C(22)-C(27)-C(26)	-171.2(3)
C(23)-C(22)-C(27)-O(2)	-171.5(3)
O(1)-C(22)-C(27)-O(2)	9.9(5)
C(28)-O(2)-C(27)-C(26)	-175.0(3)
C(28)-O(2)-C(27)-C(22)	3.9(5)
C(27)-O(2)-C(28)-C(29)	171.0(3)
C(27)-O(2)-C(28)-C(21)	-11.6(5)
O(1)-C(21)-C(28)-O(2)	5.9(5)
C(18)-C(21)-C(28)-O(2)	-171.6(3)
O(1)-C(21)-C(28)-C(29)	-176.8(3)
C(18)-C(21)-C(28)-C(29)	5.7(5)
C(30)-O(3)-C(29)-C(28)	-174.0(3)
C(30)-O(3)-C(29)-C(36)	7.9(5)
O(2)-C(28)-C(29)-O(3)	-0.3(5)
C(21)-C(28)-C(29)-O(3)	-177.7(3)
O(2)-C(28)-C(29)-C(36)	177.9(3)
C(21)-C(28)-C(29)-C(36)	0.5(6)
C(29)-O(3)-C(30)-C(31)	177.7(3)
C(29)-O(3)-C(30)-C(35)	-2.5(5)
C(35)-C(30)-C(31)-C(32)	1.8(6)
O(3)-C(30)-C(31)-C(32)	-178.4(3)
C(30)-C(31)-C(32)-C(33)	1.6(6)
C(30)-C(31)-C(32)-C(45)	-176.4(4)
C(31)-C(32)-C(33)-C(34)	-2.7(6)
C(45)-C(32)-C(33)-C(34)	175.3(4)
C(32)-C(33)-C(34)-C(35)	0.3(6)
C(32)-C(33)-C(34)-C(49)	-179.1(4)
C(31)-C(30)-C(35)-C(34)	-4.3(6)
O(3)-C(30)-C(35)-C(34)	175.9(3)
C(31)-C(30)-C(35)-O(4)	174.1(3)
O(3)-C(30)-C(35)-O(4)	-5.7(6)
C(33)-C(34)-C(35)-C(30)	3.2(6)
C(49)-C(34)-C(35)-C(30)	-177.4(4)
C(33)-C(34)-C(35)-O(4)	-175.2(3)
C(49)-C(34)-C(35)-O(4)	4.1(5)
C(36)-O(4)-C(35)-C(30)	8.4(5)
C(36)-O(4)-C(35)-C(34)	-173.2(3)
C(35)-O(4)-C(36)-C(19)	179.5(3)
C(35)-O(4)-C(36)-C(29)	-3.1(5)
C(18)-C(19)-C(36)-O(4)	-177.2(3)
C(20)-C(19)-C(36)-O(4)	1.1(6)
C(18)-C(19)-C(36)-C(29)	5.3(5)
C(20)-C(19)-C(36)-C(29)	-176.4(4)
O(3)-C(29)-C(36)-O(4)	-5.3(6)
C(28)-C(29)-C(36)-O(4)	176.6(3)
O(3)-C(29)-C(36)-C(19)	172.1(3)
C(28)-C(29)-C(36)-C(19)	-6.0(6)
C(22)-C(23)-C(37)-C(40)	-176.1(4)
C(24)-C(23)-C(37)-C(40)	1.7(5)
C(22)-C(23)-C(37)-C(38)	63.5(5)

