Electronic Supplementary Material (ESI) for CrystEngComm

Halogen bonds can direct the solid state arrangement of phenoxy-boron subphthalocyanines

Jessica D. Virdo,[†] Yazan H. Kawar,[†] Alan J. Lough[‡] and Timothy P. Bender[†,‡,*]

† - Department of Chemical Engineering and Applied Chemistry, The University of Toronto, 200 College St., Toronto, Ontario, Canada, M5S 3E5
‡ - Department of Chemistry, University of Toronto, 80 St. George St., Toronto, Ontario, Canada, M5S 3H6
** - To whom all correspondence should be addressed: tim.bender@utoronto.ca*

ELECTRONIC SUPPORTING INFORMATION.

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EXPERIMENTAL.

Materials

meta-Bromophenol was purchased from TCI Company Ltd. (Portland, Oregon). m*eta*-Fluorophenol, *meta*-chlorophenol, *meta*-iodophenol, *ortho*-fluorophenol, *ortho*-chlorophenol, *ortho*-bromophenol, *ortho*-iodophenol, pentachlorophenol and pentabromophenol were purchased from Sigma Aldrich (Mississauga, Ontario, Canada). All reagents were used as received. Other common solvents, reagents and standard basic alumina (300 mesh) were purchased from Caledon Laboratories (Caledon, Ontario, Canada) and used as received. Cl-**BsubPc** was synthesized according to a previously described procedure[1] and Br-**BsubPc** was synthesized according to a procedure previously described by Potz.[2]

Methods

The reaction progress and purity analysis was performed using a Waters 2695 high pressure liquid chromatography (HPLC) separation module with a Waters 2998 photodiode array and a Waters 4.6 mm x 100 mm SunFire C_{18} 3.5 μm column. HPLC grade acetonitrile and dimethylformamide was eluted with an isocratic flow of 80/20 acetonitrile/dimethylformamide at 0.6 mL/min during operation.

All nuclear magnetic resonance (NMR) spectra were acquired on a Varian Mercury 400 MHz system in deuterated chloroform with 0.05% (v/v) tetramethylsilane (TMS) as a ^{1}H NMR reference purchased from Cambridge Isotope Laboratories and used as received. Mass spectrometry was performed on a Waters GC time-of-flightmass spectrometer with an electron ionization probe and accurate mass determination.

X-ray diffraction results were analyzed using PLATON 40M-version 300311[3] for bond angles and lengths, and crystal packing images were generated using Mercury version 2.4.[4] All data sets were collected using a Nonius KappaCCD diffractometer equipped with an Oxford Cryostream variable temperature apparatus, with the exception of the data set for α-*m*-IPhO-**Bsubc**, which was collected using a Bruker APEX-II CCD equipped with an Oxford Cryostream variable temperature apparatus. Hydrogen positions were calculated.

Molecular modeling was performed with HyperChem for Windows OS version 8.0, using a modified set of RM1 parameter files that have been previously published.[5] The crystal state heat of formation ($\Delta H_{f,cry}$) values were obtained by isolating a single molecule from the appropriate crystallographic information file and performing a single-point calculation using the RM1 semi-empirical method. The single molecule used in the previous calculation was then optimized by using the MM+ molecular mechanics forcefield and then further refined using the RM1 semi-empirical

method in order to obtain the corresponding optimized state heat of formation value ($\Delta H_{f,opt}$). Geometric optimization was performed using the Polak-Ribiere conjugated gradient method with a 0.02 kcal/ Å mol root-mean-squared convergence limit.

Synthesis

***meta*-Fluorophenoxy-boron subphthalocyanine** (*m*-FPhO-**BsubPc**, **2a**).

Cl-**BsubPc** (**1**, 1.001 g, 0.0023 mol) was mixed with *meta*-fluorophenol (0.781 g, 0.0070 mol) in chlorobenzene (22 mL) in a round-bottom flask fitted with a reflux condenser and argon inlet. The mixture was stirred and heated at reflux under a constant pressure of argon for 20 to 40 hours. The reaction was monitored via HPLC and determined to be complete by the non-detection of **1**. The crude product was isolated by removing the solvent under rotary evaporation. Preliminary purification was achieved by dissolving the crude product in toluene (700 mL) and vigorously stirring the toluene mixture with 3.0 M KOH solution in distilled water (300 mL) overnight. The toluene phase was isolated and the solvent was removed under rotary evaporation. The product was further purified on a Kauffman column using standard basic alumina (300 mesh) as the adsorbent and dichloromethane as the eluent. The product elutes from the Kauffman column while the excess phenol remains adsorbed, as previously described.[6] The dichloromethane was then removed under rotary evaporation yielding a dark pink/magenta powder. Compound **2a** (yield 1.030 g, 88%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.26; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.11-5.14 (1H, m), 5.14-5.18 (1H, m), 6.29-6.35 (1H, m), 6.66-6.72 (1H, m), 7.88-7.92 (6H, m), 8.83-8.87 (6H, m); HRMS (EI) Calcd. for [$C_{30}H_{16}BFN_6O$] ([M]+): m/z 506.1463, found 506.1470.

***meta*-Chlorophenoxy-boron subphthalocyanine** (*m*-ClPhO-**BsubPc**, **2b**).

2b was synthesized as for **2a** except *meta*-chlorophenol (0.896 g, 0.0070 mol) was used in place of *meta*-fluorophenol, yielding compound **2b** (1.013 g, 83%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.55; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.18-5.21 (1H, m), 5.46-5.47 (1H, t), 6.57-6.60 (1H, m), 6.65-6.69 (1H, t), 7.87-7.92 (6H, m), 8.83-8.88 (6H, m); HRMS (EI) Calcd. for [$C_{30}H_{16}BClN_6O$] ([M]+): m/z 522.1167, found 522.1168.

***meta*-Bromophenoxy-boron subphthalocyanine** (*m*-BrPhO-**BsubPc**, **2c**).

2c was synthesized as for **2a** except *meta*-bromophenol (1.206 g, 0.0070 mol) was used in place of *meta*-fluorophenol, yielding compound **2c** (1.159 g, 88%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.63; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.23-5.26 (1H, m), 5.64-5.65 (1H, t), 6.60-

6.64 (1H, t), 6.74-6.77 (1H, m), 7.89-7.94 (6H, m), 8.84-8.89 (6H, m); HRMS (EI) Calcd. for $[C_{30}H_{16}BBrN_6O]$ ([M]+): m/z 566.0662, found 566.0668.

***meta*-Iodophenoxy-boron subphthalocyanine** (*m*-IPhO-**BsubPc**, **2d**).

2d was synthesized as for **2a** except *meta*-iodophenol (1.206 g, 0.0070 mol) was used in place of *meta*-fluorophenol, yielding compound **2d** (1.173 g, 82%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.71; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.26-5.29 (1H, m), 5.83-5.84 (1H, t), 6.46-6.50 (1H, t), 6.94-6.96 (1H, m), 7.90-7.95 (6H, m), 8.85-8.90 (6H, m); HRMS (EI) Calcd. for $[C_{30}H_{16}BIN_6O]$ ([M]+): m/z 614.0523, found 614.0533.

***ortho*-Fluorophenoxy-boron subphthalocyanine** (*o*-FPhO-**BsubPc**, **4a**).

In a manner similar to the synthesis of **2a**, Br-**BsubPc** (**3**, 1.200 g, 0.0025 mol) was mixed with *ortho*-fluorophenol (0.849 g, 0.0076 mol) in chlorobenzene (26 mL) and heated at reflux under a constant pressure of argon. The reaction was monitored via HPLC and determined to be complete by the non-detection of **3**. The crude product was isolated and purified as described in the synthesis of **2a**, yielding compound **4a** (0.857 g, 67%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.07; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.40-5.45 (1H, t), 6.50-6.60 (3H, m), 7.89-7.94 (6H, m), 8.83-8.89 (6H, m); HRMS (EI) Calcd. for $[C_{30}H_{16}BFN_6O]$ ([M]+): m/z 506.1463, found 506.1458.

***ortho*-Chlorophenoxy-boron subphthalocyanine** (*o*-ClPhO-**BsubPc**, **4b**).

4b was synthesized as for **4a** except *ortho*-chlorophenol (0.974 g, 0.0076 mol) was used in place of *ortho*-fluorophenol, yielding compound **4b** (1.002 g, 76%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 561.0, R_T (min) = 2.21; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.32-5.36 (1H, m), 6.57-6.62 (1H, m), 6.65-6.71 (1H, m), 6.81-6.84 (1H, m), 7.90-7.95 (6H, m), 8.84-8.89 (6H, m); HRMS (EI) Calcd. for $[C_{30}H_{16}BClN_6O]$ ([M]+): m/z 522.1167, found 522.1172.

***ortho*-Bromophenoxy-boron subphthalocyanine** (*o*-BrPhO-**BsubPc**, **4c**).

4c was synthesized as for **4a** except *ortho*-bromophenol (1.311 g, 0.0076 mol) was used in place of *ortho*-fluorophenol, yielding compound **4c** (0.764 g, 53%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 562.2, R_T (min) = 2.25; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.29-5.32 (1H, m), 6.50-6.55 (1H, m), 6.69-6.75 (1H, m), 6.98-7.01 (1H, m), 7.89-7.95 (6H, m), 8.83-8.89 (6H, m); HRMS (EI) Calcd. for $[C_{30}H_{16}BBrN_6O]$ ([M]+): m/z 566.0662, found 566.0667.

***ortho*-Iodophenoxy-boron subphthalocyanine** (*o*-IPhO-**BsubPc**, **4d**).

4d was synthesized as for **4a** except *ortho*-iodophenol (1.667 g, 0.0076 mol) was used in place of *ortho*-fluorophenol, yielding compound **4d** (0.945 g, 61%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 562.2, R_T (min) = 2.29; δ_H (400 MHz; $CDCl_3$; Me_4Si) 5.19-5.22 (1H, m), 6.36-6.41 (1H, m), 6.72-6.78 (1H, m), 7.22-7.25 (1H, m), 7.89-7.95 (6H, m), 8.84-8.90 (6H, m); HRMS (EI) Calcd. for [$C_{30}H_{16}BIN_6O$] ([M]+): m/z 614.0523, found 614.0529.

Pentachlorophenoxy-boron subphthalocyanine (Cl_5PhO-**BsubPc**, **4e**).

4e was synthesized as for **4a** except pentachlorophenol (2.018 g, 0.0076 mol) was used in place of *ortho*-fluorophenol, yielding compound **4e** (1.075 g, 64%). Purity by HPLC (> 99%, max plot). HPLC λ_{max} (nm) = 564.7, R_T (min) = 4.51; δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.92-7.97 (6H, m), 8.86-8.90 (6H, m); HRMS (EI) Calcd. for [$C_{30}H_{12}BCl_5N_6O$] ([M]+): m/z 657.9608, found 657.9626.

Pentabromophenoxy-boron subphthalocyanine (Br_5PhO-**BsubPc**, **4f**).

4f was synthesized as for **4a** except pentabromophenol (3.702 g, 0.0076 mol) was used in place of *ortho*-fluorophenol, yielding compound **4f** (0.803 g, 39%). Purity by HPLC (97.6%, max plot, with the remainder being pentabromophenol). HPLC λ_{max} (nm) = 565.9, R_T (min) = 3.902; δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.94-7.96 (6H, m), 8.87-8.89 (6H, m); HRMS (EI) Calcd. for [$C_{30}H_{12}BBr_5N_6O$] ([M]+): m/z 877.7082, found 877.7088.

Preparation of single crystals

Slow diffusion crystallization was performed using two solvent systems. In the first solvent system, benzene was used as the good solvent and heptane was used as the diffusing solvent. In the second solvent system, dichloromethane was used as the good solvent and pentane was used as the diffusing solvent. Samples of **2a-d** and **4a-d** were prepared by dissolving the appropriate phenoxy-**BsubPc** compound (0.040 g) in a good solvent (8 mL of benzene or dichloromethane). Due to the lower solubility of **4e** and **4f**, samples of these compounds were prepared by dissolving the appropriate phenoxy-**BsubPc** compound (0.025 g) in a good solvent (10 mL of benzene or dichloromethane). The sample solution was then transferred to a 20-mL vial. The opening of the vial was covered with aluminum foil, and the foil was punctured with small holes. The vial was sealed in a larger airtight chair with the appropriate diffusing solvent (150 mL of heptane or pentane). Single crystals of high quality suitable for X-ray diffraction were obtained within 1-2 weeks.

Schematics and instructions for use for the train sublimation apparatus have been previously disclosed.[6] Briefly, samples to be crystallized were placed in a small boat constructed of aluminum

foil and inserted into the hot zone of the sublimation chamber. The chamber was evacuated and the internal temperature of the hot zone was increased to 120 °C for 10 minutes, then to 180 °C for 10 minutes, and then to 220 °C for approximately 1 hour in order to remove small molecule contaminants. Next, the nitrogen flow was set with the needle valve creating an internal pressure of $1x10^{-1}$ Torr. With the cooling water circulating, the interal temperature of the hot zone was slowly incremented at a rate of 10 °C/10 minutes until the material began to sublime (between 300 °C and 340 °C). The temperature was maintained at the sublimation point for 1 hour in order to seed crystals. The temperature was then increased at a rate of 3°C/10 minutes until the temperature was 100 °C past the sublimation point and held at that temperature for 2 hours before being cooled to room temperature. Finally, the crystals produced from the sublimation process were scraped from the sublimation tube and analyzed.

SUPPLEMENTARY RESULTS AND DISCUSSION.

Single crystal structure determination

The CheckCIF routine reports C- and G-level alerts related to missing reflections, but this does not raise alerts regarding the completeness of the data for any of these structures: data completeness is >95% for all structures, and is >99% for most. The integration software routinely rejects outlier reflections and reflections which are in the shadow of the beamstop, leading to some missing reflections. The missing reflections in the reported structures constitute a very small percentage in terms of the complete data set, and will have a negligible effect on the precision of the structure.

Five of the reported CIFs (**2b**, **4b**, unsolvated **4d**, solvated **4d**, and unsolvated **4f**) raise C-level alerts due to a large scale factor (K) in the Analysis of Variance section. Based on the Analysis of Variance output from the SHELXL output, these high K values are related to the weakest reflections (i.e., the reflections collected at the highest angle) for each structure. When the K values are investigated in terms of ‘resolution’, they do not appear to be out of the ordinary. For these reasons, the authors are not concerned about the large K values. It is our strategy to collect as much high angle data as possible, typically to approximately 27 degrees in theta. Although the K values can be lowered by collecting data to a lower angle, the high angle data and resulting weak reflections still contain useful information about the structure, which is mainly related to the displacement parameters of the non-hydrogen atoms.

Two of the reported structures (**4c** and unsolvated **4d**) have relatively high R values. Both of these structures contain disorder in the phenoxy moiety, as described in the manuscript. The high R values are likely due to the disorder, which was difficult to model, but may also reflect the quality of the crystals. Apart from the disorder, there did not appear to be any other issues with these crystals. The CheckCIF report for **4c** includes a C-level alert regarding a relatively high max:min residual electron density value. The highest electron density peak is in the vicinity of the disordered phenoxy moiety.

Analysis of carbon-halogen bonds

The length of the carbon-halogen (C-X) bonds observed for compounds **2b-d** and **4a-f** are provided in Table S1, and are compared with the C-X bond lengths observed for *para*-substituted halo-phenoxy-**BsubPcs**[7]. The change in bond length (Δ bond length) has also been calculated, with negative values representing bond compression and positive values representing bond stretching. The C-X metrics for halogens which are not participating in halogen-nitrogen interactions have been included for reference.

For many of the C-X bonds listed in Table S1, the change in bond length is too minor to be considered significant (-0.01 Å < Δ bond length < 0.01 Å). This category includes the motifs *m*-ClPhO-**BsubPc**, *m*-BrPhO-**BsubPc**, *o*-ClPhO-**BsubPc**, solvated *o*-IPhO-**BsubPc**, all of the C-X bonds in solvated Br_5PhO-**BsubPc** and all but one of the C-X bonds in unsolvated Br_5PhO-**BsubPc**. Notable exceptions are the C-X bonds for both solvated and unsolvated *m*-IPhO-**BsubPc**, which are involved in halogen bonding and which display significant bond stretching of approximately 0.01 Å and 0.02 Å, respectively. The remaining C-X bonds, some of which participate in halogen bonding, display mild to significant bond compression (Δ bond length < -0.01). In sum, the presence of a halogen bond, as determined by a significantly short X···N distance and a nearly linear C-X···N angle, has been observed to occur alongside both C-X bond stretching and C-X bond compression. With regards to the crystal structures for compounds **2b-d** and **4a-f**, there does not appear to be a significant correlation between halogen bonding and distortions in the C-X bond.

Table S1. Halogen-carbon covalent bond distances.

	Motif	C-X [a]	C-X distance observed/Å	C-X distance expected/Å [c]	Δ Bond length/Å
2b	*m*-ClPhO-**BsubPc**	C27-Cl1	1.731(3)	1.739(2)	-0.008(5)
2c	*m*-BrPhO-**BsubPc**	C27-Br1	1.899(3)	1.893(3)	0.006(6)
2d	*m*-IPhO-**BsubPc**	C27-I1	2.114(7)	2.094(3)	0.02(1)
	m-IPhO-**BsubPc** solvate	C27-I1	2.105(2)	2.094(3)	0.011(5)
4a	*o*-FPhO-**BsubPc**	C26-F1 [b]	1.344(3)	1.363(2)	-0.019(5)
4b	*o*-ClPhO-**BsubPc**	C26A-ClA	1.729(3)	1.739(2)	-0.010(5)
		C26B-C1B [b]	1.738(3)	1.739(2)	-0.001(5)
4c	*o*-BrPhO-**BsubPc**	C26-Br1 [b]	1.811(7)	1.893(3)	-0.082(10)
4d	*o*-IPhO-**BsubPc**	C26-I1 [b]	2.05(1)	2.094(3)	-0.04(1)
	o-IPhO-**BsubPc** solvate	C26-I1	2.089(4)	2.094(3)	-0.005(7)
4e	Cl_5PhO-**BsubPc**	C26-Cl1 [b]	1.726(3)	1.739(2)	-0.013(5)
		C27- Cl2 [b]	1.723(4)	1.739(2)	-0.016(6)
		C28- Cl3	1.718(5)	1.739(2)	-0.021(7)
		C29-Cl4 [b]	1.725(4)	1.739(2)	-0.014(6)
		C30-Cl5 [b]	1.719(4)	1.739(2)	-0.020(6)
4f	Br_5PhO-**BsubPc**	C26-Br1	1.87(1)	1.893(3)	-0.02(1)
		C27-Br2 [b]	1.90(1)	1.893(3)	0.01(1)
		C28-Br3	1.88(1)	1.893(3)	-0.01(1)
		C29-Br4 [b]	1.89(1)	1.893(3)	0.00(1)
		C30-Br5 [b]	1.90(1)	1.893(3)	0.01(1)
	Br_5PhO-**BsubPc** solvate	C26-Br1 [b]	1.890(4)	1.893(3)	-0.003(7)
		C27-Br2	1.887(4)	1.893(3)	-0.006(7)
		C28-Br3 [b]	1.899(4)	1.893(3)	0.006(7)
		C29-Br4	1.885(5)	1.893(3)	-0.008(8)
		C30-Br5 [b]	1.897(4)	1.893(3)	0.004(7)

[a] Atoms numbered according to the thermal ellipsoid plots provided in the Electronic supplementary information (ESI).

[b] These C-X distances correspond to halogens which are not participating in halogen-nitrogen interactions.

[c] C-X bond lengths observed for *para*-substituted halo-phenoxy-**BsubPcs**,[7] which do not exhibit halogen bonding.

Table S2. Comparison of intramolecular metrics for optimized *meta*- and *para*-phenoxy-**BsubPcs**.

	Bowl depth /Å	B-O bond length/Å	O-C bond length/Å	B-O-C angle/°
Comparison of *m*-ClPhO-**BsubPc** and *p*-ClPhO-**BsubPc**				
m-ClPhO-**BsubPc**	2.711	1.418	1.367	116.20
p-ClPhO-**BsubPc**	2.716	1.417	1.367	116.19
% Difference	0.18%	0.07%	0.00%	0.01%
Comparison of *m-Br*PhO-**BsubPc** and *p*-BrPhO-**BsubPc**				
m-BrPhO-**BsubPc**	2.711	1.418	1.366	116.19
p-BrPhO-**BsubPc**	2.716	1.417	1.368	116.23
% Difference	0.18%	0.07%	0.15%	0.03%
Comparison of β-*m-I*PhO-**BsubPc** and *p*-IPhO-**BsubPc**				
m-IPhO-**BsubPc**	2.714	1.417	1.367	116.00
p-IPhO-**BsubPc**	2.716	1.416	1.368	116.17
% Difference	0.07%	0.07%	0.07%	0.15%

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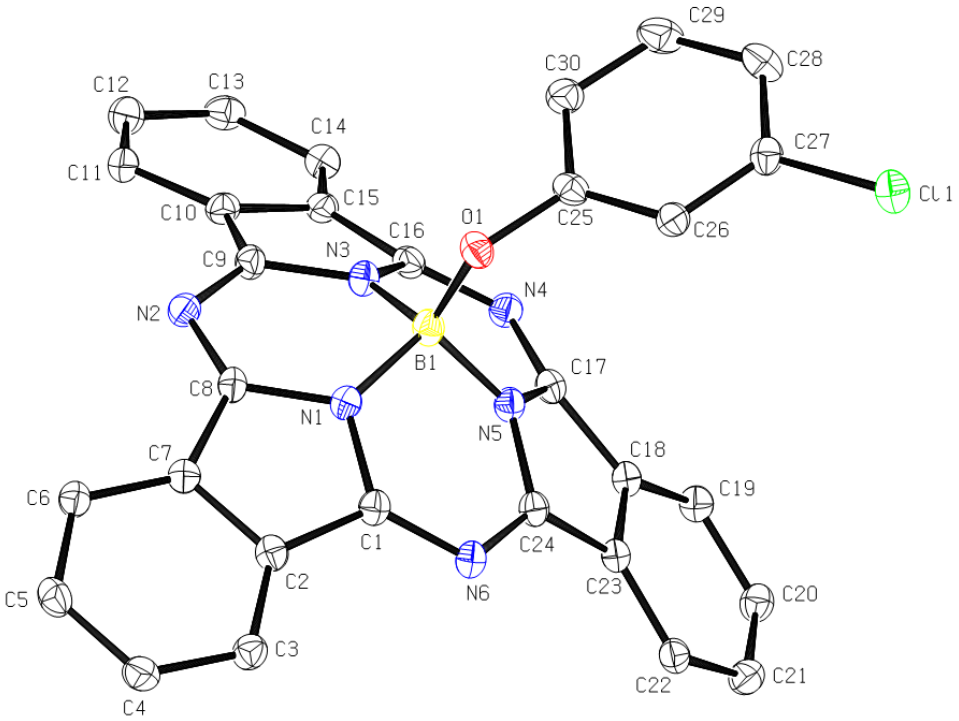

Figure S1. Anisotropic displacement ellipsoid plot of *m*-ClPhO-**BsubPc** (compound **2b**).

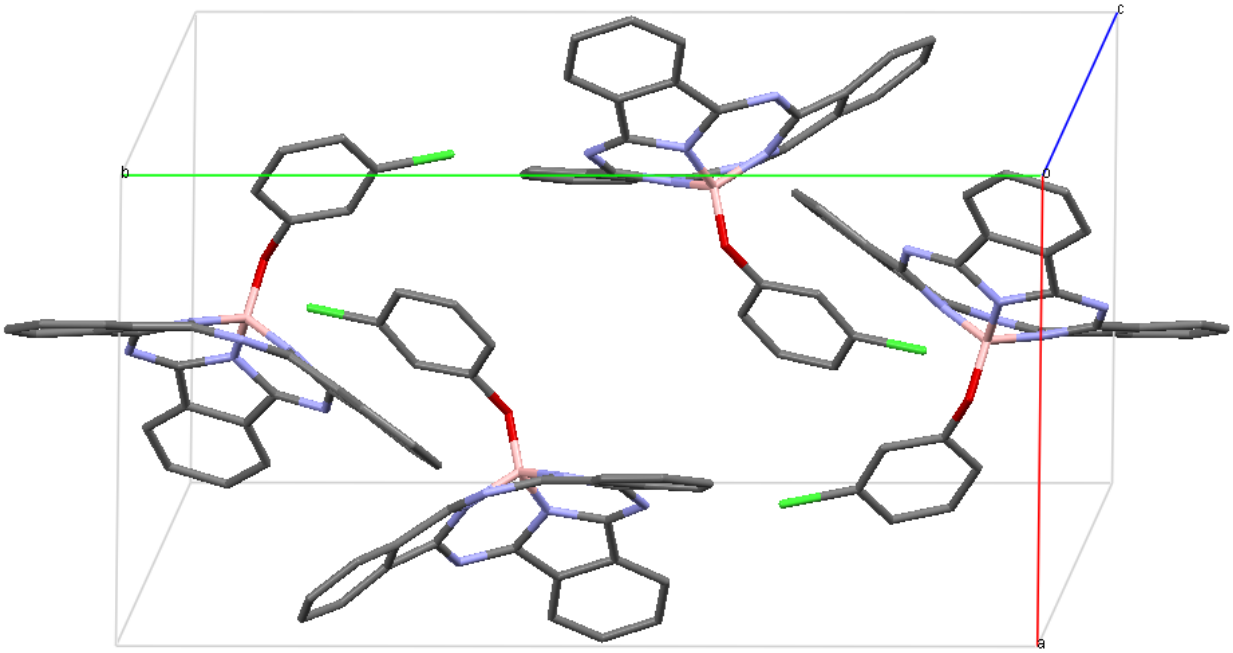

Figure S2. Populated unit cell of *m*-ClPhO-**BsubPc** (compound **2b**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; chlorine = green. Hydrogens are omitted for clarity.

Table S3. Crystal data and structure refinement for *m*-ClPhO-**BsubPc** (compound **2b**).

Identification code	k1139	
Empirical formula	C30 H16 B Cl N6 O	
Formula weight	522.75	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.6086(7) Å	α= 90°.
	b = 21.0572(7) Å	β= 112.680(2)°.
	c = 11.4521(7) Å	γ = 90°.
Volume	2360.4(2) $Å^3$	
Z	4	
Density (calculated)	1.471 Mg/m^3	
Absorption coefficient	0.202 mm^{-1}	
F(000)	1072	
Crystal size	0.16 x 0.14 x 0.08 mm^3	
Theta range for data collection	2.73 to 27.53°.	
Index ranges	-13<=h<=12, -26<=k<=27, -11<=l<=14	
Reflections collected	15224	
Independent reflections	5309 [R(int) = 0.0760]	
Completeness to theta = 25.00°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.892	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5309 / 0 / 352	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0609, wR2 = 0.1242	
R indices (all data)	R1 = 0.1475, wR2 = 0.1591	
Largest diff. peak and hole	0.321 and -0.432 $e.Å^{-3}$	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *m*-ClPhO-**BsubPc** (compound **2b**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	9914(1)	3447(1)	8452(1)	40(1)
O(1)	7349(2)	1364(1)	7490(2)	31(1)
N(1)	5019(2)	987(1)	6732(2)	25(1)
N(2)	5313(2)	-109(1)	7267(2)	28(1)
N(3)	6454(3)	682(1)	8789(2)	27(1)
N(4)	6692(3)	1362(1)	10513(2)	29(1)
N(5)	5701(3)	1738(1)	8393(2)	27(1)
N(6)	3816(2)	1972(1)	6469(2)	28(1)
C(1)	3977(3)	1389(1)	6052(3)	27(1)
C(2)	3014(3)	998(1)	5046(3)	28(1)
C(3)	1815(3)	1143(1)	4033(3)	31(1)
C(4)	1089(3)	657(1)	3245(3)	36(1)
C(5)	1556(3)	28(1)	3483(3)	34(1)
C(6)	2734(3)	-127(1)	4501(3)	29(1)
C(7)	3478(3)	361(1)	5287(3)	26(1)
C(8)	4707(3)	361(1)	6440(3)	26(1)
C(9)	6126(3)	61(1)	8456(3)	27(1)
C(10)	6572(3)	-289(1)	9644(3)	28(1)
C(11)	6600(3)	-935(1)	9917(3)	31(1)
C(12)	7132(3)	-1115(1)	11172(3)	35(1)
C(13)	7588(3)	-672(1)	12157(3)	34(1)
C(14)	7491(3)	-27(1)	11905(3)	32(1)
C(15)	7010(3)	164(1)	10639(3)	26(1)
C(16)	6805(3)	787(1)	10054(3)	27(1)
C(17)	6055(3)	1818(1)	9663(3)	26(1)
C(18)	5347(3)	2387(1)	9798(3)	26(1)
C(19)	5350(3)	2718(1)	10851(3)	30(1)
C(20)	4504(3)	3243(1)	10645(3)	32(1)

C(21)	3651(3)	3426(1)	9429(3)	32(1)
C(22)	3595(3)	3090(1)	8368(3)	28(1)
C(23)	4463(3)	2574(1)	8554(3)	26(1)
C(24)	4648(3)	2121(1)	7673(3)	26(1)
C(25)	8455(3)	1696(1)	8326(3)	29(1)
C(26)	8588(3)	2331(1)	8073(3)	28(1)
C(27)	9724(3)	2664(1)	8814(3)	30(1)
C(28)	10735(3)	2381(2)	9852(3)	39(1)
C(29)	10563(3)	1754(2)	10121(3)	42(1)
C(30)	9450(3)	1407(1)	9359(3)	34(1)
B(1)	6224(4)	1206(2)	7846(3)	29(1)

Table S5. Bond lengths [Å] and angles [°] for *m*-ClPhO-**BsubPc** (compound **2b**).

Cl(1)-C(27)	1.731(3)
O(1)-C(25)	1.384(3)
O(1)-B(1)	1.442(4)
N(1)-C(8)	1.370(3)
N(1)-C(1)	1.371(3)
N(1)-B(1)	1.488(4)
N(2)-C(8)	1.349(3)
N(2)-C(9)	1.350(3)
N(3)-C(9)	1.367(3)
N(3)-C(16)	1.368(3)
N(3)-B(1)	1.497(4)
N(4)-C(16)	1.344(3)
N(4)-C(17)	1.348(3)
N(5)-C(17)	1.365(3)
N(5)-C(24)	1.368(4)
N(5)-B(1)	1.490(4)
N(6)-C(1)	1.352(3)
N(6)-C(24)	1.356(3)
C(1)-C(2)	1.464(4)
C(2)-C(3)	1.385(4)
C(2)-C(7)	1.419(4)
C(3)-C(4)	1.386(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.403(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.379(4)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.393(4)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.455(4)
C(9)-C(10)	1.457(4)
C(10)-C(11)	1.393(4)

C(10)-C(15)	1.420(4)
C(11)-C(12)	1.379(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.399(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.385(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.398(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.450(4)
C(17)-C(18)	1.454(4)
C(18)-C(19)	1.393(4)
C(18)-C(23)	1.427(4)
C(19)-C(20)	1.385(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.391(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.388(4)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.386(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.455(4)
C(25)-C(26)	1.386(4)
C(25)-C(30)	1.386(4)
C(26)-C(27)	1.370(4)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.391(4)
C(28)-C(29)	1.383(4)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.377(4)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500

C(25)-O(1)-B(1)	119.6(2)

C(8)-N(1)-C(1)	112.9(2)
C(8)-N(1)-B(1)	123.7(2)
C(1)-N(1)-B(1)	122.3(2)
C(8)-N(2)-C(9)	117.3(2)
C(9)-N(3)-C(16)	112.7(2)
C(9)-N(3)-B(1)	123.4(2)
C(16)-N(3)-B(1)	123.1(2)
C(16)-N(4)-C(17)	117.0(2)
C(17)-N(5)-C(24)	113.3(2)
C(17)-N(5)-B(1)	123.1(2)
C(24)-N(5)-B(1)	122.7(2)
C(1)-N(6)-C(24)	116.6(2)
N(6)-C(1)-N(1)	122.9(3)
N(6)-C(1)-C(2)	130.1(3)
N(1)-C(1)-C(2)	105.4(2)
C(3)-C(2)-C(7)	120.6(3)
C(3)-C(2)-C(1)	132.2(3)
C(7)-C(2)-C(1)	107.1(3)
C(2)-C(3)-C(4)	118.8(3)
C(2)-C(3)-H(3A)	120.6
C(4)-C(3)-H(3A)	120.6
C(3)-C(4)-C(5)	120.3(3)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
C(6)-C(5)-C(4)	121.7(3)
C(6)-C(5)-H(5A)	119.2
C(4)-C(5)-H(5A)	119.2
C(5)-C(6)-C(7)	118.3(3)
C(5)-C(6)-H(6A)	120.8
C(7)-C(6)-H(6A)	120.8
C(6)-C(7)-C(2)	120.2(3)
C(6)-C(7)-C(8)	132.3(3)
C(2)-C(7)-C(8)	107.4(2)
N(2)-C(8)-N(1)	122.0(3)

N(2)-C(8)-C(7)	130.9(2)
N(1)-C(8)-C(7)	105.6(2)
N(2)-C(9)-N(3)	122.0(2)
N(2)-C(9)-C(10)	131.2(3)
N(3)-C(9)-C(10)	105.5(2)
C(11)-C(10)-C(15)	120.2(3)
C(11)-C(10)-C(9)	132.4(3)
C(15)-C(10)-C(9)	107.3(2)
C(12)-C(11)-C(10)	117.9(3)
C(12)-C(11)-H(11A)	121.1
C(10)-C(11)-H(11A)	121.1
C(11)-C(12)-C(13)	122.1(3)
C(11)-C(12)-H(12A)	118.9
C(13)-C(12)-H(12A)	118.9
C(14)-C(13)-C(12)	120.8(3)
C(14)-C(13)-H(13A)	119.6
C(12)-C(13)-H(13A)	119.6
C(13)-C(14)-C(15)	117.8(3)
C(13)-C(14)-H(14A)	121.1
C(15)-C(14)-H(14A)	121.1
C(14)-C(15)-C(10)	121.0(2)
C(14)-C(15)-C(16)	132.0(3)
C(10)-C(15)-C(16)	107.0(2)
N(4)-C(16)-N(3)	122.1(2)
N(4)-C(16)-C(15)	130.8(3)
N(3)-C(16)-C(15)	105.9(2)
N(4)-C(17)-N(5)	122.5(2)
N(4)-C(17)-C(18)	130.2(3)
N(5)-C(17)-C(18)	105.9(2)
C(19)-C(18)-C(23)	120.5(3)
C(19)-C(18)-C(17)	132.6(3)
C(23)-C(18)-C(17)	106.8(2)
C(20)-C(19)-C(18)	117.9(3)
C(20)-C(19)-H(19A)	121.0

C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.3(3)
C(19)-C(20)-H(20A)	119.3
C(21)-C(20)-H(20A)	119.3
C(22)-C(21)-C(20)	121.8(3)
C(22)-C(21)-H(21A)	119.1
C(20)-C(21)-H(21A)	119.1
C(23)-C(22)-C(21)	117.7(3)
C(23)-C(22)-H(22A)	121.2
C(21)-C(22)-H(22A)	121.2
C(22)-C(23)-C(18)	120.8(3)
C(22)-C(23)-C(24)	131.8(3)
C(18)-C(23)-C(24)	107.4(2)
N(6)-C(24)-N(5)	122.4(2)
N(6)-C(24)-C(23)	130.4(3)
N(5)-C(24)-C(23)	105.4(2)
O(1)-C(25)-C(26)	118.0(3)
O(1)-C(25)-C(30)	122.1(3)
C(26)-C(25)-C(30)	119.8(3)
C(27)-C(26)-C(25)	120.1(3)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(26)-C(27)-C(28)	120.9(3)
C(26)-C(27)-Cl(1)	119.7(2)
C(28)-C(27)-Cl(1)	119.3(2)
C(29)-C(28)-C(27)	118.3(3)
C(29)-C(28)-H(28A)	120.8
C(27)-C(28)-H(28A)	120.8
C(30)-C(29)-C(28)	121.3(3)
C(30)-C(29)-H(29A)	119.3
C(28)-C(29)-H(29A)	119.3
C(29)-C(30)-C(25)	119.5(3)
C(29)-C(30)-H(30A)	120.3
C(25)-C(30)-H(30A)	120.3

O(1)-B(1)-N(1)	111.1(2)
O(1)-B(1)-N(5)	115.3(2)
N(1)-B(1)-N(5)	104.9(3)
O(1)-B(1)-N(3)	116.9(3)
N(1)-B(1)-N(3)	103.7(2)
N(5)-B(1)-N(3)	103.6(2)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *m*-ClPhO-**BsubPc** (compound **2b**). 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)	42(1)	34(1)	42(1)	-3(1)	15(1)	-8(1)
O(1)	29(1)	33(1)	32(1)	-5(1)	14(1)	-6(1)
N(1)	30(2)	24(1)	24(1)	0(1)	12(1)	0(1)
N(2)	29(2)	25(1)	31(2)	0(1)	13(1)	1(1)
N(3)	31(2)	24(1)	26(2)	-2(1)	11(1)	-2(1)
N(4)	30(2)	27(1)	27(2)	0(1)	9(1)	1(1)
N(5)	29(2)	24(1)	25(2)	-1(1)	9(1)	-2(1)
N(6)	34(2)	24(1)	26(2)	-2(1)	12(1)	-3(1)
C(1)	32(2)	25(2)	24(2)	1(1)	11(2)	-1(1)
C(2)	31(2)	30(2)	24(2)	-4(1)	12(2)	-3(1)
C(3)	34(2)	30(2)	29(2)	-3(1)	12(2)	2(1)
C(4)	28(2)	38(2)	37(2)	-5(2)	8(2)	0(2)
C(5)	33(2)	37(2)	32(2)	-10(1)	11(2)	-8(2)
C(6)	32(2)	26(2)	31(2)	-3(1)	15(2)	-2(1)
C(7)	29(2)	27(2)	25(2)	-1(1)	14(2)	-1(1)
C(8)	30(2)	22(2)	28(2)	-4(1)	14(2)	-4(1)
C(9)	29(2)	25(2)	29(2)	-6(1)	12(2)	-2(1)
C(10)	26(2)	28(2)	33(2)	3(1)	14(2)	2(1)
C(11)	30(2)	24(2)	39(2)	-1(1)	13(2)	-2(1)
C(12)	36(2)	30(2)	40(2)	7(2)	15(2)	-1(1)
C(13)	30(2)	39(2)	32(2)	9(2)	12(2)	4(1)
C(14)	30(2)	32(2)	33(2)	0(1)	11(2)	0(1)
C(15)	23(2)	25(2)	32(2)	2(1)	12(1)	0(1)
C(16)	24(2)	29(2)	24(2)	-3(1)	6(1)	-2(1)
C(17)	27(2)	27(2)	24(2)	-3(1)	9(1)	-4(1)
C(18)	28(2)	24(2)	27(2)	-2(1)	10(1)	-4(1)
C(19)	32(2)	29(2)	28(2)	0(1)	11(2)	-1(1)
C(20)	37(2)	29(2)	32(2)	-3(1)	16(2)	-1(1)
C(21)	34(2)	30(2)	36(2)	0(1)	16(2)	2(1)

C(22)	28(2)	25(2)	28(2)	0(1)	8(2)	-4(1)
C(23)	26(2)	23(2)	29(2)	-3(1)	9(2)	-3(1)
C(24)	29(2)	24(2)	26(2)	0(1)	11(2)	-4(1)
C(25)	24(2)	37(2)	28(2)	-3(1)	13(2)	-2(1)
C(26)	29(2)	29(2)	25(2)	-2(1)	8(2)	1(1)
C(27)	36(2)	28(2)	28(2)	-4(1)	16(2)	-3(1)
C(28)	28(2)	50(2)	34(2)	1(2)	6(2)	-7(2)
C(29)	31(2)	52(2)	38(2)	11(2)	6(2)	4(2)
C(30)	32(2)	33(2)	38(2)	4(1)	14(2)	2(1)
B(1)	33(2)	26(2)	22(2)	-2(1)	6(2)	-2(2)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *m*-ClPhO-**BsubPc** (compound **2b**).

	x	y	z	U(eq)
H(3A)	1497	1569	3881	38
H(4A)	271	750	2541	43
H(5A)	1049	-298	2930	41
H(6A)	3030	-555	4661	34
H(11A)	6263	-1241	9260	37
H(12A)	7192	-1555	11373	42
H(13A)	7968	-816	13009	41
H(14A)	7744	276	12571	38
H(19A)	5914	2589	11684	36
H(20A)	4506	3483	11349	38
H(21A)	3092	3791	9322	39
H(22A)	2983	3208	7544	34
H(26A)	7890	2535	7386	34
H(28A)	11524	2612	10363	47
H(29A)	11225	1560	10847	51
H(30A)	9365	972	9539	41

Table S8. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *m*-ClPhO-**BsubPc** (compound **2b**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(3)-H(3A)	->	Cg(9)	2.80	2.67	17.34	125	3.435(3)	51
C(12)-H(12A)	->	Cg(3)	2.78	-2.71	13.38	115	3.304(4)	38
C(13)-H(13A)	->	Cg(1)	2.84	-2.76	14.16	111	3.303(4)	35

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(5) --> C(17) --> C(18) --> C(23) --> C(24) -->

6-Membered Ring (9) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

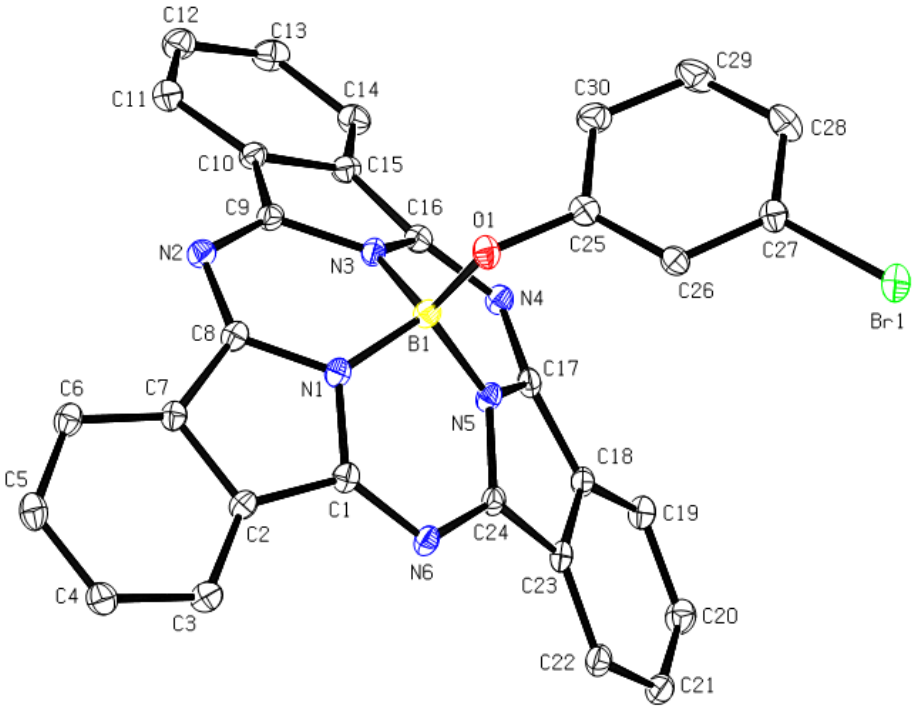

Figure S3. Anisotropic displacement ellipsoid plot of *m*-BrPhO-**BsubPc** (compound **2c**).

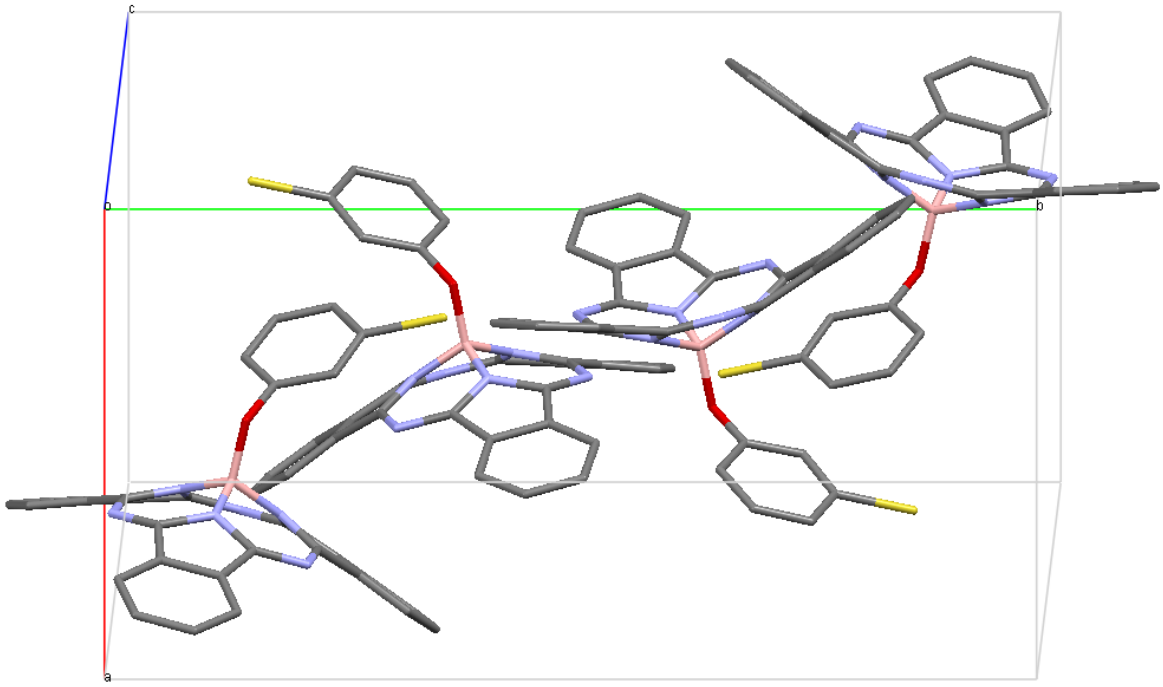

Figure S4. Populated unit cell of *m*-BrPhO-**BsubPc** (compound **2c**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow. Hydrogens are omitted for clarity.

Table S9. Crystal data and structure refinement for *m*-BrPhO-**BsubPc** (compound **2c**).

Identification code	k10270	
Empirical formula	C30 H16 B Br N6 O	
Formula weight	567.21	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.6874(3) Å	α= 90°.
	b = 21.2084(5) Å	β= 113.0790(13)°.
	c = 11.4373(3) Å	γ = 90°.
Volume	2384.93(11) $Å^3$	
Z	4	
Density (calculated)	1.580 Mg/m^3	
Absorption coefficient	1.763 mm^{-1}	
F(000)	1144	
Crystal size	0.20 x 0.16 x 0.14 mm^3	
Theta range for data collection	2.73 to 27.45°.	
Index ranges	-13<=h<=13, -27<=k<=26, -14<=l<=14	
Reflections collected	21186	
Independent reflections	5429 [R(int) = 0.0738]	
Completeness to theta = 27.45°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.786 and 0.714	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5429 / 0 / 352	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.0940	
R indices (all data)	R1 = 0.0983, wR2 = 0.1113	
Largest diff. peak and hole	0.701 and -0.676 e.$Å^{-3}$	

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *m*-BrPhO-**BsubPc** (compound **2c**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	5058(1)	3462(1)	6569(1)	31(1)
O(1)	7632(2)	1325(1)	7475(2)	24(1)
N(1)	9966(2)	972(1)	8240(2)	20(1)
N(2)	9699(2)	-119(1)	7697(2)	22(1)
N(3)	8540(2)	663(1)	6170(2)	20(1)
N(4)	8268(2)	1346(1)	4446(2)	22(1)
N(5)	9253(2)	1718(1)	6572(2)	20(1)
N(6)	11129(2)	1951(1)	8507(2)	21(1)
C(1)	10999(3)	1372(1)	8924(3)	21(1)
C(2)	11970(3)	991(1)	9931(3)	20(1)
C(3)	13166(3)	1142(2)	10949(3)	25(1)
C(4)	13889(3)	660(2)	11734(3)	28(1)
C(5)	13455(3)	32(2)	11506(3)	29(1)
C(6)	12277(3)	-129(1)	10485(3)	25(1)
C(7)	11524(3)	351(1)	9689(3)	20(1)
C(8)	10296(3)	352(1)	8528(3)	21(1)
C(9)	8884(3)	50(1)	6506(3)	21(1)
C(10)	8427(3)	-298(1)	5304(3)	21(1)
C(11)	8411(3)	-936(1)	5021(3)	28(1)
C(12)	7860(3)	-1111(2)	3758(3)	30(1)
C(13)	7386(3)	-668(2)	2777(3)	29(1)
C(14)	7463(3)	-31(2)	3037(3)	25(1)
C(15)	7970(3)	158(1)	4307(3)	22(1)
C(16)	8162(3)	775(1)	4901(3)	22(1)
C(17)	8891(3)	1802(1)	5301(3)	20(1)
C(18)	9590(3)	2367(1)	5178(3)	21(1)
C(19)	9572(3)	2697(1)	4114(3)	24(1)
C(20)	10406(3)	3223(2)	4318(3)	28(1)

C(21)	11258(3)	3411(1)	5546(3)	26(1)
C(22)	11316(3)	3076(1)	6601(3)	24(1)
C(23)	10468(3)	2559(1)	6421(3)	21(1)
C(24)	10295(3)	2100(1)	7301(3)	20(1)
C(25)	6525(3)	1651(1)	6642(3)	22(1)
C(26)	6396(3)	2283(1)	6896(3)	22(1)
C(27)	5241(3)	2609(1)	6159(3)	24(1)
C(28)	4223(3)	2323(2)	5140(3)	33(1)
C(29)	4380(3)	1705(2)	4869(3)	36(1)
C(30)	5522(3)	1359(2)	5621(3)	30(1)
B(1)	8756(4)	1183(2)	7120(3)	21(1)

Table S11. Bond lengths [Å] and angles [°] for *m*-BrPhO-**BsubPc** (compound **2c**).

Br(1)-C(27)	1.898(3)
O(1)-C(25)	1.380(4)
O(1)-B(1)	1.443(4)
N(1)-C(8)	1.368(4)
N(1)-C(1)	1.369(4)
N(1)-B(1)	1.488(4)
N(2)-C(9)	1.347(4)
N(2)-C(8)	1.354(4)
N(3)-C(9)	1.365(4)
N(3)-C(16)	1.367(4)
N(3)-B(1)	1.501(4)
N(4)-C(16)	1.341(4)
N(4)-C(17)	1.350(4)
N(5)-C(17)	1.363(4)
N(5)-C(24)	1.366(4)
N(5)-B(1)	1.490(4)
N(6)-C(1)	1.345(4)
N(6)-C(24)	1.353(4)
C(1)-C(2)	1.456(4)
C(2)-C(3)	1.388(4)
C(2)-C(7)	1.428(4)
C(3)-C(4)	1.381(4)
C(4)-C(5)	1.400(4)
C(5)-C(6)	1.383(4)
C(6)-C(7)	1.392(4)
C(7)-C(8)	1.456(4)
C(9)-C(10)	1.464(4)
C(10)-C(11)	1.390(4)
C(10)-C(15)	1.427(4)
C(11)-C(12)	1.381(4)
C(12)-C(13)	1.397(5)
C(13)-C(14)	1.379(4)

C(14)-C(15)	1.394(4)
C(15)-C(16)	1.453(4)
C(17)-C(18)	1.447(4)
C(18)-C(19)	1.398(4)
C(18)-C(23)	1.422(4)
C(19)-C(20)	1.388(4)
C(20)-C(21)	1.399(4)
C(21)-C(22)	1.380(4)
C(22)-C(23)	1.385(4)
C(23)-C(24)	1.465(4)
C(25)-C(30)	1.384(4)
C(25)-C(26)	1.389(4)
C(26)-C(27)	1.377(4)
C(27)-C(28)	1.383(4)
C(28)-C(29)	1.373(5)
C(29)-C(30)	1.395(5)

C(25)-O(1)-B(1)	119.6(2)
C(8)-N(1)-C(1)	112.6(2)
C(8)-N(1)-B(1)	123.5(2)
C(1)-N(1)-B(1)	122.6(2)
C(9)-N(2)-C(8)	117.0(2)
C(9)-N(3)-C(16)	113.5(2)
C(9)-N(3)-B(1)	123.3(2)
C(16)-N(3)-B(1)	122.6(2)
C(16)-N(4)-C(17)	117.3(3)
C(17)-N(5)-C(24)	113.3(2)
C(17)-N(5)-B(1)	123.3(2)
C(24)-N(5)-B(1)	122.3(2)
C(1)-N(6)-C(24)	117.1(2)
N(6)-C(1)-N(1)	122.4(3)
N(6)-C(1)-C(2)	130.3(3)
N(1)-C(1)-C(2)	105.8(2)
C(3)-C(2)-C(7)	120.6(3)

C(3)-C(2)-C(1)	132.2(3)
C(7)-C(2)-C(1)	107.1(3)
C(4)-C(3)-C(2)	118.1(3)
C(3)-C(4)-C(5)	121.6(3)
C(6)-C(5)-C(4)	121.1(3)
C(5)-C(6)-C(7)	118.2(3)
C(6)-C(7)-C(2)	120.3(3)
C(6)-C(7)-C(8)	132.8(3)
C(2)-C(7)-C(8)	106.8(2)
N(2)-C(8)-N(1)	122.3(3)
N(2)-C(8)-C(7)	130.4(3)
N(1)-C(8)-C(7)	106.0(2)
N(2)-C(9)-N(3)	122.3(3)
N(2)-C(9)-C(10)	131.4(3)
N(3)-C(9)-C(10)	105.2(2)
C(11)-C(10)-C(15)	120.2(3)
C(11)-C(10)-C(9)	132.7(3)
C(15)-C(10)-C(9)	107.1(2)
C(12)-C(11)-C(10)	117.9(3)
C(11)-C(12)-C(13)	122.0(3)
C(14)-C(13)-C(12)	120.9(3)
C(13)-C(14)-C(15)	118.1(3)
C(14)-C(15)-C(10)	120.7(3)
C(14)-C(15)-C(16)	132.2(3)
C(10)-C(15)-C(16)	107.1(3)
N(4)-C(16)-N(3)	122.3(3)
N(4)-C(16)-C(15)	130.6(3)
N(3)-C(16)-C(15)	105.6(2)
N(4)-C(17)-N(5)	122.2(3)
N(4)-C(17)-C(18)	130.5(3)
N(5)-C(17)-C(18)	105.7(2)
C(19)-C(18)-C(23)	120.3(3)
C(19)-C(18)-C(17)	131.9(3)
C(23)-C(18)-C(17)	107.7(3)

C(20)-C(19)-C(18)	117.9(3)
C(19)-C(20)-C(21)	121.4(3)
C(22)-C(21)-C(20)	121.3(3)
C(21)-C(22)-C(23)	118.3(3)
C(22)-C(23)-C(18)	120.9(3)
C(22)-C(23)-C(24)	132.5(3)
C(18)-C(23)-C(24)	106.5(2)
N(6)-C(24)-N(5)	122.5(3)
N(6)-C(24)-C(23)	130.2(3)
N(5)-C(24)-C(23)	105.5(2)
O(1)-C(25)-C(30)	121.9(3)
O(1)-C(25)-C(26)	117.9(3)
C(30)-C(25)-C(26)	120.1(3)
C(27)-C(26)-C(25)	119.6(3)
C(26)-C(27)-C(28)	121.1(3)
C(26)-C(27)-Br(1)	118.8(2)
C(28)-C(27)-Br(1)	120.2(2)
C(29)-C(28)-C(27)	118.9(3)
C(28)-C(29)-C(30)	121.2(3)
C(25)-C(30)-C(29)	119.0(3)
O(1)-B(1)-N(1)	111.0(3)
O(1)-B(1)-N(5)	115.6(3)
N(1)-B(1)-N(5)	105.0(2)
O(1)-B(1)-N(3)	116.6(3)
N(1)-B(1)-N(3)	103.7(2)
N(5)-B(1)-N(3)	103.6(3)

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *m*-BrPhO-**BsubPc** (compound **2c**). 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}
Br(1)	36(1)	26(1)	33(1)	4(1)	15(1)	8(1)
O(1)	26(1)	25(1)	22(1)	5(1)	10(1)	6(1)
N(1)	24(1)	18(1)	18(1)	0(1)	10(1)	1(1)
N(2)	23(1)	20(1)	22(2)	1(1)	9(1)	-1(1)
N(3)	21(1)	16(1)	21(2)	1(1)	7(1)	2(1)
N(4)	24(1)	21(1)	18(1)	1(1)	7(1)	0(1)
N(5)	26(1)	16(1)	16(1)	-1(1)	6(1)	0(1)
N(6)	27(1)	15(1)	20(1)	-1(1)	7(1)	1(1)
C(1)	26(2)	19(2)	17(2)	-1(1)	8(1)	1(1)
C(2)	26(2)	19(2)	18(2)	1(1)	10(1)	-1(1)
C(3)	30(2)	25(2)	20(2)	0(1)	9(2)	-4(1)
C(4)	27(2)	31(2)	23(2)	4(1)	5(2)	0(2)
C(5)	32(2)	30(2)	24(2)	9(2)	10(2)	8(2)
C(6)	31(2)	22(2)	26(2)	2(1)	15(2)	2(1)
C(7)	23(2)	19(2)	20(2)	2(1)	11(1)	2(1)
C(8)	26(2)	19(2)	20(2)	1(1)	12(2)	1(1)
C(9)	20(2)	19(2)	25(2)	0(1)	11(1)	-1(1)
C(10)	22(2)	19(2)	22(2)	-2(1)	8(1)	-2(1)
C(11)	25(2)	26(2)	32(2)	-1(2)	11(2)	1(1)
C(12)	28(2)	26(2)	37(2)	-9(2)	13(2)	-2(2)
C(13)	31(2)	32(2)	26(2)	-11(2)	13(2)	-6(2)
C(14)	24(2)	30(2)	20(2)	0(1)	7(1)	-1(1)
C(15)	21(2)	22(2)	24(2)	-2(1)	9(1)	-2(1)
C(16)	21(2)	22(2)	22(2)	0(1)	7(1)	0(1)
C(17)	20(2)	19(2)	20(2)	2(1)	5(1)	5(1)
C(18)	21(2)	17(2)	22(2)	2(1)	7(1)	4(1)
C(19)	28(2)	22(2)	23(2)	1(1)	11(2)	4(1)
C(20)	32(2)	27(2)	28(2)	6(1)	15(2)	3(2)

C(21)	27(2)	20(2)	34(2)	2(1)	15(2)	1(1)
C(22)	27(2)	18(2)	25(2)	-1(1)	8(2)	3(1)
C(23)	24(2)	16(2)	23(2)	3(1)	10(1)	6(1)
C(24)	23(2)	16(2)	19(2)	-2(1)	6(1)	3(1)
C(25)	24(2)	28(2)	20(2)	4(1)	12(2)	0(1)
C(26)	21(2)	25(2)	18(2)	1(1)	5(1)	1(1)
C(27)	26(2)	26(2)	20(2)	3(1)	10(2)	3(1)
C(28)	24(2)	44(2)	28(2)	0(2)	5(2)	6(2)
C(29)	26(2)	46(2)	29(2)	-9(2)	2(2)	-3(2)
C(30)	28(2)	28(2)	34(2)	-9(2)	12(2)	-4(2)
B(1)	24(2)	19(2)	18(2)	0(1)	7(2)	-2(2)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *m*-BrPhO-**BsubPc** (compound **2c**).

	x	y	z	U(eq)
H(3A)	13478	1566	11101	30
H(4A)	14700	756	12445	34
H(5A)	13979	-289	12062	35
H(6A)	11989	-555	10330	30
H(11A)	8769	-1241	5676	33
H(12A)	7802	-1546	3548	37
H(13A)	7005	-807	1920	35
H(14A)	7179	271	2370	30
H(19A)	9008	2567	3278	29
H(20A)	10397	3459	3610	34
H(21A)	11808	3776	5655	31
H(22A)	11922	3198	7430	29
H(26A)	7100	2489	7575	27
H(28A)	3429	2551	4637	40
H(29A)	3699	1509	4156	43
H(30A)	5610	928	5436	36

Table S14. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *m*-BrPhO-**BsubPc** (compound **2c**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(3)-H(3A)	->	Cg(9)	2.79	-2.68	16.62	126	3.439(4)	50
C(12)-H(12A)	->	Cg(3)	2.82	2.73	14.62	115	3.330(4)	38
C(13)-H(13A)	->	Cg(1)	2.82	2.71	15.86	109	3.256(4)	35

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(5) --> C(17) --> C(18) --> C(23) --> C(24) -->

6-Membered Ring (9) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

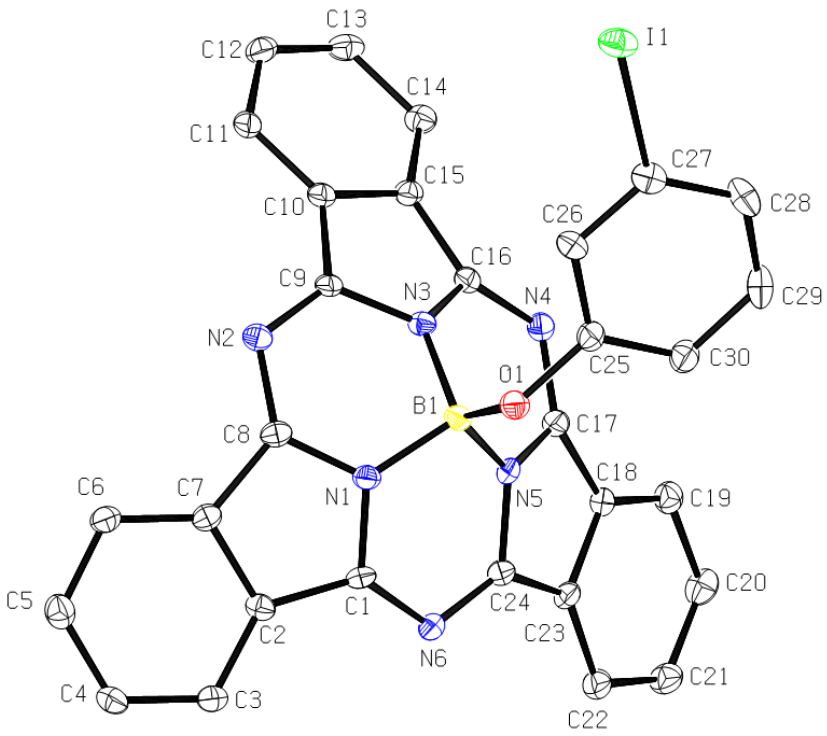

Figure S5. Anisotropic displacement ellipsoid plot of *m*-IPhO-**BsubPc** (compound **2d**).

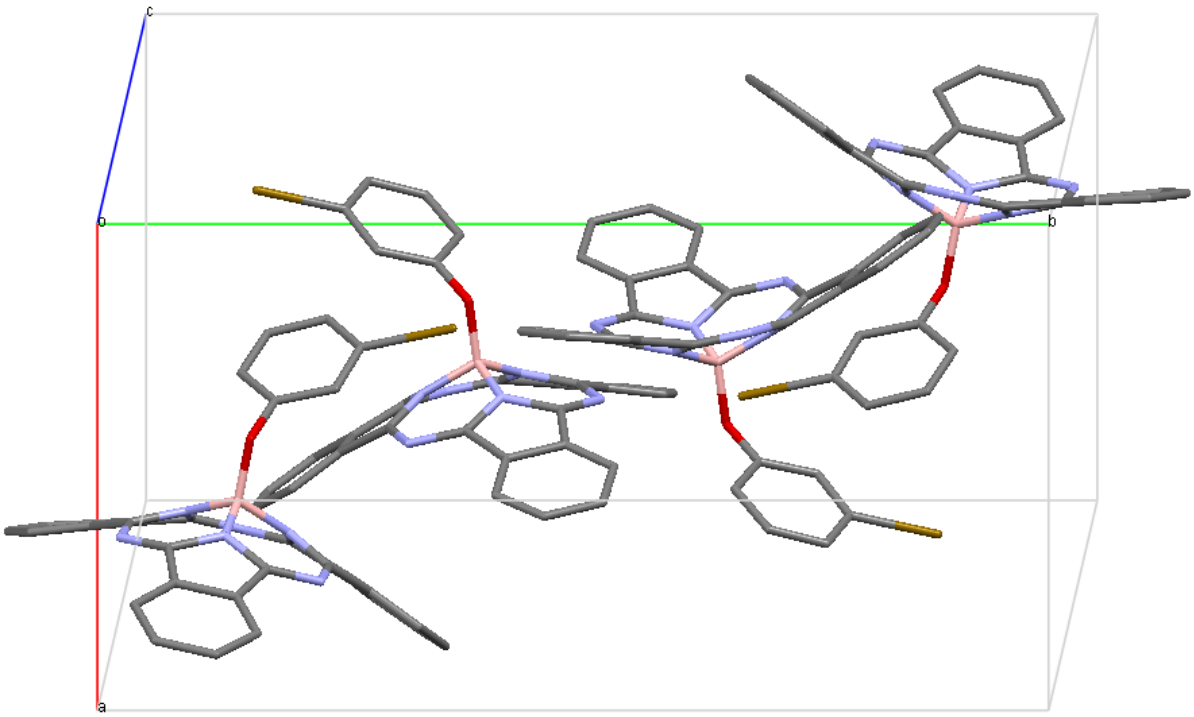

Figure S6. Populated unit cell of *m*-IPhO-**BsubPc** (compound **2d**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; iodine = brown. Hydrogens are omitted for clarity.

Table S15. Crystal data and structure refinement for *m*-IPhO-**BsubPc** (compound **2d**).

Identification code	k11109	
Empirical formula	C30 H16 B I N6 O	
Formula weight	614.20	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.8999(4) Å	α= 90°.
	b = 21.4167(6) Å	β= 114.2670(15)°.
	c = 11.4529(4) Å	γ = 90°.
Volume	2437.33(14) $Å^3$	
Z	4	
Density (calculated)	1.674 Mg/m^3	
Absorption coefficient	1.353 mm^{-1}	
F(000)	1216	
Crystal size	0.20 x 0.14 x 0.14 mm^3	
Theta range for data collection	2.72 to 27.39°.	
Index ranges	-14<=h<=12, -27<=k<=27, -14<=l<=14	
Reflections collected	16082	
Independent reflections	5505 [R(int) = 0.0656]	
Completeness to theta = 27.39°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.834 and 0.766	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5505 / 0 / 352	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0572, wR2 = 0.1365	
R indices (all data)	R1 = 0.1224, wR2 = 0.1769	
Largest diff. peak and hole	2.035 and -1.585 e.$Å^{-3}$	

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *m*-IPhO-**BsubPc** (compound **2d**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	-33(1)	1600(1)	1536(1)	36(1)
O(1)	2643(4)	3777(2)	2472(4)	27(1)
N(1)	4964(4)	4081(2)	3240(4)	23(1)
N(2)	6035(5)	3091(2)	3527(4)	24(1)
N(3)	4172(5)	3332(2)	1580(4)	21(1)
N(4)	3193(5)	3692(2)	-576(4)	25(1)
N(5)	3555(5)	4381(2)	1144(4)	23(1)
N(6)	4755(5)	5153(2)	2663(4)	24(1)
C(1)	5332(5)	4689(2)	3522(5)	22(1)
C(2)	6560(6)	4682(2)	4689(5)	23(1)
C(3)	7358(6)	5149(3)	5478(5)	26(1)
C(4)	8532(6)	4981(3)	6495(6)	32(1)
C(5)	8920(6)	4353(3)	6735(6)	33(1)
C(6)	8154(6)	3880(3)	5961(5)	27(1)
C(7)	6958(6)	4045(2)	4944(5)	24(1)
C(8)	5950(6)	3671(2)	3926(5)	24(1)
C(9)	5195(5)	2944(2)	2324(5)	22(1)
C(10)	5324(6)	2475(3)	1449(5)	26(1)
C(11)	6149(6)	1962(2)	1638(6)	29(1)
C(12)	6076(6)	1629(2)	572(6)	31(1)
C(13)	5237(6)	1813(3)	-657(6)	31(1)
C(14)	4415(6)	2337(2)	-871(5)	27(1)
C(15)	4451(5)	2666(2)	195(5)	24(1)
C(16)	3808(6)	3238(2)	307(5)	24(1)
C(17)	3144(6)	4262(2)	-131(5)	25(1)
C(18)	2965(5)	4873(2)	-744(5)	23(1)
C(19)	2434(6)	5046(3)	-2034(6)	30(1)
C(20)	2371(6)	5676(3)	-2316(6)	34(1)

C(21)	2894(6)	6123(3)	-1344(6)	34(1)
C(22)	3475(6)	5958(3)	-52(6)	32(1)
C(23)	3475(6)	5328(2)	257(5)	25(1)
C(24)	3929(6)	4991(2)	1473(5)	24(1)
C(25)	1505(6)	3474(3)	1640(6)	26(1)
C(26)	1353(6)	2849(3)	1863(5)	28(1)
C(27)	176(6)	2545(3)	1113(6)	31(1)
C(28)	-844(6)	2844(3)	111(6)	38(2)
C(29)	-649(7)	3461(3)	-126(6)	41(2)
C(30)	509(6)	3777(3)	646(6)	32(1)
B(1)	3747(7)	3885(3)	2114(6)	24(1)

Table S17. Bond lengths [Å] and angles [°] for *m*-IPhO-**BsubPc** (compound **2d**).

I(1)-C(27)	2.114(6)
O(1)-C(25)	1.376(7)
O(1)-B(1)	1.441(7)
N(1)-C(8)	1.360(7)
N(1)-C(1)	1.361(7)
N(1)-B(1)	1.481(8)
N(2)-C(8)	1.340(7)
N(2)-C(9)	1.342(7)
N(3)-C(16)	1.360(7)
N(3)-C(9)	1.371(7)
N(3)-B(1)	1.491(8)
N(4)-C(17)	1.334(7)
N(4)-C(16)	1.363(7)
N(5)-C(17)	1.364(7)
N(5)-C(24)	1.375(7)
N(5)-B(1)	1.487(8)
N(6)-C(24)	1.334(7)
N(6)-C(1)	1.358(7)
C(1)-C(2)	1.452(8)
C(2)-C(3)	1.388(7)
C(2)-C(7)	1.425(7)
C(3)-C(4)	1.378(8)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.403(8)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.377(8)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.390(8)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.467(8)
C(9)-C(10)	1.465(8)
C(10)-C(11)	1.379(8)

C(10)-C(15)	1.418(8)
C(11)-C(12)	1.388(8)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.383(9)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.394(8)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.395(7)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.443(7)
C(17)-C(18)	1.460(7)
C(18)-C(19)	1.397(8)
C(18)-C(23)	1.430(7)
C(19)-C(20)	1.383(8)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.399(9)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.395(8)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.396(7)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.462(7)
C(25)-C(30)	1.371(8)
C(25)-C(26)	1.387(8)
C(26)-C(27)	1.379(8)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.384(9)
C(28)-C(29)	1.381(9)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.384(9)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500

C(25)-O(1)-B(1)	119.9(4)

C(8)-N(1)-C(1)	113.2(4)
C(8)-N(1)-B(1)	122.2(5)
C(1)-N(1)-B(1)	123.3(5)
C(8)-N(2)-C(9)	117.0(5)
C(16)-N(3)-C(9)	112.4(4)
C(16)-N(3)-B(1)	123.7(5)
C(9)-N(3)-B(1)	122.5(5)
C(17)-N(4)-C(16)	117.0(5)
C(17)-N(5)-C(24)	113.6(4)
C(17)-N(5)-B(1)	123.4(5)
C(24)-N(5)-B(1)	122.6(5)
C(24)-N(6)-C(1)	117.8(5)
N(6)-C(1)-N(1)	121.7(5)
N(6)-C(1)-C(2)	130.6(5)
N(1)-C(1)-C(2)	106.2(4)
C(3)-C(2)-C(7)	120.0(5)
C(3)-C(2)-C(1)	133.3(5)
C(7)-C(2)-C(1)	106.6(4)
C(4)-C(3)-C(2)	118.6(5)
C(4)-C(3)-H(3A)	120.7
C(2)-C(3)-H(3A)	120.7
C(3)-C(4)-C(5)	121.1(5)
C(3)-C(4)-H(4A)	119.5
C(5)-C(4)-H(4A)	119.5
C(6)-C(5)-C(4)	121.6(6)
C(6)-C(5)-H(5A)	119.2
C(4)-C(5)-H(5A)	119.2
C(5)-C(6)-C(7)	117.7(5)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	121.0(5)
C(6)-C(7)-C(8)	131.8(5)
C(2)-C(7)-C(8)	107.1(5)
N(2)-C(8)-N(1)	123.4(5)

N(2)-C(8)-C(7)	129.9(5)
N(1)-C(8)-C(7)	105.3(4)
N(2)-C(9)-N(3)	122.2(5)
N(2)-C(9)-C(10)	130.3(5)
N(3)-C(9)-C(10)	105.8(5)
C(11)-C(10)-C(15)	120.8(5)
C(11)-C(10)-C(9)	132.6(5)
C(15)-C(10)-C(9)	106.4(5)
C(10)-C(11)-C(12)	118.2(6)
C(10)-C(11)-H(11A)	120.9
C(12)-C(11)-H(11A)	120.9
C(13)-C(12)-C(11)	121.6(5)
C(13)-C(12)-H(12A)	119.2
C(11)-C(12)-H(12A)	119.2
C(12)-C(13)-C(14)	121.1(5)
C(12)-C(13)-H(13A)	119.5
C(14)-C(13)-H(13A)	119.5
C(13)-C(14)-C(15)	117.9(5)
C(13)-C(14)-H(14A)	121.1
C(15)-C(14)-H(14A)	121.1
C(14)-C(15)-C(10)	120.4(5)
C(14)-C(15)-C(16)	131.7(5)
C(10)-C(15)-C(16)	107.6(5)
N(3)-C(16)-N(4)	121.8(5)
N(3)-C(16)-C(15)	106.4(5)
N(4)-C(16)-C(15)	130.4(5)
N(4)-C(17)-N(5)	122.2(5)
N(4)-C(17)-C(18)	131.0(5)
N(5)-C(17)-C(18)	105.6(4)
C(19)-C(18)-C(23)	121.5(5)
C(19)-C(18)-C(17)	131.4(5)
C(23)-C(18)-C(17)	107.1(5)
C(20)-C(19)-C(18)	117.7(5)
C(20)-C(19)-H(19A)	121.2

C(18)-C(19)-H(19A)	121.2
C(19)-C(20)-C(21)	121.1(6)
C(19)-C(20)-H(20A)	119.4
C(21)-C(20)-H(20A)	119.4
C(22)-C(21)-C(20)	122.0(5)
C(22)-C(21)-H(21A)	119.0
C(20)-C(21)-H(21A)	119.0
C(21)-C(22)-C(23)	117.8(5)
C(21)-C(22)-H(22A)	121.1
C(23)-C(22)-H(22A)	121.1
C(22)-C(23)-C(18)	119.7(5)
C(22)-C(23)-C(24)	133.1(5)
C(18)-C(23)-C(24)	107.2(5)
N(6)-C(24)-N(5)	121.8(5)
N(6)-C(24)-C(23)	131.9(5)
N(5)-C(24)-C(23)	105.2(5)
C(30)-C(25)-O(1)	122.2(5)
C(30)-C(25)-C(26)	119.8(5)
O(1)-C(25)-C(26)	117.9(5)
C(27)-C(26)-C(25)	119.5(6)
C(27)-C(26)-H(26A)	120.3
C(25)-C(26)-H(26A)	120.3
C(26)-C(27)-C(28)	121.5(6)
C(26)-C(27)-I(1)	118.0(5)
C(28)-C(27)-I(1)	120.5(4)
C(29)-C(28)-C(27)	118.0(6)
C(29)-C(28)-H(28A)	121.0
C(27)-C(28)-H(28A)	121.0
C(28)-C(29)-C(30)	121.1(6)
C(28)-C(29)-H(29A)	119.5
C(30)-C(29)-H(29A)	119.5
C(25)-C(30)-C(29)	120.1(6)
C(25)-C(30)-H(30A)	120.0
C(29)-C(30)-H(30A)	120.0

O(1)-B(1)-N(1)	110.6(5)
O(1)-B(1)-N(5)	116.8(5)
N(1)-B(1)-N(5)	104.4(4)
O(1)-B(1)-N(3)	115.2(5)
N(1)-B(1)-N(3)	105.3(5)
N(5)-B(1)-N(3)	103.5(5)

Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *m*-IPhO-**BsubPc** (compound **2d**). 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}
I(1)	41(1)	30(1)	46(1)	-8(1)	25(1)	-9(1)
O(1)	25(2)	26(2)	32(2)	-2(2)	14(2)	-1(2)
N(1)	23(3)	19(2)	27(3)	-3(2)	11(2)	-2(2)
N(2)	26(3)	23(2)	26(3)	0(2)	12(2)	-3(2)
N(3)	26(3)	18(2)	18(2)	0(2)	9(2)	-2(2)
N(4)	23(3)	25(2)	26(3)	1(2)	8(2)	0(2)
N(5)	20(2)	19(2)	26(3)	3(2)	5(2)	4(2)
N(6)	24(3)	21(2)	25(3)	1(2)	8(2)	3(2)
C(1)	29(3)	15(3)	24(3)	-2(2)	14(3)	1(2)
C(2)	29(3)	24(3)	16(3)	-1(2)	9(3)	-3(2)
C(3)	29(3)	21(3)	30(3)	-2(2)	14(3)	-1(2)
C(4)	30(3)	29(3)	32(3)	-10(3)	8(3)	-5(3)
C(5)	29(3)	41(4)	28(3)	-3(3)	9(3)	1(3)
C(6)	29(3)	21(3)	34(3)	-1(3)	15(3)	1(2)
C(7)	27(3)	23(3)	25(3)	-1(2)	14(3)	2(2)
C(8)	30(3)	21(3)	26(3)	-1(2)	16(3)	0(2)
C(9)	24(3)	15(2)	26(3)	0(2)	8(3)	-4(2)
C(10)	26(3)	18(3)	29(3)	0(2)	6(3)	-4(2)
C(11)	24(3)	20(3)	36(4)	3(3)	5(3)	-4(2)
C(12)	28(3)	19(3)	48(4)	-1(3)	18(3)	0(2)
C(13)	37(4)	24(3)	40(4)	-7(3)	24(3)	-4(3)
C(14)	33(3)	24(3)	25(3)	3(2)	12(3)	-2(2)
C(15)	24(3)	21(3)	28(3)	-2(2)	12(3)	-2(2)
C(16)	21(3)	21(3)	27(3)	0(2)	6(3)	-3(2)
C(17)	22(3)	22(3)	30(3)	-1(2)	10(3)	0(2)
C(18)	20(3)	24(3)	24(3)	1(2)	7(2)	2(2)
C(19)	25(3)	33(3)	31(3)	-1(3)	12(3)	2(2)
C(20)	37(4)	33(3)	35(4)	14(3)	19(3)	5(3)

C(21)	35(4)	25(3)	43(4)	6(3)	16(3)	1(3)
C(22)	26(3)	25(3)	39(4)	4(3)	10(3)	0(2)
C(23)	24(3)	20(3)	29(3)	4(2)	9(3)	4(2)
C(24)	25(3)	19(3)	27(3)	2(2)	9(3)	0(2)
C(25)	22(3)	30(3)	30(3)	-4(3)	13(3)	3(2)
C(26)	29(3)	29(3)	25(3)	-5(3)	10(3)	-5(2)
C(27)	35(4)	33(3)	32(3)	-3(3)	20(3)	-5(3)
C(28)	28(4)	51(4)	31(4)	-2(3)	7(3)	-13(3)
C(29)	24(4)	57(4)	34(4)	8(3)	4(3)	7(3)
C(30)	26(3)	29(3)	41(4)	7(3)	14(3)	1(3)
B(1)	26(4)	21(3)	21(3)	-2(3)	6(3)	-2(3)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *m*-IPhO-**BsubPc** (compound **2d**).

	x	y	z	U(eq)
H(3A)	7100	5575	5321	31
H(4A)	9089	5295	7043	38
H(5A)	9730	4251	7448	40
H(6A)	8433	3457	6118	33
H(11A)	6751	1840	2477	35
H(12A)	6617	1267	690	37
H(13A)	5220	1577	-1366	37
H(14A)	3849	2467	-1715	33
H(19A)	2126	4741	-2695	36
H(20A)	1967	5808	-3184	41
H(21A)	2852	6551	-1571	41
H(22A)	3857	6265	597	38
H(26A)	2054	2631	2528	33
H(28A)	-1654	2632	-399	46
H(29A)	-1320	3671	-830	49
H(30A)	613	4205	487	39

Table S20. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *m*-IPhO-**BsubPc** (compound **2d**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(6)-H(6A)	->	Cg(8)	2.79	-2.70	14.91	127	3.444(7)	48
C(20)-H(20A)	->	Cg(1)	2.84	2.70	18.03	106	3.223(7)	34
C(21)-H(21A)	->	Cg(2)	2.86	2.75	16.08	113	3.349(7)	38

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (2) N(3) --> C(9) --> C(10) --> C(15) --> C(16) -->

6-Membered Ring (8) C(10) --> C(11) --> C(12) --> C(13) --> C(14) --> C(15) -->

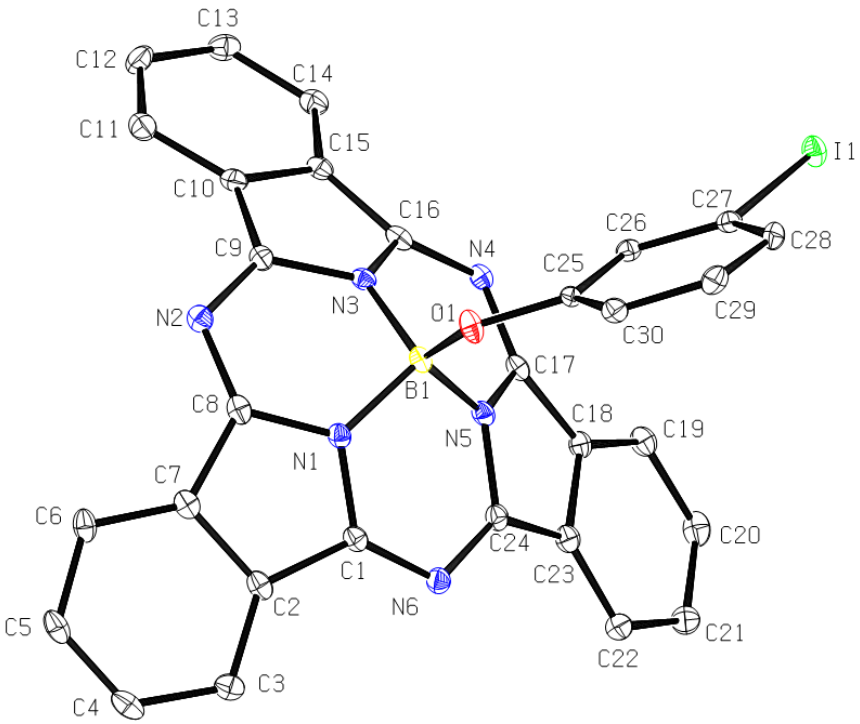

Figure S7. Anisotropic displacement ellipsoid plot of solvated *m*-IPhO-**BsubPc** (compound **2d** solvate).

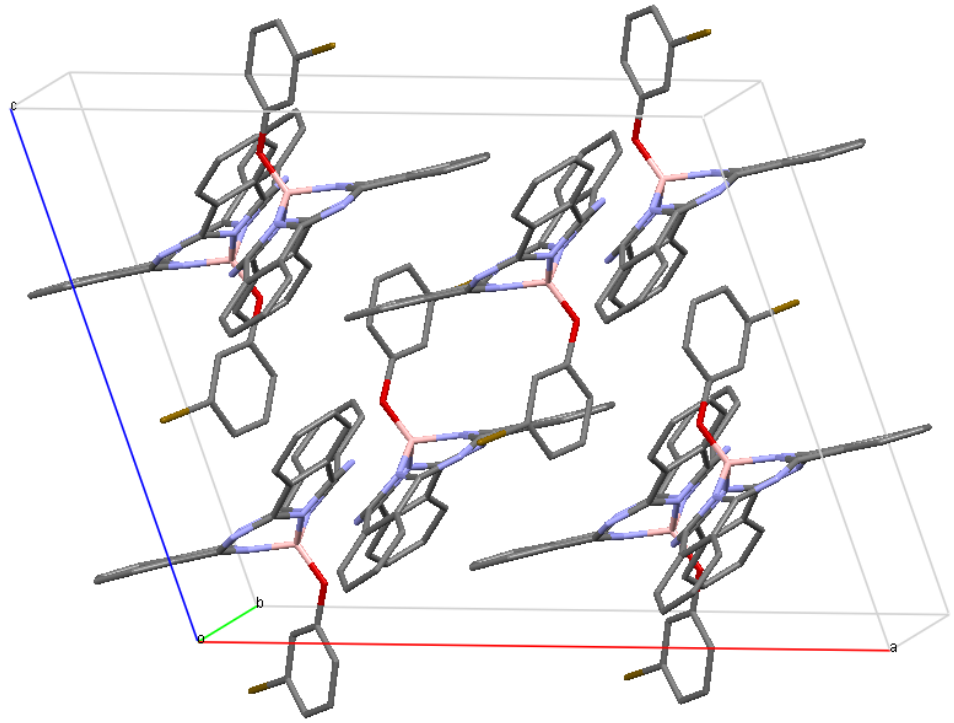

Figure S8. Populated unit cell of solvated *m*-IPhO-**BsubPc** (compound **2d**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; iodine = brown. Hydrogens are omitted for clarity.

Table S21. Crystal data and structure refinement for solvated *m*-IPhO-**BsubPc** (compound **2d**).

Identification code	k1153	
Empirical formula	C30 H16 B I N6 O	
Formula weight	614.20	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 20.5800(4) Å	α= 90°.
	b = 17.0942(4) Å	β= 109.811(1)°.
	c = 16.7268(4) Å	γ = 90°.
Volume	5536.2(2) $Å^3$	
Z	8	
Density (calculated)	1.474 Mg/m^3	
Absorption coefficient	1.191 mm^{-1}	
F(000)	2432	
Crystal size	0.14 x 0.12 x 0.04 mm^3	
Theta range for data collection	1.59 to 27.01°.	
Index ranges	-26<=h<=24, -18<=k<=21, -21<=l<=21	
Reflections collected	23563	
Independent reflections	6052 [R(int) = 0.0438]	
Completeness to theta = 27.01°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6890	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6052 / 0 / 352	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0292, wR2 = 0.0663	
R indices (all data)	R1 = 0.0416, wR2 = 0.0694	
Largest diff. peak and hole	0.437 and -0.554 e.$Å^{-3}$	

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for solvated *m*-IPhO-**BsubPc** (compound **2d**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	5060(1)	9492(1)	-1218(1)	23(1)
O(1)	6876(1)	7497(1)	958(1)	22(1)
N(1)	6960(1)	6918(1)	2288(1)	16(1)
N(2)	7876(1)	7655(1)	3237(1)	19(1)
N(3)	6912(1)	8297(1)	2233(1)	16(1)
N(4)	5805(1)	8902(1)	1843(1)	17(1)
N(5)	5912(1)	7553(1)	1564(1)	17(1)
N(6)	5910(1)	6200(1)	1889(1)	19(1)
C(1)	6599(1)	6253(1)	2295(2)	17(1)
C(2)	7064(1)	5756(1)	2942(2)	19(1)
C(3)	6994(1)	5010(2)	3237(2)	22(1)
C(4)	7528(1)	4732(2)	3928(2)	26(1)
C(5)	8111(1)	5168(2)	4330(2)	25(1)
C(6)	8194(1)	5909(2)	4052(2)	22(1)
C(7)	7671(1)	6203(1)	3350(2)	19(1)
C(8)	7565(1)	6969(2)	2948(2)	19(1)
C(9)	7520(1)	8309(1)	2909(2)	18(1)
C(10)	7558(1)	9085(1)	3286(2)	19(1)
C(11)	8066(1)	9444(2)	3964(2)	24(1)
C(12)	7934(1)	10185(2)	4193(2)	26(1)
C(13)	7307(1)	10562(2)	3778(2)	24(1)
C(14)	6793(1)	10203(2)	3122(2)	21(1)
C(15)	6920(1)	9464(1)	2863(2)	18(1)
C(16)	6496(1)	8923(1)	2232(2)	17(1)
C(17)	5523(1)	8201(1)	1558(2)	18(1)
C(18)	4818(1)	7917(1)	1360(1)	17(1)
C(19)	4187(1)	8296(2)	1186(2)	22(1)
C(20)	3598(1)	7846(2)	983(2)	26(1)

C(21)	3630(1)	7030(2)	978(2)	25(1)
C(22)	4252(1)	6640(2)	1194(2)	24(1)
C(23)	4852(1)	7079(2)	1367(2)	20(1)
C(24)	5576(1)	6867(1)	1576(2)	18(1)
C(25)	6527(1)	7721(1)	145(1)	15(1)
C(26)	6070(1)	8349(1)	-68(2)	16(1)
C(27)	5743(1)	8535(1)	-916(2)	18(1)
C(28)	5870(1)	8123(1)	-1558(2)	20(1)
C(29)	6337(1)	7510(1)	-1335(2)	22(1)
C(30)	6662(1)	7306(1)	-497(2)	18(1)
B(1)	6664(1)	7581(2)	1692(2)	17(1)

Table S23. Bond lengths [Å] and angles [°] for solvated *m*-IPhO-**BsubPc** (compound **2d**).

I(1)-C(27)	2.105(2)
O(1)-C(25)	1.361(3)
O(1)-B(1)	1.442(3)
N(1)-C(8)	1.359(3)
N(1)-C(1)	1.360(3)
N(1)-B(1)	1.495(3)
N(2)-C(8)	1.345(3)
N(2)-C(9)	1.348(3)
N(3)-C(16)	1.369(3)
N(3)-C(9)	1.374(3)
N(3)-B(1)	1.505(3)
N(4)-C(17)	1.345(3)
N(4)-C(16)	1.349(3)
N(5)-C(24)	1.365(3)
N(5)-C(17)	1.366(3)
N(5)-B(1)	1.489(3)
N(6)-C(24)	1.342(3)
N(6)-C(1)	1.352(3)
C(1)-C(2)	1.451(3)
C(2)-C(3)	1.395(3)
C(2)-C(7)	1.425(3)
C(3)-C(4)	1.381(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.379(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.379(4)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.391(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.454(3)
C(9)-C(10)	1.458(3)
C(10)-C(11)	1.398(3)

C(10)-C(15)	1.419(3)
C(11)-C(12)	1.377(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.399(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.383(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.389(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.451(3)
C(17)-C(18)	1.457(3)
C(18)-C(19)	1.391(3)
C(18)-C(23)	1.435(3)
C(19)-C(20)	1.378(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.398(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.378(4)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.389(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.458(3)
C(25)-C(30)	1.391(3)
C(25)-C(26)	1.392(3)
C(26)-C(27)	1.385(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.381(3)
C(28)-C(29)	1.384(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.377(3)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500

C(25)-O(1)-B(1)	127.92(19)

C(8)-N(1)-C(1)	113.5(2)
C(8)-N(1)-B(1)	123.1(2)
C(1)-N(1)-B(1)	122.6(2)
C(8)-N(2)-C(9)	116.7(2)
C(16)-N(3)-C(9)	112.6(2)
C(16)-N(3)-B(1)	123.4(2)
C(9)-N(3)-B(1)	122.35(19)
C(17)-N(4)-C(16)	116.9(2)
C(24)-N(5)-C(17)	113.50(19)
C(24)-N(5)-B(1)	122.2(2)
C(17)-N(5)-B(1)	123.6(2)
C(24)-N(6)-C(1)	116.7(2)
N(6)-C(1)-N(1)	122.3(2)
N(6)-C(1)-C(2)	130.6(2)
N(1)-C(1)-C(2)	105.7(2)
C(3)-C(2)-C(7)	120.0(2)
C(3)-C(2)-C(1)	132.7(2)
C(7)-C(2)-C(1)	107.1(2)
C(4)-C(3)-C(2)	117.6(2)
C(4)-C(3)-H(3A)	121.2
C(2)-C(3)-H(3A)	121.2
C(5)-C(4)-C(3)	122.4(2)
C(5)-C(4)-H(4A)	118.8
C(3)-C(4)-H(4A)	118.8
C(4)-C(5)-C(6)	121.3(2)
C(4)-C(5)-H(5A)	119.4
C(6)-C(5)-H(5A)	119.4
C(5)-C(6)-C(7)	117.9(2)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.8(2)
C(6)-C(7)-C(8)	131.9(2)
C(2)-C(7)-C(8)	106.9(2)
N(2)-C(8)-N(1)	122.8(2)

N(2)-C(8)-C(7)	129.8(2)
N(1)-C(8)-C(7)	105.7(2)
N(2)-C(9)-N(3)	122.8(2)
N(2)-C(9)-C(10)	129.5(2)
N(3)-C(9)-C(10)	105.6(2)
C(11)-C(10)-C(15)	121.0(2)
C(11)-C(10)-C(9)	131.8(2)
C(15)-C(10)-C(9)	107.2(2)
C(12)-C(11)-C(10)	117.8(2)
C(12)-C(11)-H(11A)	121.1
C(10)-C(11)-H(11A)	121.1
C(11)-C(12)-C(13)	121.4(2)
C(11)-C(12)-H(12A)	119.3
C(13)-C(12)-H(12A)	119.3
C(14)-C(13)-C(12)	121.2(2)
C(14)-C(13)-H(13A)	119.4
C(12)-C(13)-H(13A)	119.4
C(13)-C(14)-C(15)	118.5(2)
C(13)-C(14)-H(14A)	120.7
C(15)-C(14)-H(14A)	120.7
C(14)-C(15)-C(10)	120.0(2)
C(14)-C(15)-C(16)	132.5(2)
C(10)-C(15)-C(16)	107.3(2)
N(4)-C(16)-N(3)	122.4(2)
N(4)-C(16)-C(15)	130.1(2)
N(3)-C(16)-C(15)	106.0(2)
N(4)-C(17)-N(5)	122.6(2)
N(4)-C(17)-C(18)	130.8(2)
N(5)-C(17)-C(18)	105.5(2)
C(19)-C(18)-C(23)	120.4(2)
C(19)-C(18)-C(17)	132.8(2)
C(23)-C(18)-C(17)	106.9(2)
C(20)-C(19)-C(18)	118.2(2)
C(20)-C(19)-H(19A)	120.9

C(18)-C(19)-H(19A)	120.9
C(19)-C(20)-C(21)	121.4(2)
C(19)-C(20)-H(20A)	119.3
C(21)-C(20)-H(20A)	119.3
C(22)-C(21)-C(20)	121.5(2)
C(22)-C(21)-H(21A)	119.3
C(20)-C(21)-H(21A)	119.3
C(21)-C(22)-C(23)	118.3(2)
C(21)-C(22)-H(22A)	120.8
C(23)-C(22)-H(22A)	120.8
C(22)-C(23)-C(18)	120.1(2)
C(22)-C(23)-C(24)	132.9(2)
C(18)-C(23)-C(24)	107.0(2)
N(6)-C(24)-N(5)	122.7(2)
N(6)-C(24)-C(23)	130.7(2)
N(5)-C(24)-C(23)	105.3(2)
O(1)-C(25)-C(30)	116.9(2)
O(1)-C(25)-C(26)	123.7(2)
C(30)-C(25)-C(26)	119.4(2)
C(27)-C(26)-C(25)	119.3(2)
C(27)-C(26)-H(26A)	120.3
C(25)-C(26)-H(26A)	120.3
C(28)-C(27)-C(26)	121.7(2)
C(28)-C(27)-I(1)	119.81(18)
C(26)-C(27)-I(1)	118.46(17)
C(27)-C(28)-C(29)	118.2(2)
C(27)-C(28)-H(28A)	120.9
C(29)-C(28)-H(28A)	120.9
C(30)-C(29)-C(28)	121.3(2)
C(30)-C(29)-H(29A)	119.4
C(28)-C(29)-H(29A)	119.4
C(29)-C(30)-C(25)	120.0(2)
C(29)-C(30)-H(30A)	120.0
C(25)-C(30)-H(30A)	120.0

O(1)-B(1)-N(5)	118.2(2)
O(1)-B(1)-N(1)	108.6(2)
N(5)-B(1)-N(1)	103.9(2)
O(1)-B(1)-N(3)	117.0(2)
N(5)-B(1)-N(3)	103.68(19)
N(1)-B(1)-N(3)	103.82(19)

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for solvated *m*-IPhO-**BsubPc** (compound **2d**). 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}
I(1)	22(1)	23(1)	19(1)	1(1)	4(1)	7(1)
O(1)	21(1)	29(1)	16(1)	4(1)	7(1)	10(1)
N(1)	17(1)	14(1)	17(1)	1(1)	4(1)	4(1)
N(2)	16(1)	19(1)	22(1)	1(1)	7(1)	4(1)
N(3)	15(1)	14(1)	20(1)	4(1)	7(1)	2(1)
N(4)	18(1)	17(1)	16(1)	3(1)	6(1)	4(1)
N(5)	18(1)	14(1)	17(1)	2(1)	5(1)	5(1)
N(6)	20(1)	17(1)	18(1)	-1(1)	4(1)	2(1)
C(1)	21(1)	16(1)	16(1)	0(1)	7(1)	4(1)
C(2)	23(1)	18(1)	18(1)	2(1)	8(1)	8(1)
C(3)	26(1)	18(1)	24(1)	-1(1)	12(1)	2(1)
C(4)	37(2)	19(1)	26(2)	7(1)	16(1)	8(1)
C(5)	31(2)	24(1)	20(1)	6(1)	7(1)	12(1)
C(6)	22(1)	25(1)	17(1)	-1(1)	4(1)	9(1)
C(7)	21(1)	19(1)	17(1)	0(1)	9(1)	6(1)
C(8)	18(1)	24(1)	18(1)	2(1)	8(1)	6(1)
C(9)	15(1)	21(1)	18(1)	3(1)	6(1)	2(1)
C(10)	20(1)	17(1)	22(1)	3(1)	9(1)	-1(1)
C(11)	22(1)	25(1)	24(1)	4(1)	8(1)	2(1)
C(12)	26(1)	27(1)	23(1)	-6(1)	4(1)	-9(1)
C(13)	30(2)	19(1)	28(1)	-4(1)	14(1)	-2(1)
C(14)	21(1)	19(1)	25(1)	4(1)	10(1)	2(1)
C(15)	20(1)	18(1)	19(1)	4(1)	10(1)	1(1)
C(16)	21(1)	16(1)	19(1)	5(1)	11(1)	5(1)
C(17)	21(1)	20(1)	14(1)	4(1)	7(1)	3(1)
C(18)	18(1)	20(1)	14(1)	0(1)	6(1)	2(1)
C(19)	22(1)	23(1)	21(1)	2(1)	8(1)	5(1)

C(20)	18(1)	38(2)	23(1)	2(1)	9(1)	6(1)
C(21)	19(1)	32(2)	24(1)	3(1)	10(1)	-4(1)
C(22)	26(1)	23(1)	21(1)	0(1)	6(1)	-5(1)
C(23)	22(1)	22(1)	16(1)	0(1)	7(1)	1(1)
C(24)	20(1)	19(1)	14(1)	0(1)	5(1)	2(1)
C(25)	14(1)	16(1)	14(1)	3(1)	4(1)	-3(1)
C(26)	17(1)	16(1)	17(1)	-2(1)	8(1)	-2(1)
C(27)	16(1)	15(1)	22(1)	1(1)	6(1)	-2(1)
C(28)	22(1)	22(1)	14(1)	-2(1)	2(1)	-2(1)
C(29)	24(1)	20(1)	20(1)	-8(1)	7(1)	-1(1)
C(30)	18(1)	14(1)	22(1)	0(1)	7(1)	3(1)
B(1)	18(1)	18(1)	15(1)	3(1)	5(1)	3(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for solvated *m*-IPhO-**BsubPc** (compound **2d**).

	x	y	z	U(eq)
H(3A)	6594	4703	2973	26
H(4A)	7492	4222	4135	31
H(5A)	8463	4954	4807	30
H(6A)	8596	6208	4331	27
H(11A)	8488	9185	4258	28
H(12A)	8277	10446	4642	31
H(13A)	7232	11075	3950	29
H(14A)	6363	10456	2855	26
H(19A)	4163	8851	1208	26
H(20A)	3161	8096	843	31
H(21A)	3213	6737	822	30
H(22A)	4270	6085	1224	29
H(26A)	5982	8647	364	19
H(28A)	5643	8256	-2137	25
H(29A)	6435	7225	-1768	26
H(30A)	6978	6881	-358	22

Table S26. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for solvated *m*-IPhO-**BsubPc** (compound **2d**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(13)-H(13A)	->	Cg(10)	2.93	2.85	13.55	143	3.735(3)	50
C(20)-H(20A)	->	Cg(2)	2.91	-2.83	13.7	114	3.406(3)	36
C(21)-H(21A)	->	Cg(1)	2.79	-2.7	14.62	111	3.253(3)	35

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (2) N(3) --> C(9) --> C(10) --> C(15) --> C(16) -->

6-Membered Ring (10) C(25) --> C(26) --> C(27) --> C(28) --> C(29) --> C(30) -->

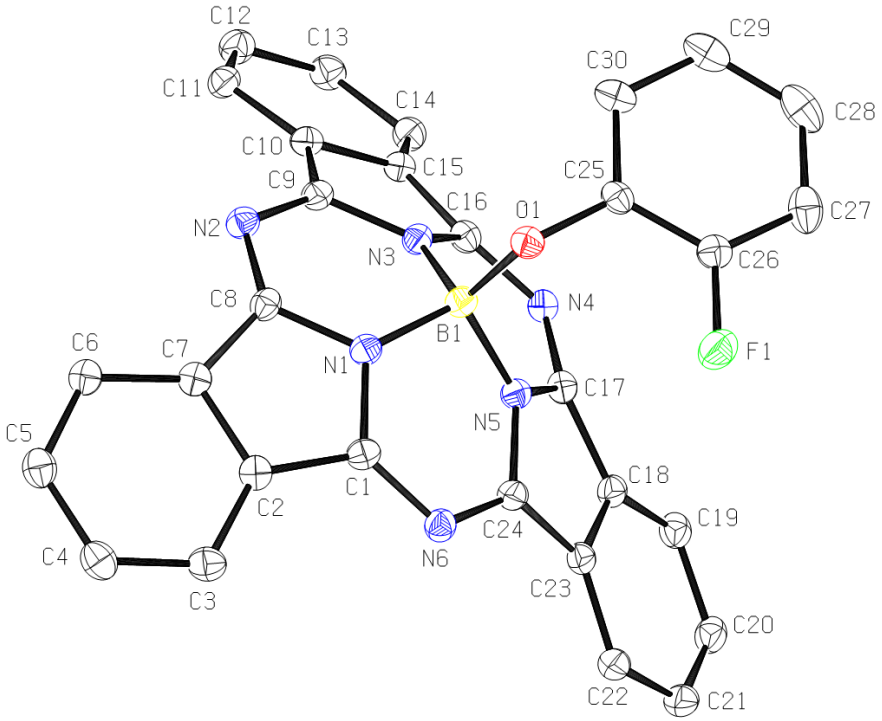

Figure S9. Anisotropic displacement ellipsoid plot of *o*-FPhO-**BsubPc** (compound **4a**).

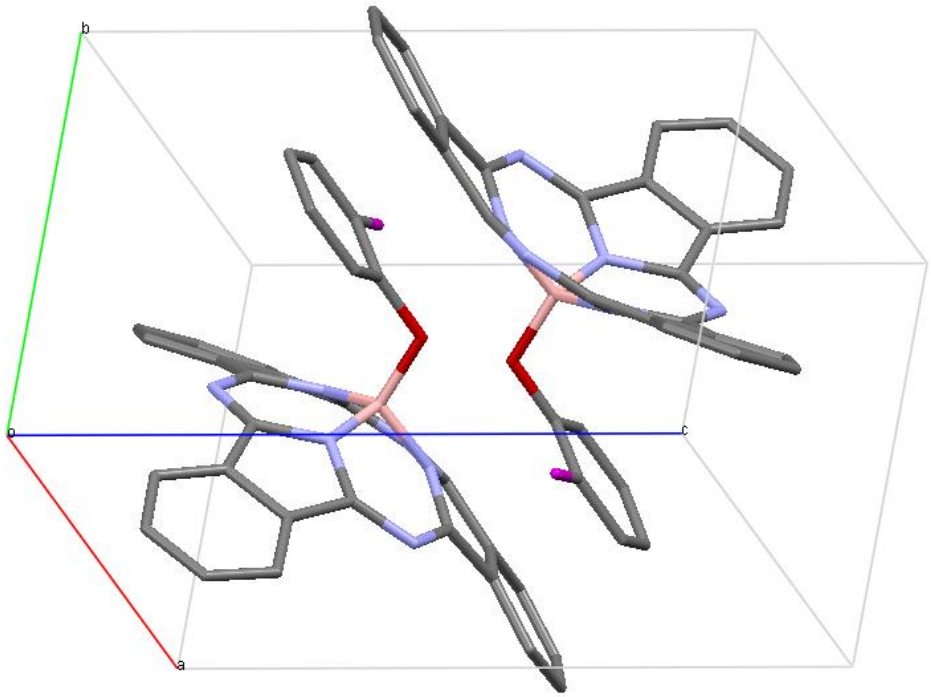

Figure S10. Populated unit cell of *o*-FPhO-**BsubPc** (compound **4a**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; fluorine = magenta. Hydrogens are omitted for clarity.

Table S27. Crystal data and structure refinement for *o*-FPhO-**BsubPc** (compound **4a**).

Identification code	k11169	
Empirical formula	C30 H16 B F N6 O	
Formula weight	506.30	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.1276(3) Å	α= 86.4627(15)°.
	b = 10.8350(3) Å	β= 77.0822(13)°.
	c = 11.8593(4) Å	γ = 64.9040(15)°.
Volume	1147.87(6) $Å^3$	
Z	2	
Density (calculated)	1.465 Mg/m^3	
Absorption coefficient	0.098 mm^{-1}	
F(000)	520	
Crystal size	0.35 x 0.30 x 0.26 mm^3	
Theta range for data collection	2.56 to 27.44°.	
Index ranges	-13<=h<=13, -13<=k<=14, -15<=l<=15	
Reflections collected	23467	
Independent reflections	5219 [R(int) = 0.0701]	
Completeness to theta = 27.44°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.977 and 0.801	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5219 / 0 / 353	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1396	
R indices (all data)	R1 = 0.0897, wR2 = 0.1637	
Extinction coefficient	0.024(4)	
Largest diff. peak and hole	0.585 and -0.372 $e.Å^{-3}$	

Table S28. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *o*-FPhO-**BsubPc** (compound **4a**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	5533(2)	8399(1)	3173(1)	46(1)
O(1)	5985(2)	5868(1)	3985(1)	29(1)
N(1)	8565(2)	4136(2)	3636(1)	27(1)
N(2)	8246(2)	2074(2)	3716(1)	29(1)
N(3)	6956(2)	3890(2)	2588(1)	26(1)
N(4)	6666(2)	5035(2)	813(2)	28(1)
N(5)	7803(2)	5606(2)	2123(1)	26(1)
N(6)	9862(2)	5496(2)	2828(2)	29(1)
C(1)	9725(2)	4504(2)	3523(2)	28(1)
C(2)	10841(2)	3430(2)	4032(2)	28(1)
C(3)	12251(2)	3247(2)	4141(2)	35(1)
C(4)	13130(3)	2047(2)	4585(2)	37(1)
C(5)	12628(2)	1030(2)	4898(2)	36(1)
C(6)	11248(2)	1173(2)	4773(2)	30(1)
C(7)	10337(2)	2384(2)	4331(2)	28(1)
C(8)	8926(2)	2816(2)	3973(2)	27(1)
C(9)	7328(2)	2595(2)	2973(2)	27(1)
C(10)	6864(2)	1922(2)	2217(2)	28(1)
C(11)	6934(2)	607(2)	2177(2)	30(1)
C(12)	6476(2)	255(2)	1277(2)	34(1)
C(13)	6002(2)	1157(2)	408(2)	34(1)
C(14)	5968(2)	2451(2)	411(2)	31(1)
C(15)	6371(2)	2840(2)	1327(2)	27(1)
C(16)	6554(2)	4059(2)	1542(2)	27(1)
C(17)	7371(2)	5741(2)	1096(2)	27(1)
C(18)	8096(2)	6525(2)	384(2)	28(1)
C(19)	8021(2)	7038(2)	-717(2)	32(1)
C(20)	8867(2)	7755(2)	-1149(2)	35(1)

C(21)	9810(2)	7914(2)	-534(2)	36(1)
C(22)	9956(2)	7350(2)	538(2)	32(1)
C(23)	9070(2)	6675(2)	1007(2)	28(1)
C(24)	8935(2)	5984(2)	2096(2)	28(1)
C(25)	4734(2)	6647(2)	3573(2)	28(1)
C(26)	4503(2)	7932(2)	3150(2)	32(1)
C(27)	3272(3)	8730(2)	2725(2)	42(1)
C(28)	2210(3)	8245(3)	2711(2)	49(1)
C(29)	2401(3)	6972(3)	3118(2)	45(1)
C(30)	3650(2)	6183(2)	3553(2)	36(1)
B(1)	7237(3)	4936(2)	3138(2)	27(1)

Table S29. Bond lengths [Å] and angles [°] for *o*-FPhO-**BsubPc** (compound **4a**).

F(1)-C(26)	1.345(2)
O(1)-C(25)	1.370(2)
O(1)-B(1)	1.451(3)
N(1)-C(1)	1.370(3)
N(1)-C(8)	1.375(2)
N(1)-B(1)	1.487(3)
N(2)-C(8)	1.345(3)
N(2)-C(9)	1.348(3)
N(3)-C(9)	1.368(2)
N(3)-C(16)	1.369(3)
N(3)-B(1)	1.496(3)
N(4)-C(17)	1.345(3)
N(4)-C(16)	1.351(3)
N(5)-C(17)	1.363(3)
N(5)-C(24)	1.365(3)
N(5)-B(1)	1.498(3)
N(6)-C(24)	1.342(3)
N(6)-C(1)	1.350(3)
C(1)-C(2)	1.449(3)
C(2)-C(3)	1.391(3)
C(2)-C(7)	1.425(3)
C(3)-C(4)	1.380(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.397(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.380(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.397(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.456(3)
C(9)-C(10)	1.454(3)
C(10)-C(11)	1.399(3)

C(10)-C(15)	1.428(3)
C(11)-C(12)	1.386(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.395(3)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.388(3)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.387(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.454(3)
C(17)-C(18)	1.463(3)
C(18)-C(19)	1.392(3)
C(18)-C(23)	1.422(3)
C(19)-C(20)	1.386(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.394(3)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.387(3)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.391(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.461(3)
C(25)-C(26)	1.391(3)
C(25)-C(30)	1.392(3)
C(26)-C(27)	1.367(3)
C(27)-C(28)	1.386(4)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.381(4)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.384(3)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500

C(25)-O(1)-B(1)	115.22(16)

C(1)-N(1)-C(8)	112.74(17)
C(1)-N(1)-B(1)	122.25(16)
C(8)-N(1)-B(1)	122.99(17)
C(8)-N(2)-C(9)	117.58(17)
C(9)-N(3)-C(16)	113.25(16)
C(9)-N(3)-B(1)	123.00(17)
C(16)-N(3)-B(1)	122.79(16)
C(17)-N(4)-C(16)	116.39(17)
C(17)-N(5)-C(24)	113.75(16)
C(17)-N(5)-B(1)	123.19(17)
C(24)-N(5)-B(1)	122.60(17)
C(24)-N(6)-C(1)	116.85(17)
N(6)-C(1)-N(1)	123.18(18)
N(6)-C(1)-C(2)	129.18(19)
N(1)-C(1)-C(2)	105.91(16)
C(3)-C(2)-C(7)	120.87(19)
C(3)-C(2)-C(1)	131.38(19)
C(7)-C(2)-C(1)	107.39(17)
C(4)-C(3)-C(2)	118.4(2)
C(4)-C(3)-H(3A)	120.8
C(2)-C(3)-H(3A)	120.8
C(3)-C(4)-C(5)	120.8(2)
C(3)-C(4)-H(4A)	119.6
C(5)-C(4)-H(4A)	119.6
C(6)-C(5)-C(4)	121.9(2)
C(6)-C(5)-H(5A)	119.1
C(4)-C(5)-H(5A)	119.1
C(5)-C(6)-C(7)	118.2(2)
C(5)-C(6)-H(6A)	120.9
C(7)-C(6)-H(6A)	120.9
C(6)-C(7)-C(2)	119.80(19)
C(6)-C(7)-C(8)	132.81(19)
C(2)-C(7)-C(8)	107.08(17)
N(2)-C(8)-N(1)	122.34(18)

N(2)-C(8)-C(7)	130.18(18)
N(1)-C(8)-C(7)	105.54(17)
N(2)-C(9)-N(3)	122.06(18)
N(2)-C(9)-C(10)	130.63(18)
N(3)-C(9)-C(10)	105.55(16)
C(11)-C(10)-C(15)	119.76(19)
C(11)-C(10)-C(9)	132.78(19)
C(15)-C(10)-C(9)	107.24(17)
C(12)-C(11)-C(10)	118.13(19)
C(12)-C(11)-H(11A)	120.9
C(10)-C(11)-H(11A)	120.9
C(11)-C(12)-C(13)	121.7(2)
C(11)-C(12)-H(12A)	119.2
C(13)-C(12)-H(12A)	119.2
C(14)-C(13)-C(12)	121.2(2)
C(14)-C(13)-H(13A)	119.4
C(12)-C(13)-H(13A)	119.4
C(15)-C(14)-C(13)	117.99(19)
C(15)-C(14)-H(14A)	121.0
C(13)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	121.21(18)
C(14)-C(15)-C(16)	131.43(18)
C(10)-C(15)-C(16)	107.03(17)
N(4)-C(16)-N(3)	122.85(18)
N(4)-C(16)-C(15)	129.95(19)
N(3)-C(16)-C(15)	105.65(16)
N(4)-C(17)-N(5)	122.69(17)
N(4)-C(17)-C(18)	130.74(18)
N(5)-C(17)-C(18)	105.40(17)
C(19)-C(18)-C(23)	120.72(19)
C(19)-C(18)-C(17)	132.2(2)
C(23)-C(18)-C(17)	107.02(17)
C(20)-C(19)-C(18)	117.5(2)
C(20)-C(19)-H(19A)	121.2

C(18)-C(19)-H(19A)	121.2
C(19)-C(20)-C(21)	121.7(2)
C(19)-C(20)-H(20A)	119.1
C(21)-C(20)-H(20A)	119.1
C(22)-C(21)-C(20)	121.4(2)
C(22)-C(21)-H(21A)	119.3
C(20)-C(21)-H(21A)	119.3
C(21)-C(22)-C(23)	117.6(2)
C(21)-C(22)-H(22A)	121.2
C(23)-C(22)-H(22A)	121.2
C(22)-C(23)-C(18)	120.81(19)
C(22)-C(23)-C(24)	131.9(2)
C(18)-C(23)-C(24)	107.30(17)
N(6)-C(24)-N(5)	122.23(17)
N(6)-C(24)-C(23)	130.90(18)
N(5)-C(24)-C(23)	105.27(17)
O(1)-C(25)-C(26)	121.09(18)
O(1)-C(25)-C(30)	121.50(19)
C(26)-C(25)-C(30)	117.4(2)
F(1)-C(26)-C(27)	119.3(2)
F(1)-C(26)-C(25)	118.10(19)
C(27)-C(26)-C(25)	122.6(2)
C(26)-C(27)-C(28)	119.0(2)
C(26)-C(27)-H(27A)	120.5
C(28)-C(27)-H(27A)	120.5
C(29)-C(28)-C(27)	120.2(2)
C(29)-C(28)-H(28A)	119.9
C(27)-C(28)-H(28A)	119.9
C(28)-C(29)-C(30)	119.9(2)
C(28)-C(29)-H(29A)	120.1
C(30)-C(29)-H(29A)	120.1
C(29)-C(30)-C(25)	120.9(2)
C(29)-C(30)-H(30A)	119.5
C(25)-C(30)-H(30A)	119.5

O(1)-B(1)-N(1)	112.54(17)
O(1)-B(1)-N(3)	115.72(17)
N(1)-B(1)-N(3)	104.76(16)
O(1)-B(1)-N(5)	114.71(17)
N(1)-B(1)-N(5)	104.58(17)
N(3)-B(1)-N(5)	103.31(16)

Symmetry transformations used to generate equivalent atoms:

Table S30. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *o*-FPhO-**BsubPc** (compound **4a**). 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)	52(1)	38(1)	52(1)	5(1)	-12(1)	-24(1)
O(1)	29(1)	31(1)	27(1)	1(1)	-5(1)	-13(1)
N(1)	28(1)	27(1)	27(1)	1(1)	-6(1)	-13(1)
N(2)	31(1)	31(1)	26(1)	3(1)	-7(1)	-15(1)
N(3)	27(1)	26(1)	28(1)	4(1)	-7(1)	-12(1)
N(4)	27(1)	26(1)	31(1)	3(1)	-7(1)	-10(1)
N(5)	26(1)	26(1)	27(1)	2(1)	-6(1)	-12(1)
N(6)	30(1)	26(1)	32(1)	1(1)	-8(1)	-12(1)
C(1)	31(1)	29(1)	27(1)	-2(1)	-6(1)	-16(1)
C(2)	32(1)	29(1)	25(1)	-2(1)	-8(1)	-12(1)
C(3)	35(1)	40(1)	36(1)	0(1)	-11(1)	-20(1)
C(4)	34(1)	42(1)	37(1)	0(1)	-14(1)	-13(1)
C(5)	37(1)	35(1)	31(1)	2(1)	-11(1)	-11(1)
C(6)	35(1)	31(1)	24(1)	2(1)	-8(1)	-13(1)
C(7)	31(1)	30(1)	21(1)	-1(1)	-6(1)	-13(1)
C(8)	32(1)	25(1)	23(1)	2(1)	-4(1)	-12(1)
C(9)	28(1)	29(1)	26(1)	4(1)	-5(1)	-14(1)
C(10)	26(1)	30(1)	28(1)	0(1)	-4(1)	-14(1)
C(11)	32(1)	27(1)	30(1)	3(1)	-4(1)	-14(1)
C(12)	36(1)	32(1)	36(1)	-1(1)	-6(1)	-16(1)
C(13)	33(1)	35(1)	36(1)	-2(1)	-11(1)	-16(1)
C(14)	31(1)	32(1)	33(1)	4(1)	-12(1)	-14(1)
C(15)	25(1)	28(1)	29(1)	2(1)	-6(1)	-12(1)
C(16)	26(1)	29(1)	27(1)	1(1)	-7(1)	-10(1)
C(17)	27(1)	26(1)	27(1)	1(1)	-6(1)	-8(1)
C(18)	28(1)	22(1)	31(1)	-1(1)	-3(1)	-9(1)
C(19)	31(1)	28(1)	31(1)	-1(1)	-3(1)	-8(1)
C(20)	37(1)	29(1)	30(1)	4(1)	-1(1)	-9(1)

C(21)	32(1)	32(1)	39(1)	2(1)	2(1)	-13(1)
C(22)	28(1)	28(1)	36(1)	1(1)	-3(1)	-11(1)
C(23)	25(1)	23(1)	30(1)	1(1)	-3(1)	-7(1)
C(24)	26(1)	25(1)	32(1)	0(1)	-4(1)	-11(1)
C(25)	25(1)	32(1)	23(1)	-2(1)	-2(1)	-8(1)
C(26)	32(1)	33(1)	29(1)	-2(1)	-4(1)	-14(1)
C(27)	48(1)	36(1)	32(1)	0(1)	-12(1)	-6(1)
C(28)	34(1)	60(2)	39(1)	-11(1)	-13(1)	-4(1)
C(29)	31(1)	61(2)	39(1)	-11(1)	-3(1)	-16(1)
C(30)	29(1)	47(1)	34(1)	-5(1)	-3(1)	-17(1)
B(1)	30(1)	29(1)	26(1)	3(1)	-7(1)	-14(1)

Table S31. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *o*-FPhO-**BsubPc** (compound **4a**).

	x	y	z	U(eq)
H(3A)	12600	3931	3915	42
H(4A)	14090	1910	4678	45
H(5A)	13254	216	5206	43
H(6A)	10927	467	4981	36
H(11A)	7285	-26	2750	36
H(12A)	6484	-623	1252	41
H(13A)	5698	881	-196	40
H(14A)	5678	3052	-195	37
H(19A)	7413	6901	-1156	38
H(20A)	8802	8149	-1885	42
H(21A)	10366	8421	-856	43
H(22A)	10638	7422	937	38
H(27A)	3146	9605	2444	51
H(28A)	1348	8791	2420	58
H(29A)	1677	6638	3100	54
H(30A)	3769	5313	3843	44

Table S32. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *o*-FPhO-**BsubPc** (compound **4a**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(12)-H(12A)	->	Cg(9)	2.83	2.79	10.01	120	3.409(2)	39
C(20)-H(20A)	->	Cg(1)	2.77	-2.73	10.15	120	3.356(2)	40
C(21)-H(21A)	->	Cg(2)	2.74	2.69	11.06	116	3.267(2)	37

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (2) N(3) --> C(9) --> C(10) --> C(15) --> C(16) -->

6-Membered Ring (9) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

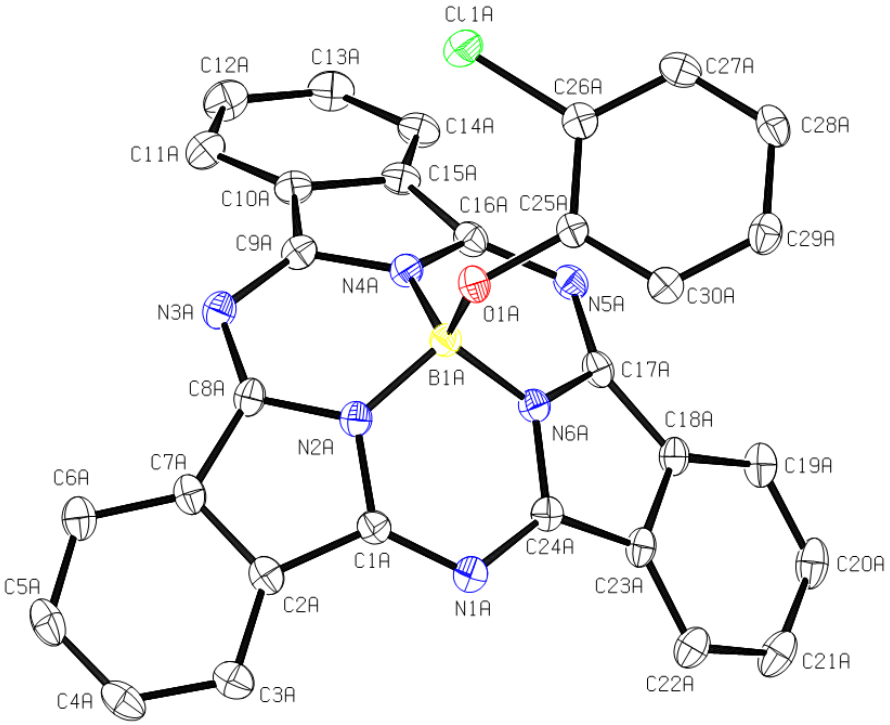

Figure S11. Anisotropic displacement ellipsoid plot for molecule A of *o*-ClPhO-**BsubPc** (compound **4b**).

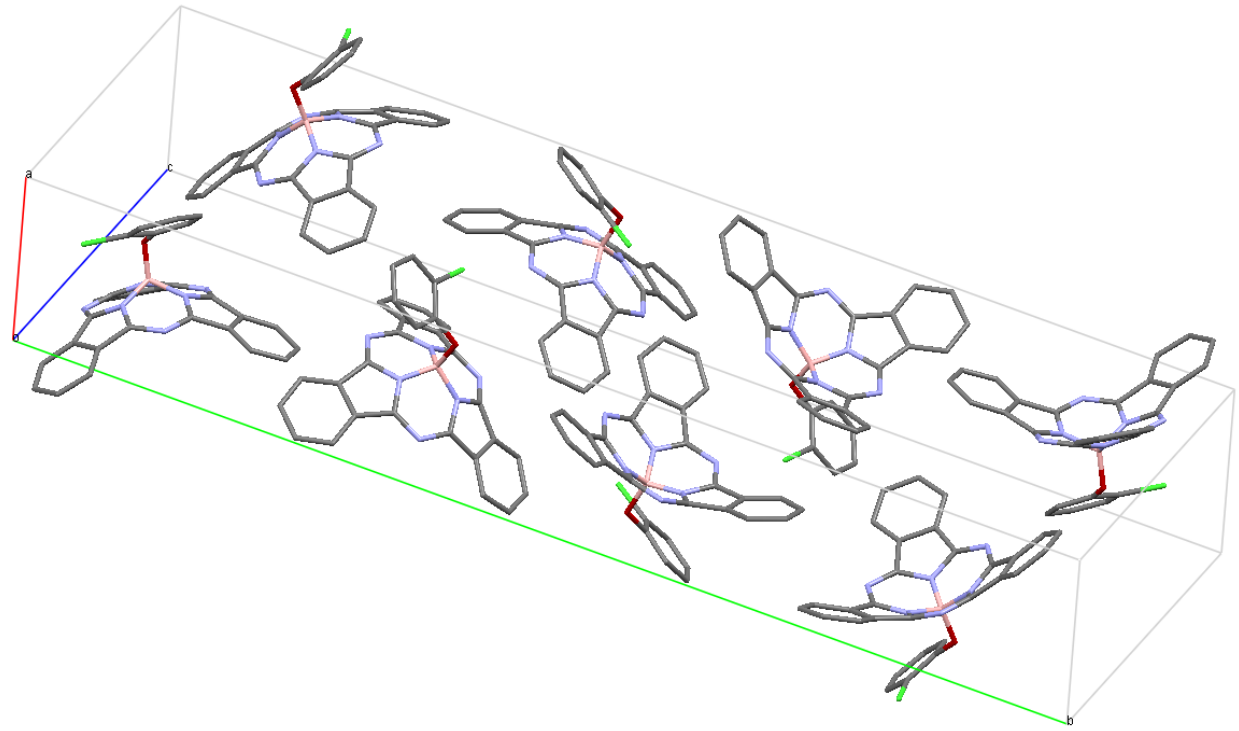

Figure S12. Populated unit cell of *o*-ClPhO-**BsubPc** (compound **4b**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; chlorine = green. Hydrogens are omitted for clarity.

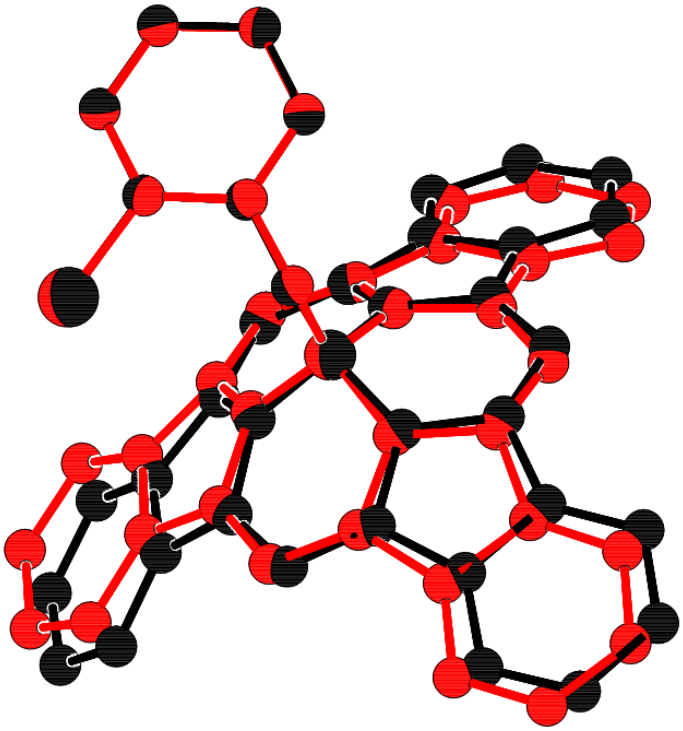

Figure S13. Overlay of the two molecules in the asymmetric unit cell of *o*-ClPhO-**BsubPc** (compound **4b**).

Table S33. Crystal data and structure refinement for *o*-ClPhO-**BsubPc** (compound **4b**).

Identification code	k11191	
Empirical formula	C30 H16 B Cl N6 O	
Formula weight	522.75	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.0880(2) Å	α= 90°.
	b = 42.9323(14) Å	β= 99.3790(15)°.
	c = 13.7269(4) Å	γ = 90°.
Volume	4702.8(2) $Å^3$	
Z	8	
Density (calculated)	1.477 Mg/m^3	
Absorption coefficient	0.202 mm^{-1}	
F(000)	2144	
Crystal size	0.50 x 0.45 x 0.24 mm^3	
Theta range for data collection	2.72 to 27.42°.	
Index ranges	-10<=h<=10, -51<=k<=55, -17<=l<=17	
Reflections collected	21445	
Independent reflections	10246 [R(int) = 0.0610]	
Completeness to theta = 25.00°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.955 and 0.551	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10246 / 0 / 703	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0609, wR2 = 0.1396	
R indices (all data)	R1 = 0.1160, wR2 = 0.1708	
Largest diff. peak and hole	0.361 and -0.497 $e.Å^{-3}$	

Table S34. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *o*-ClPhO-**BsubPc** (compound **4b**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1A)	2888(1)	6564(1)	4973(1)	42(1)
O(1A)	4993(2)	6329(1)	6816(1)	29(1)
N(1A)	8860(3)	6346(1)	8692(2)	30(1)
N(2A)	8006(3)	6251(1)	6974(2)	28(1)
N(3A)	8457(3)	6276(1)	5308(2)	32(1)
N(4A)	6857(3)	6667(1)	5963(2)	28(1)
N(5A)	6579(3)	7163(1)	6713(2)	31(1)
N(6A)	7073(3)	6704(1)	7691(2)	27(1)
C(1A)	8926(3)	6179(1)	7877(2)	29(1)
C(2A)	10154(4)	5948(1)	7674(2)	32(1)
C(3A)	11336(4)	5772(1)	8299(2)	38(1)
C(4A)	12368(4)	5579(1)	7860(3)	43(1)
C(5A)	12302(4)	5569(1)	6841(3)	44(1)
C(6A)	11147(4)	5744(1)	6211(2)	39(1)
C(7A)	10041(4)	5930(1)	6635(2)	31(1)
C(8A)	8740(4)	6145(1)	6206(2)	30(1)
C(9A)	7606(4)	6549(1)	5223(2)	30(1)
C(10A)	7705(4)	6801(1)	4533(2)	33(1)
C(11A)	8406(4)	6813(1)	3678(2)	38(1)
C(12A)	8490(4)	7102(1)	3231(2)	45(1)
C(13A)	7925(4)	7371(1)	3638(2)	44(1)
C(14A)	7266(4)	7364(1)	4498(2)	36(1)
C(15A)	7134(4)	7074(1)	4956(2)	32(1)
C(16A)	6711(3)	6986(1)	5908(2)	31(1)
C(17A)	6856(3)	7020(1)	7600(2)	29(1)
C(18A)	7434(4)	7147(1)	8578(2)	30(1)
C(19A)	7469(4)	7450(1)	8950(2)	36(1)
C(20A)	8250(4)	7502(1)	9902(3)	42(1)

C(21A)	9036(4)	7259(1)	10481(2)	42(1)
C(22A)	9026(4)	6957(1)	10132(2)	36(1)
C(23A)	8186(4)	6897(1)	9177(2)	31(1)
C(24A)	8012(3)	6618(1)	8569(2)	28(1)
C(25A)	3661(3)	6516(1)	6958(2)	27(1)
C(26A)	2617(4)	6652(1)	6166(2)	32(1)
C(27A)	1333(4)	6851(1)	6331(2)	36(1)
C(28A)	1052(4)	6907(1)	7278(2)	38(1)
C(29A)	2039(4)	6760(1)	8068(2)	38(1)
C(30A)	3337(4)	6565(1)	7909(2)	32(1)
B(1A)	6608(4)	6480(1)	6856(2)	28(1)
Cl(1B)	9441(1)	4689(1)	7066(1)	57(1)
O(1B)	8510(2)	4363(1)	8846(1)	32(1)
N(1B)	5453(3)	3901(1)	10014(2)	32(1)
N(2B)	5608(3)	4372(1)	9117(2)	29(1)
N(3B)	4390(3)	4752(1)	7952(2)	33(1)
N(4B)	6061(3)	4339(1)	7471(2)	29(1)
N(5B)	6412(3)	3839(1)	6783(2)	31(1)
N(6B)	6602(3)	3904(1)	8523(2)	29(1)
C(10B)	4548(4)	4594(1)	6184(2)	31(1)
C(11B)	3486(4)	4784(1)	5544(2)	37(1)
C(12B)	3162(4)	4707(1)	4559(2)	41(1)
C(13B)	3860(4)	4441(1)	4197(2)	40(1)
C(14B)	4865(4)	4240(1)	4828(2)	35(1)
C(15B)	5216(4)	4315(1)	5822(2)	32(1)
C(16B)	6052(4)	4147(1)	6674(2)	29(1)
C(17B)	6568(4)	3721(1)	7700(2)	31(1)
C(18B)	6289(4)	3405(1)	8019(2)	31(1)
C(19B)	6155(4)	3122(1)	7510(2)	36(1)
C(20B)	5711(4)	2860(1)	7995(2)	38(1)
C(21B)	5338(4)	2879(1)	8953(2)	36(1)
C(22B)	5449(4)	3159(1)	9464(2)	33(1)
C(23B)	5953(3)	3423(1)	9006(2)	29(1)
C(24B)	6072(4)	3751(1)	9291(2)	30(1)

C(25B)	9772(4)	4223(1)	8433(2)	32(1)
C(26B)	10276(4)	4342(1)	7587(2)	37(1)
C(27B)	11487(4)	4189(1)	7150(3)	45(1)
C(28B)	12230(4)	3923(1)	7582(3)	47(1)
C(29B)	11795(4)	3812(1)	8444(3)	46(1)
C(30B)	10568(4)	3960(1)	8871(2)	37(1)
C(1B)	5146(4)	4207(1)	9884(2)	29(1)
C(2B)	4004(4)	4408(1)	10307(2)	31(1)
C(3B)	3286(4)	4385(1)	11151(2)	34(1)
C(4B)	2234(4)	4623(1)	11359(2)	36(1)
C(5B)	1872(4)	4876(1)	10726(2)	35(1)
C(6B)	2545(3)	4900(1)	9861(2)	31(1)
C(7B)	3654(3)	4670(1)	9658(2)	29(1)
C(8B)	4599(4)	4626(1)	8855(2)	29(1)
C(9B)	5037(4)	4592(1)	7248(2)	32(1)
B(1B)	6816(4)	4251(1)	8502(2)	30(1)

Table S35. Bond lengths [Å] and angles [°] for *o*-ClPhO-**BsubPc** (compound **4b**).

Cl(1A)-C(26A)	1.730(3)
O(1A)-C(25A)	1.382(3)
O(1A)-B(1A)	1.451(4)
N(1A)-C(1A)	1.337(4)
N(1A)-C(24A)	1.352(4)
N(2A)-C(8A)	1.370(3)
N(2A)-C(1A)	1.373(4)
N(2A)-B(1A)	1.489(4)
N(3A)-C(8A)	1.340(4)
N(3A)-C(9A)	1.355(4)
N(4A)-C(9A)	1.363(4)
N(4A)-C(16A)	1.376(3)
N(4A)-B(1A)	1.507(4)
N(5A)-C(17A)	1.351(3)
N(5A)-C(16A)	1.357(4)
N(6A)-C(24A)	1.365(3)
N(6A)-C(17A)	1.371(3)
N(6A)-B(1A)	1.494(4)
C(1A)-C(2A)	1.463(4)
C(2A)-C(3A)	1.396(4)
C(2A)-C(7A)	1.416(4)
C(3A)-C(4A)	1.383(4)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.392(5)
C(4A)-H(4AA)	0.9500
C(5A)-C(6A)	1.385(5)
C(5A)-H(5AA)	0.9500
C(6A)-C(7A)	1.396(4)
C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.450(4)
C(9A)-C(10A)	1.447(4)
C(10A)-C(11A)	1.385(4)

C(10A)-C(15A)	1.420(4)
C(11A)-C(12A)	1.390(4)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.393(5)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.372(4)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.405(4)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.454(4)
C(17A)-C(18A)	1.454(4)
C(18A)-C(19A)	1.397(4)
C(18A)-C(23A)	1.428(4)
C(19A)-C(20A)	1.373(5)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.400(5)
C(20A)-H(20A)	0.9500
C(21A)-C(22A)	1.384(4)
C(21A)-H(21A)	0.9500
C(22A)-C(23A)	1.399(4)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.452(4)
C(25A)-C(30A)	1.388(4)
C(25A)-C(26A)	1.391(4)
C(26A)-C(27A)	1.392(4)
C(27A)-C(28A)	1.377(4)
C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.391(4)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.387(4)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
Cl(1B)-C(26B)	1.738(3)
O(1B)-C(25B)	1.382(3)

O(1B)-B(1B)	1.456(4)
N(1B)-C(1B)	1.345(4)
N(1B)-C(24B)	1.348(4)
N(2B)-C(1B)	1.370(4)
N(2B)-C(8B)	1.375(3)
N(2B)-B(1B)	1.485(4)
N(3B)-C(8B)	1.338(4)
N(3B)-C(9B)	1.358(4)
N(4B)-C(16B)	1.369(3)
N(4B)-C(9B)	1.373(4)
N(4B)-B(1B)	1.496(4)
N(5B)-C(17B)	1.343(4)
N(5B)-C(16B)	1.357(4)
N(6B)-C(24B)	1.370(3)
N(6B)-C(17B)	1.371(4)
N(6B)-B(1B)	1.501(4)
C(10B)-C(11B)	1.391(4)
C(10B)-C(15B)	1.435(4)
C(10B)-C(9B)	1.450(4)
C(11B)-C(12B)	1.376(4)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.402(4)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.386(4)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.386(4)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.445(4)
C(17B)-C(18B)	1.456(4)
C(18B)-C(19B)	1.397(4)
C(18B)-C(23B)	1.428(4)
C(19B)-C(20B)	1.384(4)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.399(4)

C(20B)-H(20B)	0.9500
C(21B)-C(22B)	1.388(4)
C(21B)-H(21B)	0.9500
C(22B)-C(23B)	1.390(4)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.458(4)
C(25B)-C(30B)	1.388(4)
C(25B)-C(26B)	1.389(4)
C(26B)-C(27B)	1.396(4)
C(27B)-C(28B)	1.376(5)
C(27B)-H(27B)	0.9500
C(28B)-C(29B)	1.375(5)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.385(4)
C(29B)-H(29B)	0.9500
C(30B)-H(30B)	0.9500
C(1B)-C(2B)	1.453(4)
C(2B)-C(3B)	1.381(4)
C(2B)-C(7B)	1.433(4)
C(3B)-C(4B)	1.387(4)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.394(4)
C(4B)-H(4BA)	0.9500
C(5B)-C(6B)	1.388(4)
C(5B)-H(5BA)	0.9500
C(6B)-C(7B)	1.392(4)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.452(4)

C(25A)-O(1A)-B(1A)	116.9(2)
C(1A)-N(1A)-C(24A)	116.6(2)
C(8A)-N(2A)-C(1A)	112.5(2)
C(8A)-N(2A)-B(1A)	123.6(2)
C(1A)-N(2A)-B(1A)	122.5(2)

C(8A)-N(3A)-C(9A)	116.9(2)
C(9A)-N(4A)-C(16A)	112.0(2)
C(9A)-N(4A)-B(1A)	122.9(2)
C(16A)-N(4A)-B(1A)	123.6(2)
C(17A)-N(5A)-C(16A)	117.1(2)
C(24A)-N(6A)-C(17A)	112.9(2)
C(24A)-N(6A)-B(1A)	122.6(2)
C(17A)-N(6A)-B(1A)	123.5(2)
N(1A)-C(1A)-N(2A)	123.1(3)
N(1A)-C(1A)-C(2A)	130.1(3)
N(2A)-C(1A)-C(2A)	105.3(2)
C(3A)-C(2A)-C(7A)	121.0(3)
C(3A)-C(2A)-C(1A)	131.8(3)
C(7A)-C(2A)-C(1A)	107.1(2)
C(4A)-C(3A)-C(2A)	117.2(3)
C(4A)-C(3A)-H(3AA)	121.4
C(2A)-C(3A)-H(3AA)	121.4
C(3A)-C(4A)-C(5A)	121.9(3)
C(3A)-C(4A)-H(4AA)	119.0
C(5A)-C(4A)-H(4AA)	119.0
C(6A)-C(5A)-C(4A)	121.5(3)
C(6A)-C(5A)-H(5AA)	119.3
C(4A)-C(5A)-H(5AA)	119.3
C(5A)-C(6A)-C(7A)	117.5(3)
C(5A)-C(6A)-H(6AA)	121.2
C(7A)-C(6A)-H(6AA)	121.2
C(6A)-C(7A)-C(2A)	120.7(3)
C(6A)-C(7A)-C(8A)	131.8(3)
C(2A)-C(7A)-C(8A)	107.4(2)
N(3A)-C(8A)-N(2A)	122.5(3)
N(3A)-C(8A)-C(7A)	130.2(3)
N(2A)-C(8A)-C(7A)	105.9(2)
N(3A)-C(9A)-N(4A)	122.6(3)
N(3A)-C(9A)-C(10A)	128.4(3)

N(4A)-C(9A)-C(10A)	106.8(2)
C(11A)-C(10A)-C(15A)	121.3(3)
C(11A)-C(10A)-C(9A)	131.1(3)
C(15A)-C(10A)-C(9A)	107.0(2)
C(10A)-C(11A)-C(12A)	117.7(3)
C(10A)-C(11A)-H(11A)	121.2
C(12A)-C(11A)-H(11A)	121.2
C(11A)-C(12A)-C(13A)	121.4(3)
C(11A)-C(12A)-H(12A)	119.3
C(13A)-C(12A)-H(12A)	119.3
C(14A)-C(13A)-C(12A)	121.7(3)
C(14A)-C(13A)-H(13A)	119.2
C(12A)-C(13A)-H(13A)	119.2
C(13A)-C(14A)-C(15A)	118.2(3)
C(13A)-C(14A)-H(14A)	120.9
C(15A)-C(14A)-H(14A)	120.9
C(14A)-C(15A)-C(10A)	119.7(3)
C(14A)-C(15A)-C(16A)	132.6(3)
C(10A)-C(15A)-C(16A)	107.1(2)
N(5A)-C(16A)-N(4A)	121.9(3)
N(5A)-C(16A)-C(15A)	130.4(3)
N(4A)-C(16A)-C(15A)	106.1(2)
N(5A)-C(17A)-N(6A)	122.2(3)
N(5A)-C(17A)-C(18A)	129.9(3)
N(6A)-C(17A)-C(18A)	105.8(2)
C(19A)-C(18A)-C(23A)	120.6(3)
C(19A)-C(18A)-C(17A)	132.3(3)
C(23A)-C(18A)-C(17A)	106.9(2)
C(20A)-C(19A)-C(18A)	118.5(3)
C(20A)-C(19A)-H(19A)	120.7
C(18A)-C(19A)-H(19A)	120.7
C(19A)-C(20A)-C(21A)	121.0(3)
C(19A)-C(20A)-H(20A)	119.5
C(21A)-C(20A)-H(20A)	119.5

C(22A)-C(21A)-C(20A)	121.8(3)
C(22A)-C(21A)-H(21A)	119.1
C(20A)-C(21A)-H(21A)	119.1
C(21A)-C(22A)-C(23A)	118.1(3)
C(21A)-C(22A)-H(22A)	121.0
C(23A)-C(22A)-H(22A)	121.0
C(22A)-C(23A)-C(18A)	119.9(3)
C(22A)-C(23A)-C(24A)	132.6(3)
C(18A)-C(23A)-C(24A)	107.2(2)
N(1A)-C(24A)-N(6A)	122.7(2)
N(1A)-C(24A)-C(23A)	129.8(3)
N(6A)-C(24A)-C(23A)	106.0(2)
O(1A)-C(25A)-C(30A)	119.5(2)
O(1A)-C(25A)-C(26A)	121.4(2)
C(30A)-C(25A)-C(26A)	119.1(3)
C(27A)-C(26A)-C(25A)	120.3(3)
C(27A)-C(26A)-Cl(1A)	120.0(2)
C(25A)-C(26A)-Cl(1A)	119.6(2)
C(28A)-C(27A)-C(26A)	120.2(3)
C(28A)-C(27A)-H(27A)	119.9
C(26A)-C(27A)-H(27A)	119.9
C(27A)-C(28A)-C(29A)	119.7(3)
C(27A)-C(28A)-H(28A)	120.2
C(29A)-C(28A)-H(28A)	120.2
C(30A)-C(29A)-C(28A)	120.3(3)
C(30A)-C(29A)-H(29A)	119.9
C(28A)-C(29A)-H(29A)	119.9
C(29A)-C(30A)-C(25A)	120.3(3)
C(29A)-C(30A)-H(30A)	119.9
C(25A)-C(30A)-H(30A)	119.9
O(1A)-B(1A)-N(2A)	111.8(2)
O(1A)-B(1A)-N(6A)	115.4(2)
N(2A)-B(1A)-N(6A)	104.4(2)
O(1A)-B(1A)-N(4A)	116.5(2)

N(2A)-B(1A)-N(4A)	104.0(2)
N(6A)-B(1A)-N(4A)	103.4(2)
C(25B)-O(1B)-B(1B)	116.4(2)
C(1B)-N(1B)-C(24B)	116.9(2)
C(1B)-N(2B)-C(8B)	112.7(2)
C(1B)-N(2B)-B(1B)	122.8(2)
C(8B)-N(2B)-B(1B)	123.2(2)
C(8B)-N(3B)-C(9B)	116.8(2)
C(16B)-N(4B)-C(9B)	112.0(2)
C(16B)-N(4B)-B(1B)	123.6(2)
C(9B)-N(4B)-B(1B)	123.4(2)
C(17B)-N(5B)-C(16B)	117.1(2)
C(24B)-N(6B)-C(17B)	113.1(2)
C(24B)-N(6B)-B(1B)	122.9(2)
C(17B)-N(6B)-B(1B)	122.6(2)
C(11B)-C(10B)-C(15B)	120.1(3)
C(11B)-C(10B)-C(9B)	132.6(3)
C(15B)-C(10B)-C(9B)	106.8(3)
C(12B)-C(11B)-C(10B)	118.6(3)
C(12B)-C(11B)-H(11B)	120.7
C(10B)-C(11B)-H(11B)	120.7
C(11B)-C(12B)-C(13B)	121.4(3)
C(11B)-C(12B)-H(12B)	119.3
C(13B)-C(12B)-H(12B)	119.3
C(14B)-C(13B)-C(12B)	121.0(3)
C(14B)-C(13B)-H(13B)	119.5
C(12B)-C(13B)-H(13B)	119.5
C(15B)-C(14B)-C(13B)	118.5(3)
C(15B)-C(14B)-H(14B)	120.7
C(13B)-C(14B)-H(14B)	120.7
C(14B)-C(15B)-C(10B)	120.3(3)
C(14B)-C(15B)-C(16B)	132.6(3)
C(10B)-C(15B)-C(16B)	106.8(2)
N(5B)-C(16B)-N(4B)	121.7(2)

N(5B)-C(16B)-C(15B)	129.8(3)
N(4B)-C(16B)-C(15B)	106.7(2)
N(5B)-C(17B)-N(6B)	122.9(3)
N(5B)-C(17B)-C(18B)	129.5(3)
N(6B)-C(17B)-C(18B)	105.6(2)
C(19B)-C(18B)-C(23B)	120.8(3)
C(19B)-C(18B)-C(17B)	131.7(3)
C(23B)-C(18B)-C(17B)	107.2(2)
C(20B)-C(19B)-C(18B)	118.1(3)
C(20B)-C(19B)-H(19B)	120.9
C(18B)-C(19B)-H(19B)	120.9
C(19B)-C(20B)-C(21B)	121.1(3)
C(19B)-C(20B)-H(20B)	119.4
C(21B)-C(20B)-H(20B)	119.4
C(22B)-C(21B)-C(20B)	121.4(3)
C(22B)-C(21B)-H(21B)	119.3
C(20B)-C(21B)-H(21B)	119.3
C(21B)-C(22B)-C(23B)	118.5(3)
C(21B)-C(22B)-H(22B)	120.7
C(23B)-C(22B)-H(22B)	120.7
C(22B)-C(23B)-C(18B)	120.0(3)
C(22B)-C(23B)-C(24B)	132.6(3)
C(18B)-C(23B)-C(24B)	107.1(2)
N(1B)-C(24B)-N(6B)	122.5(3)
N(1B)-C(24B)-C(23B)	130.0(3)
N(6B)-C(24B)-C(23B)	105.8(2)
O(1B)-C(25B)-C(30B)	119.8(3)
O(1B)-C(25B)-C(26B)	121.4(3)
C(30B)-C(25B)-C(26B)	118.9(3)
C(25B)-C(26B)-C(27B)	120.5(3)
C(25B)-C(26B)-Cl(1B)	120.8(2)
C(27B)-C(26B)-Cl(1B)	118.7(2)
C(28B)-C(27B)-C(26B)	119.7(3)
C(28B)-C(27B)-H(27B)	120.2

C(26B)-C(27B)-H(27B)	120.2
C(29B)-C(28B)-C(27B)	120.2(3)
C(29B)-C(28B)-H(28B)	119.9
C(27B)-C(28B)-H(28B)	119.9
C(28B)-C(29B)-C(30B)	120.4(3)
C(28B)-C(29B)-H(29B)	119.8
C(30B)-C(29B)-H(29B)	119.8
C(29B)-C(30B)-C(25B)	120.3(3)
C(29B)-C(30B)-H(30B)	119.9
C(25B)-C(30B)-H(30B)	119.9
N(1B)-C(1B)-N(2B)	122.7(3)
N(1B)-C(1B)-C(2B)	130.0(3)
N(2B)-C(1B)-C(2B)	105.7(2)
C(3B)-C(2B)-C(7B)	120.6(3)
C(3B)-C(2B)-C(1B)	132.4(3)
C(7B)-C(2B)-C(1B)	107.0(2)
C(2B)-C(3B)-C(4B)	118.4(3)
C(2B)-C(3B)-H(3BA)	120.8
C(4B)-C(3B)-H(3BA)	120.8
C(3B)-C(4B)-C(5B)	121.3(3)
C(3B)-C(4B)-H(4BA)	119.3
C(5B)-C(4B)-H(4BA)	119.3
C(6B)-C(5B)-C(4B)	121.2(3)
C(6B)-C(5B)-H(5BA)	119.4
C(4B)-C(5B)-H(5BA)	119.4
C(5B)-C(6B)-C(7B)	118.3(3)
C(5B)-C(6B)-H(6BA)	120.9
C(7B)-C(6B)-H(6BA)	120.9
C(6B)-C(7B)-C(2B)	120.1(3)
C(6B)-C(7B)-C(8B)	132.8(3)
C(2B)-C(7B)-C(8B)	107.1(2)
N(3B)-C(8B)-N(2B)	122.9(3)
N(3B)-C(8B)-C(7B)	130.4(3)
N(2B)-C(8B)-C(7B)	105.6(2)

N(3B)-C(9B)-N(4B)	122.0(3)
N(3B)-C(9B)-C(10B)	129.9(3)
N(4B)-C(9B)-C(10B)	106.5(2)
O(1B)-B(1B)-N(2B)	111.8(2)
O(1B)-B(1B)-N(4B)	116.1(2)
N(2B)-B(1B)-N(4B)	104.1(2)
O(1B)-B(1B)-N(6B)	115.2(3)
N(2B)-B(1B)-N(6B)	104.4(2)
N(4B)-B(1B)-N(6B)	103.7(2)

Symmetry transformations used to generate equivalent atoms:

Table S36. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *o*-ClPhO-**BsubPc** (compound **4b**). 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}
Cl(1A)	44(1)	51(1)	31(1)	-1(1)	5(1)	2(1)
O(1A)	30(1)	22(1)	36(1)	-1(1)	9(1)	-1(1)
N(1A)	34(1)	25(1)	31(1)	2(1)	8(1)	-3(1)
N(2A)	32(1)	23(1)	31(1)	-1(1)	7(1)	-2(1)
N(3A)	37(1)	27(1)	32(1)	-3(1)	8(1)	-3(1)
N(4A)	32(1)	23(1)	29(1)	0(1)	4(1)	0(1)
N(5A)	31(1)	24(1)	36(1)	2(1)	5(1)	2(1)
N(6A)	29(1)	23(1)	30(1)	1(1)	6(1)	0(1)
C(1A)	30(2)	27(2)	30(2)	4(1)	7(1)	1(1)
C(2A)	32(2)	21(1)	42(2)	1(1)	8(1)	-2(1)
C(3A)	35(2)	29(2)	48(2)	2(1)	2(1)	-2(1)
C(4A)	33(2)	29(2)	64(2)	7(2)	2(2)	4(1)
C(5A)	38(2)	30(2)	68(2)	-8(2)	14(2)	5(1)
C(6A)	43(2)	31(2)	46(2)	-5(2)	14(2)	0(1)
C(7A)	30(2)	22(1)	42(2)	-3(1)	11(1)	-3(1)
C(8A)	36(2)	23(1)	32(2)	-3(1)	10(1)	-4(1)
C(9A)	34(2)	26(2)	30(2)	0(1)	4(1)	-5(1)
C(10A)	33(2)	32(2)	32(2)	2(1)	2(1)	-4(1)
C(11A)	43(2)	39(2)	33(2)	0(1)	7(1)	-5(1)
C(12A)	49(2)	49(2)	37(2)	9(2)	11(2)	-8(2)
C(13A)	47(2)	39(2)	44(2)	13(2)	7(2)	-6(2)
C(14A)	34(2)	34(2)	40(2)	8(1)	2(1)	0(1)
C(15A)	29(2)	31(2)	34(2)	6(1)	1(1)	-1(1)
C(16A)	30(2)	24(2)	38(2)	0(1)	4(1)	1(1)
C(17A)	29(2)	22(1)	37(2)	2(1)	10(1)	2(1)
C(18A)	32(2)	27(2)	32(2)	-2(1)	13(1)	-2(1)
C(19A)	38(2)	29(2)	44(2)	-5(1)	17(1)	-5(1)
C(20A)	50(2)	30(2)	51(2)	-13(2)	24(2)	-10(2)

C(21A)	54(2)	41(2)	34(2)	-9(2)	16(2)	-19(2)
C(22A)	44(2)	35(2)	32(2)	-2(1)	12(1)	-7(1)
C(23A)	33(2)	29(2)	32(2)	-5(1)	14(1)	-4(1)
C(24A)	31(2)	25(2)	29(1)	2(1)	9(1)	-2(1)
C(25A)	25(1)	22(1)	34(2)	-2(1)	6(1)	-3(1)
C(26A)	31(2)	28(2)	37(2)	-1(1)	6(1)	-5(1)
C(27A)	29(2)	34(2)	43(2)	6(1)	2(1)	-3(1)
C(28A)	28(2)	33(2)	53(2)	-6(2)	11(1)	1(1)
C(29A)	37(2)	42(2)	37(2)	-7(1)	14(1)	-5(1)
C(30A)	32(2)	30(2)	34(2)	3(1)	8(1)	-3(1)
B(1A)	28(2)	26(2)	28(2)	-3(1)	4(1)	0(1)
Cl(1B)	54(1)	49(1)	71(1)	27(1)	20(1)	4(1)
O(1B)	30(1)	30(1)	38(1)	-4(1)	9(1)	-1(1)
N(1B)	38(1)	25(1)	34(1)	1(1)	9(1)	2(1)
N(2B)	33(1)	25(1)	30(1)	0(1)	6(1)	1(1)
N(3B)	38(1)	26(1)	35(1)	0(1)	8(1)	-3(1)
N(4B)	36(1)	22(1)	31(1)	0(1)	10(1)	0(1)
N(5B)	37(1)	25(1)	33(1)	-1(1)	10(1)	1(1)
N(6B)	32(1)	25(1)	30(1)	0(1)	7(1)	2(1)
C(10B)	39(2)	24(2)	32(2)	1(1)	10(1)	-7(1)
C(11B)	44(2)	28(2)	38(2)	0(1)	6(1)	1(1)
C(12B)	50(2)	30(2)	41(2)	5(1)	3(2)	-3(1)
C(13B)	51(2)	35(2)	35(2)	1(1)	5(1)	-9(2)
C(14B)	43(2)	29(2)	34(2)	0(1)	10(1)	-5(1)
C(15B)	37(2)	28(2)	32(2)	2(1)	11(1)	-4(1)
C(16B)	36(2)	25(2)	27(2)	-1(1)	9(1)	-3(1)
C(17B)	33(2)	27(2)	33(2)	-4(1)	8(1)	3(1)
C(18B)	35(2)	24(2)	34(2)	-1(1)	6(1)	4(1)
C(19B)	43(2)	31(2)	35(2)	-2(1)	7(1)	4(1)
C(20B)	46(2)	24(2)	44(2)	-3(1)	7(2)	3(1)
C(21B)	39(2)	23(2)	46(2)	4(1)	8(1)	1(1)
C(22B)	34(2)	27(2)	38(2)	4(1)	6(1)	2(1)
C(23B)	30(2)	25(1)	31(2)	1(1)	4(1)	4(1)
C(24B)	33(2)	28(2)	30(2)	3(1)	5(1)	1(1)

C(25B)	32(2)	27(2)	37(2)	-6(1)	7(1)	-2(1)
C(26B)	35(2)	33(2)	43(2)	5(1)	6(1)	-4(1)
C(27B)	41(2)	49(2)	47(2)	-3(2)	18(2)	-9(2)
C(28B)	33(2)	41(2)	71(2)	-16(2)	21(2)	-4(2)
C(29B)	30(2)	30(2)	76(3)	-1(2)	0(2)	1(1)
C(30B)	33(2)	34(2)	43(2)	2(1)	2(1)	2(1)
C(1B)	34(2)	28(2)	26(1)	1(1)	5(1)	0(1)
C(2B)	31(2)	26(2)	38(2)	-5(1)	7(1)	-1(1)
C(3B)	38(2)	29(2)	36(2)	-2(1)	11(1)	-4(1)
C(4B)	37(2)	34(2)	38(2)	-4(1)	14(1)	-4(1)
C(5B)	34(2)	30(2)	44(2)	-8(1)	9(1)	-2(1)
C(6B)	33(2)	25(2)	36(2)	-4(1)	6(1)	-2(1)
C(7B)	30(2)	26(2)	33(2)	-4(1)	7(1)	-2(1)
C(8B)	33(2)	22(1)	32(2)	-1(1)	6(1)	-2(1)
C(9B)	39(2)	25(2)	32(2)	2(1)	9(1)	-3(1)
B(1B)	37(2)	25(2)	29(2)	-1(1)	9(1)	1(1)

Table S37. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *o*-ClPhO-**BsubPc** (compound **4b**).

	x	y	z	U(eq)
H(3AA)	11427	5785	8997	45
H(4AA)	13146	5449	8267	51
H(5AA)	13066	5440	6571	53
H(6AA)	11108	5737	5516	47
H(11A)	8815	6631	3406	46
H(12A)	8942	7116	2636	54
H(13A)	7997	7565	3312	52
H(14A)	6908	7550	4776	44
H(19A)	6965	7617	8554	43
H(20A)	8257	7706	10171	50
H(21A)	9591	7303	11131	51
H(22A)	9574	6794	10531	44
H(27A)	648	6949	5788	43
H(28A)	189	7046	7391	45
H(29A)	1822	6792	8721	45
H(30A)	4008	6465	8452	38
H(11B)	2996	4964	5783	44
H(12B)	2450	4838	4113	49
H(13B)	3641	4397	3510	48
H(14B)	5303	4056	4583	42
H(19B)	6362	3110	6849	43
H(20B)	5658	2663	7671	46
H(21B)	5002	2696	9260	43
H(22B)	5187	3170	10113	39
H(27B)	11798	4267	6558	53
H(28B)	13046	3816	7282	56
H(29B)	12338	3633	8750	56
H(30B)	10270	3881	9465	45

H(3BA)	3508	4211	11578	41
H(4BA)	1752	4612	11944	43
H(5BA)	1151	5036	10890	42
H(6BA)	2256	5069	9418	37

Table S38. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *o*-ClPhO-**BsubPc** (compound **4b**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(27A)-H(27A)	->	Cg2	2.82	2.72	15.25	121	3.407(3)	43
C(27B)-H(27B)	->	Cg27	2.93	-2.73	21.16	115	3.436(4)	39
C(28A)-H(28A)	->	Cg3	2.78	2.73	11.23	124	3.407(3)	41
C(28B)-H(28B)	->	Cg28	2.98	-2.86	15.92	119	3.542(4)	40

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (2) N4A --> C9A --> C10A --> C15A --> C16A -->

5-Membered Ring (3) N6A --> C17A --> C18A --> C23A --> C24A -->

5-Membered Ring (27) N4B --> C9B --> C10B --> C15B --> C16B -->

5-Membered Ring (28) N6B --> C17B --> C18B --> C23B --> C24B -->

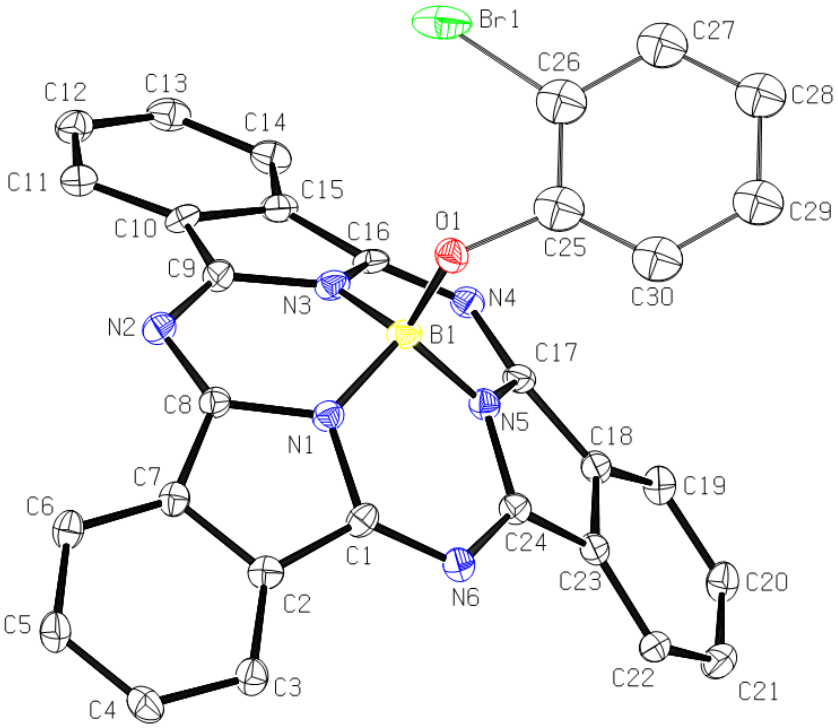

Figure S14. Anisotropic displacement ellipsoid plot of *o*-BrPhO-**BsubPc** (compound **4c**).

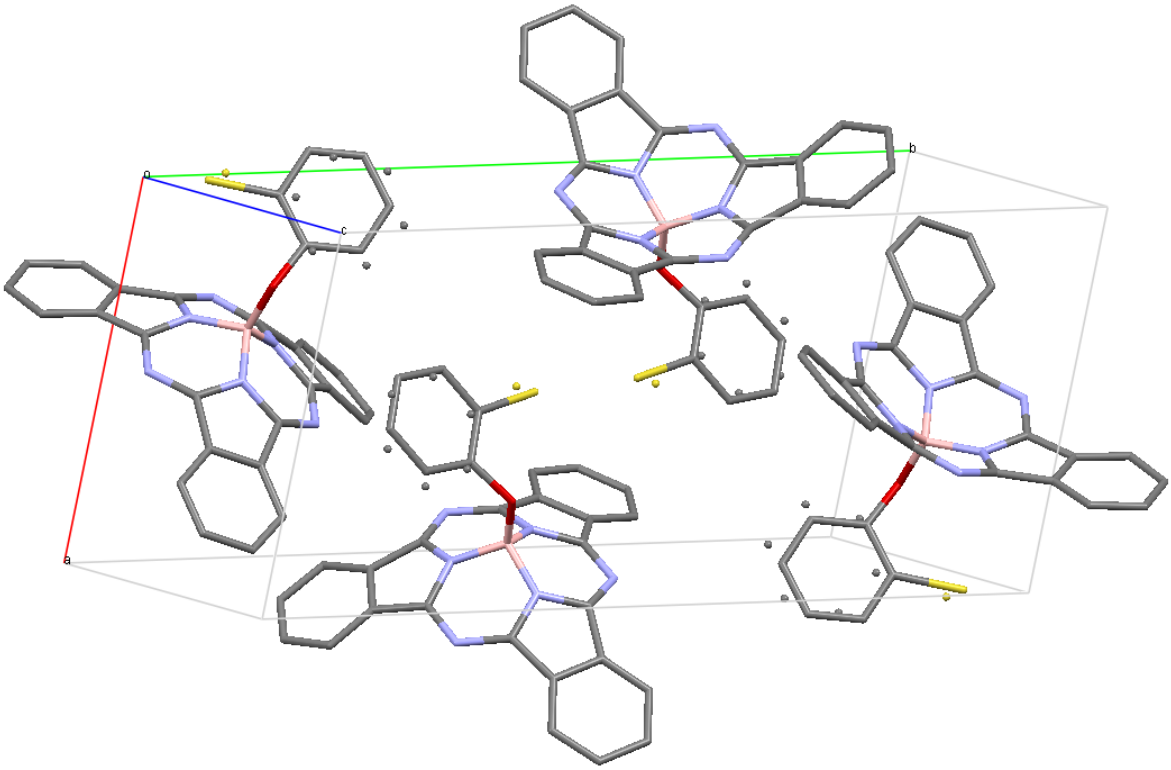

Figure S15. Populated unit cell of *o*-BrPhO-**BsubPc** (compound **4c**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow. Hydrogens are omitted for clarity.

Table S39. Crystal data and structure refinement for *o*-BrPhO-**BsubPc** (compound **4c**).

Identification code	k11190	
Empirical formula	C30 H16 B Br N6 O	
Formula weight	567.21	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.8223(5) Å	α= 90°.
	b = 20.6856(11) Å	β= 112.325(3)°.
	c = 11.5946(4) Å	γ = 90°.
Volume	2401.07(19) $Å^3$	
Z	4	
Density (calculated)	1.569 Mg/m^3	
Absorption coefficient	1.751 mm^{-1}	
F(000)	1144	
Crystal size	0.22 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.74 to 25.00°.	
Index ranges	-12<=h<=12, -24<=k<=24, -13<=l<=13	
Reflections collected	20402	
Independent reflections	4227 [R(int) = 0.0800]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.868 and 0.724	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4227 / 4 / 326	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0865, wR2 = 0.2227	
R indices (all data)	R1 = 0.1398, wR2 = 0.2668	
Largest diff. peak and hole	2.271 and -0.914 $e.Å^{-3}$	

Table S40. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *o*-BrPhO-**BsubPc** (compound **4c**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	76(4)	760(2)	387(3)	54(1)
Br(1A)	-77(8)	993(5)	302(8)	141(3)
O(1)	2570(4)	1327(2)	2441(4)	30(1)
N(1)	4892(5)	967(2)	3217(4)	25(1)
N(2)	4640(5)	-149(2)	2675(4)	27(1)
N(3)	3520(5)	663(2)	1185(4)	27(1)
N(4)	3274(5)	1365(2)	-498(4)	26(1)
N(5)	4218(5)	1738(2)	1600(4)	23(1)
N(6)	6035(5)	1970(2)	3490(4)	25(1)
C(1)	5899(6)	1375(3)	3899(5)	26(1)
C(2)	6841(6)	979(3)	4867(5)	26(1)
C(3)	8026(6)	1133(3)	5854(5)	30(1)
C(4)	8746(6)	628(3)	6588(6)	35(2)
C(5)	8303(7)	-11(3)	6371(6)	33(2)
C(6)	7146(6)	-167(3)	5379(5)	29(1)
C(7)	6399(6)	330(3)	4630(5)	25(1)
C(8)	5195(6)	329(3)	3484(5)	24(1)
C(9)	3867(6)	31(3)	1504(5)	27(1)
C(10)	3451(6)	-322(3)	333(6)	28(1)
C(11)	3471(6)	-978(3)	46(6)	33(2)
C(12)	2970(6)	-1156(3)	-1187(6)	33(2)
C(13)	2502(6)	-700(3)	-2147(6)	35(2)
C(14)	2544(6)	-46(3)	-1891(5)	33(2)
C(15)	2997(6)	147(3)	-644(6)	30(1)
C(16)	3174(5)	778(3)	-56(5)	24(1)
C(17)	3873(5)	1827(3)	340(5)	25(1)
C(18)	4576(6)	2407(3)	231(5)	26(1)
C(19)	4598(6)	2742(3)	-803(6)	31(1)

C(20)	5433(6)	3273(3)	-603(6)	34(2)
C(21)	6269(6)	3451(3)	608(6)	36(2)
C(22)	6294(6)	3119(3)	1652(5)	27(1)
C(23)	5432(6)	2600(3)	1463(5)	25(1)
C(24)	5240(6)	2127(3)	2311(5)	25(1)
C(25)	1621(9)	1809(3)	1827(11)	50(1)
C(26)	446(8)	1589(3)	908(9)	50(1)
C(27)	-592(6)	2018(4)	320(8)	50(1)
C(28)	-455(7)	2667(4)	652(9)	50(1)
C(29)	720(10)	2888(3)	1572(9)	50(1)
C(30)	1758(9)	2459(3)	2159(10)	50(1)
C(25A)	1766(10)	1879(3)	1973(15)	50(1)
C(26A)	478(9)	1746(4)	1138(12)	50(1)
C(27A)	-469(8)	2237(6)	756(11)	50(1)
C(28A)	-126(11)	2861(5)	1209(14)	50(1)
C(29A)	1162(14)	2994(3)	2044(14)	50(1)
C(30A)	2108(12)	2503(3)	2426(15)	50(1)
B(1)	3706(7)	1192(3)	2117(6)	26(2)

Table S41. Bond lengths [Å] and angles [°] for *o*-BrPhO-**BsubPc** (compound **4c**).

Br(1)-C(26)	1.810(5)
Br(1A)-C(26A)	1.812(6)
O(1)-C(25A)	1.412(6)
O(1)-C(25)	1.414(6)
O(1)-B(1)	1.443(8)
N(1)-C(8)	1.367(7)
N(1)-C(1)	1.367(7)
N(1)-B(1)	1.499(8)
N(2)-C(8)	1.337(7)
N(2)-C(9)	1.349(8)
N(3)-C(16)	1.364(7)
N(3)-C(9)	1.371(7)
N(3)-B(1)	1.497(9)
N(4)-C(16)	1.337(7)
N(4)-C(17)	1.341(7)
N(5)-C(24)	1.362(7)
N(5)-C(17)	1.376(7)
N(5)-B(1)	1.482(8)
N(6)-C(1)	1.348(7)
N(6)-C(24)	1.349(7)
C(1)-C(2)	1.449(8)
C(2)-C(3)	1.393(8)
C(2)-C(7)	1.417(8)
C(3)-C(4)	1.385(9)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.397(9)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.378(9)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.389(8)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.466(8)

C(9)-C(10)	1.454(8)
C(10)-C(11)	1.400(9)
C(10)-C(15)	1.429(9)
C(11)-C(12)	1.373(9)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.399(10)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.382(9)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.396(8)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.451(8)
C(17)-C(18)	1.451(8)
C(18)-C(19)	1.393(8)
C(18)-C(23)	1.433(8)
C(19)-C(20)	1.386(9)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.399(9)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.382(9)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.384(8)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.458(8)
C(25)-C(26)	1.3900
C(25)-C(30)	1.3900
C(26)-C(27)	1.3900
C(27)-C(28)	1.3900
C(27)-H(27A)	0.9500
C(28)-C(29)	1.3900
C(28)-H(28A)	0.9500
C(29)-C(30)	1.3900
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500

C(25A)-C(26A)	1.3900
C(25A)-C(30A)	1.3900
C(26A)-C(27A)	1.3900
C(27A)-C(28A)	1.3900
C(27A)-H(27B)	0.9500
C(28A)-C(29A)	1.3900
C(28A)-H(28B)	0.9500
C(29A)-C(30A)	1.3900
C(29A)-H(29B)	0.9500
C(30A)-H(30B)	0.9500

C(25A)-O(1)-C(25)	9.4(4)
C(25A)-O(1)-B(1)	121.2(9)
C(25)-O(1)-B(1)	122.2(8)
C(8)-N(1)-C(1)	113.2(5)
C(8)-N(1)-B(1)	123.1(5)
C(1)-N(1)-B(1)	122.5(5)
C(8)-N(2)-C(9)	116.4(5)
C(16)-N(3)-C(9)	112.9(5)
C(16)-N(3)-B(1)	122.8(5)
C(9)-N(3)-B(1)	123.7(5)
C(16)-N(4)-C(17)	117.2(5)
C(24)-N(5)-C(17)	113.2(5)
C(24)-N(5)-B(1)	123.2(5)
C(17)-N(5)-B(1)	122.6(5)
C(1)-N(6)-C(24)	117.6(5)
N(6)-C(1)-N(1)	122.0(5)
N(6)-C(1)-C(2)	130.5(5)
N(1)-C(1)-C(2)	105.8(5)
C(3)-C(2)-C(7)	120.9(5)
C(3)-C(2)-C(1)	131.7(6)
C(7)-C(2)-C(1)	107.4(5)
C(4)-C(3)-C(2)	117.4(6)
C(4)-C(3)-H(3A)	121.3

C(2)-C(3)-H(3A)	121.3
C(3)-C(4)-C(5)	121.9(6)
C(3)-C(4)-H(4A)	119.1
C(5)-C(4)-H(4A)	119.1
C(6)-C(5)-C(4)	120.8(6)
C(6)-C(5)-H(5A)	119.6
C(4)-C(5)-H(5A)	119.6
C(5)-C(6)-C(7)	118.5(6)
C(5)-C(6)-H(6A)	120.7
C(7)-C(6)-H(6A)	120.7
C(6)-C(7)-C(2)	120.4(5)
C(6)-C(7)-C(8)	132.2(5)
C(2)-C(7)-C(8)	107.2(5)
N(2)-C(8)-N(1)	123.3(5)
N(2)-C(8)-C(7)	130.1(5)
N(1)-C(8)-C(7)	105.0(5)
N(2)-C(9)-N(3)	122.4(5)
N(2)-C(9)-C(10)	131.0(5)
N(3)-C(9)-C(10)	105.7(5)
C(11)-C(10)-C(15)	120.1(6)
C(11)-C(10)-C(9)	132.9(6)
C(15)-C(10)-C(9)	106.9(5)
C(12)-C(11)-C(10)	118.1(6)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.9(6)
C(11)-C(12)-H(12A)	119.0
C(13)-C(12)-H(12A)	119.0
C(14)-C(13)-C(12)	121.1(6)
C(14)-C(13)-H(13A)	119.5
C(12)-C(13)-H(13A)	119.5
C(13)-C(14)-C(15)	118.2(6)
C(13)-C(14)-H(14A)	120.9
C(15)-C(14)-H(14A)	120.9

C(14)-C(15)-C(10)	120.4(6)
C(14)-C(15)-C(16)	132.5(6)
C(10)-C(15)-C(16)	107.1(5)
N(4)-C(16)-N(3)	122.2(5)
N(4)-C(16)-C(15)	130.7(5)
N(3)-C(16)-C(15)	105.8(5)
N(4)-C(17)-N(5)	122.4(5)
N(4)-C(17)-C(18)	130.6(5)
N(5)-C(17)-C(18)	105.2(5)
C(19)-C(18)-C(23)	120.2(6)
C(19)-C(18)-C(17)	131.8(5)
C(23)-C(18)-C(17)	107.9(5)
C(20)-C(19)-C(18)	118.3(6)
C(20)-C(19)-H(19A)	120.9
C(18)-C(19)-H(19A)	120.9
C(19)-C(20)-C(21)	120.5(6)
C(19)-C(20)-H(20A)	119.7
C(21)-C(20)-H(20A)	119.7
C(22)-C(21)-C(20)	122.6(6)
C(22)-C(21)-H(21A)	118.7
C(20)-C(21)-H(21A)	118.7
C(21)-C(22)-C(23)	117.3(5)
C(21)-C(22)-H(22A)	121.4
C(23)-C(22)-H(22A)	121.4
C(22)-C(23)-C(18)	121.1(5)
C(22)-C(23)-C(24)	132.4(5)
C(18)-C(23)-C(24)	106.3(5)
N(6)-C(24)-N(5)	122.1(5)
N(6)-C(24)-C(23)	130.2(5)
N(5)-C(24)-C(23)	106.2(5)
C(26)-C(25)-C(30)	120.0
C(26)-C(25)-O(1)	115.6(5)
C(30)-C(25)-O(1)	124.2(5)
C(25)-C(26)-C(27)	120.0

C(25)-C(26)-Br(1)	126.1(4)
C(27)-C(26)-Br(1)	113.9(4)
C(26)-C(27)-C(28)	120.0
C(26)-C(27)-H(27A)	120.0
C(28)-C(27)-H(27A)	120.0
C(29)-C(28)-C(27)	120.0
C(29)-C(28)-H(28A)	120.0
C(27)-C(28)-H(28A)	120.0
C(28)-C(29)-C(30)	120.0
C(28)-C(29)-H(29A)	120.0
C(30)-C(29)-H(29A)	120.0
C(29)-C(30)-C(25)	120.0
C(29)-C(30)-H(30A)	120.0
C(25)-C(30)-H(30A)	120.0
C(26A)-C(25A)-C(30A)	120.0
C(26A)-C(25A)-O(1)	114.6(5)
C(30A)-C(25A)-O(1)	124.6(5)
C(25A)-C(26A)-C(27A)	120.0
C(25A)-C(26A)-Br(1A)	125.7(4)
C(27A)-C(26A)-Br(1A)	113.8(4)
C(26A)-C(27A)-C(28A)	120.0
C(26A)-C(27A)-H(27B)	120.0
C(28A)-C(27A)-H(27B)	120.0
C(29A)-C(28A)-C(27A)	120.0
C(29A)-C(28A)-H(28B)	120.0
C(27A)-C(28A)-H(28B)	120.0
C(30A)-C(29A)-C(28A)	120.0
C(30A)-C(29A)-H(29B)	120.0
C(28A)-C(29A)-H(29B)	120.0
C(29A)-C(30A)-C(25A)	120.0
C(29A)-C(30A)-H(30B)	120.0
C(25A)-C(30A)-H(30B)	120.0
O(1)-B(1)-N(5)	116.3(5)
O(1)-B(1)-N(3)	115.8(5)

N(5)-B(1)-N(3)	103.6(5)
O(1)-B(1)-N(1)	112.2(5)
N(5)-B(1)-N(1)	104.5(5)
N(3)-B(1)-N(1)	102.9(5)

Symmetry transformations used to generate equivalent atoms:

Table S42. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *o*-BrPhO-**BsubPc** (compound **4c**). 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}
Br(1)	33(1)	87(2)	36(1)	4(1)	5(1)	-19(1)
Br(1A)	53(2)	242(8)	120(5)	-62(5)	23(3)	-16(4)
O(1)	28(2)	30(2)	34(2)	7(2)	12(2)	2(2)
N(1)	25(3)	24(3)	24(3)	-1(2)	8(2)	-2(2)
N(2)	28(3)	26(3)	27(3)	1(2)	12(2)	-3(2)
N(3)	26(3)	28(3)	21(3)	-1(2)	4(2)	-6(2)
N(4)	24(3)	29(3)	21(2)	0(2)	3(2)	-1(2)
N(5)	24(3)	25(3)	19(2)	0(2)	5(2)	1(2)
N(6)	28(3)	26(3)	20(2)	-2(2)	7(2)	2(2)
C(1)	33(3)	23(3)	23(3)	-2(2)	12(3)	-4(3)
C(2)	28(3)	32(3)	21(3)	2(2)	12(3)	-2(3)
C(3)	36(4)	27(3)	26(3)	0(2)	9(3)	2(3)
C(4)	29(3)	40(4)	31(3)	6(3)	6(3)	6(3)
C(5)	41(4)	26(4)	31(3)	4(3)	11(3)	6(3)
C(6)	39(4)	24(3)	26(3)	0(2)	14(3)	2(3)
C(7)	30(3)	24(3)	25(3)	2(2)	14(3)	1(3)
C(8)	24(3)	24(3)	27(3)	1(2)	12(3)	-1(2)
C(9)	27(3)	24(3)	31(3)	1(2)	12(3)	-1(3)
C(10)	26(3)	25(3)	31(3)	-3(2)	10(3)	-10(3)
C(11)	26(3)	33(4)	41(4)	1(3)	13(3)	-3(3)
C(12)	30(3)	32(4)	40(4)	-12(3)	15(3)	-4(3)
C(13)	28(3)	46(4)	31(3)	-12(3)	11(3)	-5(3)
C(14)	28(3)	42(4)	29(3)	-3(3)	11(3)	-1(3)
C(15)	22(3)	33(4)	34(3)	-3(3)	9(3)	-6(3)
C(16)	18(3)	30(3)	25(3)	0(2)	8(2)	-8(2)
C(17)	20(3)	28(3)	24(3)	2(2)	4(2)	-1(2)
C(18)	25(3)	25(3)	27(3)	1(2)	9(3)	3(2)
C(19)	36(4)	28(3)	29(3)	1(3)	12(3)	4(3)

C(20)	41(4)	27(4)	33(3)	4(3)	13(3)	3(3)
C(21)	36(4)	28(3)	40(4)	3(3)	12(3)	-6(3)
C(22)	25(3)	24(3)	29(3)	1(2)	7(3)	-2(3)
C(23)	24(3)	24(3)	26(3)	1(2)	8(3)	4(2)
C(24)	25(3)	26(3)	22(3)	-1(2)	8(3)	0(2)
C(25)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(26)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(27)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(28)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(29)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(30)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(25A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(26A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(27A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(28A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(29A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
C(30A)	50(3)	64(3)	43(3)	5(2)	26(2)	-3(2)
B(1)	22(3)	31(4)	22(3)	5(3)	5(3)	-5(3)

Table S43. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *o*-BrPhO-**BsubPc** (compound **4c**).

	x	y	z	U(eq)
H(3A)	8329	1567	6016	36
H(4A)	9564	720	7260	42
H(5A)	8805	-343	6913	40
H(6A)	6866	-604	5211	35
H(11A)	3821	-1292	687	40
H(12A)	2940	-1601	-1394	40
H(13A)	2150	-842	-2989	42
H(14A)	2272	264	-2545	40
H(19A)	4055	2609	-1625	38
H(20A)	5438	3520	-1293	41
H(21A)	6841	3813	716	43
H(22A)	6880	3243	2465	33
H(27A)	-1395	1867	-309	60
H(28A)	-1164	2960	250	60
H(29A)	814	3332	1799	60
H(30A)	2561	2609	2788	60
H(27B)	-1349	2146	185	60
H(28B)	-773	3196	947	60
H(29B)	1396	3421	2353	60
H(30B)	2989	2594	2997	60

Table S44. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *o*-BrPhO-**BsubPc** (compound **4c**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(3)-H(3A)	->	Cg(9)	2.81	-2.68	17.92	123	3.430(7)	51
C(12)-H(12A)	->	Cg(3)	2.74	2.65	14.83	116	3.268(7)	40
C(13)-H(13A)	->	Cg(1)	2.85	2.74	15.5	110	3.302(7)	36

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(5) --> C(17) --> C(18) --> C(23) --> C(24) -->

6-Membered Ring (9) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

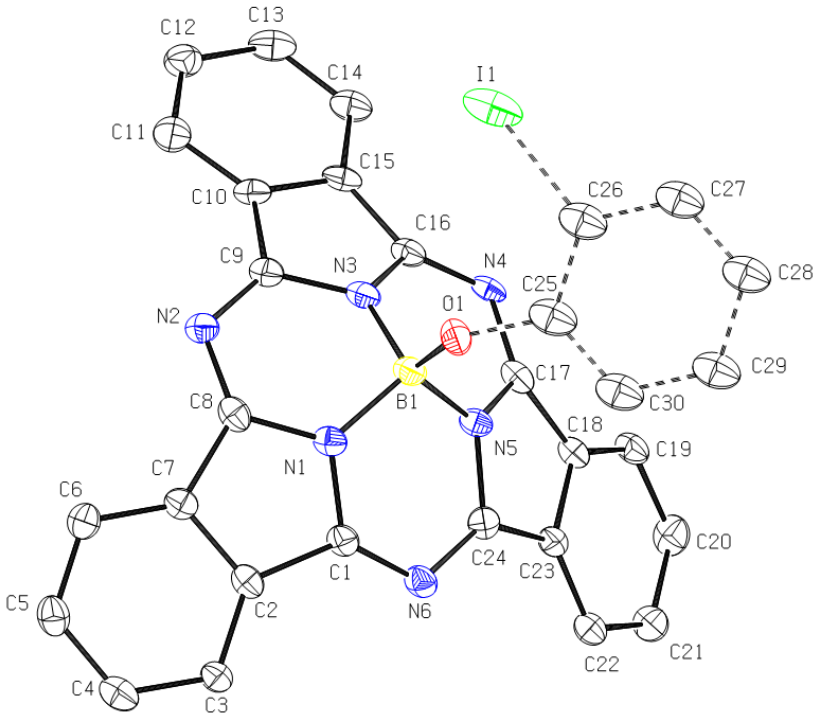

Figure S16. Anisotropic displacement ellipsoid plot of *o*-IPhO-**BsubPc** (compound **4d**).

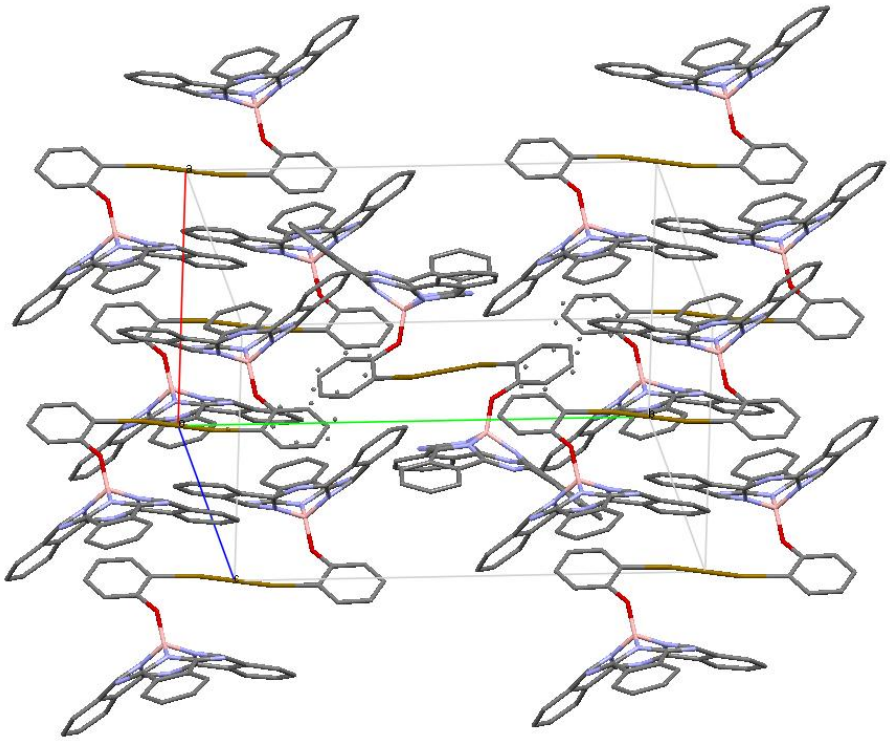

Figure S17. Populated unit cell of *o*-IPhO-**BsubPc** (compound **4d**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; iodine = brown. Hydrogens are omitted for clarity.

Table S45. Crystal data and structure refinement for *o*-IPhO-**BsubPc** (compound **4d**).

Identification code	k11175	
Empirical formula	C30 H16 B I N6 O	
Formula weight	614.20	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.0324(5) Å	α= 90°.
	b = 20.5587(8) Å	β= 112.710(2)°.
	c = 11.6778(6) Å	γ = 90°.
Volume	2443.31(19) $Å^3$	
Z	4	
Density (calculated)	1.670 Mg/m^3	
Absorption coefficient	1.349 mm^{-1}	
F(000)	1216	
Crystal size	0.18 x 0.14 x 0.12 mm^3	
Theta range for data collection	2.74 to 25.00°.	
Index ranges	-13<=h<=13, -24<=k<=24, -13<=l<=13	
Reflections collected	15379	
Independent reflections	4282 [R(int) = 0.0920]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.900 and 0.607	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4282 / 4 / 326	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0914, wR2 = 0.2426	
R indices (all data)	R1 = 0.1609, wR2 = 0.3026	
Largest diff. peak and hole	1.627 and -1.298 e.$Å^{-3}$	

Table S46. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *o*-IPhO-**BsubPc** (compound **4d**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	-14(5)	741(3)	322(4)	72(1)
I(1A)	-116(4)	1052(4)	111(6)	110(2)
O(1)	2603(5)	1320(2)	2413(5)	39(1)
N(1)	4890(6)	963(3)	3202(6)	30(2)
N(2)	4653(6)	-158(3)	2664(6)	33(2)
N(3)	3538(6)	658(3)	1180(6)	34(2)
N(4)	3285(6)	1370(3)	-497(6)	33(2)
N(5)	4213(6)	1747(3)	1588(5)	30(2)
N(6)	6041(6)	1974(3)	3475(6)	35(2)
C(1)	5893(8)	1381(4)	3876(7)	32(2)
C(2)	6821(8)	972(4)	4855(7)	32(2)
C(3)	8004(8)	1122(4)	5811(7)	35(2)
C(4)	8725(8)	618(4)	6546(8)	44(2)
C(5)	8261(9)	-28(4)	6333(8)	42(2)
C(6)	7108(8)	-178(4)	5359(8)	38(2)
C(7)	6389(8)	321(4)	4609(7)	32(2)
C(8)	5199(8)	322(4)	3466(7)	36(2)
C(9)	3887(8)	23(4)	1504(7)	33(2)
C(10)	3485(8)	-327(4)	321(7)	34(2)
C(11)	3512(9)	-985(4)	37(9)	43(2)
C(12)	3009(8)	-1167(4)	-1193(8)	43(2)
C(13)	2525(8)	-704(4)	-2156(8)	45(2)
C(14)	2566(9)	-45(4)	-1890(8)	42(2)
C(15)	3026(7)	146(4)	-647(8)	36(2)
C(16)	3203(7)	780(4)	-60(7)	33(2)
C(17)	3869(7)	1836(4)	337(7)	34(2)
C(18)	4580(7)	2426(4)	216(7)	31(2)
C(19)	4581(8)	2756(4)	-796(7)	36(2)

C(20)	5424(9)	3285(4)	-592(8)	45(2)
C(21)	6260(8)	3465(4)	611(8)	41(2)
C(22)	6284(8)	3128(4)	1646(7)	35(2)
C(23)	5414(7)	2610(3)	1440(7)	32(2)
C(24)	5248(8)	2139(3)	2312(7)	32(2)
C(25)	1685(11)	1808(4)	1945(16)	53(1)
C(26)	435(10)	1648(5)	1101(13)	53(1)
C(27)	-522(9)	2128(6)	657(13)	53(1)
C(28)	-228(11)	2767(5)	1055(14)	53(1)
C(29)	1023(13)	2927(4)	1898(14)	53(1)
C(30)	1979(11)	2447(4)	2343(15)	53(1)
C(25A)	1910(9)	1892(3)	2042(12)	53(1)
C(26A)	620(8)	1861(4)	1183(10)	53(1)
C(27A)	-175(8)	2410(5)	936(10)	53(1)
C(28A)	320(10)	2990(4)	1549(11)	53(1)
C(29A)	1609(11)	3022(3)	2408(11)	53(1)
C(30A)	2404(9)	2473(4)	2655(12)	53(1)
B(1)	3726(9)	1182(4)	2110(8)	33(2)

Table S47. Bond lengths [Å] and angles [°] for *o*-IPhO-**BsubPc** (compound **4d**).

I(1)-C(26)	2.051(7)
I(1)-I(1)#1	3.141(13)
I(1A)-C(26A)	2.050(7)
O(1)-C(25A)	1.378(7)
O(1)-C(25)	1.379(7)
O(1)-B(1)	1.442(11)
N(1)-C(8)	1.366(10)
N(1)-C(1)	1.381(10)
N(1)-B(1)	1.488(11)
N(2)-C(8)	1.334(10)
N(2)-C(9)	1.343(10)
N(3)-C(16)	1.372(10)
N(3)-C(9)	1.372(10)
N(3)-B(1)	1.487(11)
N(4)-C(16)	1.333(10)
N(4)-C(17)	1.339(10)
N(5)-C(17)	1.373(10)
N(5)-C(24)	1.386(10)
N(5)-B(1)	1.503(11)
N(6)-C(1)	1.339(9)
N(6)-C(24)	1.344(9)
C(1)-C(2)	1.469(10)
C(2)-C(3)	1.386(11)
C(2)-C(7)	1.412(11)
C(3)-C(4)	1.384(11)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.409(12)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.375(12)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.384(11)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.467(11)
C(9)-C(10)	1.467(11)
C(10)-C(11)	1.395(11)
C(10)-C(15)	1.429(12)
C(11)-C(12)	1.377(12)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.411(13)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.388(12)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.397(12)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.449(11)
C(17)-C(18)	1.481(11)
C(18)-C(19)	1.363(11)
C(18)-C(23)	1.421(10)
C(19)-C(20)	1.390(12)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.401(12)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.384(11)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.391(11)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.468(11)
C(25)-C(26)	1.3900
C(25)-C(30)	1.3900
C(26)-C(27)	1.3900
C(27)-C(28)	1.3900
C(27)-H(27A)	0.9500
C(28)-C(29)	1.3900
C(28)-H(28A)	0.9500
C(29)-C(30)	1.3900
C(29)-H(29A)	0.9500

C(30)-H(30A)	0.9500
C(25A)-C(26A)	1.3900
C(25A)-C(30A)	1.3900
C(26A)-C(27A)	1.3900
C(27A)-C(28A)	1.3900
C(27A)-H(27B)	0.9500
C(28A)-C(29A)	1.3900
C(28A)-H(28B)	0.9500
C(29A)-C(30A)	1.3900
C(29A)-H(29B)	0.9500
C(30A)-H(30B)	0.9500

C(26)-I(1)-I(1)#1	164.9(3)
C(25A)-O(1)-C(25)	12.0(6)
C(25A)-O(1)-B(1)	121.1(8)
C(25)-O(1)-B(1)	127.9(11)
C(8)-N(1)-C(1)	113.3(6)
C(8)-N(1)-B(1)	122.9(6)
C(1)-N(1)-B(1)	122.5(6)
C(8)-N(2)-C(9)	116.1(6)
C(16)-N(3)-C(9)	113.4(6)
C(16)-N(3)-B(1)	122.9(6)
C(9)-N(3)-B(1)	122.9(7)
C(16)-N(4)-C(17)	117.2(6)
C(17)-N(5)-C(24)	113.3(6)
C(17)-N(5)-B(1)	122.6(6)
C(24)-N(5)-B(1)	122.7(6)
C(1)-N(6)-C(24)	117.5(6)
N(6)-C(1)-N(1)	123.1(6)
N(6)-C(1)-C(2)	130.6(7)
N(1)-C(1)-C(2)	104.6(6)
C(3)-C(2)-C(7)	120.9(7)
C(3)-C(2)-C(1)	131.1(7)
C(7)-C(2)-C(1)	107.8(7)

C(4)-C(3)-C(2)	118.1(7)
C(4)-C(3)-H(3A)	121.0
C(2)-C(3)-H(3A)	121.0
C(3)-C(4)-C(5)	120.9(8)
C(3)-C(4)-H(4A)	119.6
C(5)-C(4)-H(4A)	119.6
C(6)-C(5)-C(4)	121.0(8)
C(6)-C(5)-H(5A)	119.5
C(4)-C(5)-H(5A)	119.5
C(5)-C(6)-C(7)	118.5(8)
C(5)-C(6)-H(6A)	120.7
C(7)-C(6)-H(6A)	120.7
C(6)-C(7)-C(2)	120.6(7)
C(6)-C(7)-C(8)	132.0(7)
C(2)-C(7)-C(8)	107.3(7)
N(2)-C(8)-N(1)	123.4(7)
N(2)-C(8)-C(7)	129.8(7)
N(1)-C(8)-C(7)	105.3(7)
N(2)-C(9)-N(3)	122.8(7)
N(2)-C(9)-C(10)	131.1(7)
N(3)-C(9)-C(10)	104.9(7)
C(11)-C(10)-C(15)	120.4(8)
C(11)-C(10)-C(9)	132.3(8)
C(15)-C(10)-C(9)	107.2(6)
C(12)-C(11)-C(10)	118.3(8)
C(12)-C(11)-H(11A)	120.8
C(10)-C(11)-H(11A)	120.8
C(11)-C(12)-C(13)	121.6(8)
C(11)-C(12)-H(12A)	119.2
C(13)-C(12)-H(12A)	119.2
C(14)-C(13)-C(12)	120.8(8)
C(14)-C(13)-H(13A)	119.6
C(12)-C(13)-H(13A)	119.6
C(13)-C(14)-C(15)	118.3(8)

C(13)-C(14)-H(14A)	120.8
C(15)-C(14)-H(14A)	120.8
C(14)-C(15)-C(10)	120.4(7)
C(14)-C(15)-C(16)	132.3(8)
C(10)-C(15)-C(16)	107.3(7)
N(4)-C(16)-N(3)	122.6(7)
N(4)-C(16)-C(15)	130.8(7)
N(3)-C(16)-C(15)	105.5(6)
N(4)-C(17)-N(5)	122.4(7)
N(4)-C(17)-C(18)	129.8(7)
N(5)-C(17)-C(18)	105.7(6)
C(19)-C(18)-C(23)	121.5(7)
C(19)-C(18)-C(17)	132.0(7)
C(23)-C(18)-C(17)	106.5(7)
C(18)-C(19)-C(20)	117.8(7)
C(18)-C(19)-H(19A)	121.1
C(20)-C(19)-H(19A)	121.1
C(19)-C(20)-C(21)	121.1(8)
C(19)-C(20)-H(20A)	119.4
C(21)-C(20)-H(20A)	119.4
C(22)-C(21)-C(20)	121.8(8)
C(22)-C(21)-H(21A)	119.1
C(20)-C(21)-H(21A)	119.1
C(21)-C(22)-C(23)	116.9(7)
C(21)-C(22)-H(22A)	121.5
C(23)-C(22)-H(22A)	121.5
C(22)-C(23)-C(18)	120.9(7)
C(22)-C(23)-C(24)	130.4(7)
C(18)-C(23)-C(24)	108.4(6)
N(6)-C(24)-N(5)	122.1(7)
N(6)-C(24)-C(23)	131.3(7)
N(5)-C(24)-C(23)	104.8(6)
O(1)-C(25)-C(26)	119.0(6)
O(1)-C(25)-C(30)	120.9(6)

C(26)-C(25)-C(30)	120.0
C(25)-C(26)-C(27)	120.0
C(25)-C(26)-I(1)	122.2(4)
C(27)-C(26)-I(1)	117.5(4)
C(26)-C(27)-C(28)	120.0
C(26)-C(27)-H(27A)	120.0
C(28)-C(27)-H(27A)	120.0
C(29)-C(28)-C(27)	120.0
C(29)-C(28)-H(28A)	120.0
C(27)-C(28)-H(28A)	120.0
C(28)-C(29)-C(30)	120.0
C(28)-C(29)-H(29A)	120.0
C(30)-C(29)-H(29A)	120.0
C(29)-C(30)-C(25)	120.0
C(29)-C(30)-H(30A)	120.0
C(25)-C(30)-H(30A)	120.0
O(1)-C(25A)-C(26A)	118.5(6)
O(1)-C(25A)-C(30A)	120.7(6)
C(26A)-C(25A)-C(30A)	120.0
C(25A)-C(26A)-C(27A)	120.0
C(25A)-C(26A)-I(1A)	122.1(4)
C(27A)-C(26A)-I(1A)	117.5(4)
C(26A)-C(27A)-C(28A)	120.0
C(26A)-C(27A)-H(27B)	120.0
C(28A)-C(27A)-H(27B)	120.0
C(29A)-C(28A)-C(27A)	120.0
C(29A)-C(28A)-H(28B)	120.0
C(27A)-C(28A)-H(28B)	120.0
C(30A)-C(29A)-C(28A)	120.0
C(30A)-C(29A)-H(29B)	120.0
C(28A)-C(29A)-H(29B)	120.0
C(29A)-C(30A)-C(25A)	120.0
C(29A)-C(30A)-H(30B)	120.0
C(25A)-C(30A)-H(30B)	120.0

O(1)-B(1)-N(3)	115.5(7)
O(1)-B(1)-N(1)	112.8(7)
N(3)-B(1)-N(1)	103.7(6)
O(1)-B(1)-N(5)	115.0(7)
N(3)-B(1)-N(5)	103.6(7)
N(1)-B(1)-N(5)	104.8(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table S48. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *o*-IPhO-**BsubPc** (compound **4d**). 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}
I(1)	44(1)	124(3)	42(1)	-6(2)	11(1)	-19(2)
I(1A)	45(1)	161(4)	114(3)	-78(3)	21(2)	-17(2)
O(1)	32(3)	39(3)	44(3)	11(2)	14(3)	5(2)
N(1)	33(4)	38(4)	19(3)	3(3)	10(3)	-5(3)
N(2)	34(4)	35(3)	30(4)	-1(3)	11(3)	-5(3)
N(3)	25(3)	41(4)	29(4)	-1(3)	4(3)	-5(3)
N(4)	25(3)	47(4)	19(3)	-1(3)	-2(3)	-2(3)
N(5)	29(3)	38(4)	20(3)	-2(3)	7(3)	-2(3)
N(6)	36(4)	40(4)	23(4)	1(3)	7(3)	2(3)
C(1)	36(4)	37(4)	20(4)	2(3)	9(3)	0(4)
C(2)	32(4)	43(5)	22(4)	7(3)	12(4)	3(3)
C(3)	34(4)	37(4)	28(4)	1(3)	6(4)	0(4)
C(4)	34(5)	59(6)	34(5)	4(4)	8(4)	-1(4)
C(5)	49(6)	44(5)	34(5)	8(4)	16(4)	10(4)
C(6)	43(5)	36(4)	38(5)	4(4)	19(4)	0(4)
C(7)	33(4)	39(4)	26(4)	-2(3)	12(4)	0(4)
C(8)	32(4)	45(5)	30(5)	8(4)	13(4)	4(4)
C(9)	29(4)	39(5)	31(5)	-1(3)	10(4)	-5(3)
C(10)	30(4)	41(5)	28(4)	-4(4)	9(4)	-13(4)
C(11)	36(5)	46(5)	50(6)	1(4)	20(4)	-3(4)
C(12)	40(5)	45(5)	44(5)	-12(4)	14(4)	-2(4)
C(13)	35(5)	67(6)	38(5)	-14(5)	20(4)	-16(4)
C(14)	37(5)	58(6)	29(5)	-4(4)	9(4)	-8(4)
C(15)	19(4)	52(5)	34(5)	-7(4)	7(4)	-8(3)
C(16)	27(4)	43(5)	24(4)	3(3)	5(3)	-5(3)
C(17)	24(4)	47(5)	28(5)	9(4)	9(3)	3(3)
C(18)	24(4)	40(4)	27(4)	3(3)	8(3)	3(3)
C(19)	32(4)	45(5)	25(4)	5(4)	4(4)	1(4)

C(20)	58(6)	44(5)	38(5)	9(4)	22(5)	0(4)
C(21)	39(5)	43(5)	41(5)	7(4)	17(4)	-3(4)
C(22)	33(4)	41(4)	28(4)	3(3)	9(4)	2(4)
C(23)	30(4)	33(4)	28(4)	3(3)	6(3)	1(3)
C(24)	38(4)	34(4)	25(4)	-3(3)	13(4)	3(3)
C(25)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(26)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(27)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(28)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(29)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(30)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(25A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(26A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(27A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(28A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(29A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
C(30A)	39(3)	78(4)	43(4)	3(3)	18(3)	-12(3)
B(1)	29(5)	38(5)	29(5)	4(4)	6(4)	-5(4)

Table S49. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *o*-IPhO-**BsubPc** (compound **4d**).

	x	y	z	U(eq)
H(3A)	8312	1558	5959	42
H(4A)	9543	708	7202	53
H(5A)	8752	-364	6870	51
H(6A)	6812	-616	5204	46
H(11A)	3868	-1299	676	52
H(12A)	2988	-1615	-1398	52
H(13A)	2168	-846	-2995	54
H(14A)	2289	269	-2538	51
H(19A)	4025	2629	-1612	43
H(20A)	5432	3528	-1280	55
H(21A)	6827	3828	720	49
H(22A)	6867	3245	2459	42
H(27A)	-1377	2018	80	63
H(28A)	-882	3095	751	63
H(29A)	1223	3364	2170	63
H(30A)	2834	2556	2919	63
H(27B)	-1056	2389	349	63
H(28B)	-224	3366	1380	63
H(29B)	1947	3419	2827	63
H(30B)	3285	2494	3242	63

Table S50. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for *o*-IPhO-**BsubPc** (compound **4d**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(3)-H(3A)	->	Cg(9)	2.83	-2.69	18.12	125	3.457(10)	53
C(12)-H(12A)	->	Cg(3)	2.73	2.63	15.65	116	3.264(10)	41
C(13)-H(13A)	->	Cg(1)	2.87	2.76	16.06	109	3.309(10)	35

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(5) --> C(17) --> C(18) --> C(23) --> C(24) -->

6-Membered Ring (9) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

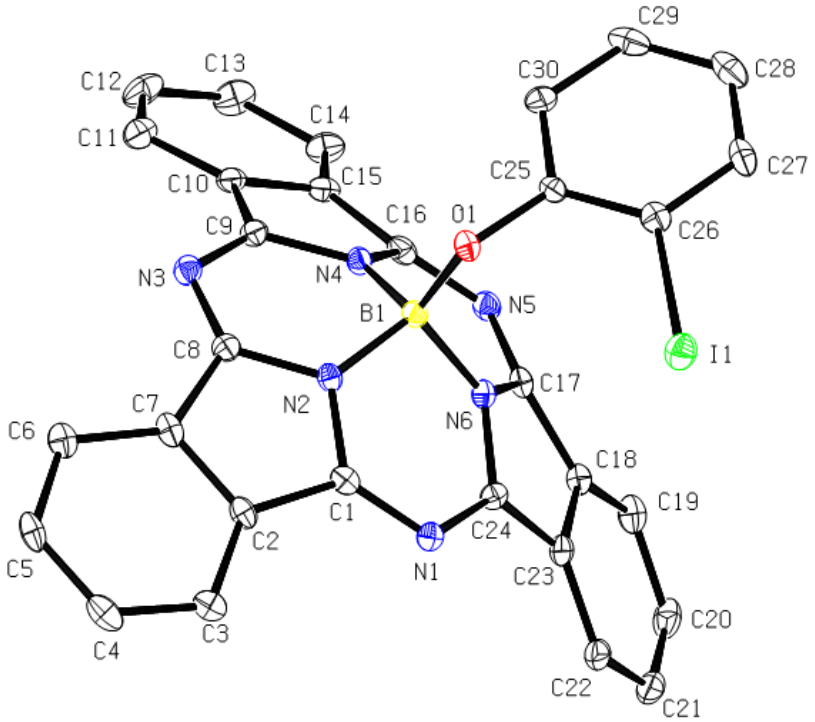

Figure S18. Anisotropic displacement ellipsoid plot of solvated *o*-IPhO-**BsubPc** (compound **4d** solvate).

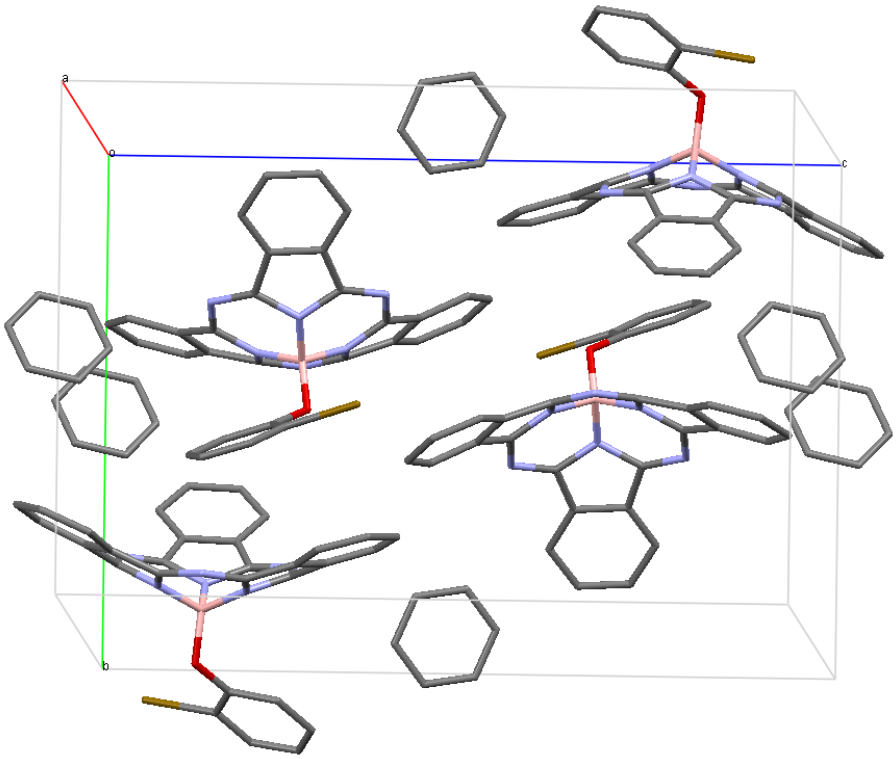

Figure S19. Populated unit cell of solvated *o*-IPhO-**BsubPc** (compound **4d**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; iodine = brown. Hydrogens are omitted for clarity.

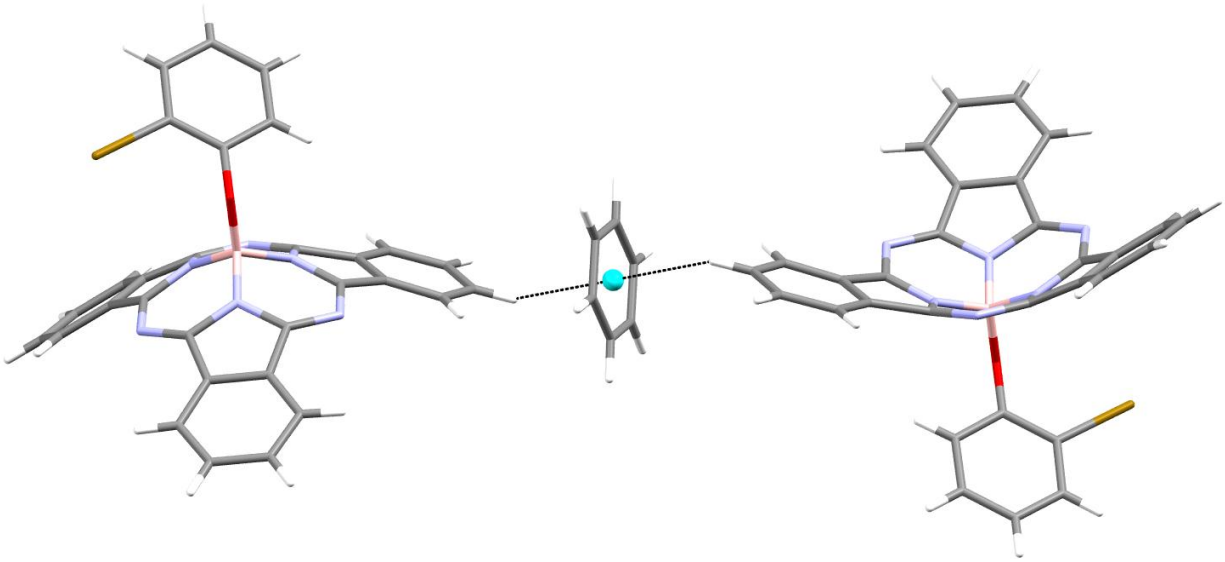

Figure S20. Illustration of the molecular packing arrangement within the single crystal (extended beyond the unit cell) of solvated *o*-IPhO-**BsubPc** (compound **4d**), showing close benzene-**BsubPc** contacts. The benzene centroid is shown in cyan. CH-π interactions are shown as black dotted lines, and occur at a distance of approximately 2.67 Å. Colours: carbon = grey; hydrogen = white; nitrogen = light blue; oxygen = red; boron = pink; iodine = brown.

Table S51. Crystal data and structure refinement for solvated *o*-IPhO-**BsubPc** (compound **4d**).

Identification code	k11197	
Empirical formula	C33 H19 B I N6 O	
Formula weight	653.25	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.1641(3) Å	α= 90°.
	b = 13.8900(4) Å	β= 97.6040(16)°.
	c = 19.3994(6) Å	γ = 90°.
Volume	2714.71(14) $Å^3$	
Z	4	
Density (calculated)	1.598 Mg/m^3	
Absorption coefficient	1.220 mm^{-1}	
F(000)	1300	
Crystal size	0.25 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.58 to 27.49°.	
Index ranges	-13<=h<=13, -17<=k<=17, -25<=l<=25	
Reflections collected	18456	
Independent reflections	6189 [R(int) = 0.0488]	
Completeness to theta = 27.49°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.890 and 0.789	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6189 / 0 / 379	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1127	
R indices (all data)	R1 = 0.0840, wR2 = 0.1317	
Largest diff. peak and hole	1.477 and -1.098 e.$Å^{-3}$	

Table S52. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for solvated *o*-IPhO-**BsubPc** (compound **4d**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	4682(1)	1265(1)	898(1)	32(1)
O(1)	7599(3)	968(2)	1762(1)	21(1)
N(1)	6921(3)	-1205(2)	669(2)	19(1)
N(2)	8723(3)	-388(2)	1320(2)	19(1)
N(3)	10803(4)	-335(2)	2048(2)	23(1)
N(4)	8768(3)	-297(2)	2533(2)	19(1)
N(5)	7030(4)	-1023(3)	3059(2)	22(1)
N(6)	6789(3)	-717(2)	1836(2)	19(1)
C(1)	8159(4)	-867(3)	732(2)	20(1)
C(2)	9264(4)	-1093(3)	353(2)	22(1)
C(3)	9326(5)	-1536(3)	-287(2)	25(1)
C(4)	10560(5)	-1663(3)	-502(2)	30(1)
C(5)	11723(5)	-1389(3)	-88(2)	28(1)
C(6)	11695(5)	-982(3)	560(2)	26(1)
C(7)	10449(4)	-811(3)	775(2)	22(1)
C(8)	10074(4)	-428(3)	1417(2)	21(1)
C(9)	10129(4)	-330(3)	2597(2)	22(1)
C(10)	10567(4)	-571(3)	3325(2)	22(1)
C(11)	11821(5)	-678(3)	3693(2)	30(1)
C(12)	11913(5)	-931(4)	4387(3)	36(1)
C(13)	10774(5)	-1102(4)	4699(2)	36(1)
C(14)	9512(5)	-1039(3)	4337(2)	30(1)
C(15)	9410(4)	-764(3)	3639(2)	23(1)
C(16)	8265(4)	-667(3)	3099(2)	23(1)
C(17)	6348(4)	-1102(3)	2418(2)	20(1)
C(18)	5281(4)	-1756(3)	2159(2)	21(1)
C(19)	4484(5)	-2363(3)	2497(2)	29(1)
C(20)	3666(5)	-3011(3)	2101(3)	33(1)

C(21)	3628(4)	-3062(3)	1382(3)	32(1)
C(22)	4418(4)	-2463(3)	1034(2)	26(1)
C(23)	5249(4)	-1807(3)	1420(2)	21(1)
C(24)	6289(4)	-1190(3)	1239(2)	19(1)
C(25)	6780(4)	1380(3)	2179(2)	20(1)
C(26)	5462(4)	1606(3)	1920(2)	24(1)
C(27)	4643(5)	2057(3)	2345(3)	31(1)
C(28)	5111(5)	2271(3)	3028(3)	36(1)
C(29)	6400(5)	2051(3)	3285(2)	33(1)
C(30)	7245(5)	1614(3)	2869(2)	26(1)
B(1)	7935(5)	-35(3)	1865(2)	19(1)
C(1S)	5576(5)	-693(4)	4626(3)	33(1)
C(2S)	5201(5)	179(4)	4321(2)	31(1)
C(3S)	4640(5)	881(4)	4696(2)	31(1)

Table S53. Bond lengths [Å] and angles [°] for solvated *o*-IPhO-**BsubPc** (compound **4d**).

I(1)-C(26)	2.090(4)
O(1)-C(25)	1.361(5)
O(1)-B(1)	1.442(6)
N(1)-C(1)	1.334(5)
N(1)-C(24)	1.351(5)
N(2)-C(8)	1.363(5)
N(2)-C(1)	1.377(5)
N(2)-B(1)	1.491(6)
N(3)-C(9)	1.340(6)
N(3)-C(8)	1.350(5)
N(4)-C(16)	1.371(5)
N(4)-C(9)	1.373(5)
N(4)-B(1)	1.496(6)
N(5)-C(16)	1.342(6)
N(5)-C(17)	1.346(5)
N(6)-C(24)	1.368(5)
N(6)-C(17)	1.376(5)
N(6)-B(1)	1.497(6)
C(1)-C(2)	1.456(6)
C(2)-C(3)	1.394(6)
C(2)-C(7)	1.419(6)
C(3)-C(4)	1.384(6)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.391(7)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.382(6)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.404(6)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.451(6)
C(9)-C(10)	1.462(6)
C(10)-C(11)	1.384(6)

C(10)-C(15)	1.420(6)
C(11)-C(12)	1.383(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.396(8)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.382(7)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.397(6)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.466(6)
C(17)-C(18)	1.452(6)
C(18)-C(19)	1.392(6)
C(18)-C(23)	1.432(6)
C(19)-C(20)	1.386(7)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.393(7)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.391(7)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.391(6)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.440(6)
C(25)-C(30)	1.398(6)
C(25)-C(26)	1.403(6)
C(26)-C(27)	1.395(6)
C(27)-C(28)	1.380(7)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.373(7)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.392(7)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
C(1S)-C(2S)	1.380(7)
C(1S)-C(3S)#1	1.388(7)

C(1S)-H(1S)	0.9500
C(2S)-C(3S)	1.384(7)
C(2S)-H(2S)	0.9500
C(3S)-C(1S)#1	1.388(7)
C(3S)-H(3S)	0.9500

C(25)-O(1)-B(1)	118.5(3)
C(1)-N(1)-C(24)	117.7(3)
C(8)-N(2)-C(1)	113.3(3)
C(8)-N(2)-B(1)	122.7(3)
C(1)-N(2)-B(1)	122.8(4)
C(9)-N(3)-C(8)	116.3(4)
C(16)-N(4)-C(9)	113.1(3)
C(16)-N(4)-B(1)	123.8(4)
C(9)-N(4)-B(1)	122.3(3)
C(16)-N(5)-C(17)	116.5(3)
C(24)-N(6)-C(17)	112.5(3)
C(24)-N(6)-B(1)	122.3(3)
C(17)-N(6)-B(1)	123.5(3)
N(1)-C(1)-N(2)	122.0(4)
N(1)-C(1)-C(2)	131.2(4)
N(2)-C(1)-C(2)	105.0(4)
C(3)-C(2)-C(7)	120.1(4)
C(3)-C(2)-C(1)	132.4(4)
C(7)-C(2)-C(1)	107.5(4)
C(4)-C(3)-C(2)	118.2(4)
C(4)-C(3)-H(3A)	120.9
C(2)-C(3)-H(3A)	120.9
C(3)-C(4)-C(5)	121.8(4)
C(3)-C(4)-H(4A)	119.1
C(5)-C(4)-H(4A)	119.1
C(6)-C(5)-C(4)	121.2(4)
C(6)-C(5)-H(5A)	119.4
C(4)-C(5)-H(5A)	119.4

C(5)-C(6)-C(7)	117.9(4)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.8(4)
C(6)-C(7)-C(8)	131.8(4)
C(2)-C(7)-C(8)	107.3(4)
N(3)-C(8)-N(2)	122.9(4)
N(3)-C(8)-C(7)	129.6(4)
N(2)-C(8)-C(7)	105.7(4)
N(3)-C(9)-N(4)	122.9(4)
N(3)-C(9)-C(10)	130.1(4)
N(4)-C(9)-C(10)	105.6(4)
C(11)-C(10)-C(15)	121.1(4)
C(11)-C(10)-C(9)	131.6(4)
C(15)-C(10)-C(9)	107.1(4)
C(12)-C(11)-C(10)	117.9(5)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	120.9(4)
C(11)-C(12)-H(12A)	119.6
C(13)-C(12)-H(12A)	119.6
C(14)-C(13)-C(12)	122.4(4)
C(14)-C(13)-H(13A)	118.8
C(12)-C(13)-H(13A)	118.8
C(13)-C(14)-C(15)	117.1(5)
C(13)-C(14)-H(14A)	121.5
C(15)-C(14)-H(14A)	121.5
C(14)-C(15)-C(10)	120.6(4)
C(14)-C(15)-C(16)	131.9(4)
C(10)-C(15)-C(16)	107.5(4)
N(5)-C(16)-N(4)	122.5(4)
N(5)-C(16)-C(15)	131.0(4)
N(4)-C(16)-C(15)	105.2(4)
N(5)-C(17)-N(6)	122.8(4)

N(5)-C(17)-C(18)	129.8(4)
N(6)-C(17)-C(18)	105.6(3)
C(19)-C(18)-C(23)	120.2(4)
C(19)-C(18)-C(17)	132.1(4)
C(23)-C(18)-C(17)	107.1(4)
C(20)-C(19)-C(18)	118.5(4)
C(20)-C(19)-H(19A)	120.8
C(18)-C(19)-H(19A)	120.8
C(19)-C(20)-C(21)	121.5(4)
C(19)-C(20)-H(20A)	119.3
C(21)-C(20)-H(20A)	119.3
C(22)-C(21)-C(20)	121.0(4)
C(22)-C(21)-H(21A)	119.5
C(20)-C(21)-H(21A)	119.5
C(23)-C(22)-C(21)	118.6(4)
C(23)-C(22)-H(22A)	120.7
C(21)-C(22)-H(22A)	120.7
C(22)-C(23)-C(18)	120.2(4)
C(22)-C(23)-C(24)	132.2(4)
C(18)-C(23)-C(24)	107.1(4)
N(1)-C(24)-N(6)	122.5(4)
N(1)-C(24)-C(23)	129.3(4)
N(6)-C(24)-C(23)	106.4(3)
O(1)-C(25)-C(30)	120.8(4)
O(1)-C(25)-C(26)	120.8(4)
C(30)-C(25)-C(26)	118.4(4)
C(27)-C(26)-C(25)	120.4(4)
C(27)-C(26)-I(1)	118.7(3)
C(25)-C(26)-I(1)	120.9(3)
C(28)-C(27)-C(26)	120.4(4)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
C(29)-C(28)-C(27)	119.5(4)
C(29)-C(28)-H(28A)	120.2

C(27)-C(28)-H(28A)	120.2
C(28)-C(29)-C(30)	121.2(5)
C(28)-C(29)-H(29A)	119.4
C(30)-C(29)-H(29A)	119.4
C(29)-C(30)-C(25)	120.0(4)
C(29)-C(30)-H(30A)	120.0
C(25)-C(30)-H(30A)	120.0
O(1)-B(1)-N(2)	111.1(3)
O(1)-B(1)-N(4)	116.8(4)
N(2)-B(1)-N(4)	103.9(3)
O(1)-B(1)-N(6)	115.9(4)
N(2)-B(1)-N(6)	104.7(3)
N(4)-B(1)-N(6)	103.1(3)
C(2S)-C(1S)-C(3S)#1	120.1(5)
C(2S)-C(1S)-H(1S)	119.9
C(3S)#1-C(1S)-H(1S)	119.9
C(1S)-C(2S)-C(3S)	120.2(4)
C(1S)-C(2S)-H(2S)	119.9
C(3S)-C(2S)-H(2S)	119.9
C(2S)-C(3S)-C(1S)#1	119.7(5)
C(2S)-C(3S)-H(3S)	120.2
C(1S)#1-C(3S)-H(3S)	120.2

Symmetry transformations used to generate equivalent atoms:

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

Table S54. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for solvated *o*-IPhO-**BsubPc** (compound **4d**). 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}
I(1)	28(1)	38(1)	30(1)	3(1)	2(1)	2(1)
O(1)	20(2)	22(2)	22(2)	2(1)	6(1)	3(1)
N(1)	20(2)	20(2)	16(2)	4(1)	0(1)	2(2)
N(2)	19(2)	21(2)	17(2)	2(1)	5(1)	2(1)
N(3)	21(2)	22(2)	27(2)	2(2)	6(2)	-2(2)
N(4)	18(2)	22(2)	19(2)	0(1)	3(1)	2(1)
N(5)	23(2)	27(2)	18(2)	-1(2)	5(2)	1(2)
N(6)	16(2)	22(2)	21(2)	1(1)	5(1)	1(1)
C(1)	26(2)	18(2)	17(2)	4(2)	4(2)	3(2)
C(2)	25(2)	22(2)	20(2)	4(2)	9(2)	5(2)
C(3)	33(3)	23(2)	19(2)	3(2)	5(2)	2(2)
C(4)	45(3)	26(2)	22(2)	5(2)	15(2)	9(2)
C(5)	27(2)	29(2)	30(2)	9(2)	16(2)	10(2)
C(6)	27(2)	22(2)	28(2)	8(2)	6(2)	5(2)
C(7)	25(2)	19(2)	26(2)	7(2)	11(2)	5(2)
C(8)	22(2)	18(2)	23(2)	2(2)	5(2)	-2(2)
C(9)	21(2)	21(2)	23(2)	-2(2)	0(2)	0(2)
C(10)	24(2)	19(2)	22(2)	-3(2)	-3(2)	1(2)
C(11)	29(2)	26(2)	32(2)	1(2)	-2(2)	-2(2)
C(12)	35(3)	35(3)	34(3)	5(2)	-15(2)	-6(2)
C(13)	43(3)	39(3)	22(2)	6(2)	-6(2)	-3(2)
C(14)	38(3)	31(3)	21(2)	1(2)	1(2)	-5(2)
C(15)	30(2)	18(2)	20(2)	-2(2)	-3(2)	2(2)
C(16)	28(2)	25(2)	16(2)	-2(2)	5(2)	5(2)
C(17)	18(2)	22(2)	20(2)	3(2)	5(2)	6(2)
C(18)	19(2)	22(2)	24(2)	2(2)	5(2)	3(2)
C(19)	25(2)	33(3)	31(2)	7(2)	9(2)	5(2)

C(20)	20(2)	29(2)	50(3)	10(2)	9(2)	-2(2)
C(21)	20(2)	23(2)	50(3)	-1(2)	-2(2)	0(2)
C(22)	19(2)	24(2)	34(2)	-1(2)	0(2)	4(2)
C(23)	17(2)	23(2)	23(2)	4(2)	-1(2)	6(2)
C(24)	20(2)	19(2)	17(2)	3(2)	-1(2)	1(2)
C(25)	22(2)	16(2)	22(2)	-1(2)	9(2)	-2(2)
C(26)	27(2)	21(2)	26(2)	3(2)	6(2)	0(2)
C(27)	27(2)	25(2)	42(3)	4(2)	15(2)	7(2)
C(28)	46(3)	22(2)	45(3)	-2(2)	24(2)	3(2)
C(29)	52(3)	23(2)	27(2)	-6(2)	17(2)	-8(2)
C(30)	26(2)	21(2)	31(2)	-3(2)	4(2)	-6(2)
B(1)	19(2)	23(2)	16(2)	-1(2)	4(2)	1(2)
C(1S)	27(3)	34(3)	39(3)	-8(2)	11(2)	-4(2)
C(2S)	30(3)	41(3)	23(2)	-2(2)	5(2)	-12(2)
C(3S)	29(3)	32(2)	33(3)	2(2)	2(2)	-4(2)

Table S55. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for solvated *o*-IPhO-**BsubPc** (compound **4d**).

	x	y	z	U(eq)
H(3A)	8541	-1745	-569	30
H(4A)	10614	-1945	-943	36
H(5A)	12552	-1483	-254	33
H(6A)	12492	-824	851	31
H(11A)	12595	-581	3475	36
H(12A)	12762	-989	4655	44
H(13A)	10871	-1268	5178	43
H(14A)	8747	-1178	4552	36
H(19A)	4500	-2334	2987	35
H(20A)	3119	-3431	2326	40
H(21A)	3054	-3512	1125	38
H(22A)	4390	-2501	544	31
H(27A)	3756	2219	2162	37
H(28A)	4546	2568	3318	43
H(29A)	6722	2199	3755	40
H(30A)	8137	1476	3054	31
H(1S)	5984	-1166	4370	39
H(2S)	5327	298	3852	37
H(3S)	4405	1488	4490	37

Table S56. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for solvated *o*-IPhO-**BsubPc** (compound **4d**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(12)-H(12A)	->	Cg(26)	2.67	-2.62	10.1	141	3.456(6)	61
C(12)-H(12A)	->	Cg(26)	2.67	2.62	10.1	141	3.456(6)	61
C(28)-H(28A)	->	Cg(3)	2.95	-2.77	20.18	115	3.463(5)	41
C(30)-H(30A)	->	Cg(1)	2.88	2.83	10.52	134	3.601(5)	34

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(2) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->

6-Membered Ring (26) C(1S) --> C(2S) --> C(3S) --> C(1S)a --> C(2S)a --> C(3S)a -->

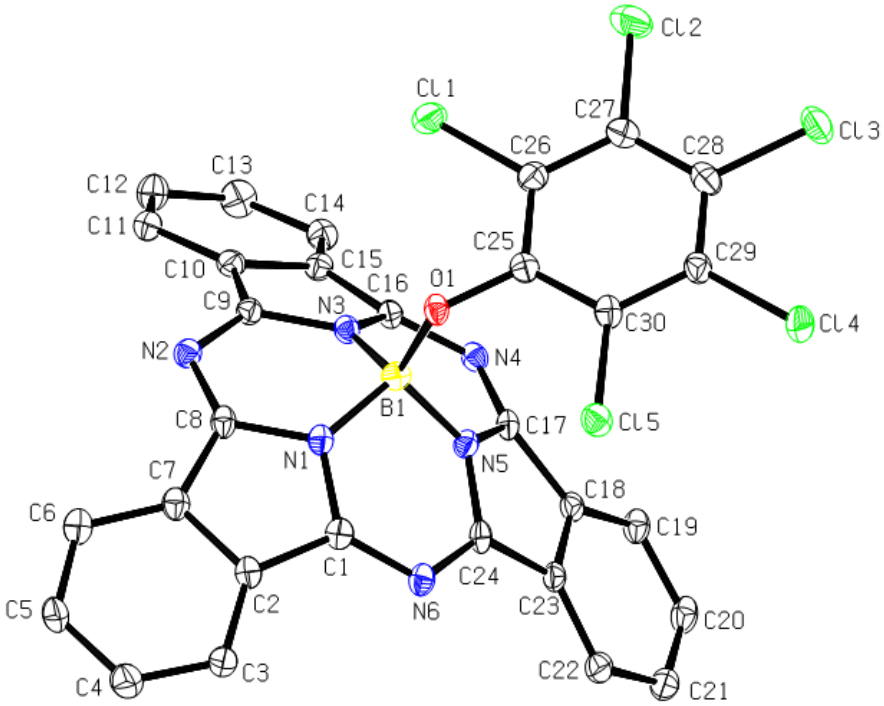

Figure S21. Anisotropic displacement ellipsoid plot of Cl_5PhO-**BsubPc** (compound **4e**).

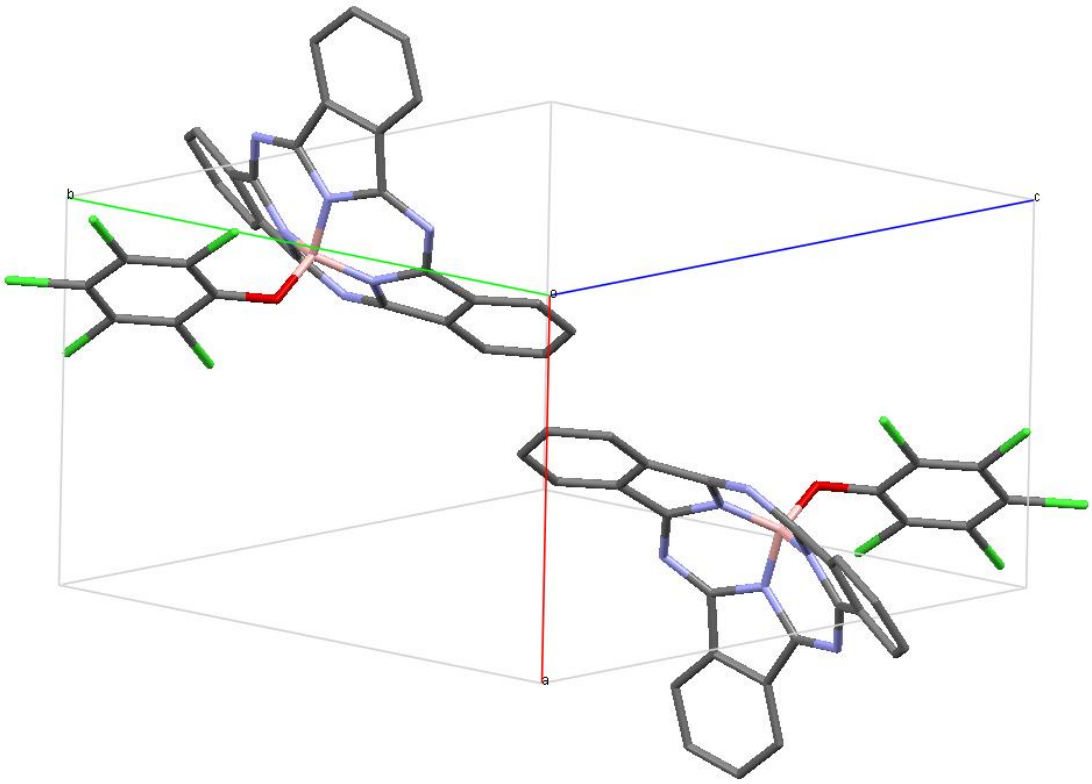

Figure S22. Populated unit cell of Cl_5PhO-**BsubPc** (compound **4e**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; chlorine = green. Hydrogens are omitted for clarity.

Table S57. Crystal data and structure refinement for Cl_5PhO-**BsubPc** (compound **4e**).

Identification code	k11121	
Empirical formula	C30 H12 B Cl5 N6 O	
Formula weight	660.52	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.5099(3) Å	α= 107.637(2)°.
	b = 12.5191(4) Å	β= 100.015(2)°.
	c = 13.8756(6) Å	γ = 99.280(3)°.
Volume	1350.77(9) $Å^3$	
Z	2	
Density (calculated)	1.624 Mg/m^3	
Absorption coefficient	0.577 mm^{-1}	
F(000)	664	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.62 to 27.53°.	
Index ranges	-11<=h<=11, -16<=k<=16, -15<=l<=18	
Reflections collected	17295	
Independent reflections	6109 [R(int) = 0.0720]	
Completeness to theta = 25.24°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.949 and 0.750	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6109 / 0 / 388	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0624, wR2 = 0.1477	
R indices (all data)	R1 = 0.1322, wR2 = 0.1882	
Largest diff. peak and hole	0.491 and -0.615 e.$Å^{-3}$	

Table S58. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Cl_5PhO-**BsubPc** (compound **4e**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	10046(1)	3622(1)	10147(1)	42(1)
Cl(2)	10324(1)	2081(1)	11540(1)	55(1)
Cl(3)	7973(1)	-344(1)	10818(1)	46(1)
Cl(4)	5362(1)	-1214(1)	8711(1)	42(1)
Cl(5)	5124(1)	344(1)	7322(1)	35(1)
O(1)	7548(3)	2537(2)	8163(2)	26(1)
N(1)	7724(3)	2922(2)	6557(2)	25(1)
N(2)	9685(3)	4717(2)	7204(2)	26(1)
N(3)	10203(3)	3149(2)	7739(2)	24(1)
N(4)	11374(3)	1537(2)	7655(2)	25(1)
N(5)	8615(3)	1295(2)	6763(2)	24(1)
N(6)	6569(3)	1067(2)	5271(2)	27(1)
C(1)	6723(4)	2213(3)	5609(3)	27(1)
C(2)	6314(4)	2960(3)	5037(3)	28(1)
C(3)	5320(4)	2746(3)	4058(3)	32(1)
C(4)	5320(5)	3639(3)	3675(3)	40(1)
C(5)	6327(5)	4727(3)	4234(3)	37(1)
C(6)	7335(5)	4965(3)	5197(3)	35(1)
C(7)	7309(4)	4079(3)	5618(3)	28(1)
C(8)	8277(4)	4018(3)	6561(3)	26(1)
C(9)	10661(4)	4256(3)	7747(3)	24(1)
C(10)	12419(4)	4610(3)	8192(3)	28(1)
C(11)	13563(4)	5637(3)	8422(3)	32(1)
C(12)	15209(5)	5663(3)	8753(3)	38(1)
C(13)	15713(5)	4682(3)	8835(3)	41(1)
C(14)	14609(4)	3659(3)	8621(3)	32(1)
C(15)	12944(4)	3624(3)	8308(3)	25(1)
C(16)	11501(4)	2686(3)	7956(3)	25(1)

C(17)	9958(4)	869(3)	7017(3)	23(1)
C(18)	9601(4)	-298(3)	6267(3)	25(1)
C(19)	10463(4)	-1166(3)	6160(3)	30(1)
C(20)	9838(5)	-2179(3)	5313(3)	34(1)
C(21)	8433(5)	-2297(3)	4564(3)	33(1)
C(22)	7582(4)	-1435(3)	4638(3)	31(1)
C(23)	8149(4)	-438(3)	5514(3)	26(1)
C(24)	7600(4)	635(3)	5818(3)	26(1)
C(25)	7674(4)	1865(3)	8770(3)	27(1)
C(26)	8792(4)	2261(3)	9734(3)	30(1)
C(27)	8903(5)	1581(3)	10364(3)	35(1)
C(28)	7856(5)	498(3)	10045(3)	35(1)
C(29)	6695(5)	113(3)	9102(3)	31(1)
C(30)	6593(4)	786(3)	8469(3)	28(1)
B(1)	8480(5)	2470(3)	7363(3)	25(1)

Table S59. Bond lengths [Å] and angles [°] for Cl_5PhO-**BsubPc** (compound **4e**).

Cl(1)-C(26)	1.726(3)
Cl(2)-C(27)	1.723(4)
Cl(3)-C(28)	1.718(4)
Cl(4)-C(29)	1.725(4)
Cl(5)-C(30)	1.719(4)
O(1)-C(25)	1.362(4)
O(1)-B(1)	1.462(5)
N(1)-C(8)	1.374(4)
N(1)-C(1)	1.380(4)
N(1)-B(1)	1.495(5)
N(2)-C(9)	1.338(4)
N(2)-C(8)	1.347(4)
N(3)-C(16)	1.357(4)
N(3)-C(9)	1.374(4)
N(3)-B(1)	1.486(5)
N(4)-C(17)	1.338(4)
N(4)-C(16)	1.351(4)
N(5)-C(24)	1.366(4)
N(5)-C(17)	1.373(4)
N(5)-B(1)	1.489(5)
N(6)-C(1)	1.344(4)
N(6)-C(24)	1.345(4)
C(1)-C(2)	1.445(5)
C(2)-C(3)	1.392(5)
C(2)-C(7)	1.423(5)
C(3)-C(4)	1.376(5)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.394(5)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.374(5)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.400(5)

C(6)-H(6A)	0.9500
C(7)-C(8)	1.450(5)
C(9)-C(10)	1.454(5)
C(10)-C(11)	1.393(5)
C(10)-C(15)	1.422(5)
C(11)-C(12)	1.388(5)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.394(6)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.376(5)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.397(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.451(4)
C(17)-C(18)	1.462(5)
C(18)-C(19)	1.392(5)
C(18)-C(23)	1.421(5)
C(19)-C(20)	1.390(5)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.395(5)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.382(5)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.397(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.458(5)
C(25)-C(26)	1.394(5)
C(25)-C(30)	1.403(5)
C(26)-C(27)	1.395(5)
C(27)-C(28)	1.392(5)
C(28)-C(29)	1.391(5)
C(29)-C(30)	1.391(5)

C(25)-O(1)-B(1)	121.1(3)

C(8)-N(1)-C(1)	112.1(3)
C(8)-N(1)-B(1)	123.1(3)
C(1)-N(1)-B(1)	122.7(3)
C(9)-N(2)-C(8)	117.3(3)
C(16)-N(3)-C(9)	112.9(3)
C(16)-N(3)-B(1)	123.3(3)
C(9)-N(3)-B(1)	123.1(3)
C(17)-N(4)-C(16)	116.7(3)
C(24)-N(5)-C(17)	113.2(3)
C(24)-N(5)-B(1)	123.7(3)
C(17)-N(5)-B(1)	122.0(3)
C(1)-N(6)-C(24)	117.6(3)
N(6)-C(1)-N(1)	122.3(3)
N(6)-C(1)-C(2)	129.8(3)
N(1)-C(1)-C(2)	106.0(3)
C(3)-C(2)-C(7)	120.3(3)
C(3)-C(2)-C(1)	132.4(3)
C(7)-C(2)-C(1)	107.0(3)
C(4)-C(3)-C(2)	118.5(3)
C(4)-C(3)-H(3A)	120.8
C(2)-C(3)-H(3A)	120.8
C(3)-C(4)-C(5)	121.1(4)
C(3)-C(4)-H(4A)	119.4
C(5)-C(4)-H(4A)	119.4
C(6)-C(5)-C(4)	121.9(4)
C(6)-C(5)-H(5A)	119.1
C(4)-C(5)-H(5A)	119.1
C(5)-C(6)-C(7)	117.9(3)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	120.3(3)
C(6)-C(7)-C(8)	131.8(3)
C(2)-C(7)-C(8)	107.6(3)
N(2)-C(8)-N(1)	122.4(3)

N(2)-C(8)-C(7)	130.1(3)
N(1)-C(8)-C(7)	105.7(3)
N(2)-C(9)-N(3)	122.3(3)
N(2)-C(9)-C(10)	130.1(3)
N(3)-C(9)-C(10)	105.6(3)
C(11)-C(10)-C(15)	120.1(3)
C(11)-C(10)-C(9)	132.6(4)
C(15)-C(10)-C(9)	107.1(3)
C(12)-C(11)-C(10)	118.4(4)
C(12)-C(11)-H(11A)	120.8
C(10)-C(11)-H(11A)	120.8
C(11)-C(12)-C(13)	121.0(3)
C(11)-C(12)-H(12A)	119.5
C(13)-C(12)-H(12A)	119.5
C(14)-C(13)-C(12)	121.8(4)
C(14)-C(13)-H(13A)	119.1
C(12)-C(13)-H(13A)	119.1
C(13)-C(14)-C(15)	118.0(4)
C(13)-C(14)-H(14A)	121.0
C(15)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	120.7(3)
C(14)-C(15)-C(16)	131.9(3)
C(10)-C(15)-C(16)	107.2(3)
N(4)-C(16)-N(3)	122.3(3)
N(4)-C(16)-C(15)	130.0(3)
N(3)-C(16)-C(15)	106.2(3)
N(4)-C(17)-N(5)	122.8(3)
N(4)-C(17)-C(18)	130.3(3)
N(5)-C(17)-C(18)	105.1(3)
C(19)-C(18)-C(23)	120.6(3)
C(19)-C(18)-C(17)	131.8(3)
C(23)-C(18)-C(17)	107.4(3)
C(20)-C(19)-C(18)	118.0(4)
C(20)-C(19)-H(19A)	121.0

C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	120.9(4)
C(19)-C(20)-H(20A)	119.6
C(21)-C(20)-H(20A)	119.6
C(22)-C(21)-C(20)	122.1(3)
C(22)-C(21)-H(21A)	118.9
C(20)-C(21)-H(21A)	118.9
C(21)-C(22)-C(23)	117.5(4)
C(21)-C(22)-H(22A)	121.2
C(23)-C(22)-H(22A)	121.2
C(22)-C(23)-C(18)	120.7(3)
C(22)-C(23)-C(24)	132.0(3)
C(18)-C(23)-C(24)	107.1(3)
N(6)-C(24)-N(5)	122.0(3)
N(6)-C(24)-C(23)	131.1(3)
N(5)-C(24)-C(23)	105.7(3)
O(1)-C(25)-C(26)	121.2(3)
O(1)-C(25)-C(30)	120.3(3)
C(26)-C(25)-C(30)	118.4(3)
C(25)-C(26)-C(27)	121.2(3)
C(25)-C(26)-Cl(1)	118.8(3)
C(27)-C(26)-Cl(1)	120.0(3)
C(28)-C(27)-C(26)	120.0(4)
C(28)-C(27)-Cl(2)	119.8(3)
C(26)-C(27)-Cl(2)	120.2(3)
C(29)-C(28)-C(27)	119.3(4)
C(29)-C(28)-Cl(3)	120.3(3)
C(27)-C(28)-Cl(3)	120.4(3)
C(28)-C(29)-C(30)	120.8(3)
C(28)-C(29)-Cl(4)	119.7(3)
C(30)-C(29)-Cl(4)	119.4(3)
C(29)-C(30)-C(25)	120.3(3)
C(29)-C(30)-Cl(5)	121.4(3)
C(25)-C(30)-Cl(5)	118.3(3)

O(1)-B(1)-N(3)	115.5(3)
O(1)-B(1)-N(5)	115.9(3)
N(3)-B(1)-N(5)	104.0(3)
O(1)-B(1)-N(1)	111.3(3)
N(3)-B(1)-N(1)	104.3(3)
N(5)-B(1)-N(1)	104.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S60. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Cl_5PhO-**BsubPc** (compound **4e**). 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}
Cl(1)	48(1)	36(1)	33(1)	6(1)	10(1)	-4(1)
Cl(2)	61(1)	64(1)	33(1)	17(1)	-1(1)	5(1)
Cl(3)	64(1)	47(1)	40(1)	27(1)	18(1)	20(1)
Cl(4)	53(1)	32(1)	44(1)	18(1)	17(1)	1(1)
Cl(5)	30(1)	37(1)	36(1)	16(1)	6(1)	1(1)
O(1)	31(1)	23(1)	31(1)	13(1)	16(1)	10(1)
N(1)	26(2)	23(2)	31(2)	12(1)	10(1)	7(1)
N(2)	26(2)	25(2)	28(2)	8(1)	8(1)	5(1)
N(3)	26(2)	23(2)	25(2)	11(1)	9(1)	9(1)
N(4)	27(2)	27(2)	27(2)	12(1)	9(1)	12(1)
N(5)	26(2)	20(2)	27(2)	8(1)	9(1)	6(1)
N(6)	26(2)	24(2)	35(2)	12(1)	11(1)	5(1)
C(1)	23(2)	27(2)	33(2)	12(2)	8(2)	7(2)
C(2)	27(2)	27(2)	33(2)	14(2)	10(2)	7(2)
C(3)	37(2)	27(2)	31(2)	10(2)	10(2)	7(2)
C(4)	47(2)	39(2)	38(2)	16(2)	9(2)	13(2)
C(5)	46(2)	31(2)	39(2)	20(2)	10(2)	12(2)
C(6)	36(2)	30(2)	43(3)	16(2)	11(2)	8(2)
C(7)	26(2)	28(2)	35(2)	14(2)	12(2)	7(2)
C(8)	27(2)	23(2)	35(2)	13(2)	15(2)	9(2)
C(9)	27(2)	22(2)	24(2)	8(2)	9(2)	6(1)
C(10)	32(2)	29(2)	23(2)	8(2)	10(2)	2(2)
C(11)	36(2)	28(2)	30(2)	11(2)	5(2)	1(2)
C(12)	32(2)	36(2)	45(3)	16(2)	10(2)	2(2)
C(13)	29(2)	46(3)	47(3)	17(2)	9(2)	6(2)
C(14)	32(2)	33(2)	32(2)	13(2)	11(2)	10(2)
C(15)	26(2)	24(2)	26(2)	7(2)	10(2)	7(1)
C(16)	29(2)	23(2)	26(2)	11(2)	8(2)	6(2)

C(17)	26(2)	20(2)	30(2)	13(2)	10(2)	7(1)
C(18)	30(2)	23(2)	27(2)	12(2)	13(2)	5(2)
C(19)	31(2)	26(2)	39(2)	15(2)	17(2)	10(2)
C(20)	40(2)	25(2)	46(3)	14(2)	25(2)	9(2)
C(21)	40(2)	26(2)	35(2)	9(2)	18(2)	7(2)
C(22)	35(2)	28(2)	31(2)	11(2)	14(2)	2(2)
C(23)	32(2)	20(2)	29(2)	12(2)	13(2)	5(2)
C(24)	23(2)	23(2)	36(2)	16(2)	9(2)	2(1)
C(25)	29(2)	29(2)	29(2)	11(2)	14(2)	12(2)
C(26)	31(2)	29(2)	30(2)	7(2)	11(2)	4(2)
C(27)	40(2)	38(2)	28(2)	12(2)	9(2)	9(2)
C(28)	44(2)	40(2)	32(2)	19(2)	16(2)	18(2)
C(29)	37(2)	28(2)	32(2)	13(2)	17(2)	8(2)
C(30)	25(2)	29(2)	36(2)	15(2)	15(2)	10(2)
B(1)	19(2)	28(2)	27(2)	8(2)	6(2)	4(2)

Table S61. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Cl_5PhO-**BsubPc** (compound **4e**).

	x	y	z	U(eq)
H(3A)	4656	2000	3664	38
H(4A)	4623	3512	3018	48
H(5A)	6315	5322	3942	44
H(6A)	8028	5707	5566	42
H(11A)	13224	6302	8354	39
H(12A)	16003	6360	8926	45
H(13A)	16850	4720	9045	49
H(14A)	14967	2998	8684	38
H(19A)	11450	-1070	6651	35
H(20A)	10373	-2798	5243	41
H(21A)	8050	-2992	3985	39
H(22A)	6647	-1518	4112	37

Table S62. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for Cl_5PhO-**BsubPc** (compound **4e**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(20)-H(20A)	->	Cg(1)	2.77	2.75	6.6	126	3.418(5)	42
C(21)-H(21A)	->	Cg(2)	2.71	-2.71	0.96	134	3.440(4)	44

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (2) N(3) --> C(9) --> C(10) --> C(15) --> C(16) -->

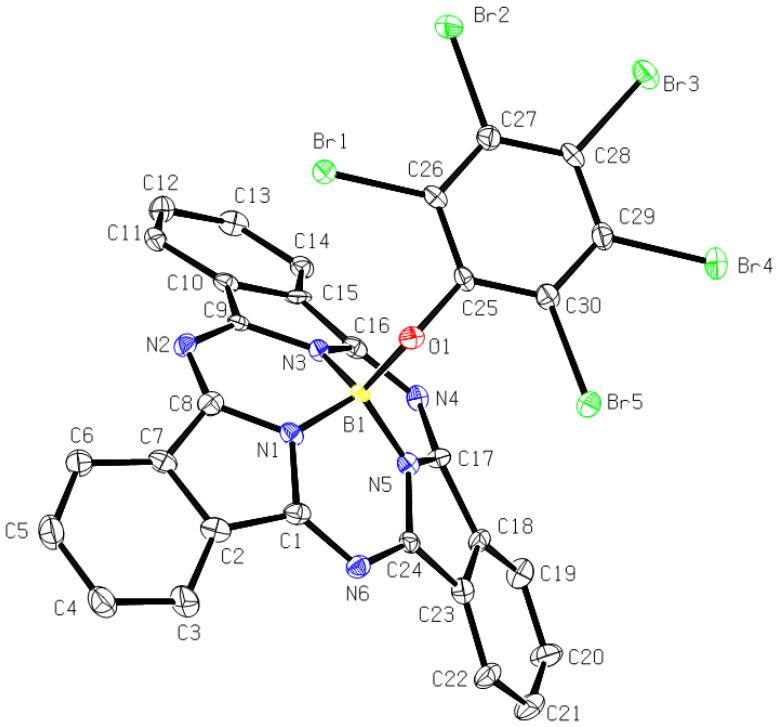

Figure S23. Anisotropic displacement ellipsoid plot of Br_5PhO-**BsubPc** (compound **4f**).

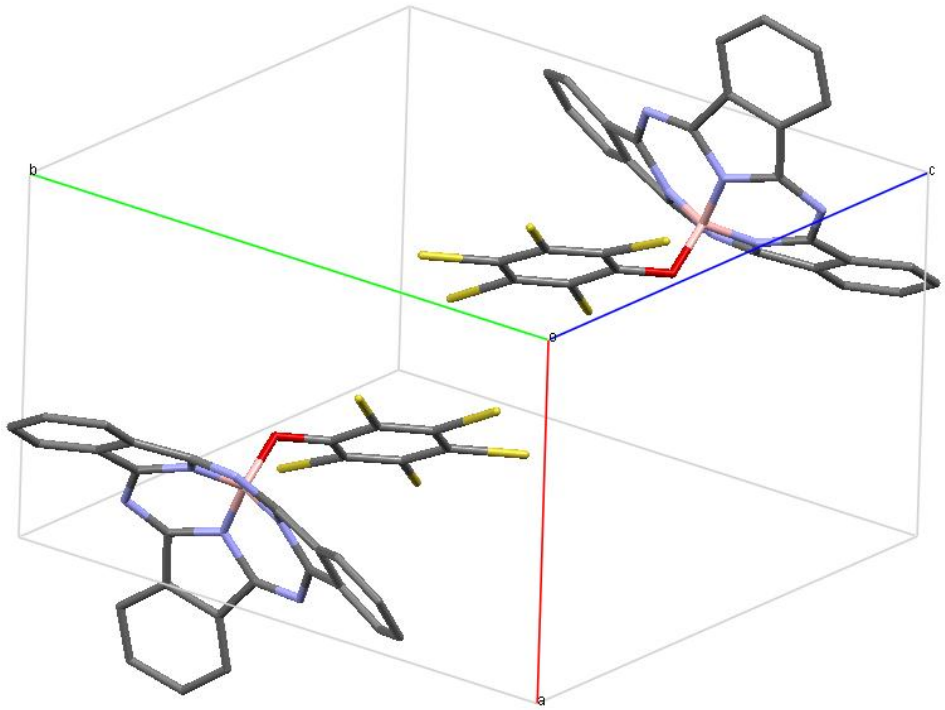

Figure S24. Populated unit cell of Br_5PhO-**BsubPc** (compound **4f**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow. Hydrogens are omitted for clarity.

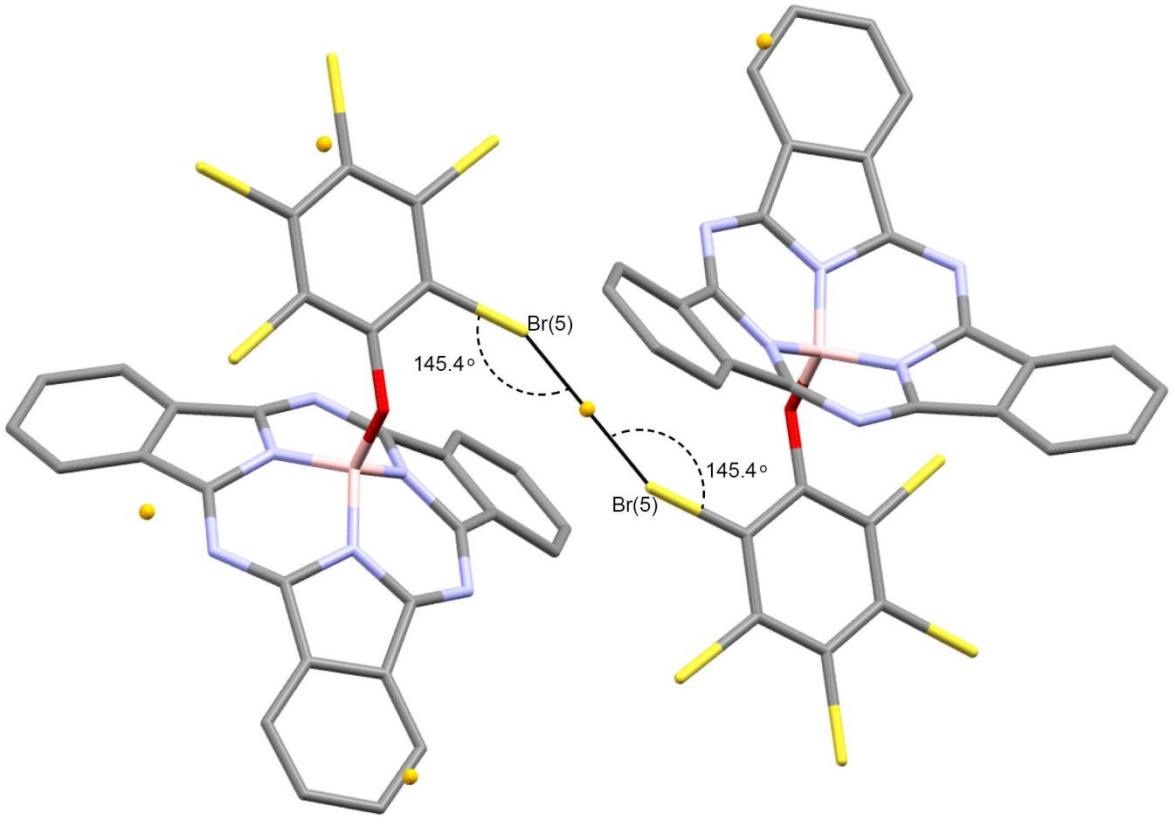

Figure S25. Illustration of the molecular packing arrangement within the single crystal (extended beyond the unit cell) of Br_5PhO-**BsubPc** (compound **4f**), showing the close Br-Br contact as a black dotted line. The Br(5)-Br(5) distance is 3.4573(17) Å. Crystallographic inversion centres are shown as orange spheres. Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow. Hydrogens are omitted for clarity.

Table S63. Crystal data and structure refinement for Br_5PhO-**BsubPc** (compound **4f**).

Identification code	k1190twin	
Empirical formula	C30 H12 B Br5 N6 O	
Formula weight	882.82	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.4976(3) Å	α= 107.2430(18)°.
	b = 12.9454(4) Å	β= 97.553(2)°.
	c = 13.9650(5) Å	γ = 101.703(2)°.
Volume	1406.21(8) $Å^3$	
Z	2	
Density (calculated)	2.085 Mg/m^3	
Absorption coefficient	7.184 mm^{-1}	
F(000)	844	
Crystal size	0.28 x 0.15 x 0.02 mm^3	
Theta range for data collection	2.64 to 25.00°.	
Index ranges	-10<=h<=10, -15<=k<=14, -15<=l<=16	
Reflections collected	4953	
Independent reflections	4953 [R(int) = 0.0000]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.871 and 0.412	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4953 / 0 / 389	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0656, wR2 = 0.1717	
R indices (all data)	R1 = 0.0984, wR2 = 0.1901	
Largest diff. peak and hole	1.015 and -1.043 e.$Å^{-3}$	

Table S64. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Br_5PhO-**BsubPc** (compound **4f**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	5007(1)	4830(1)	7795(1)	28(1)
Br(2)	4720(1)	6429(1)	6344(1)	34(1)
Br(3)	2060(2)	5425(1)	4141(1)	35(1)
Br(4)	-229(2)	2848(1)	3400(1)	44(1)
Br(5)	119(1)	1301(1)	4875(1)	33(1)
O(1)	2535(8)	2603(5)	6883(5)	23(2)
N(1)	2189(10)	2136(7)	8438(6)	22(2)
N(2)	3355(10)	3902(7)	9746(6)	25(2)
N(3)	1424(10)	3747(7)	8299(6)	22(2)
N(4)	-1262(10)	3556(7)	7407(6)	21(2)
N(5)	-213(10)	1950(7)	7273(6)	20(2)
N(6)	175(10)	401(7)	7757(7)	25(2)
C(1)	1587(13)	1056(8)	8384(8)	26(2)
C(2)	2514(13)	952(9)	9286(9)	29(3)
C(3)	2431(16)	33(10)	9634(9)	38(3)
C(4)	3383(18)	191(11)	10564(10)	46(3)
C(5)	4402(17)	1256(11)	11141(10)	45(3)
C(6)	4469(14)	2169(9)	10832(9)	31(3)
C(7)	3498(13)	2026(9)	9894(9)	28(2)
C(8)	3164(12)	2798(9)	9378(8)	26(2)
C(9)	2403(12)	4357(8)	9229(7)	18(2)
C(10)	1915(13)	5399(8)	9525(8)	23(2)
C(11)	2543(14)	6383(9)	10399(8)	28(2)
C(12)	1779(14)	7247(9)	10481(8)	29(3)
C(13)	418(13)	7152(9)	9755(9)	30(3)
C(14)	-217(13)	6179(8)	8907(8)	25(2)
C(15)	542(13)	5302(8)	8795(8)	25(2)
C(16)	132(13)	4190(8)	8055(8)	23(2)

C(17)	-1436(12)	2451(8)	7090(8)	24(2)
C(18)	-2964(13)	1525(8)	6724(8)	23(2)
C(19)	-4580(13)	1496(10)	6430(9)	33(3)
C(20)	-5739(15)	500(10)	6193(10)	40(3)
C(21)	-5297(13)	-467(10)	6285(9)	37(3)
C(22)	-3680(13)	-463(9)	6593(8)	31(3)
C(23)	-2494(13)	558(9)	6809(8)	29(3)
C(24)	-728(13)	878(8)	7260(7)	22(2)
C(25)	2417(13)	3240(8)	6267(7)	22(2)
C(26)	3452(13)	4319(8)	6565(8)	22(2)
C(27)	3328(13)	4960(9)	5939(8)	29(3)
C(28)	2228(13)	4553(9)	4995(8)	25(2)
C(29)	1242(13)	3458(10)	4680(8)	30(3)
C(30)	1357(13)	2814(9)	5325(8)	26(2)
B(1)	1537(14)	2617(9)	7679(8)	18(2)

Table S65. Bond lengths [Å] and angles [°] for Br_5PhO-**BsubPc** (compound **4f**).

Br(1)-C(26)	1.873(10)
Br(2)-C(27)	1.900(11)
Br(3)-C(28)	1.880(10)
Br(4)-C(29)	1.886(11)
Br(5)-C(30)	1.897(11)
O(1)-C(25)	1.364(12)
O(1)-B(1)	1.483(13)
N(1)-C(1)	1.363(13)
N(1)-C(8)	1.380(13)
N(1)-B(1)	1.481(14)
N(2)-C(8)	1.334(14)
N(2)-C(9)	1.347(13)
N(3)-C(9)	1.359(12)
N(3)-C(16)	1.387(13)
N(3)-B(1)	1.492(14)
N(4)-C(16)	1.334(13)
N(4)-C(17)	1.337(13)
N(5)-C(24)	1.361(13)
N(5)-C(17)	1.366(13)
N(5)-B(1)	1.499(14)
N(6)-C(24)	1.325(13)
N(6)-C(1)	1.340(13)
C(1)-C(2)	1.452(16)
C(2)-C(3)	1.404(15)
C(2)-C(7)	1.412(15)
C(3)-C(4)	1.372(17)
C(4)-C(5)	1.405(18)
C(5)-C(6)	1.366(17)
C(6)-C(7)	1.394(16)
C(7)-C(8)	1.445(15)
C(9)-C(10)	1.450(14)
C(10)-C(15)	1.403(15)

C(10)-C(11)	1.424(14)
C(11)-C(12)	1.387(16)
C(12)-C(13)	1.393(16)
C(13)-C(14)	1.397(15)
C(14)-C(15)	1.396(15)
C(15)-C(16)	1.442(14)
C(17)-C(18)	1.488(14)
C(18)-C(19)	1.371(15)
C(18)-C(23)	1.421(15)
C(19)-C(20)	1.375(16)
C(20)-C(21)	1.413(17)
C(21)-C(22)	1.384(16)
C(22)-C(23)	1.413(15)
C(23)-C(24)	1.472(15)
C(25)-C(30)	1.379(14)
C(25)-C(26)	1.400(14)
C(26)-C(27)	1.380(15)
C(27)-C(28)	1.398(15)
C(28)-C(29)	1.399(15)
C(29)-C(30)	1.404(16)

C(25)-O(1)-B(1)	121.7(8)
C(1)-N(1)-C(8)	113.1(9)
C(1)-N(1)-B(1)	123.1(9)
C(8)-N(1)-B(1)	122.1(8)
C(8)-N(2)-C(9)	117.9(9)
C(9)-N(3)-C(16)	113.1(8)
C(9)-N(3)-B(1)	123.7(8)
C(16)-N(3)-B(1)	122.4(8)
C(16)-N(4)-C(17)	116.8(9)
C(24)-N(5)-C(17)	115.3(8)
C(24)-N(5)-B(1)	122.2(9)
C(17)-N(5)-B(1)	121.2(8)
C(24)-N(6)-C(1)	117.2(9)

N(6)-C(1)-N(1)	122.5(10)
N(6)-C(1)-C(2)	130.4(10)
N(1)-C(1)-C(2)	105.0(9)
C(3)-C(2)-C(7)	121.1(11)
C(3)-C(2)-C(1)	130.7(10)
C(7)-C(2)-C(1)	107.9(9)
C(4)-C(3)-C(2)	118.5(11)
C(3)-C(4)-C(5)	119.6(12)
C(6)-C(5)-C(4)	123.0(12)
C(5)-C(6)-C(7)	118.2(11)
C(6)-C(7)-C(2)	119.6(10)
C(6)-C(7)-C(8)	132.9(10)
C(2)-C(7)-C(8)	107.4(9)
N(2)-C(8)-N(1)	122.8(10)
N(2)-C(8)-C(7)	130.4(10)
N(1)-C(8)-C(7)	105.1(9)
N(2)-C(9)-N(3)	121.5(9)
N(2)-C(9)-C(10)	132.7(9)
N(3)-C(9)-C(10)	104.8(8)
C(15)-C(10)-C(11)	120.8(10)
C(15)-C(10)-C(9)	108.2(9)
C(11)-C(10)-C(9)	131.0(10)
C(12)-C(11)-C(10)	117.5(10)
C(11)-C(12)-C(13)	121.7(10)
C(12)-C(13)-C(14)	120.8(10)
C(15)-C(14)-C(13)	118.8(10)
C(14)-C(15)-C(10)	120.4(9)
C(14)-C(15)-C(16)	132.0(10)
C(10)-C(15)-C(16)	107.6(9)
N(4)-C(16)-N(3)	122.0(9)
N(4)-C(16)-C(15)	131.9(10)
N(3)-C(16)-C(15)	104.7(9)
N(4)-C(17)-N(5)	124.4(9)
N(4)-C(17)-C(18)	129.3(10)

N(5)-C(17)-C(18)	104.6(8)
C(19)-C(18)-C(23)	121.0(10)
C(19)-C(18)-C(17)	132.6(10)
C(23)-C(18)-C(17)	106.2(9)
C(18)-C(19)-C(20)	118.4(11)
C(19)-C(20)-C(21)	121.3(11)
C(22)-C(21)-C(20)	121.8(11)
C(21)-C(22)-C(23)	116.4(11)
C(22)-C(23)-C(18)	121.0(10)
C(22)-C(23)-C(24)	130.0(10)
C(18)-C(23)-C(24)	108.5(9)
N(6)-C(24)-N(5)	123.4(9)
N(6)-C(24)-C(23)	131.2(9)
N(5)-C(24)-C(23)	103.9(9)
O(1)-C(25)-C(30)	120.9(9)
O(1)-C(25)-C(26)	119.7(9)
C(30)-C(25)-C(26)	119.2(9)
C(27)-C(26)-C(25)	119.5(9)
C(27)-C(26)-Br(1)	122.1(8)
C(25)-C(26)-Br(1)	118.4(7)
C(26)-C(27)-C(28)	122.0(10)
C(26)-C(27)-Br(2)	119.7(8)
C(28)-C(27)-Br(2)	118.3(8)
C(27)-C(28)-C(29)	118.4(10)
C(27)-C(28)-Br(3)	122.0(8)
C(29)-C(28)-Br(3)	119.6(8)
C(28)-C(29)-C(30)	119.4(10)
C(28)-C(29)-Br(4)	120.4(8)
C(30)-C(29)-Br(4)	120.1(8)
C(25)-C(30)-C(29)	121.4(10)
C(25)-C(30)-Br(5)	118.7(8)
C(29)-C(30)-Br(5)	119.8(8)
N(1)-B(1)-O(1)	112.1(9)
N(1)-B(1)-N(3)	105.1(8)

O(1)-B(1)-N(3)	115.3(8)
N(1)-B(1)-N(5)	104.7(8)
O(1)-B(1)-N(5)	114.3(8)
N(3)-B(1)-N(5)	104.4(8)

Symmetry transformations used to generate equivalent atoms:

Table S66. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Br_5PhO-**BsubPc** (compound **4f**). 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}
Br(1)	26(1)	32(1)	25(1)	11(1)	3(1)	2(1)
Br(2)	40(1)	27(1)	34(1)	13(1)	8(1)	3(1)
Br(3)	46(1)	36(1)	29(1)	18(1)	10(1)	14(1)
Br(4)	52(1)	48(1)	25(1)	13(1)	-4(1)	1(1)
Br(5)	41(1)	26(1)	24(1)	3(1)	5(1)	0(1)
O(1)	24(4)	19(4)	25(4)	3(3)	12(3)	6(3)
N(1)	31(5)	19(4)	22(5)	9(4)	10(4)	11(4)
N(2)	18(4)	28(5)	23(5)	6(4)	2(4)	1(4)
N(3)	22(4)	24(5)	18(4)	8(4)	4(4)	4(4)
N(4)	23(5)	24(5)	19(4)	5(4)	8(4)	12(4)
N(5)	24(5)	20(4)	20(4)	7(3)	7(4)	9(4)
N(6)	25(5)	21(4)	25(5)	5(4)	6(4)	4(4)
C(1)	30(6)	19(5)	30(6)	7(5)	13(5)	7(5)
C(2)	29(6)	27(6)	39(7)	15(5)	14(5)	13(5)
C(3)	58(8)	27(6)	37(7)	17(5)	7(6)	23(6)
C(4)	72(10)	35(7)	33(7)	16(6)	13(7)	15(7)
C(5)	61(9)	45(8)	29(7)	14(6)	1(6)	15(7)
C(6)	37(7)	27(6)	31(6)	10(5)	6(5)	9(5)
C(7)	34(6)	24(6)	35(6)	17(5)	11(5)	11(5)
C(8)	21(5)	29(6)	28(6)	6(5)	11(5)	6(5)
C(9)	23(5)	14(5)	19(5)	8(4)	10(4)	3(4)
C(10)	33(6)	17(5)	24(6)	8(4)	16(5)	7(4)
C(11)	36(6)	28(6)	19(5)	8(5)	9(5)	3(5)
C(12)	34(6)	25(6)	25(6)	2(5)	11(5)	8(5)
C(13)	31(6)	27(6)	39(7)	14(5)	16(5)	13(5)
C(14)	34(6)	22(5)	21(5)	7(4)	11(5)	5(5)
C(15)	26(6)	16(5)	33(6)	13(5)	9(5)	-3(4)
C(16)	29(6)	23(5)	24(6)	11(5)	14(5)	10(5)

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

Table S67. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Br_5PhO-**BsubPc** (compound **4f**).

	x	y	z	U(eq)
H(3A)	1733	-681	9234	45
H(4A)	3353	-417	10817	55
H(5A)	5076	1346	11774	54
H(6A)	5158	2881	11245	37
H(11A)	3452	6445	10906	34
H(12A)	2194	7920	11047	35
H(13A)	-86	7756	9838	36
H(14A)	-1148	6116	8415	30
H(19A)	-4892	2149	6389	39
H(20A)	-6860	460	5964	48
H(21A)	-6133	-1137	6130	44
H(22A)	-3383	-1113	6657	37

Table S68. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for Br_5PhO-**BsubPc** (compound **4f**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(12)-H(12A)	->	Cg(3)	2.72	2.72	3.19	131	3.424(12)	42
C(13)-H(13A)	->	Cg(1)	2.83	-2.82	3.47	129	3.500(12)	40

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (3) N(5) --> C(17) --> C(18) --> C(23) --> C(24) -->

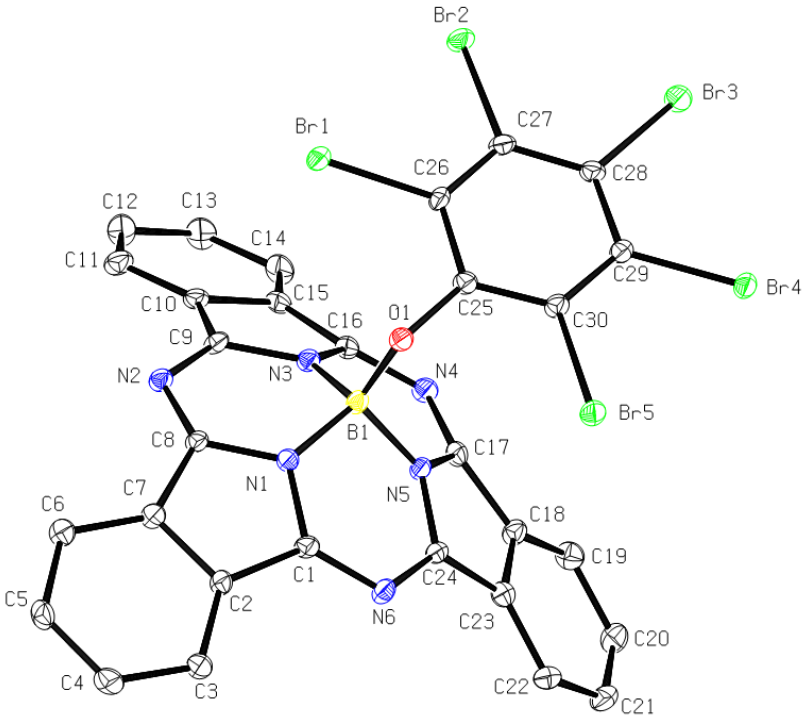

Figure S26. Anisotropic displacement ellipsoid plot of solvated Br_5PhO-**BsubPc** (compound **4f** solvate).

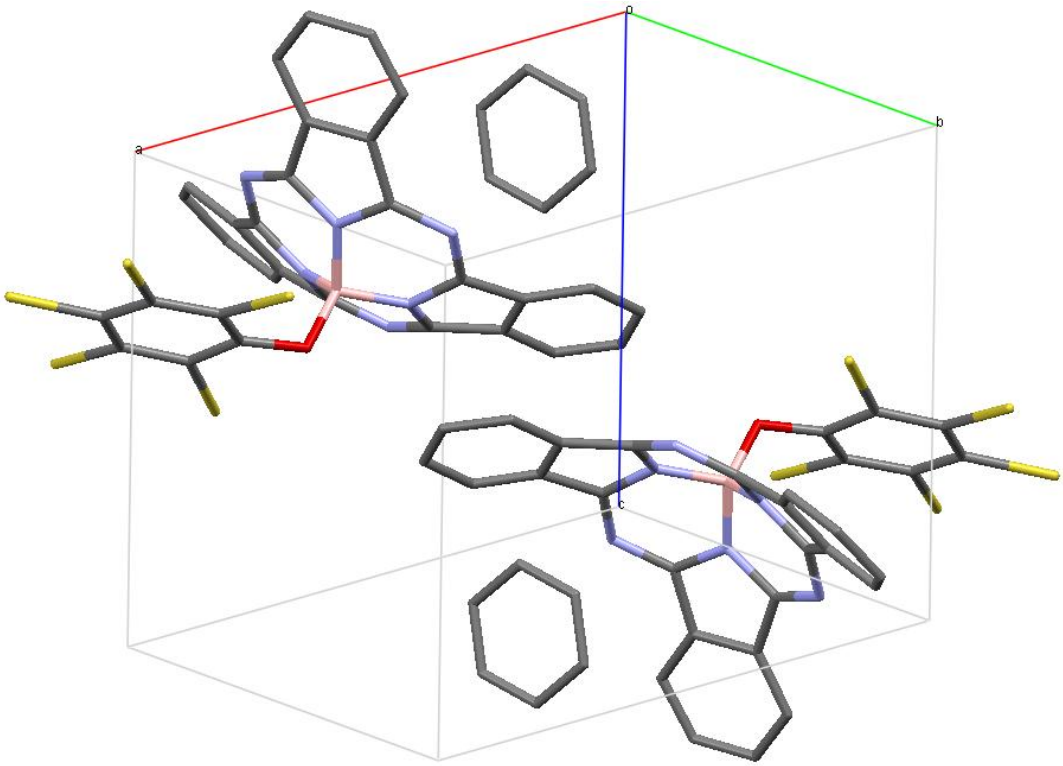

Figure S27. Populated unit cell of solvated Br_5PhO-**BsubPc** (compound **4f**). Colours: carbon = grey; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow. Hydrogens are omitted for clarity.

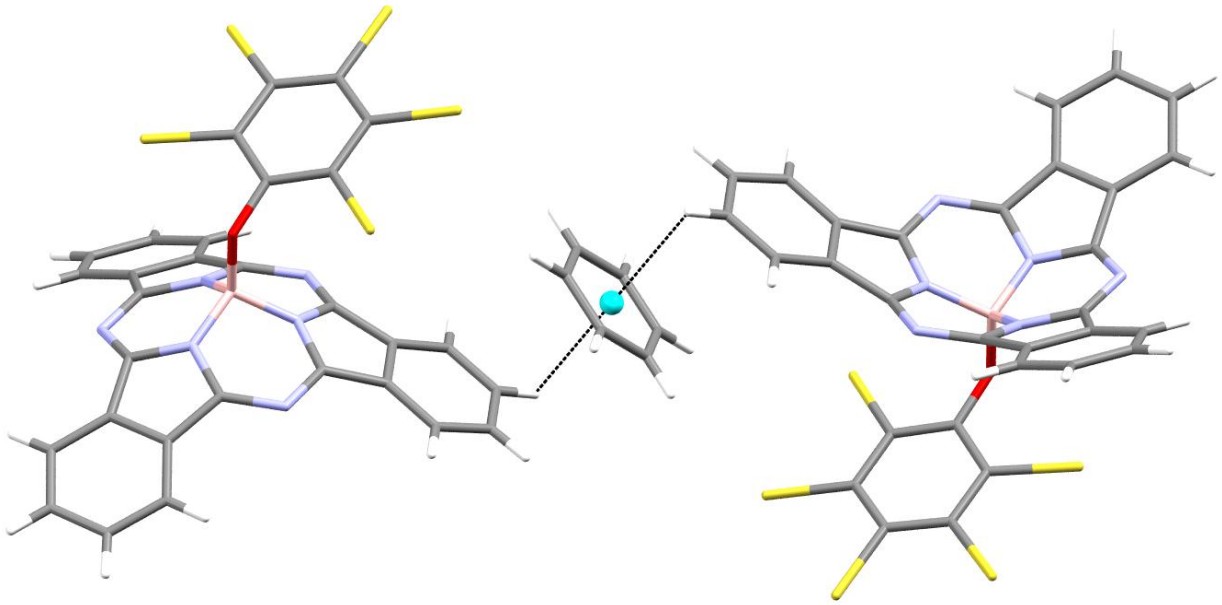

Figure S28. Illustration of the molecular packing arrangement within the single crystal (extended beyond the unit cell) of solvated Br_5PhO-**BsubPc** (compound **4f**), showing showing close benzene-**BsubPc** contacts. The benzene centroid is shown in cyan. CH-π interactions are shown as black dotted lines, and occur at a distance of approximately 2.98 Å. Colours: carbon = grey; hydrogen = white; nitrogen = light blue; oxygen = red; boron = pink; bromine = yellow.

Table S69. Crystal data and structure refinement for solvated Br_5PhO-**BsubPc** (compound **4f**).

Identification code	k1186	
Empirical formula	C33 H15 B Br5 N6 O	
Formula weight	921.87	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.0395(3) Å	α= 115.1770(18)°.
	b = 11.7114(4) Å	β= 94.9400(19)°.
	c = 13.1600(4) Å	γ = 93.6730(17)°.
Volume	1524.47(8) $Å^3$	
Z	2	
Density (calculated)	2.008 Mg/m^3	
Absorption coefficient	6.631 mm^{-1}	
F(000)	886	
Crystal size	0.30 x 0.25 x 0.08 mm^3	
Theta range for data collection	2.69 to 27.58°.	
Index ranges	-14<=h<=14, -15<=k<=13, -16<=l<=17	
Reflections collected	15993	
Independent reflections	6925 [R(int) = 0.0551]	
Completeness to theta = 25.24°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.603 and 0.439	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6925 / 0 / 415	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1036	
R indices (all data)	R1 = 0.0632, wR2 = 0.1132	
Largest diff. peak and hole	0.956 and -1.067 e.$Å^{-3}$	

Table S70. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for solvated Br_5PhO-**BsubPc** (compound **4f**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	10409(1)	3333(1)	4359(1)	28(1)
Br(2)	12275(1)	1113(1)	3391(1)	29(1)
Br(3)	11352(1)	-1818(1)	2964(1)	33(1)
Br(4)	8503(1)	-2532(1)	3268(1)	26(1)
Br(5)	6606(1)	-313(1)	3951(1)	28(1)
O(1)	7812(2)	2162(2)	4085(2)	22(1)
N(1)	6415(3)	3247(3)	3343(3)	20(1)
N(2)	7773(3)	4726(3)	3077(3)	21(1)
N(3)	8126(3)	2559(3)	2389(3)	20(1)
N(4)	8028(3)	439(3)	953(3)	24(1)
N(5)	6517(3)	1060(3)	2206(3)	20(1)
N(6)	4614(3)	1769(3)	2760(3)	23(1)
C(1)	5176(3)	2964(4)	3256(3)	22(1)
C(2)	4664(3)	4158(4)	3520(3)	21(1)
C(3)	3463(4)	4458(4)	3582(3)	25(1)
C(4)	3263(4)	5702(4)	3816(4)	30(1)
C(5)	4228(4)	6619(4)	3996(4)	28(1)
C(6)	5421(4)	6333(4)	3900(3)	25(1)
C(7)	5644(4)	5082(4)	3662(3)	22(1)
C(8)	6745(3)	4434(3)	3436(3)	20(1)
C(9)	8430(3)	3775(4)	2510(3)	21(1)
C(10)	9322(3)	3680(4)	1743(3)	23(1)
C(11)	9988(4)	4552(4)	1511(4)	30(1)
C(12)	10718(4)	4126(4)	653(4)	35(1)
C(13)	10791(4)	2833(4)	12(4)	34(1)
C(14)	10134(4)	1940(4)	221(4)	30(1)
C(15)	9394(3)	2347(4)	1091(3)	23(1)
C(16)	8558(3)	1656(4)	1471(3)	22(1)

C(17)	6974(4)	189(3)	1292(3)	22(1)
C(18)	5972(4)	-808(4)	703(3)	24(1)
C(19)	5887(4)	-1950(4)	-281(3)	29(1)
C(20)	4772(4)	-2682(4)	-651(3)	31(1)
C(21)	3745(4)	-2296(4)	-83(3)	30(1)
C(22)	3801(4)	-1158(4)	856(4)	29(1)
C(23)	4921(4)	-412(4)	1264(3)	25(1)
C(24)	5298(3)	841(4)	2185(3)	22(1)
C(25)	8618(3)	1280(4)	3910(3)	21(1)
C(26)	9856(4)	1605(4)	3903(3)	22(1)
C(27)	10667(3)	676(4)	3591(3)	24(1)
C(28)	10257(3)	-554(4)	3385(3)	24(1)
C(29)	9049(3)	-876(4)	3488(3)	22(1)
C(30)	8244(3)	57(4)	3756(3)	22(1)
B(1)	7268(4)	2248(4)	3065(4)	22(1)
C(1S)	5380(5)	5895(5)	1096(4)	42(1)
C(2S)	6216(5)	5436(5)	349(4)	40(1)
C(3S)	5853(5)	4545(5)	-752(4)	44(1)

Table S71. Bond lengths [Å] and angles [°] for solvated Br_5PhO-**BsubPc** (compound **4f**).

Br(1)-C(26)	1.890(4)
Br(2)-C(27)	1.887(4)
Br(3)-C(28)	1.899(4)
Br(4)-C(29)	1.884(4)
Br(5)-C(30)	1.897(4)
O(1)-C(25)	1.365(4)
O(1)-B(1)	1.468(6)
N(1)-C(8)	1.365(5)
N(1)-C(1)	1.370(5)
N(1)-B(1)	1.492(5)
N(2)-C(8)	1.343(5)
N(2)-C(9)	1.347(5)
N(3)-C(16)	1.372(5)
N(3)-C(9)	1.379(5)
N(3)-B(1)	1.483(6)
N(4)-C(17)	1.340(5)
N(4)-C(16)	1.355(5)
N(5)-C(24)	1.349(5)
N(5)-C(17)	1.367(4)
N(5)-B(1)	1.501(5)
N(6)-C(1)	1.345(5)
N(6)-C(24)	1.352(5)
C(1)-C(2)	1.456(5)
C(2)-C(3)	1.394(5)
C(2)-C(7)	1.420(5)
C(3)-C(4)	1.392(6)
C(4)-C(5)	1.392(6)
C(5)-C(6)	1.384(6)
C(6)-C(7)	1.405(6)
C(7)-C(8)	1.460(5)
C(9)-C(10)	1.445(5)
C(10)-C(11)	1.374(6)

C(10)-C(15)	1.438(5)
C(11)-C(12)	1.380(6)
C(12)-C(13)	1.397(6)
C(13)-C(14)	1.370(6)
C(14)-C(15)	1.397(5)
C(15)-C(16)	1.444(6)
C(17)-C(18)	1.451(5)
C(18)-C(19)	1.401(5)
C(18)-C(23)	1.425(6)
C(19)-C(20)	1.376(6)
C(20)-C(21)	1.404(6)
C(21)-C(22)	1.372(6)
C(22)-C(23)	1.388(6)
C(23)-C(24)	1.455(5)
C(25)-C(30)	1.388(6)
C(25)-C(26)	1.397(5)
C(26)-C(27)	1.401(5)
C(27)-C(28)	1.384(6)
C(28)-C(29)	1.397(5)
C(29)-C(30)	1.400(5)
C(1S)-C(2S)	1.371(7)
C(1S)-C(3S)#1	1.389(7)
C(2S)-C(3S)	1.381(7)
C(3S)-C(1S)#1	1.389(7)

C(25)-O(1)-B(1)	115.6(3)
C(8)-N(1)-C(1)	113.4(3)
C(8)-N(1)-B(1)	122.9(3)
C(1)-N(1)-B(1)	122.0(3)
C(8)-N(2)-C(9)	117.9(3)
C(16)-N(3)-C(9)	112.6(3)
C(16)-N(3)-B(1)	123.2(3)
C(9)-N(3)-B(1)	123.5(3)
C(17)-N(4)-C(16)	116.7(3)

C(24)-N(5)-C(17)	113.8(3)
C(24)-N(5)-B(1)	122.9(3)
C(17)-N(5)-B(1)	122.8(3)
C(1)-N(6)-C(24)	116.8(3)
N(6)-C(1)-N(1)	123.2(3)
N(6)-C(1)-C(2)	129.5(4)
N(1)-C(1)-C(2)	105.5(3)
C(3)-C(2)-C(7)	121.1(4)
C(3)-C(2)-C(1)	131.5(4)
C(7)-C(2)-C(1)	107.3(3)
C(4)-C(3)-C(2)	117.5(4)
C(5)-C(4)-C(3)	121.3(4)
C(6)-C(5)-C(4)	122.0(4)
C(5)-C(6)-C(7)	117.5(4)
C(6)-C(7)-C(2)	120.3(4)
C(6)-C(7)-C(8)	132.4(4)
C(2)-C(7)-C(8)	107.2(3)
N(2)-C(8)-N(1)	122.5(3)
N(2)-C(8)-C(7)	129.9(4)
N(1)-C(8)-C(7)	105.3(3)
N(2)-C(9)-N(3)	121.2(3)
N(2)-C(9)-C(10)	131.2(4)
N(3)-C(9)-C(10)	106.3(3)
C(11)-C(10)-C(15)	119.7(4)
C(11)-C(10)-C(9)	133.7(4)
C(15)-C(10)-C(9)	106.4(3)
C(10)-C(11)-C(12)	118.9(4)
C(11)-C(12)-C(13)	121.7(4)
C(14)-C(13)-C(12)	120.7(4)
C(13)-C(14)-C(15)	118.7(4)
C(14)-C(15)-C(10)	120.2(4)
C(14)-C(15)-C(16)	131.9(4)
C(10)-C(15)-C(16)	107.8(3)
N(4)-C(16)-N(3)	122.0(3)

N(4)-C(16)-C(15)	130.7(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)	130.6(3)
N(5)-C(17)-C(18)	105.1(3)
C(19)-C(18)-C(23)	120.5(4)
C(19)-C(18)-C(17)	131.8(4)
C(23)-C(18)-C(17)	107.7(3)
C(20)-C(19)-C(18)	117.5(4)
C(19)-C(20)-C(21)	121.7(4)
C(22)-C(21)-C(20)	121.5(4)
C(21)-C(22)-C(23)	118.1(4)
C(22)-C(23)-C(18)	120.7(4)
C(22)-C(23)-C(24)	132.8(4)
C(18)-C(23)-C(24)	106.4(3)
N(5)-C(24)-N(6)	122.4(3)
N(5)-C(24)-C(23)	106.2(3)
N(6)-C(24)-C(23)	129.8(3)
O(1)-C(25)-C(30)	121.6(3)
O(1)-C(25)-C(26)	120.0(3)
C(30)-C(25)-C(26)	118.4(4)
C(25)-C(26)-C(27)	120.7(4)
C(25)-C(26)-Br(1)	118.3(3)
C(27)-C(26)-Br(1)	121.1(3)
C(28)-C(27)-C(26)	119.4(4)
C(28)-C(27)-Br(2)	121.4(3)
C(26)-C(27)-Br(2)	119.1(3)
C(27)-C(28)-C(29)	120.8(3)
C(27)-C(28)-Br(3)	119.7(3)
C(29)-C(28)-Br(3)	119.5(3)
C(28)-C(29)-C(30)	118.6(4)
C(28)-C(29)-Br(4)	121.0(3)
C(30)-C(29)-Br(4)	120.3(3)
C(25)-C(30)-C(29)	121.6(4)

C(25)-C(30)-Br(5)	118.0(3)
C(29)-C(30)-Br(5)	120.5(3)
O(1)-B(1)-N(3)	116.7(3)
O(1)-B(1)-N(1)	111.6(3)
N(3)-B(1)-N(1)	104.5(3)
O(1)-B(1)-N(5)	114.9(4)
N(3)-B(1)-N(5)	103.1(3)
N(1)-B(1)-N(5)	104.7(3)
C(2S)-C(1S)-C(3S)#1	119.9(4)
C(1S)-C(2S)-C(3S)	121.0(5)
C(2S)-C(3S)-C(1S)#1	119.0(5)

Symmetry transformations used to generate equivalent atoms:

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

Table S72. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for solvated Br_5PhO-**BsubPc** (compound **4f**). 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}
Br(1)	21(1)	19(1)	39(1)	9(1)	-1(1)	-1(1)
Br(2)	16(1)	26(1)	42(1)	12(1)	6(1)	1(1)
Br(3)	22(1)	24(1)	50(1)	11(1)	9(1)	7(1)
Br(4)	22(1)	18(1)	35(1)	10(1)	5(1)	2(1)
Br(5)	18(1)	27(1)	44(1)	18(1)	10(1)	3(1)
O(1)	18(1)	17(1)	26(1)	5(1)	5(1)	4(1)
N(1)	17(2)	16(2)	24(2)	7(1)	5(1)	3(1)
N(2)	17(2)	19(2)	26(2)	7(1)	5(1)	2(1)
N(3)	17(2)	18(2)	24(2)	7(1)	4(1)	2(1)
N(4)	19(2)	22(2)	29(2)	8(2)	8(1)	6(1)
N(5)	16(2)	15(2)	27(2)	7(1)	4(1)	1(1)
N(6)	19(2)	17(2)	29(2)	7(2)	7(1)	0(1)
C(1)	15(2)	21(2)	27(2)	7(2)	7(2)	4(2)
C(2)	21(2)	15(2)	24(2)	4(2)	6(2)	4(2)
C(3)	21(2)	23(2)	32(2)	10(2)	8(2)	6(2)
C(4)	22(2)	30(2)	35(2)	10(2)	10(2)	12(2)
C(5)	32(2)	19(2)	34(2)	10(2)	8(2)	10(2)
C(6)	26(2)	21(2)	25(2)	5(2)	6(2)	5(2)
C(7)	21(2)	20(2)	23(2)	6(2)	6(2)	3(2)
C(8)	16(2)	16(2)	23(2)	4(2)	2(1)	1(1)
C(9)	17(2)	18(2)	23(2)	3(2)	2(2)	-2(1)
C(10)	13(2)	23(2)	31(2)	9(2)	3(2)	4(2)
C(11)	19(2)	27(2)	37(2)	9(2)	6(2)	1(2)
C(12)	28(2)	34(2)	51(3)	23(2)	21(2)	10(2)
C(13)	28(2)	37(3)	45(3)	20(2)	20(2)	12(2)
C(14)	28(2)	28(2)	36(2)	12(2)	15(2)	13(2)
C(15)	17(2)	25(2)	30(2)	13(2)	5(2)	8(2)

C(16)	16(2)	22(2)	29(2)	12(2)	8(2)	6(2)
C(17)	22(2)	16(2)	26(2)	7(2)	6(2)	6(2)
C(18)	24(2)	19(2)	25(2)	6(2)	4(2)	1(2)
C(19)	29(2)	29(2)	27(2)	10(2)	5(2)	6(2)
C(20)	37(3)	20(2)	26(2)	2(2)	-1(2)	0(2)
C(21)	26(2)	24(2)	34(2)	7(2)	-3(2)	-4(2)
C(22)	19(2)	29(2)	38(2)	14(2)	0(2)	0(2)
C(23)	24(2)	21(2)	30(2)	10(2)	4(2)	5(2)
C(24)	16(2)	18(2)	28(2)	8(2)	2(2)	0(1)
C(25)	18(2)	20(2)	24(2)	6(2)	4(2)	4(2)
C(26)	20(2)	14(2)	28(2)	6(2)	1(2)	-2(1)
C(27)	15(2)	24(2)	28(2)	7(2)	0(2)	0(2)
C(28)	16(2)	23(2)	29(2)	8(2)	3(2)	4(2)
C(29)	20(2)	19(2)	25(2)	8(2)	1(2)	0(2)
C(30)	18(2)	21(2)	26(2)	8(2)	6(2)	2(2)
B(1)	17(2)	17(2)	32(2)	9(2)	7(2)	2(2)
C(1S)	50(3)	38(3)	33(3)	12(2)	-3(2)	-3(2)
C(2S)	39(3)	46(3)	39(3)	24(2)	0(2)	-4(2)
C(3S)	47(3)	43(3)	45(3)	19(2)	15(2)	3(2)

Table S73. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for solvated Br_5PhO-**BsubPc** (compound **4f**).

	x	y	z	U(eq)
H(3A)	2804	3836	3469	30
H(4A)	2452	5930	3853	36
H(5A)	4062	7469	4192	34
H(6A)	6067	6958	3991	30
H(11A)	9946	5436	1934	35
H(12A)	11183	4728	493	42
H(13A)	11301	2571	-575	41
H(14A)	10182	1061	-217	36
H(19A)	6574	-2209	-678	35
H(20A)	4695	-3468	-1307	37
H(21A)	2995	-2834	-356	37
H(22A)	3095	-888	1218	35
H(1S)	5644	6512	1849	50
H(2SA)	7059	5736	591	48
H(3S)	6439	4237	-1266	53

Table S74. Selected C-H…Cg (pi-ring) interactions (H…Cg < 3.0 Å., Gamma < 30.0°) for solvated Br_5PhO-**BsubPc** (compound **4f**).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (°)	X-H..Cg (°)	X..Cg (Å)	X-H, Pi (°)
C(20)-H(20A)	->	Cg1	2.61	-2.6	3.56	131	3.303(4)	44
C(20)-H(20A)	->	Cg26	2.98	2.88	14.81	94	3.193(6)	19
C(20)-H(20A)	->	Cg26	2.98	-2.88	14.81	94	3.193(6)	19
C(21)-H(21A)	->	Cg2	2.65	-2.64	3.72	126	3.302(4)	40

Cg(J) is the center of gravity of ring J

H-Perp is the perpendicular distance of H to ring plane J

Gamma is the angle between Cg-H vector and ring J normal

X-H..Cg is the X-H-Cg angle (°)

X..Cg is the distance of X to Cg (Å)

X-H, Pi is the angle of the X-H bond with the Pi-plane (i.e., perpendicular =90°, parallel = 0°)

Cg definitions:

5-Membered Ring (1) N(1) --> C(1) --> C(2) --> C(7) --> C(8) -->

5-Membered Ring (2) N3 --> C9 --> C10 --> C15 --> C16 -->

6-Membered Ring (26) C1S --> C2S --> C3S --> C1S_a --> C2S_a --> C3S_a -->