Electronic Supplementary Information.

Process for the synthesis of symmetric and unsymmetric oxygen bridged dimers of boron subphthalocyanines (μ-oxo-(BsubPc)$_2$s).

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† these two authors contributed equally to the execution of the work described herein and to the preparation of the manuscript.

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General Experimental Methods

Materials. All ACS grade solvents, basic alumina, potassium carbonate, and sodium hydroxide were purchased from Caledon Labs (Caledon, Ontario, Canada) and used without further purification unless otherwise stated. Phthalonitrile, 4,5-dichlorophthalonitrile, and tetrafluorophthalonitrile were purchased from TCI America (Portland, Oregon, USA) and used as received. Boron tribromide, boron trichloride (1.0 M solution in heptane), dicyclohexano-18-crown-6, aluminum chloride, aluminum chloride hexahydrate, iron(III) chloride hexahydrate, tin(IV) chloride, tin(IV) chloride pentahydrate, tripotassium phosphate, decamethylferrocene, and tetrabutylammonium perchlorate were purchased from Sigma-Aldrich Chemical Company (Mississauga, Ontario, Canada) and used as received. Tetrachlorophthalonitrile was purchased from Hangzhou Dayangchem Company Limited (Hangzhou, China) and used as received. Extraction thimbles (cellulose, single thickness) and aluminum plates coated with silica (pore size of 60Å) and fluorescent indicator were purchased from Whatman International Ltd. (Kent, England). Silica Gel P60 (mesh size 40-63 μm) was purchased from SiliCycle Inc. (Quebec City, Quebec, Canada).

Methods. All reactions were performed under an atmosphere of argon gas using oven-dried glasswares. Thin layer chromatography (TLC) was performed on aluminum plates coated with silica (pore size of 60Å) and fluorescent indicator and visualized under UV (254 nm) light. Column chromatography was performed using Silica Gel P60 (mesh size 40-63 μm) or alumina (basic, mesh size 70-290 μm). Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III spectrometer at 23 °C in $CDCl_3$, operating at 400 MHz for ^1H NMR and 100 MHz for ^{13}C NMR. Chemical shifts (δ) are reported in parts per million (ppm) referenced to tetramethylsilane (0 ppm) for ^1H NMR and $CDCl_3$ (77.16 ppm) for ^{13}C NMR. Coupling constants (J) are reported in hertz (Hz). Spin multiplicities are designated by the following abbreviations: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Accurate mass determinations (HRMS) were carried out on an Agilent 6538 Q-TOF mass spectrometer equipped with an Agilent 1200 HPLC and an ESI ion source. Single crystal X-ray diffraction data were collected on a Bruker Kappa APEX-DUO diffractometer using a Copper ImuS (microsource) tube with multi-layer optics and were measured using a combination of ϕ scans and ω scans. The data were processed using APEX2 and SAINT (Bruker, 2007). Absorption corrections were carried out using SADABS (Bruker, 2007). The structures were solved and refined using SHELXTL and SHELXL-2103 (Sheldrick, 2008) for full-matrix least-squares refinement that was based on F^2. Ultraviolet-visible (UV-vis) absorption spectra were acquired on a PerkinElmer Lambda 1050 UV/VIS/NIR spectrometer using a PerkinElmer quartz cuvette with a 10 mm path length. Photoluminescence (PL) spectra were recorded on a PerkinElmer LS55 fluorescence spectrometer using a PerkinElmer quartz cuvette with a 10mm path length. High pressure liquid chromatography (HPLC) analysis was carried out on a Waters 2695 separation module with a Waters 2998 photodiode array and a Waters Styragel® HR 2 THF 4.6 x 300 mm column. The mobile phase used was HPLC grade acetonitrile (80 % by volume) and *N,N*-dimethylformamide (20 % by volume). Cyclic voltammetry was carried out using a Bioanalytical Systems C3 electrochemical workstation. The working electrode was a 1 mm platinum disk, the counter electrode was a platinum wire, and the reference electrode was $Ag/AgCl_2$ saturated salt solution. Spec-grade solvents were purged with nitrogen gas at room temperature prior to their use. Four cycles at a scan rate of 100 mV/s were measured for each sample. Tetrabutylammonium perchlorate (0.1 M) was used as the supporting electrolyte. Decamethylferrocene was used as an internal reference. All half-wave potentials were corrected to the half-wave reduction potential ($E_{1/2,red}$) of decamethylferrocene, which was previously reported to be -0.012 V vs. Ag/AgCl.[1] Soxhlet extractions were performed using single thickness cellulose extraction thimbles (33 × 118 mm, 25 × 80mm).

Synthetic Procedures

Synthetic Procedures for Starting BsubPc Materials:

Br-BsubPc. Br-BsubPc was prepared according to literature procedure.[2]

HO-BsubPc. HO-BsubPc was prepared according to literature procedure.[3]

Br-F_{12}BsubPc. Br-F_{12}BsubPc was prepared according to literature procedure.[4]

Cl-Cl_6BsubPc. Cl-Cl_6BsubPc was prepared according to literature procedure.[5]

Cl-Cl_{12}BsubPc. Cl-Cl_{12}BsubPc was prepared according to literature procedure.[6]

Attempted Synthetic Procedures for μ-Oxo-$(BsubPc)_2$:

Methods 1.1 to 1.4 (Table S1): For **1.1**, conditions were maintained as reported by Geyer *et al.*[7] For **1.2-1.4**: Br-BsubPc was used in the place of Cl-BsubPc. In **1.3**, the volume of solvent was reduced by a factor of four. In **1.4**, the amount of NaOH was reduced to a molar amount equivalent to the moles of Br-BsubPc while keeping its molar equivalence relative to dicyclohexano-18-crown-6 the same.

Table S1. μ-Oxo-$(BsubPc)_2$ syntheses adapted from Geyer *et al.*[7]

Method	Halo-BsubPc			*p*-Xylene	NaOH		Dicyclohexano-18-Crown-6	
	Halo	Mass (g)	Moles (mmol)	Volume (mL)	Mass (g)	Moles (mmol)	Mass (g)	Moles (mmol)
1.1[7]	Cl	0.14	0.325	200	0.08	2	0.28	0.75
1.2	Br	0.154	0.325	200	0.08	2	0.28	0.75
1.3	Br	0.154	0.325	50	0.08	2	0.28	0.75
1.4	Br	0.154	0.325	50	0.013	0.325	0.045	0.122

Method 2.1 - Self-Condensation of HO-BsubPc Method (Table S2): μ-Oxo-$(BsubPc)_2$ was synthesized by the self-condensation of HO-BsubPc as adapted from the method of Yamasaki & Mori.[8] 1,2-Dichlorobenzene (1.4 mL) was added to make up a 10 wt% solution of HO-BsubPc (0.200 g, 0.485 mmol) in a 4 Dram (15 mL) vial fitted with a condenser. The reaction mixture was heated to a reflux (180 °C) under an atmosphere of argon and the reaction progress was monitored by HPLC. After 120 h (5 days), full conversion was not achieved and the reaction was cooled to room temperature. The solvent was removed by rotary evaporation and the solid was

dried in a vacuum oven overnight at 40°C. The crude product was purified by Kauffman column chromatography (alumina, DCM). The first band was collected and it contained μ-oxo-$(BsubPc)_2$ and two unknown impurities (HPLC R_T: 2.0 min and 3.7 min) and the second band was a mixture of the same in addition to traces of other BsubPc impurities. The collected fractions were concentrated via rotary evaporation and dried in a vacuum oven overnight at 40°C to afford μ-oxo-$(BsubPc)_2$ (45 mg, 23 %).

Method 2.2 - '1 Pot' Reaction Method (Table S2): μ-Oxo-$(BsubPc)_2$ was synthesized as reported in (9) by the *in situ* hydrolysis of Br-BsubPc (0.200 g, 0.421 mmol) in the presence of water.

Table S2. μ-Oxo-$(BsubPc)_2$ syntheses via the self-condensation of HO-BsubPc method.

Method	BsubPc Starting Material	Mass (g)	Moles (mmol)	Volume of 1,2-Dichlorobenzene (mL)	Weight Percent (%)	Temperature (°C)	Reaction Time (h)
2.1[8]	HO-BsubPc	0.20	0.485	1.4	10	180	120
2.2[9]	Br-BsubPc	0.20	0.421	1.4	10	180	24

Methods 3.1 to 3.6 - Equimolar Method (Table S3): μ-Oxo-$(BsubPc)_2$ was synthesized by reacting equimolar quantities of HO-BsubPc and Br-BsubPc, a reaction pathway which is included in the patent application of Mori *et al.*[10] For **3.1** to **3.5**, solvent was added to HO-BsubPc (0.100 g, 0.243 mmol) and Br-BsubPc (0.115 g, 0.243 mmol) in a scintillation (20 mL) or 4 Dram (15 mL) vial fitted with a condenser, to make up a ~2 wt% or ~10 wt% solution, respectively. Each reaction was heated to a temperature (as indicated in Table S3) under an atmosphere of argon and the reaction progress was monitored by HPLC. After a certain reaction time (as indicated in Table S3), the concentration of μ-oxo-$(BsubPc)_2$ had reach steady state as determined by HPLC. The reaction was cooled to room temperature. For **3.1** to **3.3**, no further workup was done. The subsequent steps for **3.5** and **3.6** (5x scale of **3.5**) are described in (3). For **3.4**, solvent was added to the reaction mixture in an attempt to precipitate out μ-oxo-$(BsubPc)_2$. A significant quantity of cyclohexane (200 mL) was added, however no precipitate was observed until after the solution was left covered in an ice bath overnight. The recovered solids were dried in a vacuum oven overnight at 40°C (123 mg; HPLC (545nm channel): 82 % μ-oxo-$(BsubPc)_2$ by area). In a replicate of **3.4**, methanol was added to the reaction mixture and no precipitate was observed.

Table S3. μ-Oxo-$(BsubPc)_2$ syntheses via the equimolar method.

Method	Solvent	Volume (mL)	Weight Percent (wt %)	Temperature (°C)	Reaction Time (h)
3.1	*p*-xylene	10	2.4	105	139.5
3.2	nitrobenzene	10	1.8	200	31
3.3	diphenyl ether	10	2.0	200	31
3.4	diphenyl ether	1.8	10	200	15.5
3.5	1,2-dichlorobenzene	1.5	10	181	20
3.6	1,2-dichlorobenzene	7.5	10	181	20

Methods 4.1 - 4.3, 4.5 - Equimolar Tripotassium Phosphate Method (Table S4): μ-Oxo-$(BsubPc)_2$ was synthesized based on **3.5/3.6**, but with the addition of tripotassium phosphate (K_3PO_4). 1,2-Dichlorobenzene was added to make up a 10 wt% solution of equimolar HO-BsubPc and Br-BsubPc in a 4 Dram (15 mL) vial fitted with a condenser. In **4.3**, glassware were dried in an oven at 100 °C overnight and the solvent was filtered through alumina before use. A mass of K_3PO_4 equivalent to 20 % or 80 % of the solvent's mass, ground in a mortar and pestle and activated in an oven at 200 °C was added. The reaction mixture was heated to a reflux under an atmosphere of argon and the reaction progress was monitored by HPLC. Samples were filtered through glass wool prior to analysis via HPLC to remove suspended solids. After a certain reaction time (as indicated in Table S4), the reaction was cooled to room temperature. Various workup steps followed.

For **4.1**, the solvent was removed by rotary evaporation and the solid was dried in a vacuum oven overnight at 40 °C. The solids were transferred to a Soxhlet thimble and a Soxhlet extraction using toluene was carried out. The solids remaining in the thimble had a deep turquoise colour and were insoluble in a range of organic solvents. The solvent was removed from the filtrate by rotary evaporation and the solid was then dried in a vacuum oven overnight at 40 °C (60 mg, 31 %). Pure μ-oxo-$(BsubPc)_2$ was not isolated.

For **4.2**, the same sequence was followed as **4.1** with a Soxhlet extraction using toluene (130 mg, 66 %). The solids were train sublimed at 220 °C to remove small molecule impurities (70 mg, 36 %). The solids remaining in the crucible were subsequently train sublimed at 450 °C following the same procedure as **3.5**, and μ-oxo-$(BsubPc)_2$ was collected as a loosely, partially crystalline solid (16 mg, 8 %).

For **4.3**, the reaction products were not isolated.

For **4.5**, the reaction mixture was transferred directly into a Soxhlet thimble and a Soxhlet extraction using toluene was carried out. Alumina (40 g) was added to the toluene retentate (~100 mL) and stirred. The liquid was decanted into a filter, and more toluene was added to the flask containing alumina and stirred. This was repeated several times and the remaining alumina and liquid was poured into the filter and rinsed with toluene. The toluene rinse runoff remained deeply magenta coloured. The solvent was removed from the filtrate by rotary evaporation and the solid was dried in a vacuum oven overnight at 40 °C (42 mg, 21 %). HPLC R_T: 2.8 min (>99.9%, 545 nm channel). A Kauffman column was run on the retained and dried alumina using DCM as the eluent. The solvent was removed from the filtrate by rotary evaporation and the solid was dried in a vacuum oven overnight at 40 °C (14 mg, 7%). HPLC R_T: 2.8 min (>99.9%, 545 nm channel). (Total Yield: 56 mg, 29 %). μ-Oxo-$(BsubPc)_2$ could not separated from the non-BsubPc impurities.

Methods 4.4, 4.6 - 4.8 – '1 pot' Tripotassium Phosphate Method (Table S4): μ-Oxo-$(BsubPc)_2$ was synthesized based on **2.2**, but with the addition of K_3PO_4. For **4.4** and **4.6**, K_3PO_4 was grinded in a mortar and pestle and activated in an oven at 200 °C. It was then left exposed to the atmosphere to absorb water overnight or until its mass had increased by approximately 15%, at which point the dry mass equivalent of wet K_3PO_4 corresponding to 20 % of the solvent's mass was added to the reaction vial (wet mass calculated using the measured wt% of water). For **4.7** and **4.8**, a mass of dry K_3PO_4 equivalent to 20 % of the solvent's mass, ground in a mortar and pestle and activated in an oven at 200 °C, was added to the reaction vial. This was then left open to absorb water until its mass had increased by approximately 15 %. 1,2-Dichlorobenzene

was added to make up a 10 wt% solution of Br-BsubPc in the 4 Dram (15 mL) (**4.4, 4.6**) or scintillation (20 mL) (**4.7 - 4.8**) vial fitted with a condenser. The reaction was heated to a reflux under an atmosphere of argon and the reaction progress was monitored by HPLC. Samples were filtered through glass wool prior to analysis via HPLC to remove suspended solids. After a certain reaction time (as indicated in Table S4), the reaction was cooled to room temperature. Various workup steps followed.
For **4.4**, **4.6-4.8** the reaction products were not isolated.

Method 4.9 – Final Method (Table S4): μ-Oxo-$(BsubPc)_2$ was synthesized based on an adaptation of **4.5**. 1,2-Dichlorobenzene (6.9 mL) was added to make up a 10 wt% solution of HO-BsubPc (0.464 g, 1.13 mmol) and Br-BsubPc (0.535 g, 1.13 mmol) in a scintillation (20 mL) vial fitted with a condenser. A mass of K_3PO_4 equivalent to 20 % of the solvent's mass (1.801 g, 8.49 mmol), ground in a mortar and pestle and activated in an oven at 200 °C was added. The reaction was heated to a reflux under an atmosphere of argon and the reaction progress was monitored by HPLC. After 1 hour, the reaction was cooled and immediately transferred to a Soxhlet thimble. A Soxhlet extraction using toluene was carried out for 2 days. The solvents were removed by rotary evaporation and the solids were fully redissolved in DCM. A Kauffman column chromatography (alumina, DCM) was carried out. The column was left to dry overnight, after which a fresh flask of DCM was placed under the column and reflux was established. The Kauffman column was ran for another day. The solvent was removed by rotary evaporation and the solids were dried in a vacuum oven overnight at 40 °C (537 mg, 59 % overall mass yield, HPLC R_T: 2.8 min (>99.9%, at 545 nm)). The solids were train sublimed at a temperature of 450 °C (held for 5hrs 45min, total heating time 10hrs 15min), and single crystals as well as a band of μ-oxo-$(BsubPc)_2$ were collected (357 mg, overall 39 % mass yield; sublimation step yield 70%). Removed white crystals were found to be phthalimide (~10 mg) and bands containing small quantities of HO-BsubPc were also discarded (mass below collection limit). The μ-oxo-$(BsubPc)_2$ was train sublimed a second time under the same conditions. Single crystals and μ-oxo-$(BsubPc)_2$ band were collected (sublimation step yield 58 %). Overall yield: 0.204 g, 22.5 %. HPLC R_T: 2.8 min (>99.9%, MAXPlot).

Table S4. μ-Oxo-$(BsubPc)_2$ syntheses via the tripotassium phosphate method.

Method	Volume of 1,2-Dichlorobenzene (mL)	HO-BsubPc		Br-BsubPc		Mass of K_3PO_4			Reaction Time (h)
		Mass (g)	Moles (mmol)	Mass (g)	Moles (mmol)	% of Solvent Mass	Dry Mass (g)	Wet Mass (g)	
4.1	1.5	0.100	0.243	0.115	0.243	80	1.553	-	24
4.2	1.5	0.100	0.243	0.115	0.243	20	0.388	-	24
4.3	1.5	0.100	0.243	0.115	0.243	20	0.388	-	24
4.4	1.6	0	0	0.231	0.485	20	0.388	0.437	24
4.5	1.5	0.100	0.243	0.115	0.243	20	0.388	-	1
4.6	1.6	0	0	0.231	0.485	20	0.388	0.464	1
4.7	4.0	0	0	0.576	1.213	20	1.039	1.193	1.25
4.8	4.0	0	0	0.576	1.213	20	1.039	1.236	1
4.9	6.9	0.464	1.13	0.535	1.13	20	1.801	-	1

Synthetic Procedures for Asymmetric μ-Oxo-(BsubPc)$_2$ Compounds:

F$_{12}$BsubPc-O-BsubPc. To a single neck round bottom flask equipped with a condenser was added 1,2-dichlorobenzene (14 mL, ~10 w/w % relative to HO-BsubPc and Br-F$_{12}$BsubPc), HO-BsubPc (0.75 g, 1.82 mmol, 1 equiv), and Br-F$_{12}$BsubPc (1.26 g, 1.82 mmol, 1 equiv) under an argon atmosphere. To this reaction mixture was added tripotassium phosphate (3.66 g, ~20 % mass equivalent relative to 1,2-DCB), which was pre-ground and activated in an oven at 200 ºC for one hour prior to use. The reaction mixture was heated to 180 ºC and the reaction progress was monitored by HPLC. Once the reaction was complete (~19 h), the reaction was cooled to room temperature before it was concentrated to dryness via rotary evaporation. The crude product was purified by silica gel column chromatography (100% DCM to 95:5 DCM/ethyl acetate) to afford F$_{12}$BsubPc-O-BsubPc (670 mg, 36 %) as a dark purple-gold solid. The compound was further purified using train sublimation. The apparatus was operated under a vacuum with a controlled flow of carbon dioxide gas generating an internal pressure of 100 mTorr. The temperature was increased from room temperature up to ~440 °C and was held constant at that temperature overnight (~12 h). A metallic gold band was confirmed to be the title compound (71 mg, 41 % yield relative to mass placed in the train sublimation apparatus). Vapour diffusion of heptane into DCM solution produced single crystals suitable for X-ray diffraction analysis. ^{1}H NMR (400 MHz, CDCl$_3$, Me$_4$Si) δ 8.70-8.64 (m, 6H), 7.87-7.81 (m, 6H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 150.6, 147.4, 130.7, 129.8, 122.0; ^{11}B NMR (400 MHz, CDCl$_3$, BF$_3$•OEt$_2$) δ -18.3 (s); ^{19}F NMR (400 MHz, CDCl$_3$, BF$_3$•OEt$_2$) δ 15.67-14.93 (m, 6F), 4.28-3.60 (m, 6F); HRMS (ESI): *m/z* $[M+H]^+$ calcd for 1021.1397, found 1021.1368; UV-vis$_{toluene}$ λ_{max} (ε): 547 nm (89800 $M^{-1}cm^{-1}$).

Cl$_6$BsubPc-O-BsubPc. To a single neck round bottom flask equipped with a condenser was added 1,2-dichlorobenzene (13 mL, ~10 w/w % relative to HO-BsubPc and Cl-Cl$_6$BsubPc), HO-BsubPc (0.75 g, 1.82 mmol, 1 equiv), and Cl-Cl$_6$BsubPc (1.16 g, 1.82 mmol, 1 equiv) under an argon atmosphere. To this reaction mixture was added tripotassium phosphate (3.40 g, ~20 % mass equivalent relative to 1,2-DCB), which was pre-ground and activated in an oven at 200 ºC for one hour prior to use. The reaction mixture was heated to 180 ºC and the reaction progress was monitored by HPLC. Once the reaction was complete (~17 h), the reaction was cooled to room temperature before it was concentrated to dryness via rotary evaporation. The crude product was purified by silica gel column chromatography (100% DCM to 95:5 DCM/ethyl acetate) to afford Cl$_6$BsubPc-O-BsubPc (737 mg, 40 %) as a gold solid. The compound was further purified using train sublimation. The apparatus was operated under a vacuum with a controlled flow of carbon dioxide gas generating an internal pressure of 90 mTorr. The temperature was increased from room temperature up to ~440 °C and was held constant at that temperature overnight (~12 h). A metallic gold band was confirmed to be the title compound (50 mg, 35 % yield relative to mass placed in the train sublimation apparatus). Slow evaporation from DCM solution produced single crystals suitable for X-ray diffraction analysis. ^{1}H NMR (400 MHz, CDCl$_3$, Me$_4$Si) δ 8.63-8.59 (m, 12H), 7.83-7.77 (m, 6H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 150.5, 149.3, 134.4, 130.6, 129.53, 129.5, 123.5, 121.9; ^{11}B NMR (400 MHz, CDCl$_3$, BF$_3$•OEt$_2$) δ -18.2 (s); HRMS (ESI): *m/z* $[M+H]^+$ calcd for 1009.0189, found 1009.0166; UV-vis$_{toluene}$ λ_{max} (ε): 541 nm (89800 $M^{-1}cm^{-1}$).

Cl_{12}BsubPc-O-BsubPc. To a single neck round bottom flask equipped with a condenser was added 1,2-dichlorobenzene (10 mL, ~10 w/w % relative to HO-BsubPc and Cl-Cl_{12}BsubPc), HO-BsubPc (0.50 g, 1.21 mmol, 1 equiv), and Cl-Cl_{12}BsubPc (1.02 g, 1.21 mmol, 1 equiv) under an argon atmosphere. To this reaction mixture was added tripotassium phosphate (2.60 g, ~20 % mass equivalent relative to 1,2-DCB), which was pre-ground and activated in an oven at 200 ºC for one hour prior to use. The reaction mixture was heated to 180 ºC and the reaction progress was monitored by HPLC. Once the reaction was complete (~18 h), the reaction was cooled to room temperature before it was concentrated to dryness via rotary evaporation. The crude product was purified by silica gel column chromatography (100% DCM) to afford Cl_{12}BsubPc-O-BsubPc (630 mg, 43 %) as a dark purple solid. The compound was further purified using train sublimation. The apparatus was operated under a vacuum with a controlled flow of carbon dioxide gas generating an internal pressure of 90 mTorr. The temperature was increased from room temperature up to ~480 °C and was held constant at that temperature overnight (~12 h). A metallic gold band was confirmed to be the title compound (73 mg, 55 % yield relative to mass placed in the train sublimation apparatus). ^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ 8.69-8.64 (m, 6H), 7.86-7.80 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 148.1, 135.0, 130.7, 129.7, 128.5, 127.3, 122.1; ^{11}B NMR (400 MHz, $CDCl_3$, BF_3•OEt_2) δ -18.7 (s); MS (ESI): *m/z* $[M+H]^+$ calcd for 1219.8, found 1219.8; UV-vis$_{toluene}$ λ_{max} (ε): 558 nm (89600 $M^{-1}cm^{-1}$).

NMR Spectra

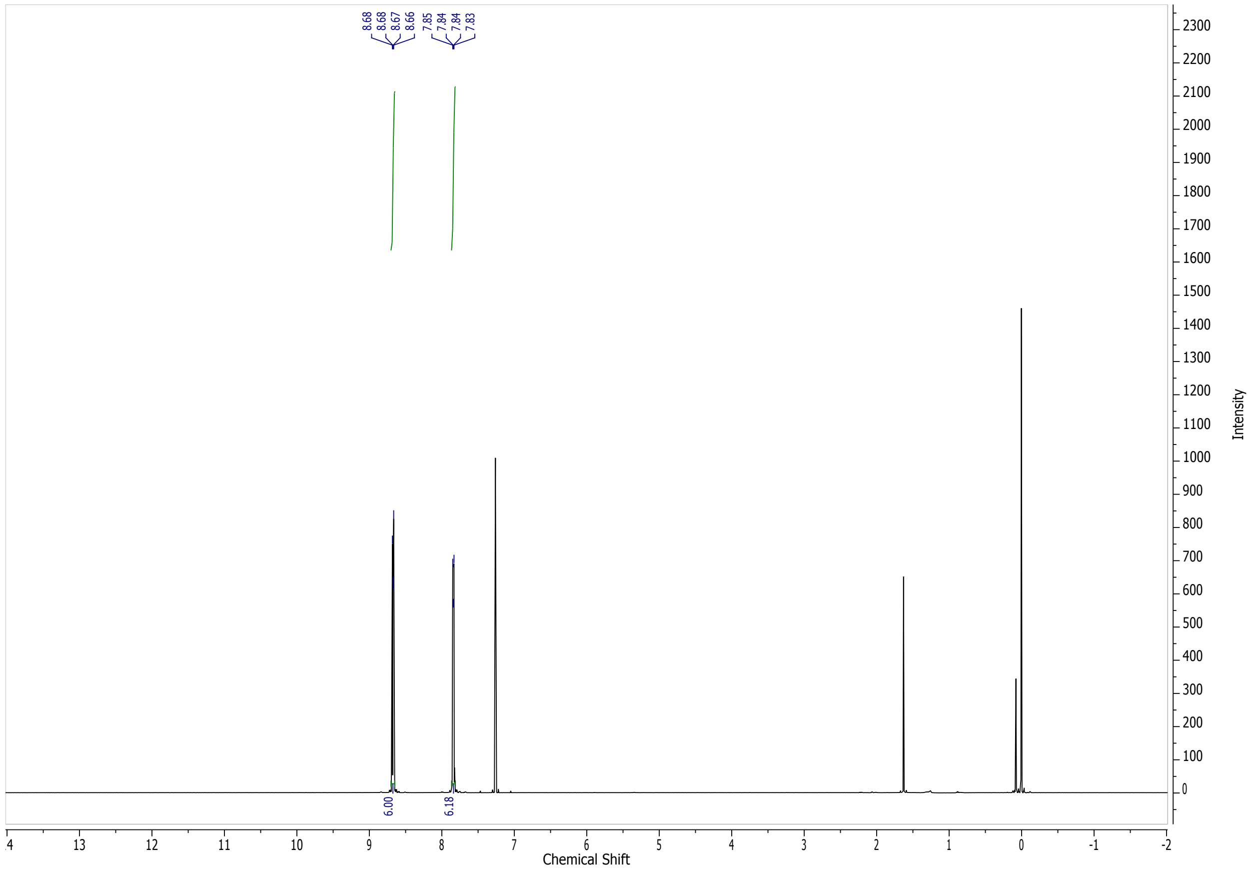


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum obtained at 296 K for F_{12}BsubPc-O-BsubPc.

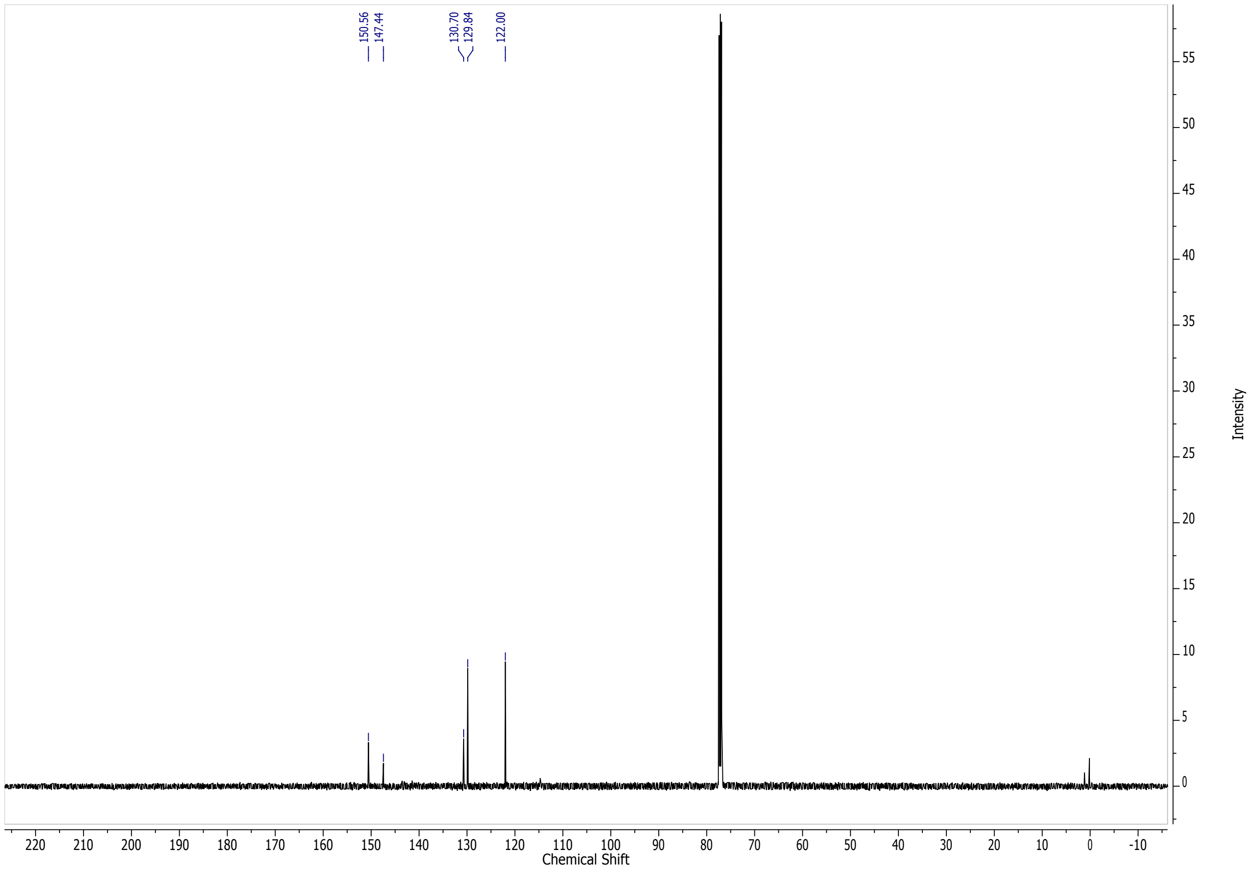


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum obtained at 296 K for F_{12}BsubPc-O-BsubPc.

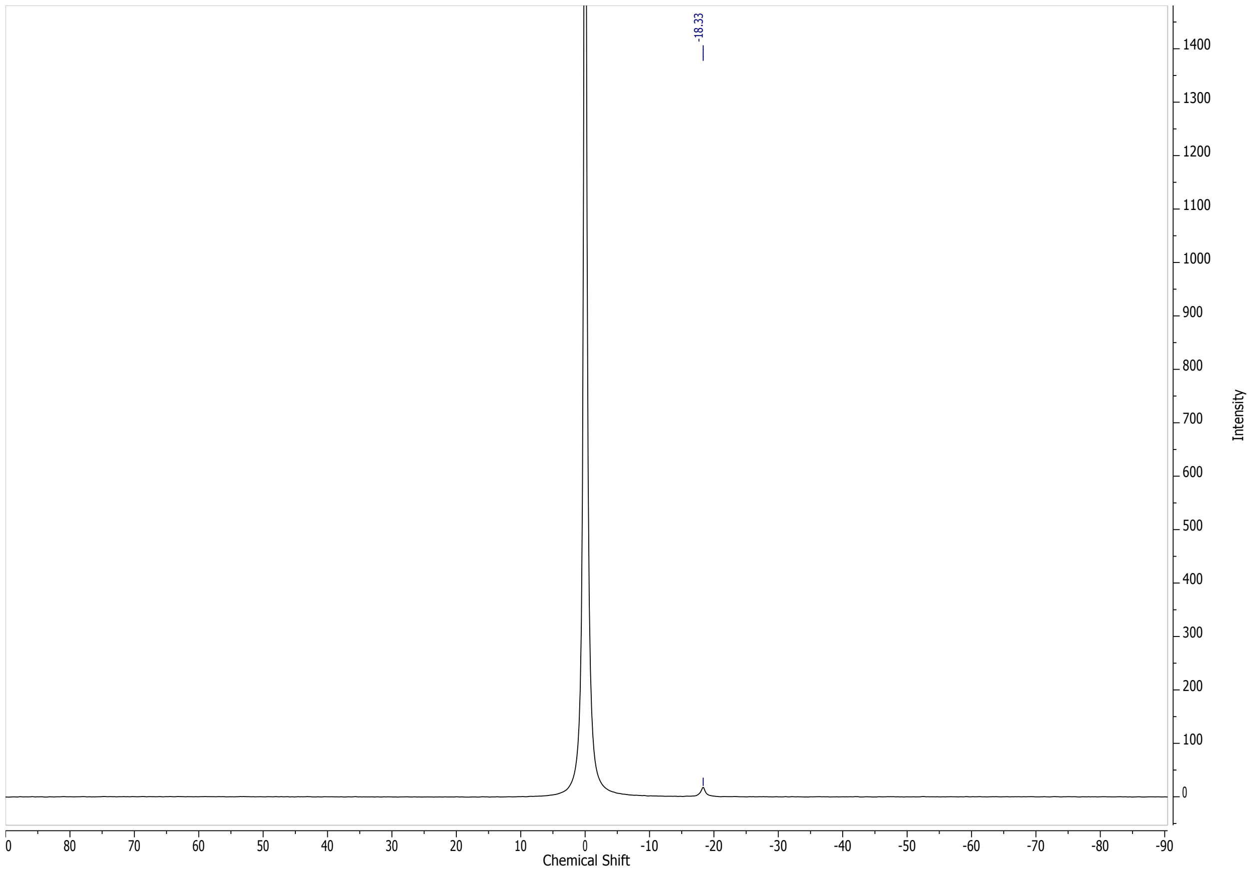


Figure S3. ^{11}B NMR (400 MHz, $CDCl_3$, referenced to BF_3•OEt_2) spectrum obtained at 296 K for F_{12}BsubPc-O-BsubPc.

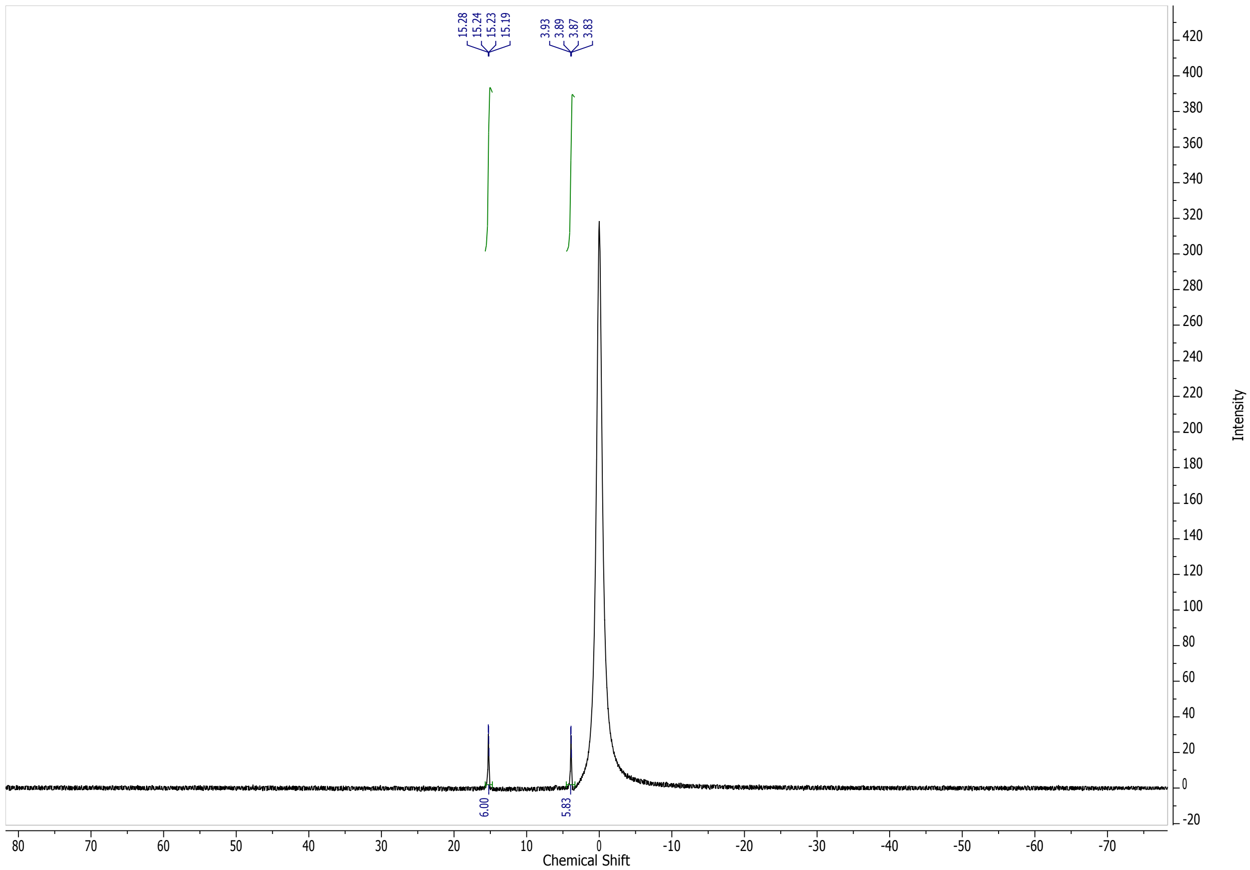


Figure S4. ^{19}F NMR (400 MHz, $CDCl_3$, referenced to BF_3•OEt_2) spectrum obtained at 296 K for F_{12}BsubPc-O-BsubPc.

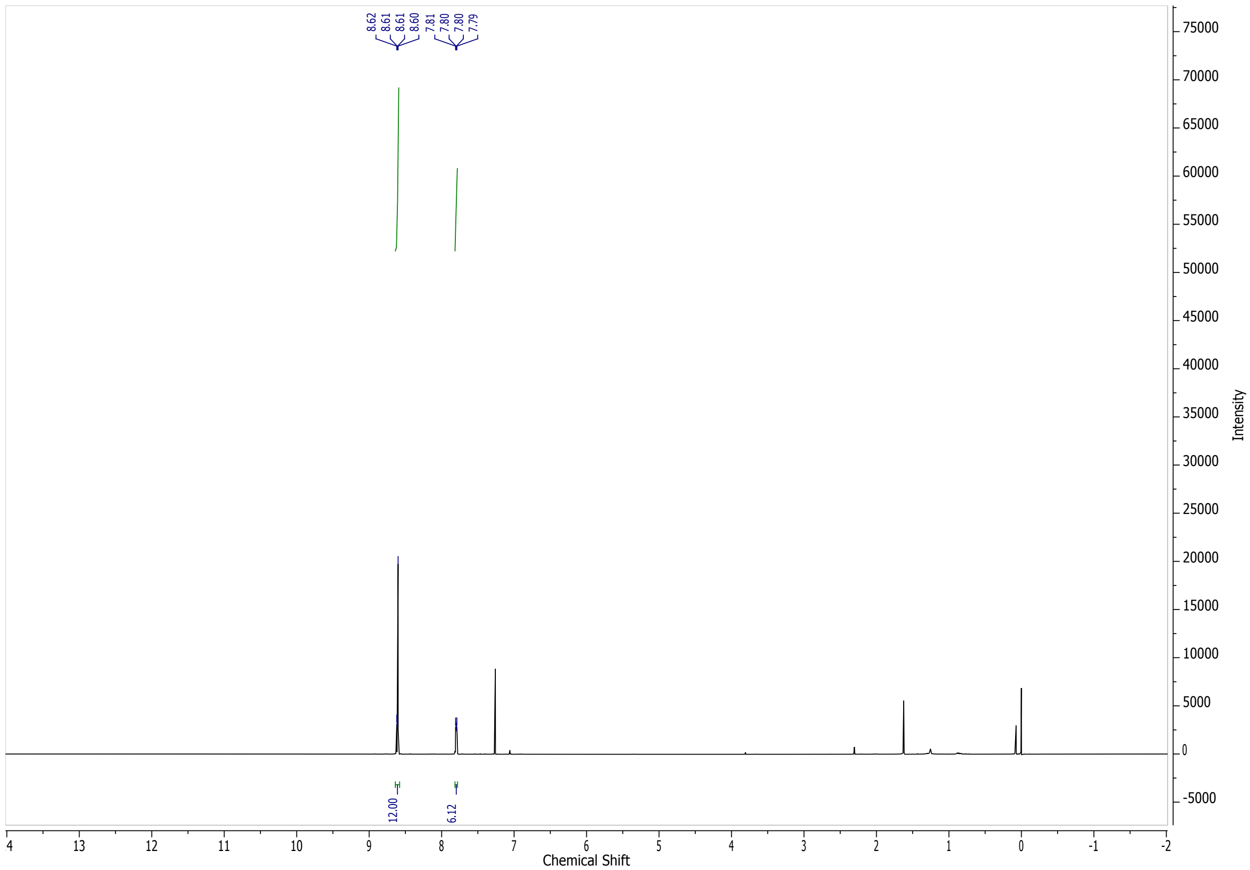


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum obtained at 296 K for Cl_6BsubPc-O-BsubPc.

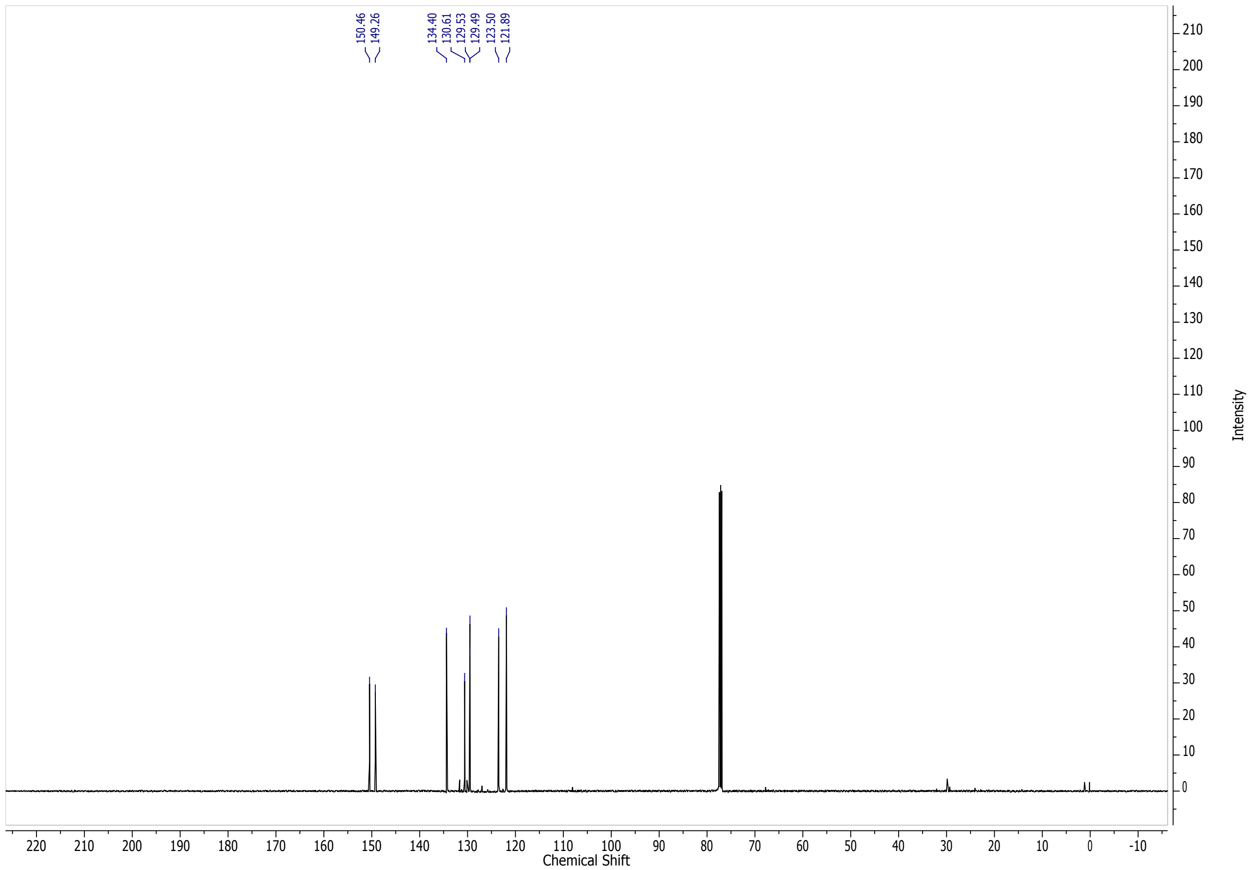


Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum obtained at 296 K for Cl_6BsubPc-O-BsubPc.

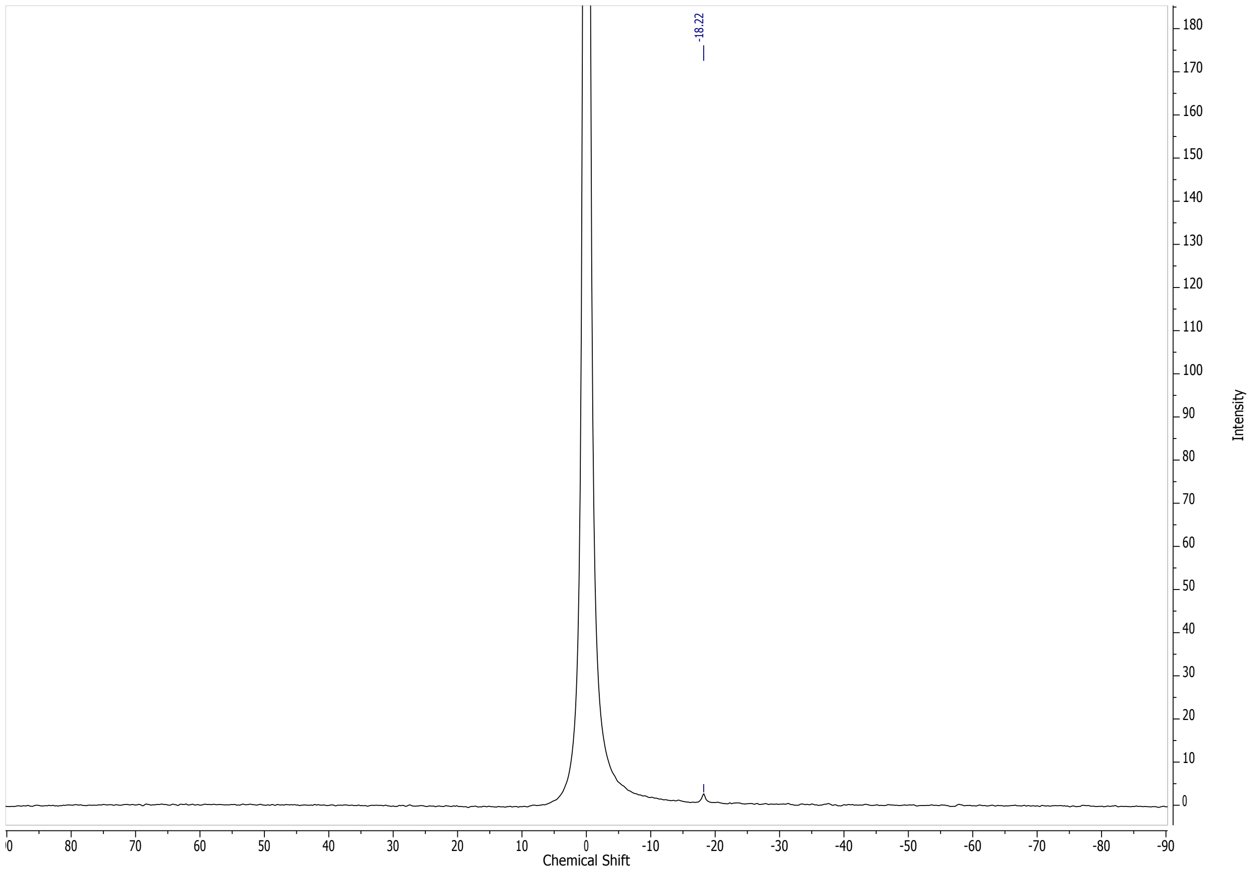


Figure S7. ^{11}B NMR (400 MHz, $CDCl_3$, referenced to BF_3•OEt_2) spectrum obtained at 296 K for Cl_6BsubPc-O-BsubPc.

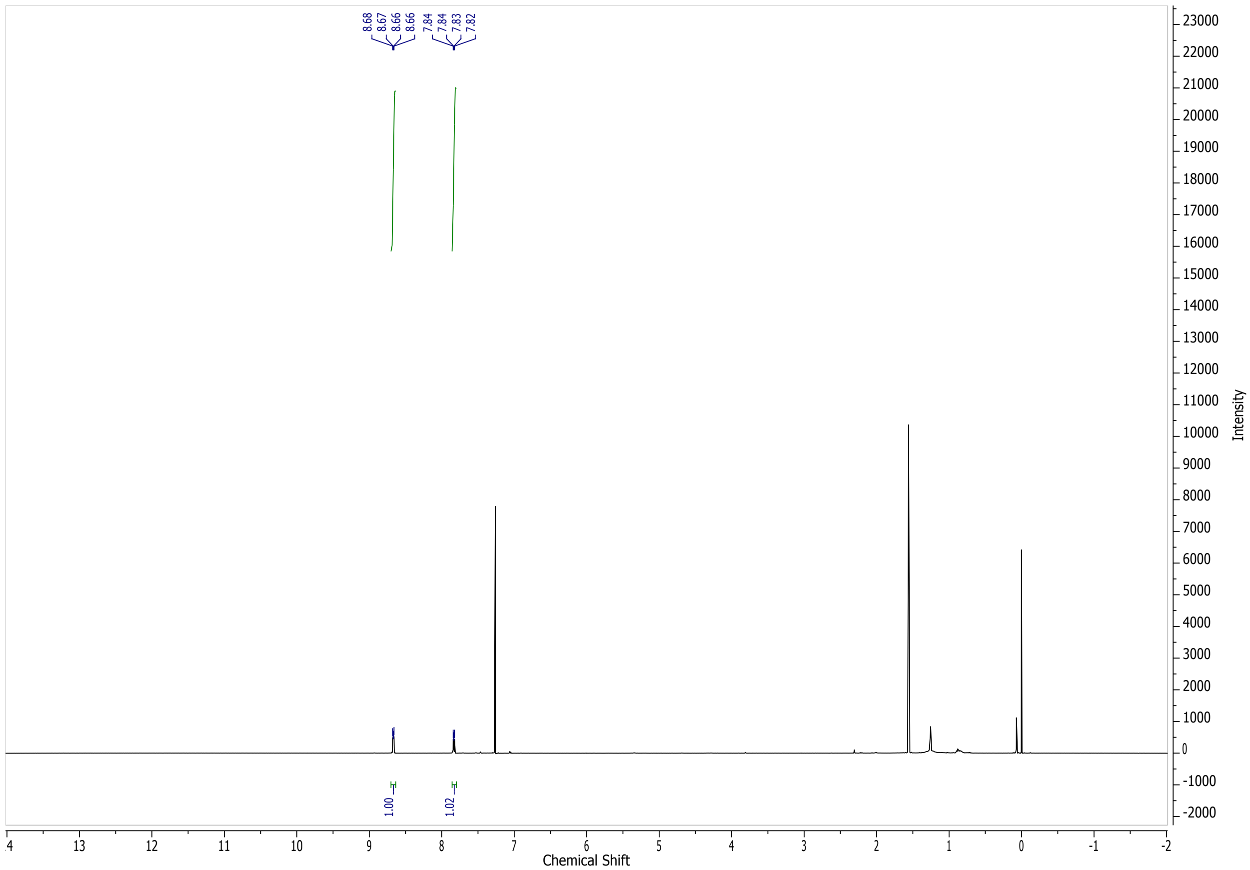


Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum obtained at 296 K for Cl_{12}BsubPc-O-BsubPc.

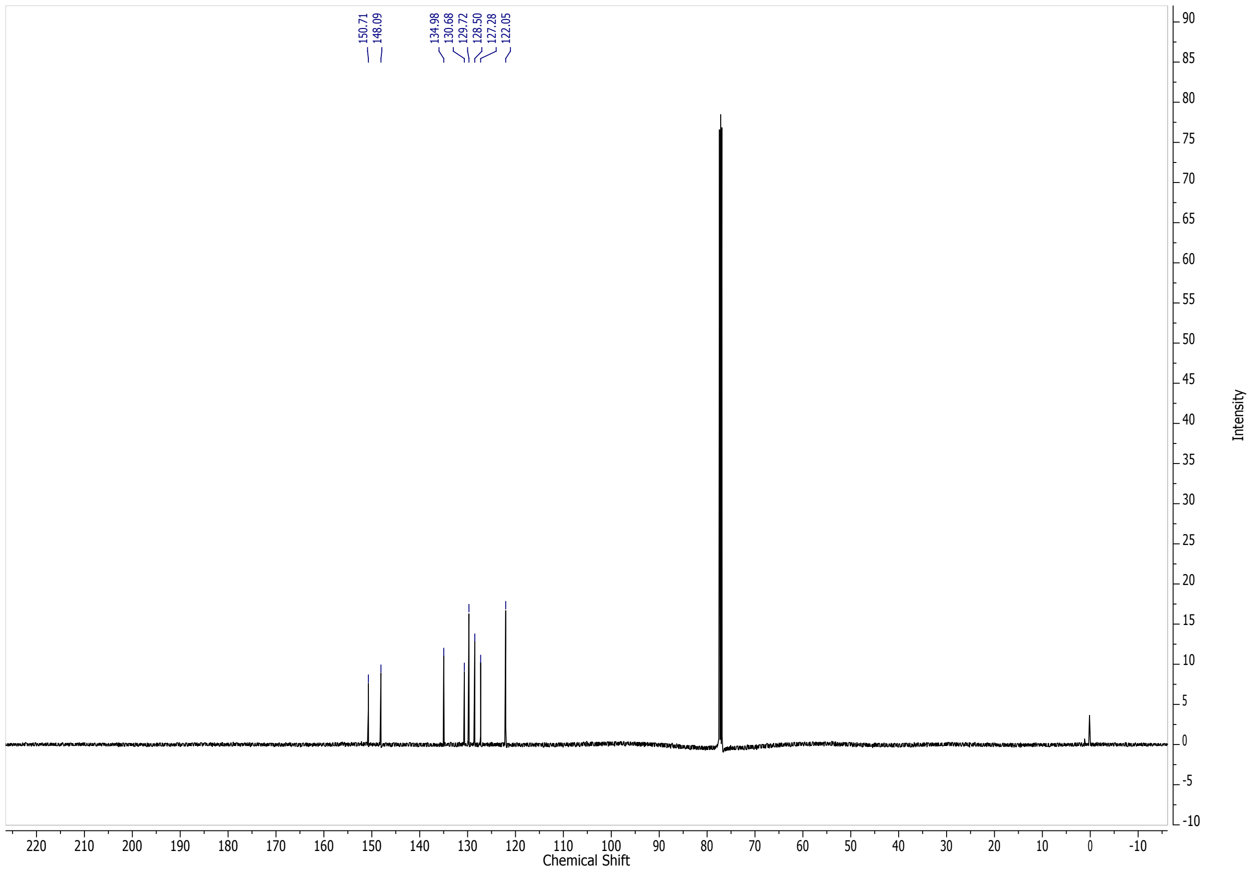


Figure S9. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum obtained at 296 K for Cl_{12}BsubPc-O-BsubPc.

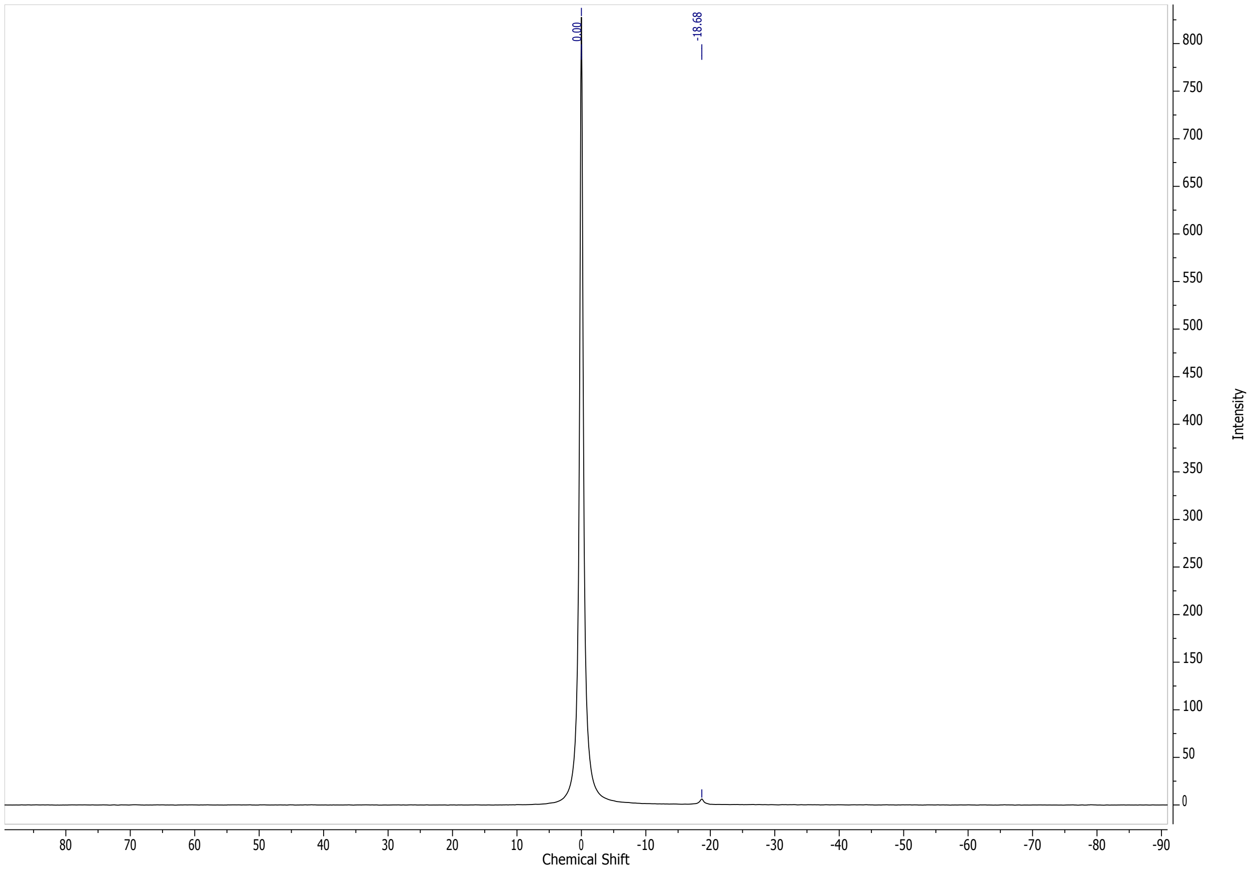


Figure S10. ^{11}B NMR (400 MHz, $CDCl_3$, referenced to BF_3•OEt_2) spectrum obtained at 296 K for Cl_{12}BsubPc-O-BsubPc.

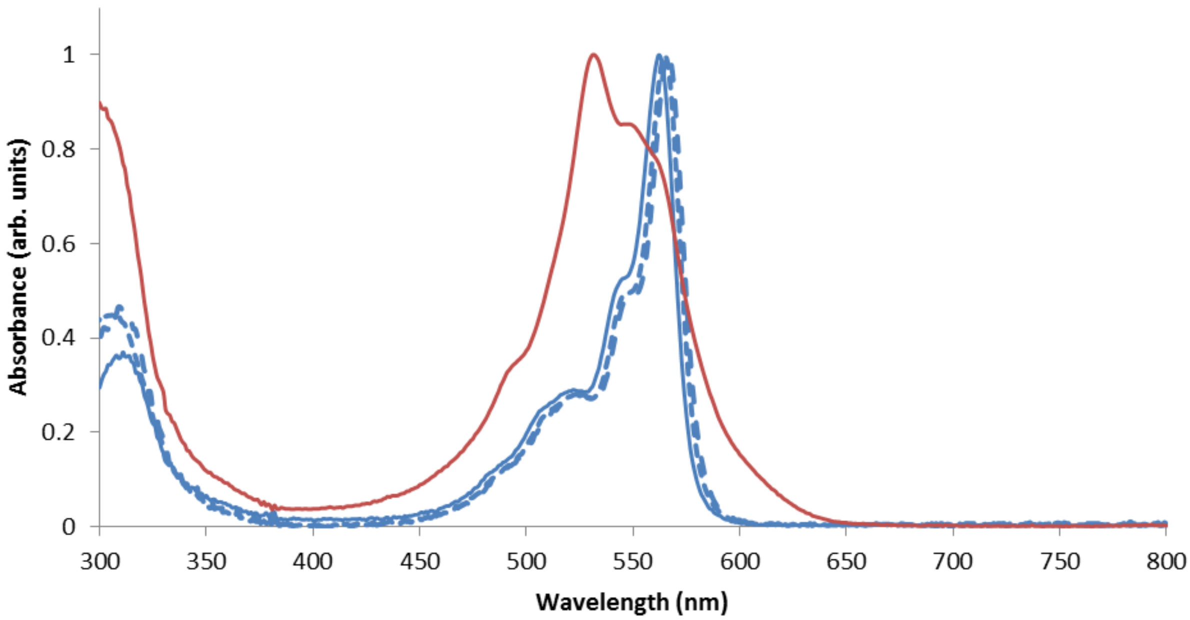
Wavelength of Maximum Absorption for Some Monomeric BsubPcs

Table S5. λ_{max} Values for Some Monomeric BsubPc Compounds

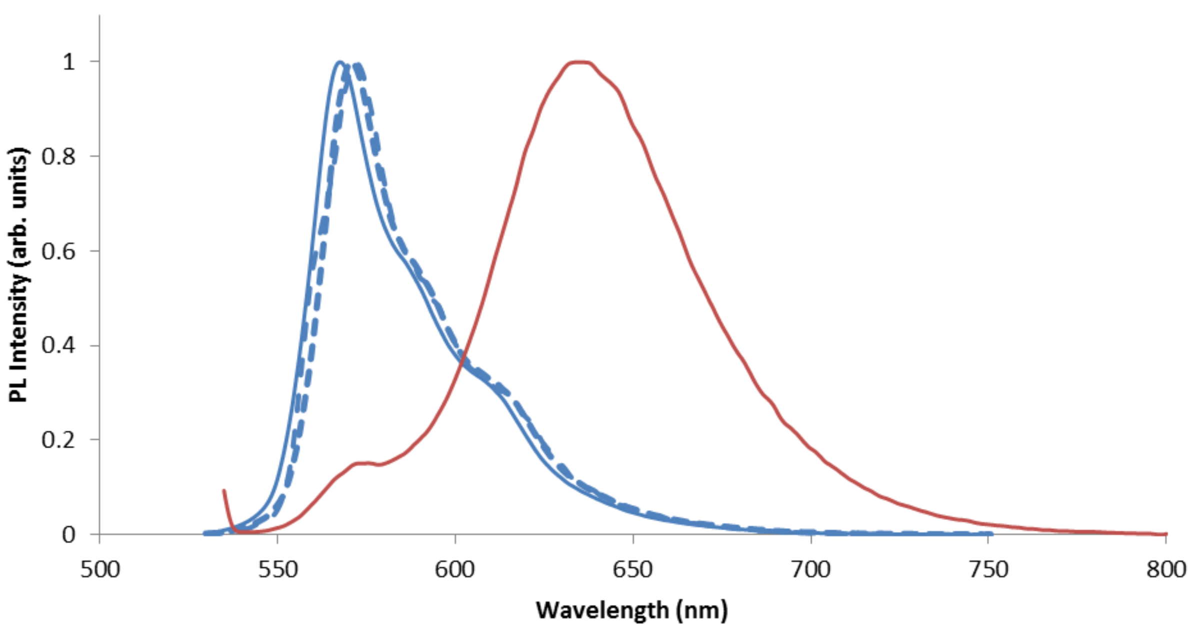
BsubPc Compound	λ_{max} (nm)
Br-BsubPc	566
Cl-BsubPc	565
F-BsubPc	562
PhO-BsubPc	563
HO-BsubPc	561
Br-F_{12}BsubPc	578
Cl-Cl_6BsubPc	574
Cl-Cl_{12}BsubPc	593

All measurements were done in toluene solutions at room temperature.

UV-vis Absorption and Photoluminescence Plots

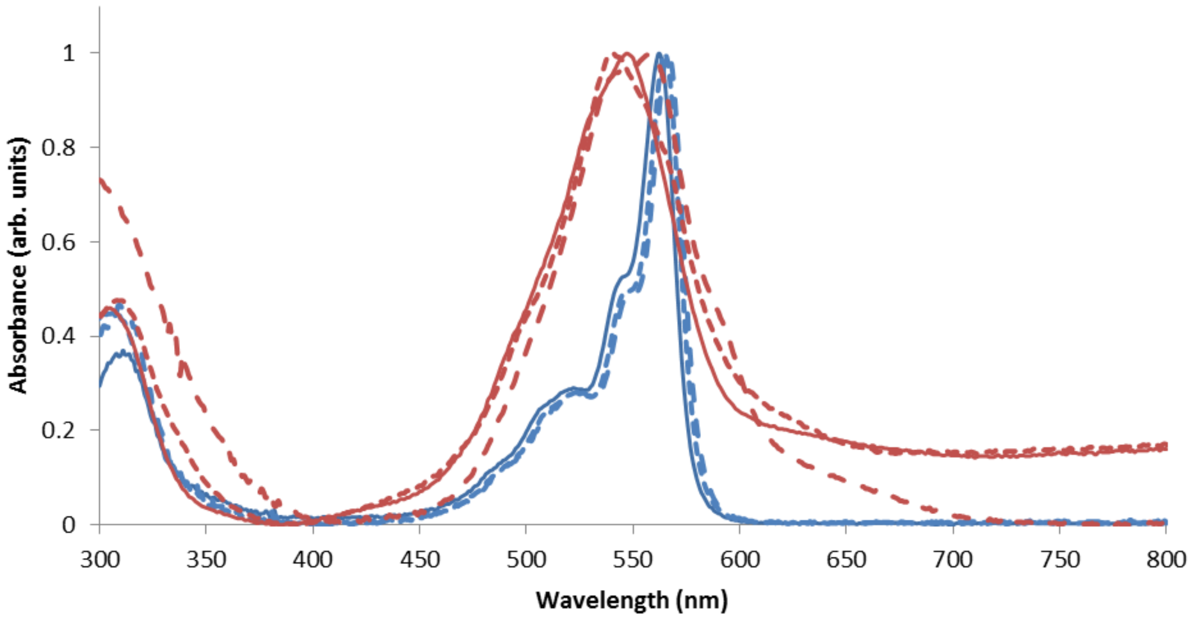


(a)

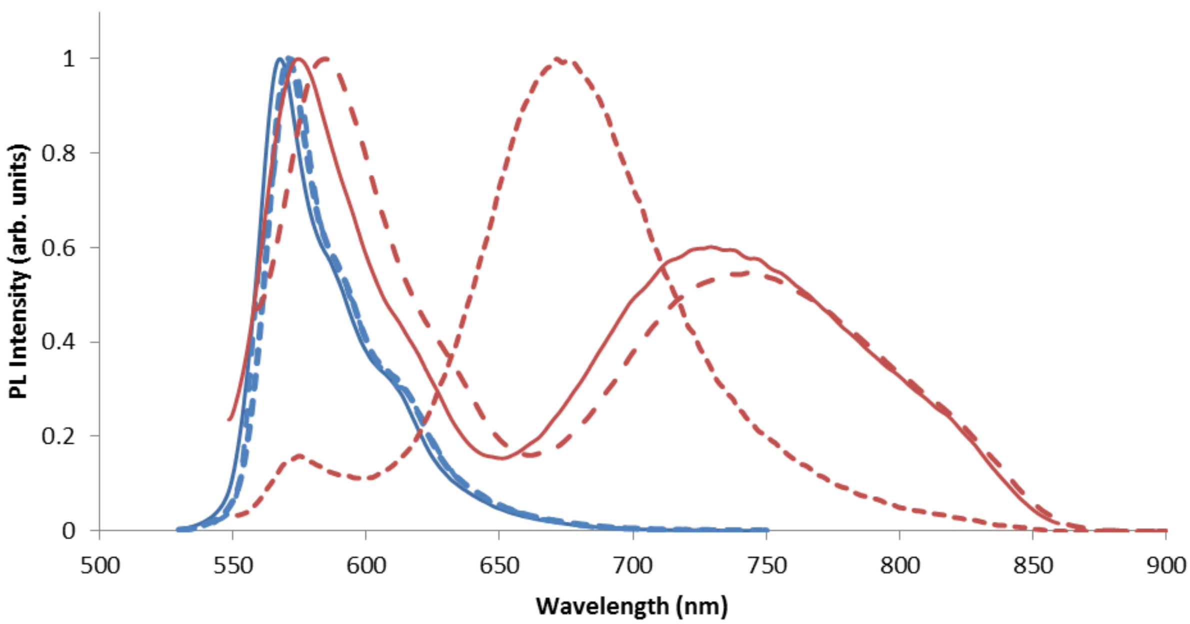


(b)

Figure S11. Overlay of μ-oxo BsubPc's (red) and the halo-BsubPc's (blue; F- solid, Cl- dotted, Br- dashed) (a) normalized absorption spectra; and (b) photoluminescence (PL) spectra.[9]



(a)



(b)

Figure S12. Overlay of F_{12}BsubPc-O-BsubPc's (solid red), Cl_6BsubPc-O-BsubPc's (dotted red), and Cl_{12}BsubPc-O-BsubPc's (dashed red) and the halo-BsubPc's (blue; F- solid, Cl- dotted, Br- dashed) (a) normalized absorption spectra; and (b) normalized photoluminescence (PL) spectra.

Determination of Fluorescence Quantum Yields

The fluorescence quantum yields (φ) were calculated using the formula below:

$$\varphi = \varphi_R \, (I / I_R)(OD_R / OD)(n^2 / n_R^2) \qquad \text{(Eq. S1)}$$

where *I* is the integrated fluorescence intensity, *OD* is the optical density (*i.e.* absorbance), and *n* is the refractive index of the solvent. The subscript $_R$ is PhO-F_{12}BsubPc, a reference fluorophore, which has previously been reported to have a φ = 0.40.[11] Integrated fluorescence intensity values were acquired from PerkinElmer FL WinLab (version 4.00.03) while the optical density values were acquired from PerkinElmer UV WinLab (version 6.02.0723).

Crystal Structure Details of F_{12}BsubPc-O-BsubPc

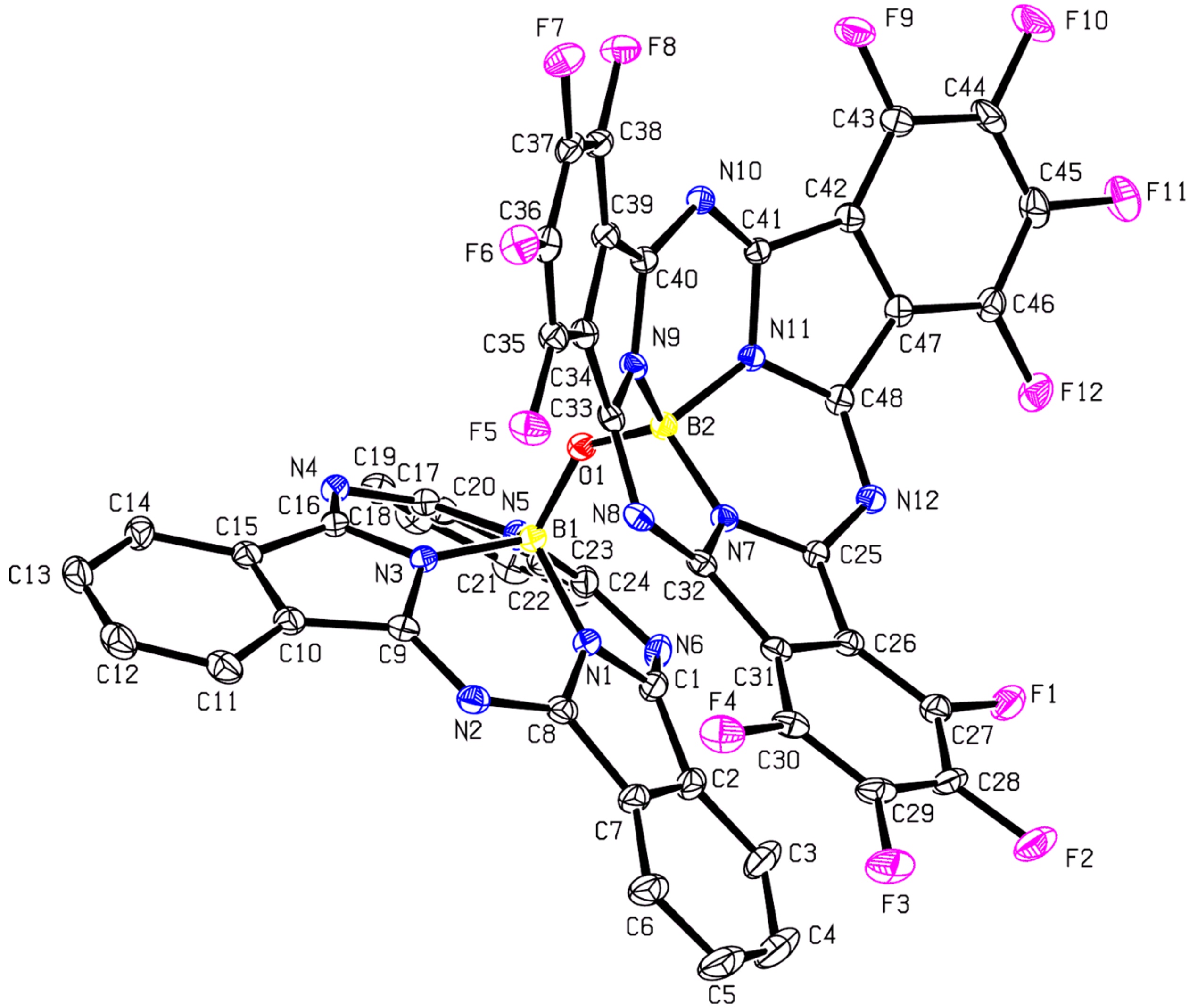


Figure S13. Thermal ellipsoid plot (50 % probability) showing the structure and atom numbering scheme of F_{12}BsubPc-O-BsubPc•C_7H_{16} (CCDC deposition number: 1018494). Hydrogen atoms and solvent inclusions have been omitted for clarity. Colors: boron - yellow; nitrogen - blue; carbon - white; oxygen - red; fluorine - magenta.

Table S6. Crystal data and structure refinement for F_{12}BsubPc-O-BsubPc.

Empirical formula	C55 H28 B2 F12 N12 O	
Formula weight	1122.51	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.5201(4) Å	a= 90°.
	b = 18.9039(7) Å	b= 99.163(2)°.
	c = 22.5091(9) Å	g = 90°.
Volume	4839.4(3) $Å^3$	
Z	4	
Density (calculated)	1.541 Mg/m^3	
Absorption coefficient	1.108 mm^{-1}	
F(000)	2272	
Crystal size	0.160 x 0.040 x 0.015 mm^3	
Theta range for data collection	3.069 to 66.755°.	
Index ranges	-13<=h<=13, -19<=k<=22, -26<=l<=26	
Reflections collected	32959	
Independent reflections	8365 [R(int) = 0.0562]	
Completeness to theta = 67.679°	95.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6549	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8365 / 17 / 739	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.1395	
R indices (all data)	R1 = 0.0760, wR2 = 0.1544	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.998 and -0.665 e.$Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for F_{12}BsubPc-O-BsubPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	6382(2)	5989(1)	387(1)	38(1)
F(2)	4239(2)	6537(1)	-39(1)	46(1)
F(3)	2295(2)	6007(1)	302(1)	47(1)
F(4)	2375(2)	4820(1)	982(1)	42(1)
F(5)	2242(1)	2337(1)	1375(1)	35(1)
F(6)	1975(1)	988(1)	972(1)	36(1)
F(7)	3835(2)	198(1)	826(1)	35(1)
F(8)	6043(1)	719(1)	1078(1)	34(1)
F(9)	9674(2)	1809(1)	695(1)	39(1)
F(10)	11273(2)	2415(1)	107(1)	48(1)
F(11)	11440(2)	3823(1)	23(1)	48(1)
F(12)	9954(2)	4684(1)	524(1)	38(1)
O(1)	7099(2)	3644(1)	2421(1)	23(1)
N(1)	6463(2)	4870(1)	2638(1)	24(1)
N(2)	4568(2)	4646(1)	2889(1)	27(1)
N(3)	6214(2)	3954(1)	3309(1)	21(1)
N(4)	7801(2)	3672(1)	4081(1)	23(1)
N(5)	8105(2)	4371(1)	3241(1)	23(1)
N(6)	8293(2)	5465(1)	2748(1)	29(1)
N(7)	5980(2)	4134(1)	1474(1)	20(1)
N(8)	4141(2)	3567(1)	1460(1)	24(1)
N(9)	5924(2)	2908(1)	1646(1)	20(1)
N(10)	7394(2)	2201(1)	1309(1)	22(1)
N(11)	7647(2)	3440(1)	1427(1)	19(1)
N(12)	7561(2)	4607(1)	1036(1)	23(1)
C(1)	7136(3)	5435(2)	2538(1)	27(1)
C(2)	6309(3)	5993(2)	2315(1)	32(1)
C(3)	6478(4)	6680(2)	2121(2)	44(1)
C(4)	5498(4)	7099(2)	1966(2)	56(1)
C(5)	4369(4)	6856(2)	2006(2)	54(1)
C(6)	4184(3)	6179(2)	2211(2)	41(1)

C(7)	5168(3)	5743(2)	2359(1)	30(1)
C(8)	5301(3)	5034(2)	2611(1)	26(1)
C(9)	5060(2)	4140(2)	3261(1)	24(1)
C(10)	4639(3)	3800(2)	3772(1)	26(1)
C(11)	3530(3)	3762(2)	3938(2)	34(1)
C(12)	3416(3)	3374(2)	4444(2)	39(1)
C(13)	4380(3)	3059(2)	4790(2)	38(1)
C(14)	5503(3)	3129(2)	4656(1)	31(1)
C(15)	5630(3)	3493(2)	4134(1)	25(1)
C(16)	6649(2)	3654(2)	3848(1)	22(1)
C(17)	8497(2)	4075(2)	3790(1)	23(1)
C(18)	9612(2)	4412(2)	4010(1)	25(1)
C(19)	10411(2)	4329(2)	4536(1)	28(1)
C(20)	11350(3)	4790(2)	4640(2)	35(1)
C(21)	11497(3)	5334(2)	4237(2)	36(1)
C(22)	10704(3)	5429(2)	3717(1)	32(1)
C(23)	9769(3)	4964(2)	3599(1)	26(1)
C(24)	8734(3)	4954(2)	3129(1)	26(1)
C(25)	6461(2)	4648(1)	1165(1)	20(1)
C(26)	5492(2)	5101(2)	913(1)	23(1)
C(27)	5426(3)	5694(2)	546(1)	28(1)
C(28)	4339(3)	5978(2)	336(1)	32(1)
C(29)	3323(3)	5691(2)	495(1)	33(1)
C(30)	3370(2)	5092(2)	845(1)	28(1)
C(31)	4449(2)	4791(2)	1054(1)	23(1)
C(32)	4781(2)	4139(2)	1378(1)	22(1)
C(33)	4719(2)	2956(2)	1558(1)	23(1)
C(34)	4307(2)	2239(2)	1421(1)	24(1)
C(35)	3185(2)	1957(2)	1298(1)	26(1)
C(36)	3046(2)	1271(2)	1102(1)	27(1)
C(37)	4013(3)	862(2)	1028(1)	26(1)
C(38)	5139(2)	1128(2)	1158(1)	25(1)
C(39)	5297(2)	1819(2)	1357(1)	23(1)
C(40)	6326(2)	2282(1)	1468(1)	20(1)
C(41)	8011(2)	2794(2)	1263(1)	20(1)
C(42)	8981(2)	2936(2)	935(1)	23(1)

C(43)	9715(2)	2512(2)	661(1)	28(1)
C(44)	10529(3)	2820(2)	357(1)	34(1)
C(45)	10620(3)	3549(2)	316(1)	34(1)
C(46)	9881(2)	3983(2)	570(1)	28(1)
C(47)	9058(2)	3683(2)	877(1)	24(1)
C(48)	8107(2)	3987(2)	1147(1)	22(1)
B(1)	6976(3)	4168(2)	2857(1)	21(1)
B(2)	6695(3)	3549(2)	1809(1)	21(1)
C(1S)	-805(11)	1495(8)	3616(7)	249(7)
C(2S)	40(20)	1634(6)	3180(11)	431(18)
C(3S)	-190(12)	2429(6)	3095(4)	213(5)
C(4S)	479(9)	2723(6)	2626(6)	219(5)
C(5S)	568(9)	3521(6)	2621(4)	187(4)
C(6S)	1445(8)	3791(7)	2246(5)	209(5)
C(7S)	1296(9)	4584(7)	2234(4)	187(4)

Table S8. Bond lengths [Å] and angles [°] for F_{12}BsubPc-O-BsubPc.

F(1)-C(27)	1.334(4)
F(2)-C(28)	1.346(4)
F(3)-C(29)	1.335(3)
F(4)-C(30)	1.338(4)
F(5)-C(35)	1.336(3)
F(6)-C(36)	1.334(3)
F(7)-C(37)	1.339(3)
F(8)-C(38)	1.332(3)
F(9)-C(43)	1.332(4)
F(10)-C(44)	1.340(3)
F(11)-C(45)	1.339(3)
F(12)-C(46)	1.333(4)
O(1)-B(2)	1.393(4)
O(1)-B(1)	1.418(4)
N(1)-C(1)	1.360(4)
N(1)-C(8)	1.366(4)
N(1)-B(1)	1.503(4)
N(2)-C(9)	1.337(4)
N(2)-C(8)	1.345(4)
N(3)-C(16)	1.360(4)
N(3)-C(9)	1.362(4)
N(3)-B(1)	1.502(4)
N(4)-C(16)	1.348(4)
N(4)-C(17)	1.349(4)
N(5)-C(24)	1.364(4)
N(5)-C(17)	1.367(4)
N(5)-B(1)	1.492(4)
N(6)-C(24)	1.338(4)
N(6)-C(1)	1.343(4)
N(7)-C(32)	1.363(3)
N(7)-C(25)	1.364(4)
N(7)-B(2)	1.507(4)
N(8)-C(33)	1.332(4)
N(8)-C(32)	1.339(4)

N(9)-C(40)	1.355(4)
N(9)-C(33)	1.373(3)
N(9)-B(2)	1.512(4)
N(10)-C(41)	1.339(4)
N(10)-C(40)	1.344(3)
N(11)-C(41)	1.361(4)
N(11)-C(48)	1.362(4)
N(11)-B(2)	1.512(4)
N(12)-C(48)	1.336(4)
N(12)-C(25)	1.347(3)
C(1)-C(2)	1.456(4)
C(2)-C(3)	1.393(5)
C(2)-C(7)	1.415(5)
C(3)-C(4)	1.378(6)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.396(6)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.388(5)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.398(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.455(4)
C(9)-C(10)	1.465(4)
C(10)-C(11)	1.390(4)
C(10)-C(15)	1.417(4)
C(11)-C(12)	1.379(5)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.386(5)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.381(5)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.389(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.458(4)
C(17)-C(18)	1.448(4)
C(18)-C(19)	1.388(4)

C(18)-C(23)	1.424(4)
C(19)-C(20)	1.380(5)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.400(5)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.377(5)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.384(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.463(4)
C(25)-C(26)	1.448(4)
C(26)-C(27)	1.388(4)
C(26)-C(31)	1.418(4)
C(27)-C(28)	1.375(4)
C(28)-C(29)	1.388(5)
C(29)-C(30)	1.375(5)
C(30)-C(31)	1.380(4)
C(31)-C(32)	1.452(4)
C(33)-C(34)	1.453(4)
C(34)-C(35)	1.385(4)
C(34)-C(39)	1.416(4)
C(35)-C(36)	1.372(4)
C(36)-C(37)	1.388(4)
C(37)-C(38)	1.378(4)
C(38)-C(39)	1.382(4)
C(39)-C(40)	1.463(4)
C(41)-C(42)	1.459(4)
C(42)-C(43)	1.380(4)
C(42)-C(47)	1.423(4)
C(43)-C(44)	1.376(4)
C(44)-C(45)	1.386(5)
C(45)-C(46)	1.372(4)
C(46)-C(47)	1.381(4)
C(47)-C(48)	1.453(4)
C(1S)-C(2S)	1.511(5)
C(1S)-H(1SA)	0.9800

C(1S)-H(1SB)	0.9800
C(1S)-H(1SC)	0.9800
C(2S)-C(3S)	1.532(5)
C(2S)-H(2SA)	0.9900
C(2S)-H(2SB)	0.9900
C(3S)-C(4S)	1.509(5)
C(3S)-H(3SA)	0.9900
C(3S)-H(3SB)	0.9900
C(4S)-C(5S)	1.513(5)
C(4S)-H(4SA)	0.9900
C(4S)-H(4SB)	0.9900
C(5S)-C(6S)	1.504(5)
C(5S)-H(5SA)	0.9900
C(5S)-H(5SB)	0.9900
C(6S)-C(7S)	1.509(5)
C(6S)-H(6SA)	0.9900
C(6S)-H(6SB)	0.9900
C(7S)-H(7SA)	0.9800
C(7S)-H(7SB)	0.9800
C(7S)-H(7SC)	0.9800

B(2)-O(1)-B(1)	136.1(2)
C(1)-N(1)-C(8)	113.2(2)
C(1)-N(1)-B(1)	122.9(2)
C(8)-N(1)-B(1)	123.1(2)
C(9)-N(2)-C(8)	116.5(2)
C(16)-N(3)-C(9)	113.3(2)
C(16)-N(3)-B(1)	123.0(2)
C(9)-N(3)-B(1)	123.0(2)
C(16)-N(4)-C(17)	116.7(2)
C(24)-N(5)-C(17)	112.9(2)
C(24)-N(5)-B(1)	122.7(2)
C(17)-N(5)-B(1)	123.4(2)
C(24)-N(6)-C(1)	116.7(3)
C(32)-N(7)-C(25)	113.4(2)
C(32)-N(7)-B(2)	122.9(2)

C(25)-N(7)-B(2)	123.0(2)
C(33)-N(8)-C(32)	116.8(2)
C(40)-N(9)-C(33)	113.6(2)
C(40)-N(9)-B(2)	123.8(2)
C(33)-N(9)-B(2)	121.5(2)
C(41)-N(10)-C(40)	116.4(2)
C(41)-N(11)-C(48)	113.4(2)
C(41)-N(11)-B(2)	124.0(2)
C(48)-N(11)-B(2)	122.1(2)
C(48)-N(12)-C(25)	116.2(2)
N(6)-C(1)-N(1)	122.3(3)
N(6)-C(1)-C(2)	130.4(3)
N(1)-C(1)-C(2)	105.6(3)
C(3)-C(2)-C(7)	120.7(3)
C(3)-C(2)-C(1)	131.9(3)
C(7)-C(2)-C(1)	107.3(3)
C(4)-C(3)-C(2)	117.8(4)
C(4)-C(3)-H(3A)	121.1
C(2)-C(3)-H(3A)	121.1
C(3)-C(4)-C(5)	121.9(3)
C(3)-C(4)-H(4A)	119.1
C(5)-C(4)-H(4A)	119.1
C(6)-C(5)-C(4)	121.3(4)
C(6)-C(5)-H(5A)	119.4
C(4)-C(5)-H(5A)	119.4
C(5)-C(6)-C(7)	117.4(4)
C(5)-C(6)-H(6A)	121.3
C(7)-C(6)-H(6A)	121.3
C(6)-C(7)-C(2)	120.9(3)
C(6)-C(7)-C(8)	131.8(3)
C(2)-C(7)-C(8)	107.2(3)
N(2)-C(8)-N(1)	122.6(3)
N(2)-C(8)-C(7)	130.5(3)
N(1)-C(8)-C(7)	105.5(3)
N(2)-C(9)-N(3)	123.1(3)
N(2)-C(9)-C(10)	130.2(3)

N(3)-C(9)-C(10)	105.3(2)
C(11)-C(10)-C(15)	121.0(3)
C(11)-C(10)-C(9)	131.8(3)
C(15)-C(10)-C(9)	107.1(2)
C(12)-C(11)-C(10)	117.5(3)
C(12)-C(11)-H(11A)	121.2
C(10)-C(11)-H(11A)	121.2
C(11)-C(12)-C(13)	121.4(3)
C(11)-C(12)-H(12A)	119.3
C(13)-C(12)-H(12A)	119.3
C(14)-C(13)-C(12)	122.0(3)
C(14)-C(13)-H(13A)	119.0
C(12)-C(13)-H(13A)	119.0
C(13)-C(14)-C(15)	117.5(3)
C(13)-C(14)-H(14A)	121.3
C(15)-C(14)-H(14A)	121.3
C(14)-C(15)-C(10)	120.4(3)
C(14)-C(15)-C(16)	132.7(3)
C(10)-C(15)-C(16)	106.9(2)
N(4)-C(16)-N(3)	122.5(2)
N(4)-C(16)-C(15)	130.2(3)
N(3)-C(16)-C(15)	105.8(2)
N(4)-C(17)-N(5)	122.3(2)
N(4)-C(17)-C(18)	130.2(3)
N(5)-C(17)-C(18)	106.1(2)
C(19)-C(18)-C(23)	120.1(3)
C(19)-C(18)-C(17)	132.3(3)
C(23)-C(18)-C(17)	107.3(2)
C(20)-C(19)-C(18)	118.0(3)
C(20)-C(19)-H(19A)	121.0
C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.7(3)
C(19)-C(20)-H(20A)	119.1
C(21)-C(20)-H(20A)	119.1
C(22)-C(21)-C(20)	121.0(3)
C(22)-C(21)-H(21A)	119.5

C(20)-C(21)-H(21A)	119.5
C(21)-C(22)-C(23)	118.1(3)
C(21)-C(22)-H(22A)	121.0
C(23)-C(22)-H(22A)	121.0
C(22)-C(23)-C(18)	121.1(3)
C(22)-C(23)-C(24)	131.8(3)
C(18)-C(23)-C(24)	106.7(2)
N(6)-C(24)-N(5)	122.9(3)
N(6)-C(24)-C(23)	129.5(3)
N(5)-C(24)-C(23)	105.8(2)
N(12)-C(25)-N(7)	122.8(2)
N(12)-C(25)-C(26)	130.0(2)
N(7)-C(25)-C(26)	105.7(2)
C(27)-C(26)-C(31)	119.9(3)
C(27)-C(26)-C(25)	132.6(3)
C(31)-C(26)-C(25)	107.2(2)
F(1)-C(27)-C(28)	119.3(3)
F(1)-C(27)-C(26)	121.9(3)
C(28)-C(27)-C(26)	118.8(3)
F(2)-C(28)-C(27)	120.3(3)
F(2)-C(28)-C(29)	118.5(3)
C(27)-C(28)-C(29)	121.2(3)
F(3)-C(29)-C(30)	120.4(3)
F(3)-C(29)-C(28)	118.9(3)
C(30)-C(29)-C(28)	120.7(3)
F(4)-C(30)-C(29)	119.5(3)
F(4)-C(30)-C(31)	121.4(3)
C(29)-C(30)-C(31)	119.1(3)
C(30)-C(31)-C(26)	120.1(3)
C(30)-C(31)-C(32)	132.3(3)
C(26)-C(31)-C(32)	107.3(2)
N(8)-C(32)-N(7)	122.6(2)
N(8)-C(32)-C(31)	130.5(2)
N(7)-C(32)-C(31)	105.4(2)
N(8)-C(33)-N(9)	123.2(3)
N(8)-C(33)-C(34)	129.4(2)

N(9)-C(33)-C(34)	104.9(2)
C(35)-C(34)-C(39)	120.3(3)
C(35)-C(34)-C(33)	131.7(3)
C(39)-C(34)-C(33)	107.7(2)
F(5)-C(35)-C(36)	119.6(3)
F(5)-C(35)-C(34)	121.3(3)
C(36)-C(35)-C(34)	119.1(3)
F(6)-C(36)-C(35)	120.5(3)
F(6)-C(36)-C(37)	118.9(3)
C(35)-C(36)-C(37)	120.7(3)
F(7)-C(37)-C(38)	120.2(3)
F(7)-C(37)-C(36)	118.6(3)
C(38)-C(37)-C(36)	121.2(3)
F(8)-C(38)-C(37)	119.2(3)
F(8)-C(38)-C(39)	121.8(3)
C(37)-C(38)-C(39)	119.0(3)
C(38)-C(39)-C(34)	119.8(3)
C(38)-C(39)-C(40)	133.0(3)
C(34)-C(39)-C(40)	106.9(2)
N(10)-C(40)-N(9)	123.3(2)
N(10)-C(40)-C(39)	129.6(2)
N(9)-C(40)-C(39)	105.5(2)
N(10)-C(41)-N(11)	122.7(2)
N(10)-C(41)-C(42)	130.6(3)
N(11)-C(41)-C(42)	105.4(2)
C(43)-C(42)-C(47)	118.9(3)
C(43)-C(42)-C(41)	133.9(3)
C(47)-C(42)-C(41)	107.1(2)
F(9)-C(43)-C(44)	119.0(3)
F(9)-C(43)-C(42)	121.5(3)
C(44)-C(43)-C(42)	119.4(3)
F(10)-C(44)-C(43)	119.9(3)
F(10)-C(44)-C(45)	118.7(3)
C(43)-C(44)-C(45)	121.3(3)
F(11)-C(45)-C(46)	120.5(3)
F(11)-C(45)-C(44)	119.0(3)

C(46)-C(45)-C(44)	120.5(3)
F(12)-C(46)-C(45)	120.7(3)
F(12)-C(46)-C(47)	120.3(3)
C(45)-C(46)-C(47)	119.0(3)
C(46)-C(47)-C(42)	120.8(3)
C(46)-C(47)-C(48)	132.1(3)
C(42)-C(47)-C(48)	107.0(2)
N(12)-C(48)-N(11)	123.2(2)
N(12)-C(48)-C(47)	129.3(3)
N(11)-C(48)-C(47)	105.6(2)
O(1)-B(1)-N(5)	114.0(2)
O(1)-B(1)-N(3)	114.6(2)
N(5)-B(1)-N(3)	103.1(2)
O(1)-B(1)-N(1)	117.8(2)
N(5)-B(1)-N(1)	102.9(2)
N(3)-B(1)-N(1)	102.6(2)
O(1)-B(2)-N(7)	118.0(2)
O(1)-B(2)-N(9)	115.8(2)
N(7)-B(2)-N(9)	102.3(2)
O(1)-B(2)-N(11)	114.9(2)
N(7)-B(2)-N(11)	101.8(2)
N(9)-B(2)-N(11)	101.7(2)
C(2S)-C(1S)-H(1SA)	109.5
C(2S)-C(1S)-H(1SB)	109.5
H(1SA)-C(1S)-H(1SB)	109.5
C(2S)-C(1S)-H(1SC)	109.5
H(1SA)-C(1S)-H(1SC)	109.5
H(1SB)-C(1S)-H(1SC)	109.5
C(1S)-C(2S)-C(3S)	97.8(10)
C(1S)-C(2S)-H(2SA)	112.2
C(3S)-C(2S)-H(2SA)	112.2
C(1S)-C(2S)-H(2SB)	112.2
C(3S)-C(2S)-H(2SB)	112.2
H(2SA)-C(2S)-H(2SB)	109.8
C(4S)-C(3S)-C(2S)	110.5(8)
C(4S)-C(3S)-H(3SA)	109.5

C(2S)-C(3S)-H(3SA)	109.5
C(4S)-C(3S)-H(3SB)	109.5
C(2S)-C(3S)-H(3SB)	109.5
H(3SA)-C(3S)-H(3SB)	108.1
C(3S)-C(4S)-C(5S)	114.5(10)
C(3S)-C(4S)-H(4SA)	108.6
C(5S)-C(4S)-H(4SA)	108.6
C(3S)-C(4S)-H(4SB)	108.6
C(5S)-C(4S)-H(4SB)	108.6
H(4SA)-C(4S)-H(4SB)	107.6
C(6S)-C(5S)-C(4S)	113.3(8)
C(6S)-C(5S)-H(5SA)	108.9
C(4S)-C(5S)-H(5SA)	108.9
C(6S)-C(5S)-H(5SB)	108.9
C(4S)-C(5S)-H(5SB)	108.9
H(5SA)-C(5S)-H(5SB)	107.7
C(5S)-C(6S)-C(7S)	105.2(8)
C(5S)-C(6S)-H(6SA)	110.7
C(7S)-C(6S)-H(6SA)	110.7
C(5S)-C(6S)-H(6SB)	110.7
C(7S)-C(6S)-H(6SB)	110.7
H(6SA)-C(6S)-H(6SB)	108.8
C(6S)-C(7S)-H(7SA)	109.5
C(6S)-C(7S)-H(7SB)	109.5
H(7SA)-C(7S)-H(7SB)	109.5
C(6S)-C(7S)-H(7SC)	109.5
H(7SA)-C(7S)-H(7SC)	109.5
H(7SB)-C(7S)-H(7SC)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3) for F_{12}BsubPc-O-BsubPc. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	41(1)	28(1)	45(1)	10(1)	11(1)	1(1)
F(2)	57(1)	30(1)	47(1)	11(1)	-4(1)	13(1)
F(3)	36(1)	48(1)	52(1)	0(1)	-10(1)	21(1)
F(4)	21(1)	49(1)	55(1)	-2(1)	4(1)	6(1)
F(5)	19(1)	39(1)	50(1)	-5(1)	10(1)	1(1)
F(6)	26(1)	36(1)	45(1)	-1(1)	5(1)	-9(1)
F(7)	36(1)	22(1)	45(1)	0(1)	0(1)	-5(1)
F(8)	28(1)	24(1)	49(1)	-1(1)	9(1)	3(1)
F(9)	36(1)	31(1)	54(1)	-4(1)	20(1)	7(1)
F(10)	37(1)	55(1)	60(1)	-8(1)	31(1)	8(1)
F(11)	34(1)	60(1)	58(1)	5(1)	31(1)	-5(1)
F(12)	30(1)	35(1)	50(1)	13(1)	15(1)	-2(1)
O(1)	27(1)	22(1)	21(1)	1(1)	2(1)	5(1)
N(1)	31(1)	20(1)	21(1)	1(1)	6(1)	3(1)
N(2)	29(1)	25(1)	26(1)	-3(1)	3(1)	3(1)
N(3)	24(1)	18(1)	21(1)	-1(1)	5(1)	-1(1)
N(4)	26(1)	20(1)	24(1)	1(1)	6(1)	-1(1)
N(5)	26(1)	22(1)	21(1)	1(1)	5(1)	-2(1)
N(6)	38(1)	27(1)	23(1)	4(1)	7(1)	-4(1)
N(7)	17(1)	22(1)	21(1)	0(1)	4(1)	2(1)
N(8)	20(1)	26(1)	25(1)	-3(1)	7(1)	2(1)
N(9)	18(1)	22(1)	22(1)	-1(1)	6(1)	1(1)
N(10)	20(1)	23(1)	22(1)	2(1)	5(1)	3(1)
N(11)	16(1)	21(1)	20(1)	2(1)	3(1)	2(1)
N(12)	21(1)	23(1)	24(1)	0(1)	4(1)	1(1)
C(1)	41(2)	21(2)	21(1)	1(1)	5(1)	-1(1)
C(2)	51(2)	24(2)	20(1)	2(1)	2(1)	4(2)
C(3)	67(2)	24(2)	37(2)	10(1)	-1(2)	-1(2)
C(4)	83(3)	26(2)	54(2)	14(2)	-5(2)	2(2)
C(5)	74(3)	32(2)	50(2)	6(2)	-9(2)	19(2)
C(6)	54(2)	33(2)	32(2)	1(1)	-5(2)	14(2)

C(7)	43(2)	25(2)	21(1)	1(1)	-1(1)	8(1)
C(8)	31(2)	24(2)	21(1)	-4(1)	3(1)	4(1)
C(9)	24(1)	21(2)	26(2)	-4(1)	5(1)	2(1)
C(10)	32(2)	19(2)	29(2)	-5(1)	10(1)	-4(1)
C(11)	32(2)	33(2)	40(2)	-7(1)	15(1)	-3(1)
C(12)	37(2)	38(2)	48(2)	-7(2)	25(2)	-7(2)
C(13)	53(2)	31(2)	37(2)	-2(1)	24(2)	-8(2)
C(14)	43(2)	23(2)	27(2)	-1(1)	10(1)	-7(1)
C(15)	31(2)	17(1)	28(2)	-5(1)	10(1)	-5(1)
C(16)	28(2)	17(1)	23(1)	-1(1)	6(1)	0(1)
C(17)	26(1)	21(1)	23(1)	0(1)	5(1)	3(1)
C(18)	22(1)	25(2)	29(2)	-3(1)	7(1)	2(1)
C(19)	24(2)	30(2)	32(2)	-1(1)	5(1)	4(1)
C(20)	23(2)	45(2)	36(2)	-4(2)	3(1)	4(1)
C(21)	20(2)	40(2)	46(2)	-7(2)	7(1)	-6(1)
C(22)	29(2)	30(2)	40(2)	-2(1)	14(1)	-5(1)
C(23)	25(2)	27(2)	28(2)	-2(1)	9(1)	-1(1)
C(24)	30(2)	26(2)	23(1)	1(1)	7(1)	-3(1)
C(25)	22(1)	20(1)	18(1)	1(1)	3(1)	2(1)
C(26)	25(2)	22(2)	21(1)	-3(1)	1(1)	4(1)
C(27)	32(2)	25(2)	26(2)	-2(1)	4(1)	3(1)
C(28)	45(2)	19(2)	30(2)	2(1)	-3(1)	10(1)
C(29)	32(2)	32(2)	33(2)	-6(1)	-6(1)	16(1)
C(30)	21(2)	29(2)	32(2)	-8(1)	2(1)	5(1)
C(31)	23(1)	24(2)	22(1)	-6(1)	2(1)	4(1)
C(32)	18(1)	26(2)	22(1)	-3(1)	4(1)	4(1)
C(33)	19(1)	28(2)	23(1)	-1(1)	9(1)	0(1)
C(34)	22(1)	25(2)	26(1)	1(1)	8(1)	-2(1)
C(35)	21(1)	29(2)	29(2)	2(1)	8(1)	0(1)
C(36)	21(1)	31(2)	29(2)	3(1)	4(1)	-9(1)
C(37)	32(2)	21(2)	26(2)	4(1)	3(1)	-3(1)
C(38)	25(2)	22(2)	28(2)	4(1)	6(1)	1(1)
C(39)	20(1)	23(2)	25(1)	2(1)	5(1)	1(1)
C(40)	20(1)	21(2)	20(1)	1(1)	3(1)	2(1)
C(41)	18(1)	22(2)	19(1)	3(1)	2(1)	4(1)
C(42)	16(1)	28(2)	25(1)	2(1)	4(1)	3(1)

C(43)	22(1)	30(2)	32(2)	-1(1)	5(1)	3(1)
C(44)	22(2)	47(2)	36(2)	-4(2)	14(1)	8(2)
C(45)	20(1)	50(2)	33(2)	6(2)	11(1)	-1(1)
C(46)	21(1)	33(2)	30(2)	8(1)	6(1)	1(1)
C(47)	17(1)	31(2)	23(1)	4(1)	2(1)	2(1)
C(48)	16(1)	26(2)	24(1)	2(1)	2(1)	-1(1)
B(1)	25(2)	18(2)	21(2)	0(1)	5(1)	1(1)
B(2)	18(2)	23(2)	22(2)	2(1)	5(1)	2(1)
C(1S)	167(10)	283(15)	299(18)	-41(12)	45(10)	-93(11)
C(2S)	520(40)	243(14)	630(40)	-30(19)	390(30)	60(20)
C(3S)	300(14)	234(9)	110(7)	13(7)	45(7)	189(9)
C(4S)	134(8)	260(10)	253(14)	-41(10)	1(8)	88(8)
C(5S)	177(9)	261(9)	130(7)	-56(8)	50(6)	85(9)
C(6S)	89(5)	374(13)	158(9)	-92(10)	7(5)	35(9)
C(7S)	128(7)	356(12)	88(5)	-55(8)	52(5)	-25(10)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for F_{12}BsubPc-O-BsubPc.

	x	y	z	U(eq)
H(3A)	7243	6853	2096	53
H(4A)	5593	7568	1828	68
H(5A)	3714	7159	1891	64
H(6A)	3418	6017	2249	49
H(11A)	2874	3995	3711	41
H(12A)	2661	3321	4557	47
H(13A)	4265	2786	5131	46
H(14A)	6163	2935	4911	37
H(19A)	10315	3965	4815	34
H(20A)	11911	4737	4995	42
H(21A)	12154	5642	4323	43
H(22A)	10796	5804	3447	38
H(1SA)	-1219	1048	3511	373
H(1SB)	-1376	1882	3593	373
H(1SC)	-367	1464	4026	373
H(2SA)	-171	1367	2799	518
H(2SB)	865	1532	3358	518
H(3SA)	-1042	2512	2969	256
H(3SB)	57	2677	3482	256
H(4SA)	90	2563	2224	263
H(4SB)	1283	2522	2694	263
H(5SA)	-215	3721	2463	224
H(5SB)	795	3691	3039	224
H(6SA)	1283	3593	1834	250
H(6SB)	2255	3659	2430	250
H(7SA)	1803	4792	1970	281
H(7SB)	1515	4773	2642	281
H(7SC)	474	4702	2083	281

Table S11. Torsion angles [°] for F_{12}BsubPc-O-BsubPc.

C(24)-N(6)-C(1)-N(1)	-8.4(4)
C(24)-N(6)-C(1)-C(2)	154.6(3)
C(8)-N(1)-C(1)-N(6)	155.4(3)
B(1)-N(1)-C(1)-N(6)	-15.1(4)
C(8)-N(1)-C(1)-C(2)	-11.2(3)
B(1)-N(1)-C(1)-C(2)	178.3(2)
N(6)-C(1)-C(2)-C(3)	17.0(5)
N(1)-C(1)-C(2)-C(3)	-177.9(3)
N(6)-C(1)-C(2)-C(7)	-158.8(3)
N(1)-C(1)-C(2)-C(7)	6.3(3)
C(7)-C(2)-C(3)-C(4)	-1.0(5)
C(1)-C(2)-C(3)-C(4)	-176.3(3)
C(2)-C(3)-C(4)-C(5)	0.7(6)
C(3)-C(4)-C(5)-C(6)	0.7(6)
C(4)-C(5)-C(6)-C(7)	-1.8(5)
C(5)-C(6)-C(7)-C(2)	1.5(5)
C(5)-C(6)-C(7)-C(8)	176.4(3)
C(3)-C(2)-C(7)-C(6)	-0.1(5)
C(1)-C(2)-C(7)-C(6)	176.2(3)
C(3)-C(2)-C(7)-C(8)	-176.1(3)
C(1)-C(2)-C(7)-C(8)	0.2(3)
C(9)-N(2)-C(8)-N(1)	8.5(4)
C(9)-N(2)-C(8)-C(7)	-156.0(3)
C(1)-N(1)-C(8)-N(2)	-156.4(3)
B(1)-N(1)-C(8)-N(2)	14.0(4)
C(1)-N(1)-C(8)-C(7)	11.4(3)
B(1)-N(1)-C(8)-C(7)	-178.2(2)
C(6)-C(7)-C(8)-N(2)	-15.6(5)
C(2)-C(7)-C(8)-N(2)	159.8(3)
C(6)-C(7)-C(8)-N(1)	177.9(3)
C(2)-C(7)-C(8)-N(1)	-6.6(3)
C(8)-N(2)-C(9)-N(3)	-8.1(4)
C(8)-N(2)-C(9)-C(10)	156.5(3)
C(16)-N(3)-C(9)-N(2)	155.6(3)

B(1)-N(3)-C(9)-N(2)	-14.8(4)
C(16)-N(3)-C(9)-C(10)	-12.2(3)
B(1)-N(3)-C(9)-C(10)	177.4(2)
N(2)-C(9)-C(10)-C(11)	17.8(5)
N(3)-C(9)-C(10)-C(11)	-175.5(3)
N(2)-C(9)-C(10)-C(15)	-160.0(3)
N(3)-C(9)-C(10)-C(15)	6.6(3)
C(15)-C(10)-C(11)-C(12)	-4.5(4)
C(9)-C(10)-C(11)-C(12)	177.9(3)
C(10)-C(11)-C(12)-C(13)	2.8(5)
C(11)-C(12)-C(13)-C(14)	1.4(5)
C(12)-C(13)-C(14)-C(15)	-3.9(5)
C(13)-C(14)-C(15)-C(10)	2.2(4)
C(13)-C(14)-C(15)-C(16)	-178.4(3)
C(11)-C(10)-C(15)-C(14)	2.0(4)
C(9)-C(10)-C(15)-C(14)	-179.9(3)
C(11)-C(10)-C(15)-C(16)	-177.5(3)
C(9)-C(10)-C(15)-C(16)	0.6(3)
C(17)-N(4)-C(16)-N(3)	7.7(4)
C(17)-N(4)-C(16)-C(15)	-156.3(3)
C(9)-N(3)-C(16)-N(4)	-154.7(3)
B(1)-N(3)-C(16)-N(4)	15.8(4)
C(9)-N(3)-C(16)-C(15)	12.7(3)
B(1)-N(3)-C(16)-C(15)	-176.9(2)
C(14)-C(15)-C(16)-N(4)	-21.1(5)
C(10)-C(15)-C(16)-N(4)	158.3(3)
C(14)-C(15)-C(16)-N(3)	172.9(3)
C(10)-C(15)-C(16)-N(3)	-7.6(3)
C(16)-N(4)-C(17)-N(5)	-9.2(4)
C(16)-N(4)-C(17)-C(18)	155.0(3)
C(24)-N(5)-C(17)-N(4)	156.2(3)
B(1)-N(5)-C(17)-N(4)	-12.7(4)
C(24)-N(5)-C(17)-C(18)	-11.4(3)
B(1)-N(5)-C(17)-C(18)	179.8(2)
N(4)-C(17)-C(18)-C(19)	13.9(5)
N(5)-C(17)-C(18)-C(19)	-179.9(3)

N(4)-C(17)-C(18)-C(23)	-159.6(3)
N(5)-C(17)-C(18)-C(23)	6.5(3)
C(23)-C(18)-C(19)-C(20)	-0.4(4)
C(17)-C(18)-C(19)-C(20)	-173.3(3)
C(18)-C(19)-C(20)-C(21)	0.8(5)
C(19)-C(20)-C(21)-C(22)	0.0(5)
C(20)-C(21)-C(22)-C(23)	-1.2(5)
C(21)-C(22)-C(23)-C(18)	1.6(4)
C(21)-C(22)-C(23)-C(24)	173.5(3)
C(19)-C(18)-C(23)-C(22)	-0.8(4)
C(17)-C(18)-C(23)-C(22)	173.7(3)
C(19)-C(18)-C(23)-C(24)	-174.5(3)
C(17)-C(18)-C(23)-C(24)	0.0(3)
C(1)-N(6)-C(24)-N(5)	9.1(4)
C(1)-N(6)-C(24)-C(23)	-153.9(3)
C(17)-N(5)-C(24)-N(6)	-155.1(3)
B(1)-N(5)-C(24)-N(6)	13.8(4)
C(17)-N(5)-C(24)-C(23)	11.3(3)
B(1)-N(5)-C(24)-C(23)	-179.7(2)
C(22)-C(23)-C(24)-N(6)	-14.1(5)
C(18)-C(23)-C(24)-N(6)	158.7(3)
C(22)-C(23)-C(24)-N(5)	-179.3(3)
C(18)-C(23)-C(24)-N(5)	-6.5(3)
C(48)-N(12)-C(25)-N(7)	9.7(4)
C(48)-N(12)-C(25)-C(26)	-154.3(3)
C(32)-N(7)-C(25)-N(12)	-158.0(2)
B(2)-N(7)-C(25)-N(12)	12.9(4)
C(32)-N(7)-C(25)-C(26)	9.3(3)
B(2)-N(7)-C(25)-C(26)	-179.8(2)
N(12)-C(25)-C(26)-C(27)	-11.9(5)
N(7)-C(25)-C(26)-C(27)	-178.0(3)
N(12)-C(25)-C(26)-C(31)	161.7(3)
N(7)-C(25)-C(26)-C(31)	-4.4(3)
C(31)-C(26)-C(27)-F(1)	-177.9(2)
C(25)-C(26)-C(27)-F(1)	-5.0(5)
C(31)-C(26)-C(27)-C(28)	1.3(4)

C(25)-C(26)-C(27)-C(28)	174.2(3)
F(1)-C(27)-C(28)-F(2)	1.7(4)
C(26)-C(27)-C(28)-F(2)	-177.5(3)
F(1)-C(27)-C(28)-C(29)	-179.4(3)
C(26)-C(27)-C(28)-C(29)	1.4(4)
F(2)-C(28)-C(29)-F(3)	-4.3(4)
C(27)-C(28)-C(29)-F(3)	176.8(3)
F(2)-C(28)-C(29)-C(30)	175.8(3)
C(27)-C(28)-C(29)-C(30)	-3.2(5)
F(3)-C(29)-C(30)-F(4)	1.2(4)
C(28)-C(29)-C(30)-F(4)	-178.8(3)
F(3)-C(29)-C(30)-C(31)	-177.8(3)
C(28)-C(29)-C(30)-C(31)	2.1(4)
F(4)-C(30)-C(31)-C(26)	-178.5(2)
C(29)-C(30)-C(31)-C(26)	0.5(4)
F(4)-C(30)-C(31)-C(32)	7.6(5)
C(29)-C(30)-C(31)-C(32)	-173.4(3)
C(27)-C(26)-C(31)-C(30)	-2.3(4)
C(25)-C(26)-C(31)-C(30)	-176.8(2)
C(27)-C(26)-C(31)-C(32)	173.1(2)
C(25)-C(26)-C(31)-C(32)	-1.5(3)
C(33)-N(8)-C(32)-N(7)	-9.5(4)
C(33)-N(8)-C(32)-C(31)	153.9(3)
C(25)-N(7)-C(32)-N(8)	156.7(2)
B(2)-N(7)-C(32)-N(8)	-14.1(4)
C(25)-N(7)-C(32)-C(31)	-10.2(3)
B(2)-N(7)-C(32)-C(31)	178.9(2)
C(30)-C(31)-C(32)-N(8)	15.8(5)
C(26)-C(31)-C(32)-N(8)	-158.7(3)
C(30)-C(31)-C(32)-N(7)	-178.6(3)
C(26)-C(31)-C(32)-N(7)	6.8(3)
C(32)-N(8)-C(33)-N(9)	7.8(4)
C(32)-N(8)-C(33)-C(34)	-151.7(3)
C(40)-N(9)-C(33)-N(8)	-151.6(3)
B(2)-N(9)-C(33)-N(8)	17.2(4)
C(40)-N(9)-C(33)-C(34)	12.1(3)

B(2)-N(9)-C(33)-C(34)	-179.0(2)
N(8)-C(33)-C(34)-C(35)	-18.5(5)
N(9)-C(33)-C(34)-C(35)	179.1(3)
N(8)-C(33)-C(34)-C(39)	154.7(3)
N(9)-C(33)-C(34)-C(39)	-7.6(3)
C(39)-C(34)-C(35)-F(5)	177.7(3)
C(33)-C(34)-C(35)-F(5)	-9.8(5)
C(39)-C(34)-C(35)-C(36)	-1.4(4)
C(33)-C(34)-C(35)-C(36)	171.1(3)
F(5)-C(35)-C(36)-F(6)	1.9(4)
C(34)-C(35)-C(36)-F(6)	-179.0(3)
F(5)-C(35)-C(36)-C(37)	-178.9(3)
C(34)-C(35)-C(36)-C(37)	0.3(4)
F(6)-C(36)-C(37)-F(7)	0.4(4)
C(35)-C(36)-C(37)-F(7)	-178.8(3)
F(6)-C(36)-C(37)-C(38)	-179.9(3)
C(35)-C(36)-C(37)-C(38)	0.9(4)
F(7)-C(37)-C(38)-F(8)	0.0(4)
C(36)-C(37)-C(38)-F(8)	-179.7(3)
F(7)-C(37)-C(38)-C(39)	178.9(2)
C(36)-C(37)-C(38)-C(39)	-0.8(4)
F(8)-C(38)-C(39)-C(34)	178.5(2)
C(37)-C(38)-C(39)-C(34)	-0.4(4)
F(8)-C(38)-C(39)-C(40)	6.6(5)
C(37)-C(38)-C(39)-C(40)	-172.3(3)
C(35)-C(34)-C(39)-C(38)	1.5(4)
C(33)-C(34)-C(39)-C(38)	-172.7(2)
C(35)-C(34)-C(39)-C(40)	175.3(3)
C(33)-C(34)-C(39)-C(40)	1.1(3)
C(41)-N(10)-C(40)-N(9)	-7.7(4)
C(41)-N(10)-C(40)-C(39)	155.8(3)
C(33)-N(9)-C(40)-N(10)	155.4(2)
B(2)-N(9)-C(40)-N(10)	-13.1(4)
C(33)-N(9)-C(40)-C(39)	-11.5(3)
B(2)-N(9)-C(40)-C(39)	180.0(2)
C(38)-C(39)-C(40)-N(10)	12.8(5)

C(34)-C(39)-C(40)-N(10)	-159.9(3)
C(38)-C(39)-C(40)-N(9)	178.5(3)
C(34)-C(39)-C(40)-N(9)	5.9(3)
C(40)-N(10)-C(41)-N(11)	6.6(4)
C(40)-N(10)-C(41)-C(42)	-158.4(3)
C(48)-N(11)-C(41)-N(10)	-156.2(2)
B(2)-N(11)-C(41)-N(10)	15.3(4)
C(48)-N(11)-C(41)-C(42)	12.1(3)
B(2)-N(11)-C(41)-C(42)	-176.4(2)
N(10)-C(41)-C(42)-C(43)	-13.6(5)
N(11)-C(41)-C(42)-C(43)	179.5(3)
N(10)-C(41)-C(42)-C(47)	161.6(3)
N(11)-C(41)-C(42)-C(47)	-5.4(3)
C(47)-C(42)-C(43)-F(9)	-179.3(3)
C(41)-C(42)-C(43)-F(9)	-4.7(5)
C(47)-C(42)-C(43)-C(44)	2.2(4)
C(41)-C(42)-C(43)-C(44)	176.8(3)
F(9)-C(43)-C(44)-F(10)	-0.8(5)
C(42)-C(43)-C(44)-F(10)	177.7(3)
F(9)-C(43)-C(44)-C(45)	-179.0(3)
C(42)-C(43)-C(44)-C(45)	-0.5(5)
F(10)-C(44)-C(45)-F(11)	0.7(5)
C(43)-C(44)-C(45)-F(11)	178.9(3)
F(10)-C(44)-C(45)-C(46)	-179.5(3)
C(43)-C(44)-C(45)-C(46)	-1.3(5)
F(11)-C(45)-C(46)-F(12)	0.8(5)
C(44)-C(45)-C(46)-F(12)	-179.0(3)
F(11)-C(45)-C(46)-C(47)	-179.0(3)
C(44)-C(45)-C(46)-C(47)	1.2(5)
F(12)-C(46)-C(47)-C(42)	-179.2(2)
C(45)-C(46)-C(47)-C(42)	0.6(4)
F(12)-C(46)-C(47)-C(48)	6.1(5)
C(45)-C(46)-C(47)-C(48)	-174.1(3)
C(43)-C(42)-C(47)-C(46)	-2.3(4)
C(41)-C(42)-C(47)-C(46)	-178.2(3)
C(43)-C(42)-C(47)-C(48)	173.6(3)

C(41)-C(42)-C(47)-C(48)	-2.4(3)
C(25)-N(12)-C(48)-N(11)	-6.2(4)
C(25)-N(12)-C(48)-C(47)	155.4(3)
C(41)-N(11)-C(48)-N(12)	151.7(3)
B(2)-N(11)-C(48)-N(12)	-20.0(4)
C(41)-N(11)-C(48)-C(47)	-13.6(3)
B(2)-N(11)-C(48)-C(47)	174.7(2)
C(46)-C(47)-C(48)-N(12)	20.4(5)
C(42)-C(47)-C(48)-N(12)	-154.8(3)
C(46)-C(47)-C(48)-N(11)	-175.5(3)
C(42)-C(47)-C(48)-N(11)	9.3(3)
B(2)-O(1)-B(1)-N(5)	-133.5(3)
B(2)-O(1)-B(1)-N(3)	108.1(3)
B(2)-O(1)-B(1)-N(1)	-12.7(5)
C(24)-N(5)-B(1)-O(1)	97.6(3)
C(17)-N(5)-B(1)-O(1)	-94.6(3)
C(24)-N(5)-B(1)-N(3)	-137.6(3)
C(17)-N(5)-B(1)-N(3)	30.2(3)
C(24)-N(5)-B(1)-N(1)	-31.2(3)
C(17)-N(5)-B(1)-N(1)	136.6(3)
C(16)-N(3)-B(1)-O(1)	92.8(3)
C(9)-N(3)-B(1)-O(1)	-97.7(3)
C(16)-N(3)-B(1)-N(5)	-31.7(3)
C(9)-N(3)-B(1)-N(5)	137.8(2)
C(16)-N(3)-B(1)-N(1)	-138.3(3)
C(9)-N(3)-B(1)-N(1)	31.1(3)
C(1)-N(1)-B(1)-O(1)	-94.4(3)
C(8)-N(1)-B(1)-O(1)	96.0(3)
C(1)-N(1)-B(1)-N(5)	31.9(3)
C(8)-N(1)-B(1)-N(5)	-137.6(2)
C(1)-N(1)-B(1)-N(3)	138.8(2)
C(8)-N(1)-B(1)-N(3)	-30.8(3)
B(1)-O(1)-B(2)-N(7)	3.5(5)
B(1)-O(1)-B(2)-N(9)	-118.2(3)
B(1)-O(1)-B(2)-N(11)	123.6(3)
C(32)-N(7)-B(2)-O(1)	-95.6(3)

C(25)-N(7)-B(2)-O(1)	94.5(3)
C(32)-N(7)-B(2)-N(9)	32.8(3)
C(25)-N(7)-B(2)-N(9)	-137.2(2)
C(32)-N(7)-B(2)-N(11)	137.7(2)
C(25)-N(7)-B(2)-N(11)	-32.2(3)
C(40)-N(9)-B(2)-O(1)	-96.6(3)
C(33)-N(9)-B(2)-O(1)	95.8(3)
C(40)-N(9)-B(2)-N(7)	133.7(2)
C(33)-N(9)-B(2)-N(7)	-34.0(3)
C(40)-N(9)-B(2)-N(11)	28.7(3)
C(33)-N(9)-B(2)-N(11)	-138.9(2)
C(41)-N(11)-B(2)-O(1)	96.0(3)
C(48)-N(11)-B(2)-O(1)	-93.2(3)
C(41)-N(11)-B(2)-N(7)	-135.2(2)
C(48)-N(11)-B(2)-N(7)	35.6(3)
C(41)-N(11)-B(2)-N(9)	-29.9(3)
C(48)-N(11)-B(2)-N(9)	140.9(2)
C(1S)-C(2S)-C(3S)-C(4S)	-175.2(14)
C(2S)-C(3S)-C(4S)-C(5S)	-165.0(15)
C(3S)-C(4S)-C(5S)-C(6S)	167.6(10)
C(4S)-C(5S)-C(6S)-C(7S)	173.1(10)

Symmetry transformations used to generate equivalent atoms:

Crystal Structure Details of Cl_6BsubPc-O-BsubPc

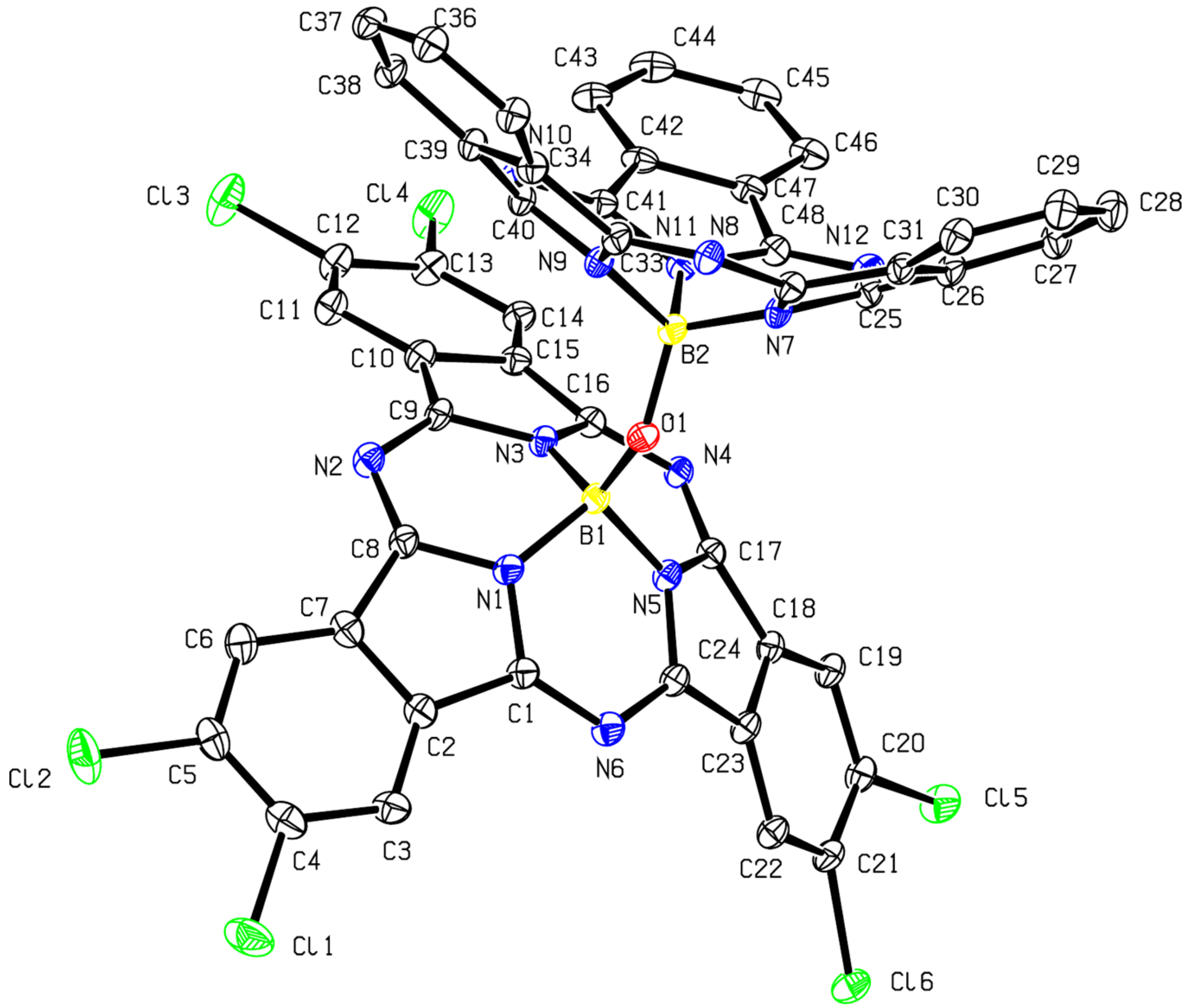


Figure S14. Ellipsoid plot (50 % probability) showing the structure and atom numbering scheme of Cl_6BsubPc-O-BsubPc (CCDC deposition number: 1018458). Hydrogen atoms have been omitted for clarity. Colors: boron - yellow; nitrogen - blue; carbon - white; oxygen - red; chlorine - green.

Table S12. Crystal data and structure refinement for Cl_6BsubPc-O-BsubPc.

Empirical formula	C48 H18 B2 Cl6 N12 O	
Formula weight	1013.06	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 19.7916(7) Å	a= 90°.
	b = 11.6134(3) Å	b= 117.050(2)°.
	c = 20.9120(7) Å	g = 90°.
Volume	4280.8(2) Å^3	
Z	4	
Density (calculated)	1.572 Mg/m^3	
Absorption coefficient	4.133 mm^{-1}	
F(000)	2040	
Crystal size	0.330 x 0.100 x 0.020 mm^3	
Theta range for data collection	2.550 to 66.822°.	
Index ranges	-23<=h<=23, -13<=k<=13, -24<=l<=24	
Reflections collected	61032	
Independent reflections	7540 [R(int) = 0.1163]	
Completeness to theta = 67.679°	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.5170	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7540 / 0 / 622	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1200	
R indices (all data)	R1 = 0.0783, wR2 = 0.1319	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.288 and -0.479 e.Å^{-3}	

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Cl_6BsubPc-O-BsubPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3551(1)	8329(1)	10629(1)	60(1)
Cl(2)	4882(1)	6744(1)	10755(1)	60(1)
Cl(3)	8340(1)	9595(1)	8645(1)	52(1)
Cl(4)	8034(1)	12024(1)	7884(1)	47(1)
Cl(5)	3771(1)	16893(1)	7605(1)	38(1)
Cl(6)	3051(1)	16025(1)	8586(1)	35(1)
O(1)	3608(1)	9728(2)	6772(1)	24(1)
N(1)	4134(2)	9795(2)	8083(2)	24(1)
N(2)	5334(2)	8911(2)	8430(2)	28(1)
N(3)	4906(2)	10441(2)	7579(2)	23(1)
N(4)	4833(2)	12395(2)	7231(2)	25(1)
N(5)	3867(2)	11559(2)	7464(2)	23(1)
N(6)	3331(2)	11153(2)	8256(2)	29(1)
N(7)	2961(2)	9545(2)	5457(2)	24(1)
N(8)	2575(2)	7577(2)	5302(2)	26(1)
N(9)	3832(2)	8095(2)	6131(2)	23(1)
N(10)	5143(2)	8349(2)	6436(2)	25(1)
N(11)	4275(2)	9919(2)	6010(2)	23(1)
N(12)	3442(2)	11171(2)	5094(2)	27(1)
C(1)	3706(2)	10147(3)	8404(2)	26(1)
C(2)	3909(2)	9391(3)	9020(2)	29(1)
C(3)	3620(3)	9316(3)	9507(2)	35(1)
C(4)	3931(3)	8489(3)	10043(2)	38(1)
C(5)	4532(3)	7792(4)	10099(2)	38(1)
C(6)	4847(2)	7907(3)	9631(2)	36(1)
C(7)	4521(2)	8704(3)	9077(2)	30(1)
C(8)	4701(2)	9050(3)	8501(2)	26(1)
C(9)	5448(2)	9665(3)	7997(2)	25(1)
C(10)	6145(2)	10042(3)	8002(2)	28(1)
C(11)	6865(2)	9570(3)	8312(2)	31(1)
C(12)	7444(2)	10186(3)	8266(2)	33(1)

C(13)	7304(2)	11267(3)	7917(2)	31(1)
C(14)	6582(2)	11737(3)	7605(2)	26(1)
C(15)	5995(2)	11122(3)	7640(2)	24(1)
C(16)	5207(2)	11397(3)	7418(2)	23(1)
C(17)	4196(2)	12485(3)	7307(2)	22(1)
C(18)	3856(2)	13502(3)	7454(2)	25(1)
C(19)	3972(2)	14668(3)	7398(2)	27(1)
C(20)	3669(2)	15436(3)	7705(2)	29(1)
C(21)	3291(2)	15061(3)	8096(2)	28(1)
C(22)	3143(2)	13896(3)	8125(2)	28(1)
C(23)	3414(2)	13116(3)	7790(2)	25(1)
C(24)	3470(2)	11874(3)	7825(2)	25(1)
C(25)	2870(2)	10459(3)	5010(2)	26(1)
C(26)	2152(2)	10271(3)	4373(2)	28(1)
C(27)	1786(2)	10875(3)	3729(2)	32(1)
C(28)	1148(2)	10393(3)	3179(2)	39(1)
C(29)	885(2)	9304(3)	3259(2)	37(1)
C(30)	1252(2)	8681(3)	3884(2)	31(1)
C(31)	1881(2)	9173(3)	4448(2)	27(1)
C(32)	2439(2)	8699(3)	5118(2)	25(1)
C(33)	3284(2)	7294(3)	5770(2)	24(1)
C(34)	3674(2)	6206(3)	5844(2)	26(1)
C(35)	3408(2)	5115(3)	5564(2)	29(1)
C(36)	3939(2)	4263(3)	5681(2)	32(1)
C(37)	4716(2)	4486(3)	6049(2)	31(1)
C(38)	4989(2)	5576(3)	6303(2)	29(1)
C(39)	4462(2)	6443(3)	6204(2)	24(1)
C(40)	4547(2)	7679(3)	6335(2)	23(1)
C(41)	4978(2)	9448(3)	6220(2)	24(1)
C(42)	5396(2)	10264(3)	6004(2)	26(1)
C(43)	6137(2)	10279(3)	6108(2)	30(1)
C(44)	6363(2)	11200(3)	5820(2)	35(1)
C(45)	5843(2)	12043(3)	5408(2)	35(1)
C(46)	5093(2)	12015(3)	5275(2)	32(1)
C(47)	4867(2)	11136(3)	5589(2)	27(1)
C(48)	4140(2)	10843(3)	5558(2)	25(1)

B(1)	4087(2)	10327(3)	7405(2)	24(1)
B(2)	3668(2)	9362(3)	6153(2)	23(1)

Table S14. Bond lengths [Å] and angles [°] for Cl_6BsubPc-O-BsubPc.

Cl(1)-C(4)	1.717(4)
Cl(2)-C(5)	1.726(4)
Cl(3)-C(12)	1.722(4)
Cl(4)-C(13)	1.720(4)
Cl(5)-C(20)	1.727(4)
Cl(6)-C(21)	1.724(4)
O(1)-B(1)	1.412(5)
O(1)-B(2)	1.417(5)
N(1)-C(1)	1.362(4)
N(1)-C(8)	1.372(5)
N(1)-B(1)	1.511(5)
N(2)-C(8)	1.336(5)
N(2)-C(9)	1.351(5)
N(3)-C(9)	1.370(4)
N(3)-C(16)	1.373(4)
N(3)-B(1)	1.495(5)
N(4)-C(16)	1.335(4)
N(4)-C(17)	1.344(5)
N(5)-C(24)	1.364(5)
N(5)-C(17)	1.373(4)
N(5)-B(1)	1.517(5)
N(6)-C(1)	1.342(5)
N(6)-C(24)	1.346(5)
N(7)-C(32)	1.366(5)
N(7)-C(25)	1.371(4)
N(7)-B(2)	1.507(5)
N(8)-C(33)	1.336(5)
N(8)-C(32)	1.351(4)
N(9)-C(33)	1.367(5)
N(9)-C(40)	1.367(5)
N(9)-B(2)	1.512(5)
N(10)-C(41)	1.344(4)
N(10)-C(40)	1.346(5)
N(11)-C(41)	1.368(5)

N(11)-C(48)	1.374(4)
N(11)-B(2)	1.509(5)
N(12)-C(48)	1.333(5)
N(12)-C(25)	1.346(5)
C(1)-C(2)	1.456(5)
C(2)-C(3)	1.378(5)
C(2)-C(7)	1.411(5)
C(3)-C(4)	1.390(6)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.399(6)
C(5)-C(6)	1.385(6)
C(6)-C(7)	1.392(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.458(5)
C(9)-C(10)	1.442(5)
C(10)-C(11)	1.383(5)
C(10)-C(15)	1.425(5)
C(11)-C(12)	1.391(5)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.415(5)
C(13)-C(14)	1.385(5)
C(14)-C(15)	1.394(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.445(5)
C(17)-C(18)	1.460(5)
C(18)-C(19)	1.387(5)
C(18)-C(23)	1.421(5)
C(19)-C(20)	1.386(5)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.405(5)
C(21)-C(22)	1.391(5)
C(22)-C(23)	1.394(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.446(5)
C(25)-C(26)	1.457(5)
C(26)-C(27)	1.394(5)

C(26)-C(31)	1.419(5)
C(27)-C(28)	1.382(6)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.406(6)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.377(6)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.389(5)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.443(5)
C(33)-C(34)	1.452(5)
C(34)-C(35)	1.395(5)
C(34)-C(39)	1.418(5)
C(35)-C(36)	1.382(5)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.396(6)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.384(5)
C(37)-H(37A)	0.9500
C(38)-C(39)	1.396(5)
C(38)-H(38A)	0.9500
C(39)-C(40)	1.456(5)
C(41)-C(42)	1.459(5)
C(42)-C(43)	1.381(5)
C(42)-C(47)	1.431(5)
C(43)-C(44)	1.397(5)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.397(6)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.381(6)
C(45)-H(45A)	0.9500
C(46)-C(47)	1.393(5)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.452(5)
B(1)-O(1)-B(2)	134.7(3)

C(1)-N(1)-C(8)	112.8(3)
C(1)-N(1)-B(1)	123.7(3)
C(8)-N(1)-B(1)	122.7(3)
C(8)-N(2)-C(9)	116.6(3)
C(9)-N(3)-C(16)	112.7(3)
C(9)-N(3)-B(1)	123.1(3)
C(16)-N(3)-B(1)	123.8(3)
C(16)-N(4)-C(17)	117.3(3)
C(24)-N(5)-C(17)	112.2(3)
C(24)-N(5)-B(1)	123.9(3)
C(17)-N(5)-B(1)	122.3(3)
C(1)-N(6)-C(24)	115.9(3)
C(32)-N(7)-C(25)	111.7(3)
C(32)-N(7)-B(2)	123.4(3)
C(25)-N(7)-B(2)	123.0(3)
C(33)-N(8)-C(32)	116.8(3)
C(33)-N(9)-C(40)	112.4(3)
C(33)-N(9)-B(2)	123.4(3)
C(40)-N(9)-B(2)	122.8(3)
C(41)-N(10)-C(40)	115.7(3)
C(41)-N(11)-C(48)	112.6(3)
C(41)-N(11)-B(2)	123.4(3)
C(48)-N(11)-B(2)	123.2(3)
C(48)-N(12)-C(25)	116.8(3)
N(6)-C(1)-N(1)	123.3(3)
N(6)-C(1)-C(2)	129.1(3)
N(1)-C(1)-C(2)	105.8(3)
C(3)-C(2)-C(7)	122.1(4)
C(3)-C(2)-C(1)	130.7(4)
C(7)-C(2)-C(1)	107.2(3)
C(2)-C(3)-C(4)	117.3(4)
C(2)-C(3)-H(3A)	121.3
C(4)-C(3)-H(3A)	121.3
C(3)-C(4)-C(5)	121.0(4)
C(3)-C(4)-Cl(1)	118.3(3)
C(5)-C(4)-Cl(1)	120.7(3)

C(6)-C(5)-C(4)	121.6(4)
C(6)-C(5)-Cl(2)	118.9(3)
C(4)-C(5)-Cl(2)	119.5(3)
C(5)-C(6)-C(7)	117.7(4)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.1(4)
C(6)-C(7)-C(8)	132.5(4)
C(2)-C(7)-C(8)	107.3(3)
N(2)-C(8)-N(1)	122.8(3)
N(2)-C(8)-C(7)	130.7(3)
N(1)-C(8)-C(7)	105.3(3)
N(2)-C(9)-N(3)	122.2(3)
N(2)-C(9)-C(10)	130.0(3)
N(3)-C(9)-C(10)	106.0(3)
C(11)-C(10)-C(15)	121.3(3)
C(11)-C(10)-C(9)	131.4(3)
C(15)-C(10)-C(9)	107.2(3)
C(10)-C(11)-C(12)	118.0(4)
C(10)-C(11)-H(11A)	121.0
C(12)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.3(3)
C(11)-C(12)-Cl(3)	118.1(3)
C(13)-C(12)-Cl(3)	120.7(3)
C(14)-C(13)-C(12)	120.7(3)
C(14)-C(13)-Cl(4)	119.1(3)
C(12)-C(13)-Cl(4)	120.3(3)
C(13)-C(14)-C(15)	118.7(3)
C(13)-C(14)-H(14A)	120.6
C(15)-C(14)-H(14A)	120.6
C(14)-C(15)-C(10)	120.1(3)
C(14)-C(15)-C(16)	132.3(3)
C(10)-C(15)-C(16)	107.4(3)
N(4)-C(16)-N(3)	121.9(3)
N(4)-C(16)-C(15)	131.3(3)
N(3)-C(16)-C(15)	105.6(3)

N(4)-C(17)-N(5)	122.7(3)
N(4)-C(17)-C(18)	129.4(3)
N(5)-C(17)-C(18)	105.6(3)
C(19)-C(18)-C(23)	120.9(3)
C(19)-C(18)-C(17)	131.4(3)
C(23)-C(18)-C(17)	107.2(3)
C(20)-C(19)-C(18)	117.7(3)
C(20)-C(19)-H(19A)	121.1
C(18)-C(19)-H(19A)	121.1
C(19)-C(20)-C(21)	121.8(3)
C(19)-C(20)-Cl(5)	118.4(3)
C(21)-C(20)-Cl(5)	119.8(3)
C(22)-C(21)-C(20)	120.4(3)
C(22)-C(21)-Cl(6)	119.0(3)
C(20)-C(21)-Cl(6)	120.5(3)
C(21)-C(22)-C(23)	118.2(3)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	120.5(3)
C(22)-C(23)-C(24)	131.4(3)
C(18)-C(23)-C(24)	106.9(3)
N(6)-C(24)-N(5)	123.2(3)
N(6)-C(24)-C(23)	128.3(3)
N(5)-C(24)-C(23)	106.8(3)
N(12)-C(25)-N(7)	123.0(3)
N(12)-C(25)-C(26)	128.6(3)
N(7)-C(25)-C(26)	106.1(3)
C(27)-C(26)-C(31)	120.1(3)
C(27)-C(26)-C(25)	132.1(3)
C(31)-C(26)-C(25)	107.2(3)
C(28)-C(27)-C(26)	118.5(4)
C(28)-C(27)-H(27A)	120.7
C(26)-C(27)-H(27A)	120.7
C(27)-C(28)-C(29)	120.8(4)
C(27)-C(28)-H(28A)	119.6
C(29)-C(28)-H(28A)	119.6

C(30)-C(29)-C(28)	121.4(4)
C(30)-C(29)-H(29A)	119.3
C(28)-C(29)-H(29A)	119.3
C(29)-C(30)-C(31)	118.1(4)
C(29)-C(30)-H(30A)	120.9
C(31)-C(30)-H(30A)	120.9
C(30)-C(31)-C(26)	120.9(3)
C(30)-C(31)-C(32)	131.5(3)
C(26)-C(31)-C(32)	106.8(3)
N(8)-C(32)-N(7)	122.7(3)
N(8)-C(32)-C(31)	127.6(3)
N(7)-C(32)-C(31)	107.1(3)
N(8)-C(33)-N(9)	122.9(3)
N(8)-C(33)-C(34)	128.4(3)
N(9)-C(33)-C(34)	106.5(3)
C(35)-C(34)-C(39)	120.9(3)
C(35)-C(34)-C(33)	131.8(3)
C(39)-C(34)-C(33)	106.9(3)
C(36)-C(35)-C(34)	117.8(4)
C(36)-C(35)-H(35A)	121.1
C(34)-C(35)-H(35A)	121.1
C(35)-C(36)-C(37)	121.5(3)
C(35)-C(36)-H(36A)	119.2
C(37)-C(36)-H(36A)	119.2
C(38)-C(37)-C(36)	121.5(3)
C(38)-C(37)-H(37A)	119.3
C(36)-C(37)-H(37A)	119.3
C(37)-C(38)-C(39)	117.9(4)
C(37)-C(38)-H(38A)	121.1
C(39)-C(38)-H(38A)	121.1
C(38)-C(39)-C(34)	120.4(3)
C(38)-C(39)-C(40)	131.9(3)
C(34)-C(39)-C(40)	107.3(3)
N(10)-C(40)-N(9)	123.6(3)
N(10)-C(40)-C(39)	128.1(3)
N(9)-C(40)-C(39)	105.9(3)

N(10)-C(41)-N(11)	123.0(3)
N(10)-C(41)-C(42)	129.5(3)
N(11)-C(41)-C(42)	106.2(3)
C(43)-C(42)-C(47)	121.2(3)
C(43)-C(42)-C(41)	132.1(4)
C(47)-C(42)-C(41)	106.6(3)
C(42)-C(43)-C(44)	117.8(4)
C(42)-C(43)-H(43A)	121.1
C(44)-C(43)-H(43A)	121.1
C(43)-C(44)-C(45)	120.8(4)
C(43)-C(44)-H(44A)	119.6
C(45)-C(44)-H(44A)	119.6
C(46)-C(45)-C(44)	122.0(4)
C(46)-C(45)-H(45A)	119.0
C(44)-C(45)-H(45A)	119.0
C(45)-C(46)-C(47)	117.9(4)
C(45)-C(46)-H(46A)	121.1
C(47)-C(46)-H(46A)	121.1
C(46)-C(47)-C(42)	120.1(4)
C(46)-C(47)-C(48)	132.4(4)
C(42)-C(47)-C(48)	107.4(3)
N(12)-C(48)-N(11)	122.4(3)
N(12)-C(48)-C(47)	130.1(3)
N(11)-C(48)-C(47)	105.9(3)
O(1)-B(1)-N(3)	117.7(3)
O(1)-B(1)-N(1)	114.0(3)
N(3)-B(1)-N(1)	102.1(3)
O(1)-B(1)-N(5)	116.4(3)
N(3)-B(1)-N(5)	102.5(3)
N(1)-B(1)-N(5)	101.9(3)
O(1)-B(2)-N(7)	114.5(3)
O(1)-B(2)-N(11)	117.3(3)
N(7)-B(2)-N(11)	102.7(3)
O(1)-B(2)-N(9)	115.4(3)
N(7)-B(2)-N(9)	103.0(3)
N(11)-B(2)-N(9)	102.0(3)

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2$x 10^3) for Cl_6BsubPc-O-BsubPc. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	103(1)	46(1)	53(1)	7(1)	56(1)	0(1)
Cl(2)	58(1)	68(1)	47(1)	32(1)	17(1)	5(1)
Cl(3)	32(1)	40(1)	84(1)	22(1)	27(1)	10(1)
Cl(4)	35(1)	34(1)	78(1)	12(1)	29(1)	0(1)
Cl(5)	52(1)	14(1)	52(1)	-2(1)	28(1)	-3(1)
Cl(6)	40(1)	23(1)	46(1)	-5(1)	22(1)	1(1)
O(1)	26(1)	20(1)	28(1)	-3(1)	13(1)	-1(1)
N(1)	31(2)	14(1)	30(2)	1(1)	16(1)	0(1)
N(2)	33(2)	18(2)	35(2)	4(1)	16(2)	0(1)
N(3)	28(2)	14(1)	28(2)	1(1)	12(1)	1(1)
N(4)	32(2)	16(1)	27(2)	2(1)	13(1)	2(1)
N(5)	24(2)	16(1)	29(2)	2(1)	13(1)	-1(1)
N(6)	35(2)	18(2)	35(2)	1(1)	18(2)	-1(1)
N(7)	28(2)	12(1)	30(2)	2(1)	12(1)	2(1)
N(8)	26(2)	18(2)	32(2)	1(1)	12(1)	-1(1)
N(9)	26(2)	14(1)	29(2)	0(1)	12(1)	0(1)
N(10)	28(2)	18(2)	30(2)	-3(1)	14(1)	-2(1)
N(11)	32(2)	12(1)	26(2)	-1(1)	13(1)	-1(1)
N(12)	38(2)	13(1)	32(2)	-2(1)	16(2)	-1(1)
C(1)	32(2)	17(2)	32(2)	1(2)	18(2)	-2(2)
C(2)	40(2)	16(2)	32(2)	1(2)	17(2)	-4(2)
C(3)	53(3)	20(2)	39(2)	-2(2)	28(2)	-3(2)
C(4)	57(3)	29(2)	34(2)	-3(2)	24(2)	-12(2)
C(5)	43(2)	35(2)	30(2)	7(2)	11(2)	-6(2)
C(6)	38(2)	30(2)	36(2)	7(2)	14(2)	0(2)
C(7)	36(2)	24(2)	29(2)	1(2)	13(2)	-6(2)
C(8)	32(2)	16(2)	30(2)	2(2)	13(2)	1(2)
C(9)	26(2)	15(2)	31(2)	0(1)	11(2)	3(1)
C(10)	34(2)	18(2)	32(2)	0(2)	15(2)	2(2)
C(11)	29(2)	26(2)	39(2)	4(2)	15(2)	2(2)
C(12)	28(2)	28(2)	45(2)	5(2)	17(2)	5(2)

C(13)	28(2)	24(2)	42(2)	-2(2)	17(2)	-3(2)
C(14)	29(2)	20(2)	30(2)	-2(2)	14(2)	-1(2)
C(15)	28(2)	19(2)	27(2)	-4(1)	13(2)	-2(1)
C(16)	27(2)	16(2)	26(2)	-1(1)	12(2)	-4(1)
C(17)	27(2)	16(2)	24(2)	1(1)	12(2)	-2(1)
C(18)	26(2)	19(2)	28(2)	3(1)	10(2)	2(1)
C(19)	28(2)	18(2)	33(2)	1(2)	12(2)	2(2)
C(20)	31(2)	15(2)	37(2)	1(2)	13(2)	0(2)
C(21)	29(2)	20(2)	34(2)	-2(2)	14(2)	4(2)
C(22)	29(2)	20(2)	35(2)	1(2)	15(2)	1(2)
C(23)	24(2)	17(2)	34(2)	1(2)	13(2)	1(1)
C(24)	27(2)	18(2)	30(2)	1(2)	12(2)	0(1)
C(25)	33(2)	13(2)	28(2)	0(1)	12(2)	1(2)
C(26)	34(2)	14(2)	32(2)	0(2)	13(2)	3(2)
C(27)	41(2)	18(2)	34(2)	3(2)	13(2)	3(2)
C(28)	43(2)	29(2)	36(2)	4(2)	11(2)	5(2)
C(29)	36(2)	28(2)	35(2)	-4(2)	7(2)	-1(2)
C(30)	30(2)	23(2)	37(2)	-3(2)	12(2)	-2(2)
C(31)	30(2)	19(2)	29(2)	-1(2)	12(2)	3(2)
C(32)	30(2)	17(2)	29(2)	-2(1)	13(2)	-2(1)
C(33)	30(2)	14(2)	30(2)	2(1)	14(2)	-1(1)
C(34)	32(2)	16(2)	31(2)	2(2)	17(2)	-2(2)
C(35)	33(2)	15(2)	36(2)	-2(2)	14(2)	-4(2)
C(36)	44(2)	12(2)	40(2)	-3(2)	20(2)	-3(2)
C(37)	39(2)	18(2)	37(2)	-2(2)	19(2)	4(2)
C(38)	34(2)	18(2)	38(2)	4(2)	19(2)	3(2)
C(39)	28(2)	16(2)	29(2)	2(1)	12(2)	0(1)
C(40)	25(2)	17(2)	26(2)	2(1)	11(2)	2(1)
C(41)	28(2)	17(2)	27(2)	-5(1)	14(2)	-4(1)
C(42)	38(2)	18(2)	28(2)	-7(2)	22(2)	-7(2)
C(43)	36(2)	23(2)	36(2)	-11(2)	20(2)	-8(2)
C(44)	43(2)	30(2)	43(2)	-15(2)	28(2)	-14(2)
C(45)	52(3)	24(2)	39(2)	-8(2)	30(2)	-14(2)
C(46)	51(3)	17(2)	33(2)	-5(2)	25(2)	-8(2)
C(47)	42(2)	14(2)	29(2)	-6(1)	21(2)	-7(2)
C(48)	39(2)	11(2)	27(2)	-1(1)	15(2)	-2(2)

B(1)	28(2)	16(2)	27(2)	2(2)	12(2)	3(2)
B(2)	28(2)	13(2)	29(2)	2(2)	15(2)	0(2)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Cl_6BsubPc-O-BsubPc.

	x	y	z	U(eq)
H(3A)	3225	9811	9477	42
H(6A)	5272	7457	9687	43
H(11A)	6962	8847	8551	38
H(14A)	6489	12464	7373	31
H(19A)	4251	14930	7157	33
H(22A)	2864	13640	8367	33
H(27A)	1971	11601	3670	39
H(28A)	884	10802	2741	47
H(29A)	444	8991	2873	44
H(30A)	1080	7936	3929	37
H(35A)	2880	4963	5301	34
H(36A)	3771	3507	5508	38
H(37A)	5065	3877	6127	37
H(38A)	5519	5729	6537	35
H(43A)	6482	9682	6366	36
H(44A)	6876	11255	5905	42
H(45A)	6011	12655	5214	42
H(46A)	4741	12577	4978	38

Table S17. Torsion angles [°] for Cl_6BsubPc-O-BsubPc.

C(24)-N(6)-C(1)-N(1)	-7.4(5)
C(24)-N(6)-C(1)-C(2)	155.1(4)
C(8)-N(1)-C(1)-N(6)	153.5(3)
B(1)-N(1)-C(1)-N(6)	-15.9(5)
C(8)-N(1)-C(1)-C(2)	-12.4(4)
B(1)-N(1)-C(1)-C(2)	178.2(3)
N(6)-C(1)-C(2)-C(3)	19.4(7)
N(1)-C(1)-C(2)-C(3)	-175.8(4)
N(6)-C(1)-C(2)-C(7)	-158.2(4)
N(1)-C(1)-C(2)-C(7)	6.6(4)
C(7)-C(2)-C(3)-C(4)	-3.2(6)
C(1)-C(2)-C(3)-C(4)	179.5(4)
C(2)-C(3)-C(4)-C(5)	2.3(6)
C(2)-C(3)-C(4)-Cl(1)	-176.8(3)
C(3)-C(4)-C(5)-C(6)	0.9(6)
Cl(1)-C(4)-C(5)-C(6)	-180.0(3)
C(3)-C(4)-C(5)-Cl(2)	-178.0(3)
Cl(1)-C(4)-C(5)-Cl(2)	1.2(5)
C(4)-C(5)-C(6)-C(7)	-3.2(6)
Cl(2)-C(5)-C(6)-C(7)	175.7(3)
C(5)-C(6)-C(7)-C(2)	2.3(6)
C(5)-C(6)-C(7)-C(8)	179.6(4)
C(3)-C(2)-C(7)-C(6)	0.9(6)
C(1)-C(2)-C(7)-C(6)	178.7(3)
C(3)-C(2)-C(7)-C(8)	-177.0(3)
C(1)-C(2)-C(7)-C(8)	0.8(4)
C(9)-N(2)-C(8)-N(1)	9.5(5)
C(9)-N(2)-C(8)-C(7)	-155.8(4)
C(1)-N(1)-C(8)-N(2)	-155.7(3)
B(1)-N(1)-C(8)-N(2)	13.9(5)
C(1)-N(1)-C(8)-C(7)	12.8(4)
B(1)-N(1)-C(8)-C(7)	-177.6(3)
C(6)-C(7)-C(8)-N(2)	-18.2(7)
C(2)-C(7)-C(8)-N(2)	159.4(4)

C(6)-C(7)-C(8)-N(1)	174.5(4)
C(2)-C(7)-C(8)-N(1)	-7.9(4)
C(8)-N(2)-C(9)-N(3)	-8.0(5)
C(8)-N(2)-C(9)-C(10)	154.1(4)
C(16)-N(3)-C(9)-N(2)	154.9(3)
B(1)-N(3)-C(9)-N(2)	-17.4(5)
C(16)-N(3)-C(9)-C(10)	-10.9(4)
B(1)-N(3)-C(9)-C(10)	176.8(3)
N(2)-C(9)-C(10)-C(11)	18.3(7)
N(3)-C(9)-C(10)-C(11)	-177.4(4)
N(2)-C(9)-C(10)-C(15)	-158.0(4)
N(3)-C(9)-C(10)-C(15)	6.3(4)
C(15)-C(10)-C(11)-C(12)	0.4(6)
C(9)-C(10)-C(11)-C(12)	-175.4(4)
C(10)-C(11)-C(12)-C(13)	0.5(6)
C(10)-C(11)-C(12)-Cl(3)	-179.4(3)
C(11)-C(12)-C(13)-C(14)	-0.6(6)
Cl(3)-C(12)-C(13)-C(14)	179.3(3)
C(11)-C(12)-C(13)-Cl(4)	178.6(3)
Cl(3)-C(12)-C(13)-Cl(4)	-1.5(5)
C(12)-C(13)-C(14)-C(15)	-0.3(6)
Cl(4)-C(13)-C(14)-C(15)	-179.5(3)
C(13)-C(14)-C(15)-C(10)	1.2(5)
C(13)-C(14)-C(15)-C(16)	175.2(4)
C(11)-C(10)-C(15)-C(14)	-1.2(5)
C(9)-C(10)-C(15)-C(14)	175.5(3)
C(11)-C(10)-C(15)-C(16)	-176.6(3)
C(9)-C(10)-C(15)-C(16)	0.1(4)
C(17)-N(4)-C(16)-N(3)	9.5(5)
C(17)-N(4)-C(16)-C(15)	-155.7(4)
C(9)-N(3)-C(16)-N(4)	-157.6(3)
B(1)-N(3)-C(16)-N(4)	14.6(5)
C(9)-N(3)-C(16)-C(15)	11.0(4)
B(1)-N(3)-C(16)-C(15)	-176.9(3)
C(14)-C(15)-C(16)-N(4)	-14.0(7)
C(10)-C(15)-C(16)-N(4)	160.6(4)

C(14)-C(15)-C(16)-N(3)	179.0(4)
C(10)-C(15)-C(16)-N(3)	-6.4(4)
C(16)-N(4)-C(17)-N(5)	-9.7(5)
C(16)-N(4)-C(17)-C(18)	150.5(4)
C(24)-N(5)-C(17)-N(4)	152.2(3)
B(1)-N(5)-C(17)-N(4)	-13.7(5)
C(24)-N(5)-C(17)-C(18)	-12.1(4)
B(1)-N(5)-C(17)-C(18)	-178.0(3)
N(4)-C(17)-C(18)-C(19)	16.8(7)
N(5)-C(17)-C(18)-C(19)	179.6(4)
N(4)-C(17)-C(18)-C(23)	-154.7(4)
N(5)-C(17)-C(18)-C(23)	8.1(4)
C(23)-C(18)-C(19)-C(20)	2.4(5)
C(17)-C(18)-C(19)-C(20)	-168.0(4)
C(18)-C(19)-C(20)-C(21)	3.4(6)
C(18)-C(19)-C(20)-Cl(5)	-177.1(3)
C(19)-C(20)-C(21)-C(22)	-6.5(6)
Cl(5)-C(20)-C(21)-C(22)	174.0(3)
C(19)-C(20)-C(21)-Cl(6)	169.9(3)
Cl(5)-C(20)-C(21)-Cl(6)	-9.6(5)
C(20)-C(21)-C(22)-C(23)	3.3(6)
Cl(6)-C(21)-C(22)-C(23)	-173.1(3)
C(21)-C(22)-C(23)-C(18)	2.5(6)
C(21)-C(22)-C(23)-C(24)	168.1(4)
C(19)-C(18)-C(23)-C(22)	-5.5(6)
C(17)-C(18)-C(23)-C(22)	167.0(3)
C(19)-C(18)-C(23)-C(24)	-174.3(3)
C(17)-C(18)-C(23)-C(24)	-1.7(4)
C(1)-N(6)-C(24)-N(5)	10.0(5)
C(1)-N(6)-C(24)-C(23)	-153.3(4)
C(17)-N(5)-C(24)-N(6)	-155.3(3)
B(1)-N(5)-C(24)-N(6)	10.3(5)
C(17)-N(5)-C(24)-C(23)	11.1(4)
B(1)-N(5)-C(24)-C(23)	176.7(3)
C(22)-C(23)-C(24)-N(6)	-7.0(7)
C(18)-C(23)-C(24)-N(6)	160.1(4)

C(22)-C(23)-C(24)-N(5)	-172.4(4)
C(18)-C(23)-C(24)-N(5)	-5.4(4)
C(48)-N(12)-C(25)-N(7)	11.2(5)
C(48)-N(12)-C(25)-C(26)	-149.3(4)
C(32)-N(7)-C(25)-N(12)	-153.9(3)
B(2)-N(7)-C(25)-N(12)	10.8(5)
C(32)-N(7)-C(25)-C(26)	10.4(4)
B(2)-N(7)-C(25)-C(26)	175.0(3)
N(12)-C(25)-C(26)-C(27)	-13.0(7)
N(7)-C(25)-C(26)-C(27)	-176.1(4)
N(12)-C(25)-C(26)-C(31)	157.6(4)
N(7)-C(25)-C(26)-C(31)	-5.4(4)
C(31)-C(26)-C(27)-C(28)	1.7(6)
C(25)-C(26)-C(27)-C(28)	171.3(4)
C(26)-C(27)-C(28)-C(29)	-1.7(6)
C(27)-C(28)-C(29)-C(30)	-0.1(6)
C(28)-C(29)-C(30)-C(31)	2.0(6)
C(29)-C(30)-C(31)-C(26)	-2.0(6)
C(29)-C(30)-C(31)-C(32)	-170.2(4)
C(27)-C(26)-C(31)-C(30)	0.2(6)
C(25)-C(26)-C(31)-C(30)	-171.8(3)
C(27)-C(26)-C(31)-C(32)	171.0(3)
C(25)-C(26)-C(31)-C(32)	-1.0(4)
C(33)-N(8)-C(32)-N(7)	-8.8(5)
C(33)-N(8)-C(32)-C(31)	150.5(4)
C(25)-N(7)-C(32)-N(8)	151.9(3)
B(2)-N(7)-C(32)-N(8)	-12.7(5)
C(25)-N(7)-C(32)-C(31)	-11.1(4)
B(2)-N(7)-C(32)-C(31)	-175.7(3)
C(30)-C(31)-C(32)-N(8)	14.7(7)
C(26)-C(31)-C(32)-N(8)	-154.8(4)
C(30)-C(31)-C(32)-N(7)	176.5(4)
C(26)-C(31)-C(32)-N(7)	7.1(4)
C(32)-N(8)-C(33)-N(9)	9.0(5)
C(32)-N(8)-C(33)-C(34)	-151.9(4)
C(40)-N(9)-C(33)-N(8)	-154.7(3)

B(2)-N(9)-C(33)-N(8)	12.2(5)
C(40)-N(9)-C(33)-C(34)	9.8(4)
B(2)-N(9)-C(33)-C(34)	176.7(3)
N(8)-C(33)-C(34)-C(35)	-13.5(7)
N(9)-C(33)-C(34)-C(35)	-176.8(4)
N(8)-C(33)-C(34)-C(39)	158.4(4)
N(9)-C(33)-C(34)-C(39)	-5.0(4)
C(39)-C(34)-C(35)-C(36)	3.2(5)
C(33)-C(34)-C(35)-C(36)	174.1(4)
C(34)-C(35)-C(36)-C(37)	-1.8(6)
C(35)-C(36)-C(37)-C(38)	-1.0(6)
C(36)-C(37)-C(38)-C(39)	2.4(6)
C(37)-C(38)-C(39)-C(34)	-1.0(5)
C(37)-C(38)-C(39)-C(40)	-172.8(4)
C(35)-C(34)-C(39)-C(38)	-1.8(5)
C(33)-C(34)-C(39)-C(38)	-174.8(3)
C(35)-C(34)-C(39)-C(40)	171.8(3)
C(33)-C(34)-C(39)-C(40)	-1.1(4)
C(41)-N(10)-C(40)-N(9)	-9.8(5)
C(41)-N(10)-C(40)-C(39)	150.2(4)
C(33)-N(9)-C(40)-N(10)	153.3(3)
B(2)-N(9)-C(40)-N(10)	-13.7(5)
C(33)-N(9)-C(40)-C(39)	-10.5(4)
B(2)-N(9)-C(40)-C(39)	-177.4(3)
C(38)-C(39)-C(40)-N(10)	16.7(7)
C(34)-C(39)-C(40)-N(10)	-156.0(4)
C(38)-C(39)-C(40)-N(9)	179.4(4)
C(34)-C(39)-C(40)-N(9)	6.8(4)
C(40)-N(10)-C(41)-N(11)	9.5(5)
C(40)-N(10)-C(41)-C(42)	-155.1(4)
C(48)-N(11)-C(41)-N(10)	-155.7(3)
B(2)-N(11)-C(41)-N(10)	14.4(5)
C(48)-N(11)-C(41)-C(42)	11.9(4)
B(2)-N(11)-C(41)-C(42)	-178.0(3)
N(10)-C(41)-C(42)-C(43)	-17.5(6)
N(11)-C(41)-C(42)-C(43)	176.0(4)

N(10)-C(41)-C(42)-C(47)	159.6(4)
N(11)-C(41)-C(42)-C(47)	-6.9(4)
C(47)-C(42)-C(43)-C(44)	2.7(5)
C(41)-C(42)-C(43)-C(44)	179.4(4)
C(42)-C(43)-C(44)-C(45)	-3.4(5)
C(43)-C(44)-C(45)-C(46)	0.8(6)
C(44)-C(45)-C(46)-C(47)	2.6(6)
C(45)-C(46)-C(47)-C(42)	-3.3(5)
C(45)-C(46)-C(47)-C(48)	-179.2(4)
C(43)-C(42)-C(47)-C(46)	0.7(5)
C(41)-C(42)-C(47)-C(46)	-176.8(3)
C(43)-C(42)-C(47)-C(48)	177.5(3)
C(41)-C(42)-C(47)-C(48)	0.0(4)
C(25)-N(12)-C(48)-N(11)	-9.2(5)
C(25)-N(12)-C(48)-C(47)	154.5(4)
C(41)-N(11)-C(48)-N(12)	155.3(3)
B(2)-N(11)-C(48)-N(12)	-14.8(5)
C(41)-N(11)-C(48)-C(47)	-11.8(4)
B(2)-N(11)-C(48)-C(47)	178.0(3)
C(46)-C(47)-C(48)-N(12)	17.3(6)
C(42)-C(47)-C(48)-N(12)	-159.0(4)
C(46)-C(47)-C(48)-N(11)	-176.9(4)
C(42)-C(47)-C(48)-N(11)	6.8(4)
B(2)-O(1)-B(1)-N(3)	-14.8(6)
B(2)-O(1)-B(1)-N(1)	-134.4(4)
B(2)-O(1)-B(1)-N(5)	107.5(4)
C(9)-N(3)-B(1)-O(1)	-91.4(4)
C(16)-N(3)-B(1)-O(1)	97.2(4)
C(9)-N(3)-B(1)-N(1)	34.2(4)
C(16)-N(3)-B(1)-N(1)	-137.2(3)
C(9)-N(3)-B(1)-N(5)	139.4(3)
C(16)-N(3)-B(1)-N(5)	-31.9(4)
C(1)-N(1)-B(1)-O(1)	-96.1(4)
C(8)-N(1)-B(1)-O(1)	95.5(4)
C(1)-N(1)-B(1)-N(3)	135.9(3)
C(8)-N(1)-B(1)-N(3)	-32.5(4)

C(1)-N(1)-B(1)-N(5)	30.2(4)
C(8)-N(1)-B(1)-N(5)	-138.2(3)
C(24)-N(5)-B(1)-O(1)	97.1(4)
C(17)-N(5)-B(1)-O(1)	-98.7(4)
C(24)-N(5)-B(1)-N(3)	-133.0(3)
C(17)-N(5)-B(1)-N(3)	31.2(4)
C(24)-N(5)-B(1)-N(1)	-27.5(4)
C(17)-N(5)-B(1)-N(1)	136.7(3)
B(1)-O(1)-B(2)-N(7)	-137.7(4)
B(1)-O(1)-B(2)-N(11)	-17.2(5)
B(1)-O(1)-B(2)-N(9)	103.0(4)
C(32)-N(7)-B(2)-O(1)	-97.7(4)
C(25)-N(7)-B(2)-O(1)	99.4(4)
C(32)-N(7)-B(2)-N(11)	134.0(3)
C(25)-N(7)-B(2)-N(11)	-28.8(4)
C(32)-N(7)-B(2)-N(9)	28.3(4)
C(25)-N(7)-B(2)-N(9)	-134.6(3)
C(41)-N(11)-B(2)-O(1)	95.4(4)
C(48)-N(11)-B(2)-O(1)	-95.5(4)
C(41)-N(11)-B(2)-N(7)	-138.2(3)
C(48)-N(11)-B(2)-N(7)	30.9(4)
C(41)-N(11)-B(2)-N(9)	-31.6(4)
C(48)-N(11)-B(2)-N(9)	137.4(3)
C(33)-N(9)-B(2)-O(1)	97.3(4)
C(40)-N(9)-B(2)-O(1)	-97.1(4)
C(33)-N(9)-B(2)-N(7)	-28.1(4)
C(40)-N(9)-B(2)-N(7)	137.4(3)
C(33)-N(9)-B(2)-N(11)	-134.4(3)
C(40)-N(9)-B(2)-N(11)	31.2(4)

Symmetry transformations used to generate equivalent atoms:

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