C(24)-C(23)-C(37)-C(38)	-118.7(4)
C(22)-C(23)-C(37)-C(39)	-57.7(5)
C(24)-C(23)-C(37)-C(39)	120.1(4)
C(26)-C(25)-C(41)-C(43)	60.2(5)
C(24)-C(25)-C(41)-C(43)	-120.1(4)
C(26)-C(25)-C(41)-C(42)	-60.2(5)
C(24)-C(25)-C(41)-C(42)	119.5(4)
C(26)-C(25)-C(41)-C(44)	-179.9(4)
C(24)-C(25)-C(41)-C(44)	-0.2(6)
C(31)-C(32)-C(45)-C(47)	-173.7(6)
C(33)-C(32)-C(45)-C(47)	8.3(7)
C(31)-C(32)-C(45)-C(48)	-53.4(6)
C(33)-C(32)-C(45)-C(48)	128.7(5)
C(31)-C(32)-C(45)-C(46)	63.3(6)
C(33)-C(32)-C(45)-C(46)	-114.7(5)
C(35)-C(34)-C(49)-C(50)	177.3(4)
C(33)-C(34)-C(49)-C(50)	-3.4(5)
C(35)-C(34)-C(49)-C(51)	57.5(5)
C(33)-C(34)-C(49)-C(51)	-123.1(4)
C(35)-C(34)-C(49)-C(52)	-63.6(5)
C(33)-C(34)-C(49)-C(52)	115.7(4)
B(1)-O(5)-C(53)-C(58)	97.4(5)
B(1)-O(5)-C(53)-C(54)	-88.0(5)
O(5)-C(53)-C(54)-F(1)	4.5(6)
C(58)-C(53)-C(54)-F(1)	179.2(4)
O(5)-C(53)-C(54)-C(55)	-173.9(4)
C(58)-C(53)-C(54)-C(55)	0.9(7)
F(1)-C(54)-C(55)-F(2)	1.5(7)
C(53)-C(54)-C(55)-F(2)	179.8(4)
F(1)-C(54)-C(55)-C(56)	-177.3(4)
C(53)-C(54)-C(55)-C(56)	1.0(7)
F(2)-C(55)-C(56)-F(3)	0.3(8)
C(54)-C(55)-C(56)-F(3)	179.1(5)
F(2)-C(55)-C(56)-C(57)	178.9(5)
C(54)-C(55)-C(56)-C(57)	-2.3(8)
F(3)-C(56)-C(57)-F(4)	0.2(8)
C(55)-C(56)-C(57)-F(4)	-178.4(5)
F(3)-C(56)-C(57)-C(58)	-179.8(5)
C(55)-C(56)-C(57)-C(58)	1.6(8)
O(5)-C(53)-C(58)-F(5)	-6.1(6)
C(54)-C(53)-C(58)-F(5)	179.1(4)
O(5)-C(53)-C(58)-C(57)	173.2(4)
C(54)-C(53)-C(58)-C(57)	-1.6(7)
F(4)-C(57)-C(58)-F(5)	-0.3(7)
C(56)-C(57)-C(58)-F(5)	179.7(4)
F(4)-C(57)-C(58)-C(53)	-179.6(4)
C(56)-C(57)-C(58)-C(53)	0.3(7)
C(53)-O(5)-B(1)-N(6)	169.2(4)
C(53)-O(5)-B(1)-N(2)	-72.5(5)
C(53)-O(5)-B(1)-N(4)	51.0(5)
C(17)-N(6)-B(1)-O(5)	-94.8(4)
C(20)-N(6)-B(1)-O(5)	95.3(4)
C(17)-N(6)-B(1)-N(2)	140.1(4)

C(20)-N(6)-B(1)-N(2)	-29.8(5)
C(17)-N(6)-B(1)-N(4)	29.8(5)
C(20)-N(6)-B(1)-N(4)	-140.1(4)
C(1)-N(2)-B(1)-O(5)	-92.8(5)
C(8)-N(2)-B(1)-O(5)	103.2(5)
C(1)-N(2)-B(1)-N(6)	27.7(5)
C(8)-N(2)-B(1)-N(6)	-136.3(4)
C(1)-N(2)-B(1)-N(4)	138.4(4)
C(8)-N(2)-B(1)-N(4)	-25.7(5)
C(16)-N(4)-B(1)-O(5)	92.9(5)
C(9)-N(4)-B(1)-O(5)	-104.6(5)
C(16)-N(4)-B(1)-N(6)	-27.5(5)
C(9)-N(4)-B(1)-N(6)	135.1(4)
C(16)-N(4)-B(1)-N(2)	-137.9(4)
C(9)-N(4)-B(1)-N(2)	24.7(5)

Symmetry transformations used to generate equivalent atoms: