

Analysis of the Solvent Effects on the Crystal Growth of Peripherally Chlorinated Boron Subphthalocyanines

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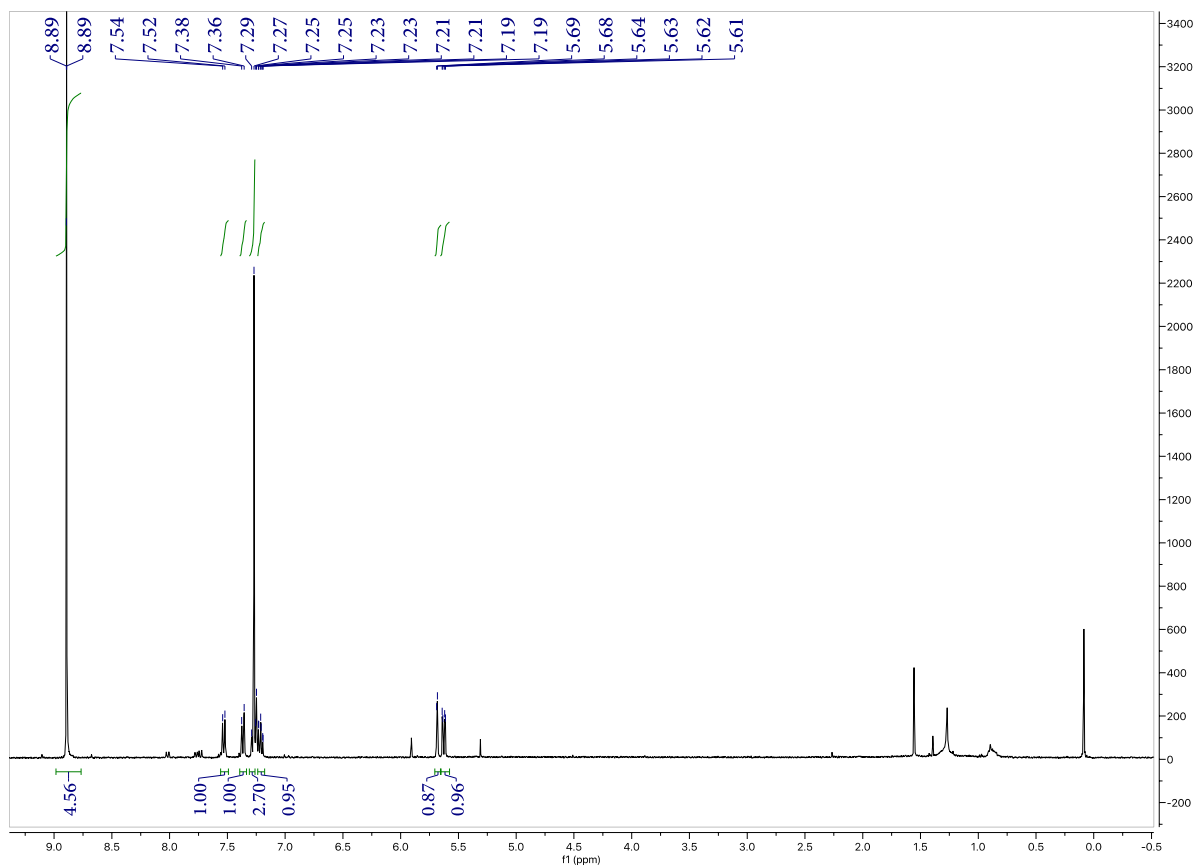


Figure S1: ^1H NMR spectrum of NaphO-Cl₆BsubPc.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

3477 formula(e) evaluated with 103 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-500 H: 0-1000 B: 1-1 N: 0-10 O: 0-10 Cl: 5-6 74Ge: 0-2

kw-02-35 column 1

UofT GCT

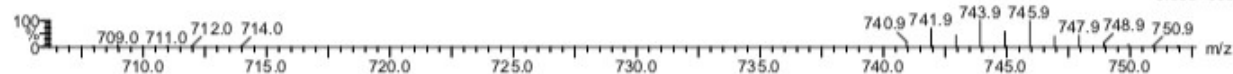
07-Oct-2019

14:40:09

TOF MS E+

5.89e+005

191007_2644 468 (7.801) Cm (444:468-35:80x3.000)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
741.9376	741.9375	0.1	0.1	21.0	1692.1	C23 H12 B N10 O8 Cl5
	741.9375	0.1	0.1	29.0	9813.5	C34 H13 B N6 O Cl6
	741.9377	-0.1	-0.1	4.5	33294.7	C22 H35 B N3 O2 Cl6 74Ge2
	741.9378	-0.2	-0.3	21.0	20189.8	C32 H22 B N2 O3 Cl5 74Ge
	741.9372	0.4	0.5	9.0	43730.0	C25 H32 B N2 O3 Cl5 74Ge2
	741.9370	0.6	0.8	9.0	17804.5	C16 H22 B N10 O8 Cl5 74Ge
	741.9370	0.6	0.8	33.5	3186.9	C37 H10 B N5 O2 Cl5
	741.9383	-0.7	-0.9	16.5	11685.1	C29 H25 B N3 O2 Cl6 74Ge
	741.9383	-0.7	-0.9	8.5	17734.7	C18 H24 B N7 O9 Cl5 74Ge
	741.9369	0.7	0.9	17.0	11365.0	C27 H23 B N6 O Cl6 74Ge
	741.9384	-0.8	-1.1	33.0	3608.4	C39 H12 B N2 O3 Cl5
	741.9364	1.2	1.6	5.0	33064.6	C20 H33 B N6 O Cl6 74Ge2
	741.9388	-1.2	-1.6	28.5	10150.5	C36 H15 B N3 O2 Cl6
	741.9364	1.2	1.6	21.5	19876.4	C30 H20 B N5 O2 Cl5 74Ge
	741.9388	-1.2	-1.6	4.0	9702.8	C15 H27 B N8 O8 Cl6 74Ge
	741.9389	-1.3	-1.8	20.5	1781.7	C25 H14 B N7 O9 Cl5
	741.9362	1.4	1.9	29.5	9525.5	C32 H11 B N9 Cl6
	741.9362	1.4	1.9	24.0	9636.0	C33 H17 B N2 O5 Cl6
	741.9390	-1.4	-1.9	4.0	33488.9	C24 H37 B O3 Cl6 74Ge2
	741.9359	1.7	2.3	9.5	43642.1	C23 H30 B N5 O2 Cl5 74Ge2
	741.9394	-1.8	-2.4	16.0	9659.3	C22 H17 B N8 O8 Cl6
	741.9357	1.9	2.6	34.0	2765.9	C35 H8 B N8 O Cl5
	741.9357	1.9	2.6	28.5	2652.0	C36 H14 B N O6 Cl5
	741.9356	2.0	2.7	17.5	11069.3	C25 H21 B N9 Cl6 74Ge
	741.9396	-2.0	-2.7	16.0	12115.5	C31 H27 B O3 Cl6 74Ge
	741.9396	-2.0	-2.7	8.0	17726.7	C20 H26 B N4 O10 Cl5 74Ge
	741.9356	2.0	2.7	12.0	10600.5	C26 H27 B N2 O5 Cl6 74Ge
	741.9399	-2.3	-3.1	13.5	44872.3	C28 H30 B N3 Cl5 74Ge2
	741.9353	2.3	3.1	12.0	10301.2	C17 H17 B N10 O10 Cl6
	741.9351	2.5	3.4	22.0	19608.9	C28 H18 B N8 O Cl5 74Ge
	741.9351	2.5	3.4	16.5	18935.7	C29 H24 B N O6 Cl5 74Ge
	741.9401	-2.5	-3.4	3.5	9719.8	C17 H29 B N5 O9 Cl6 74Ge
	741.9402	-2.6	-3.5	20.0	1929.4	C27 H16 B N4 O10 Cl5
	741.9350	2.6	3.5	0.0	32464.3	C19 H37 B N2 O5 Cl6 74Ge2
	741.9350	2.6	3.5	5.5	32959.8	C18 H31 B N9 Cl6 74Ge2
	741.9402	-2.6	-3.5	28.0	10623.0	C38 H17 B O3 Cl6
	741.9404	-2.8	-3.8	1.0	42932.6	C14 H32 B N8 O6 Cl5 74Ge2
	741.9348	2.8	3.8	24.5	9392.2	C31 H15 B N5 O4 Cl6
	741.9348	2.8	3.8	0.0	10311.4	C10 H27 B N10 O10 Cl6 74Ge
	741.9405	-2.9	-3.9	25.5	21755.2	C35 H20 B N3 Cl5 74Ge
	741.9407	-3.1	-4.2	15.5	9744.5	C24 H19 B N5 O9 Cl6
	741.9345	3.1	4.2	4.5	42914.3	C22 H34 B N O6 Cl5 74Ge2
	741.9345	3.1	4.2	10.0	43443.4	C21 H28 B N8 O Cl5 74Ge2
	741.9343	3.3	4.4	29.0	2344.7	C34 H12 B N4 O5 Cl5
	741.9343	3.3	4.4	12.5	10382.3	C24 H25 B N5 O4 Cl6 74Ge
	741.9410	-3.4	-4.6	37.5	4912.3	C42 H10 B N3 Cl5
	741.9410	-3.4	-4.6	13.0	18242.8	C21 H22 B N8 O6 Cl5 74Ge
	741.9412	-3.6	-4.9	13.0	45203.9	C30 H32 B O Cl5 74Ge2
	741.9338	3.8	5.1	17.0	18770.6	C27 H22 B N4 O5 Cl5 74Ge
	741.9415	-3.9	-5.3	25.0	2040.6	C28 H12 B N8 O6 Cl5
	741.9415	-3.9	-5.3	3.0	9777.7	C19 H31 B N2 O10 Cl6 74Ge
	741.9337	3.9	5.3	0.5	32370.0	C17 H35 B N5 O4 Cl6 74Ge2
	741.9415	-3.9	-5.3	8.5	10019.4	C18 H25 B N9 O5 Cl6 74Ge
	741.9335	4.1	5.5	19.5	9385.1	C30 H19 B N O8 Cl6
	741.9335	4.1	5.5	25.0	9173.4	C29 H13 B N8 O3 Cl6

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
741.9417	-4.1	-5.5	8.5	34825.4	C27 H35 B N C16 74Ge2	
741.9418	-4.2	-5.7	0.5	42828.0	C16 H34 B N5 O7 C15 74Ge2	
741.9418	-4.2	-5.7	25.0	22274.6	C37 H22 B O C15 74Ge	
741.9332	4.4	5.9	5.0	42875.0	C20 H32 B N4 O5 C15 74Ge2	
741.9420	-4.4	-5.9	15.0	9931.2	C26 H21 B N2 O10 C16	
741.9420	-4.4	-5.9	20.5	9630.0	C25 H15 B N9 O5 C16	
741.9330	4.6	6.2	29.5	2066.3	C32 H10 B N7 O4 C15	
741.9330	4.6	6.2	24.0	2031.8	C33 H16 B O9 C15	
741.9329	4.7	6.3	7.5	9833.2	C23 H29 B N O8 C16 74Ge	
741.9423	-4.7	-6.3	12.5	18379.6	C23 H24 B N5 O7 C15 74Ge	
741.9423	-4.7	-6.3	20.5	13670.1	C34 H25 B N C16 74Ge	
741.9329	4.7	6.3	13.0	10224.1	C22 H23 B N8 O3 C16 74Ge	
741.9424	-4.8	-6.5	37.0	5524.9	C44 H12 B O C15	
741.9428	-5.2	-7.0	8.0	10192.1	C20 H27 B N6 O6 C16 74Ge	
741.9324	5.2	7.0	12.0	18083.8	C26 H26 B O9 C15 74Ge	
741.9324	5.2	7.0	17.5	18599.6	C25 H20 B N7 O4 C15 74Ge	
741.9429	-5.3	-7.1	24.5	2347.3	C30 H14 B N5 O7 C15	
741.9429	-5.3	-7.1	32.5	11595.9	C41 H15 B N C16	
741.9323	5.3	7.1	1.0	32439.5	C15 H33 B N8 O3 C16 74Ge2	
741.9321	5.5	7.4	20.0	9318.0	C28 H17 B N4 O7 C16	
741.9431	-5.5	-7.4	0.0	42910.4	C18 H36 B N2 O8 C15 74Ge2	
741.9431	-5.5	-7.4	5.5	43394.3	C17 H30 B N9 O3 C15 74Ge2	
741.9319	5.7	7.7	5.5	42907.8	C18 H30 B N7 O4 C15 74Ge2	
741.9319	5.7	7.7	0.0	42383.2	C19 H36 B O9 C15 74Ge2	
741.9434	-5.8	-7.8	20.0	9849.6	C27 H17 B N6 O6 C16	
741.9317	5.9	8.0	30.0	1878.2	C30 H8 B N10 O3 C15	
741.9317	5.9	8.0	24.5	1866.6	C31 H14 B N3 O8 C15	
741.9316	6.0	8.1	8.0	9774.2	C21 H27 B N4 O7 C16 74Ge	
741.9436	-6.0	-8.1	1.0	32861.5	C14 H33 B N10 O2 C16 74Ge2	
741.9437	-6.1	-8.2	12.0	18674.0	C25 H26 B N2 O8 C15 74Ge	
741.9437	-6.1	-8.2	17.5	19187.7	C24 H20 B N9 O3 C15 74Ge	
741.9441	-6.5	-8.8	13.0	10802.7	C21 H23 B N10 O2 C16 74Ge	
741.9311	6.5	8.8	18.0	18517.4	C23 H18 B N10 O3 C15 74Ge	
741.9311	6.5	8.8	12.5	18012.4	C24 H24 B N3 O8 C15 74Ge	
741.9442	-6.6	-8.9	29.5	2713.6	C31 H10 B N9 O3 C15	
741.9442	-6.6	-8.9	7.5	10444.4	C22 H29 B N3 O7 C16 74Ge	
741.9442	-6.6	-8.9	24.0	2721.6	C32 H16 B N2 O8 C15	
741.9308	6.8	9.2	20.5	9252.5	C26 H15 B N7 O6 C16	
741.9444	-6.8	-9.2	5.0	43548.2	C19 H32 B N6 O4 C15 74Ge2	
741.9305	7.1	9.6	6.0	42980.1	C16 H28 B N10 O3 C15 74Ge2	
741.9447	-7.1	-9.6	19.5	10106.6	C29 H19 B N3 O7 C16	
741.9305	7.1	9.6	0.5	42487.7	C17 H34 B N3 O8 C15 74Ge2	
741.9447	-7.1	-9.6	25.0	9876.4	C28 H13 B N10 O2 C16	
741.9449	-7.3	-9.8	0.5	33061.1	C16 H35 B N7 O3 C16 74Ge2	
741.9303	7.3	9.8	33.0	10809.8	C40 H13 B N2 C16	
741.9303	7.3	9.8	25.0	1746.8	C29 H12 B N6 O7 C15	
741.9450	-7.4	-10.0	17.0	19501.0	C26 H22 B N6 O4 C15 74Ge	
741.9302	7.4	10.0	8.5	9786.9	C19 H25 B N7 O6 C16 74Ge	

Figure S2: EI+ Mass Spectrum of NaphO-Cl₆SubPc.

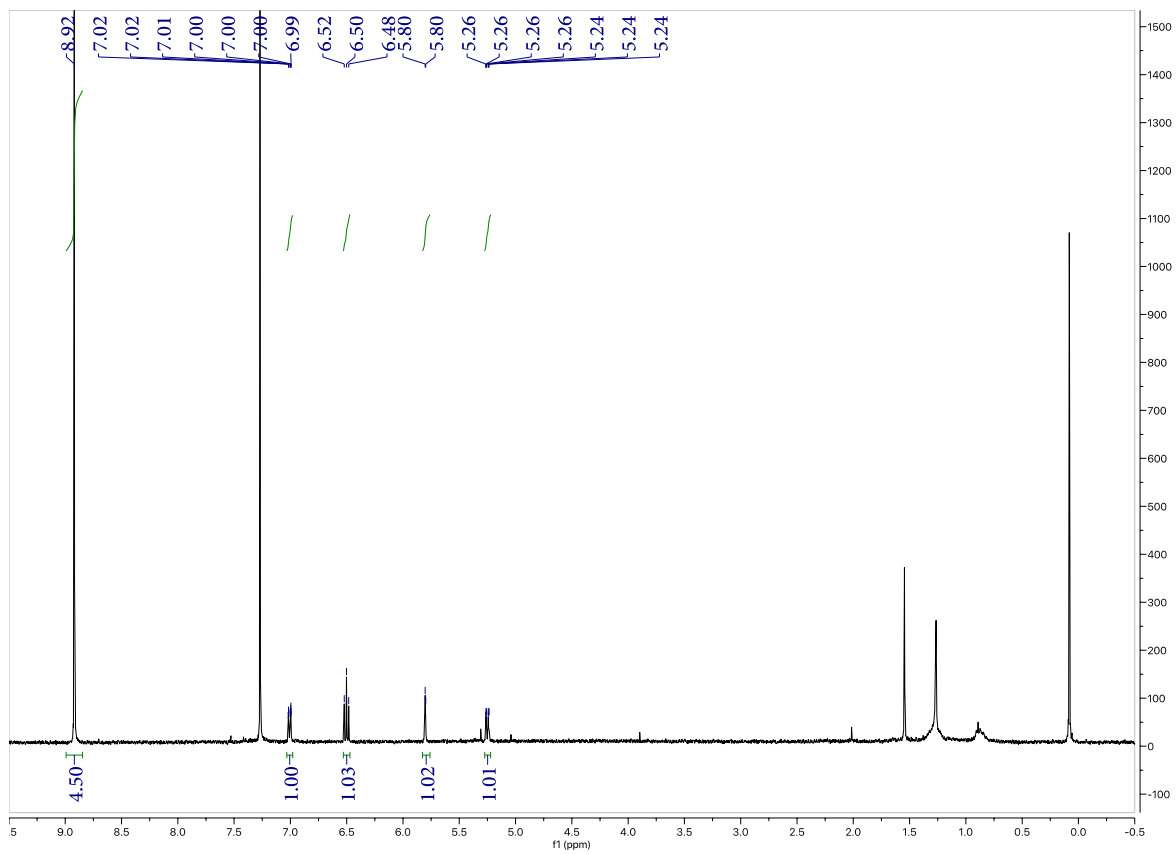
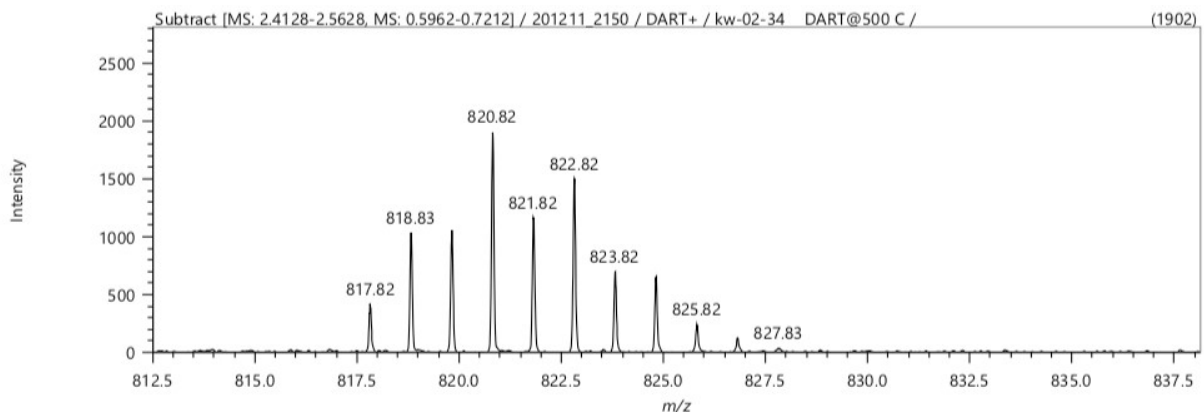


Figure S3: ^1H NMR Spectrum of *mIPhO-Cl₆BsubPc*.



Elemental Composition

Parameters

Tolerance: ± 10.00 mDa
 Electron: Odd/Even
 Charge: +1
 DBE: -1.5 - 100.0

Elements Set 1:

Symbol	C	H	O	N	B	Cl	I
Min	0	0	1	0	0	4	0
Max	100	100	1	6	1	6	1

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
818.82665	1035.05	C45 B N3 O Cl6	818.82601	0.64	0.78	45.0
		C30 H11 B N6 O Cl6 I	818.82578	0.88	1.07	25.5
		C41 H5 B N2 O Cl4 I	818.82882	-2.17	-2.65	38.5
		C43 H6 N O Cl4 I	818.82427	2.38	2.91	39.0
		C40 H10 B O Cl5 I	818.83065	-4.00	-4.89	33.5
		C47 H N2 O Cl6	818.82146	5.20	6.35	45.5
		C34 H9 N6 O Cl5 I	818.83197	-5.32	-6.49	30.5
		C32 H12 N5 O Cl6 I	818.82122	5.43	6.63	26.0
		C33 H14 N4 O Cl6 I	818.83380	-7.15	-8.73	25.5
		C48 H3 N O Cl6	818.83403	-7.38	-9.01	45.0
		C39 H8 B N O Cl5 I	818.81808	8.57	10.47	34.0

Figure S4: DART Mass Spectrum of NaphO-Cl₆BsubPc.

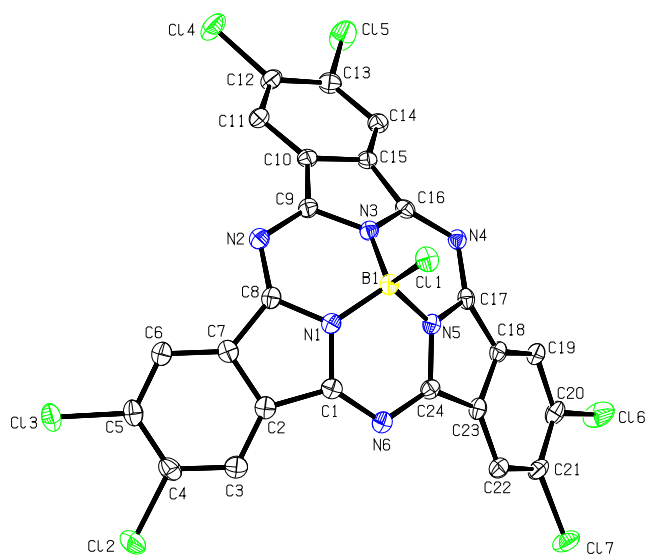


Figure S5: Anisotropic displacement ellipsoid plots of Cl-Cl₆ BsubPc (Toluene:Heptane; CCDC deposit 2087092).

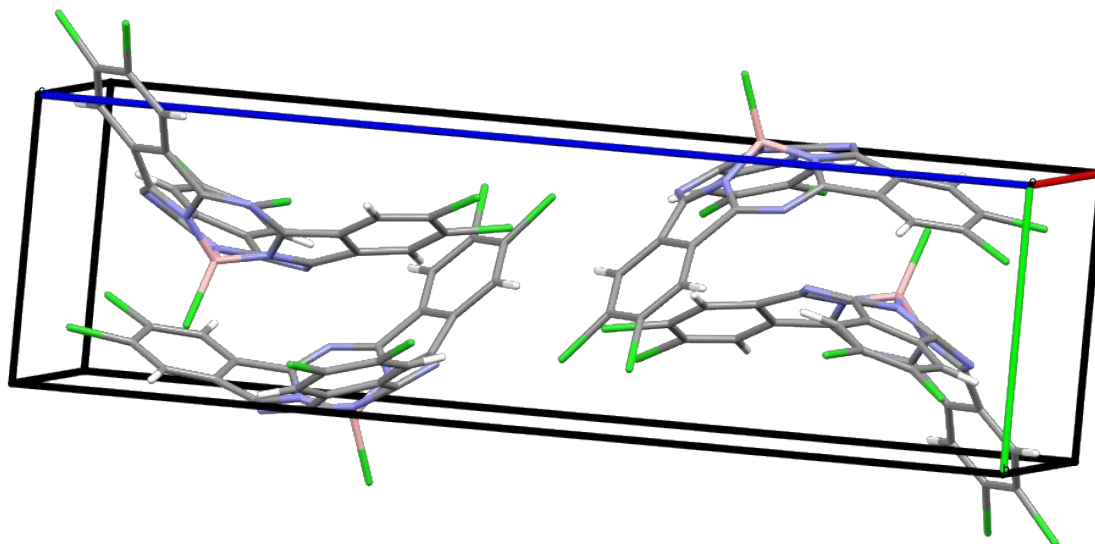


Figure S6: Populated unit cell of Cl-Cl₆ BsubPc (Toluene:Heptane; CCDC deposit 2087092).

Table S 1. Crystal data and structure refinement for **Cl-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087092)**.

Identification code	d19183_a	
Empirical formula	C ₂₄ H ₆ B Cl ₇ N ₆	
Formula weight	637.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 13.0905(3) Å	α = 90°.
	b = 7.4207(2) Å	β = 99.499(1)°.
	c = 25.4832(6) Å	γ = 90°.
Volume	2441.51(10) Å ³	
Z	4	
Density (calculated)	1.734 Mg/m ³	
Absorption coefficient	0.844 mm ⁻¹	
F(000)	1264	
Crystal size	0.230 x 0.130 x 0.050 mm ³	
Theta range for data collection	1.620 to 27.556°.	
Index ranges	-8 ≤ h ≤ 17, -9 ≤ k ≤ 9, -33 ≤ l ≤ 33	
Reflections collected	29765	
Independent reflections	5627 [R(int) = 0.0297]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6857	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5627 / 0 / 343	
Goodness-of-fit on F ²	1.022	
Final R indices [I > 2σ(I)]	R1 = 0.0291, wR2 = 0.0664	
R indices (all data)	R1 = 0.0405, wR2 = 0.0715	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.341 and -0.358 e.Å ⁻³	

Table S 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087092)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6127(1)	-2521(1)	3389(1)	23(1)
Cl(2)	3567(1)	7803(1)	4092(1)	44(1)
Cl(3)	5624(1)	7811(1)	4920(1)	29(1)
Cl(4)	12062(1)	2783(1)	4100(1)	33(1)
Cl(5)	12098(1)	1658(1)	2915(1)	36(1)
Cl(6)	6011(1)	1844(1)	242(1)	35(1)
Cl(7)	3779(1)	2926(1)	436(1)	30(1)
N(1)	6029(1)	1212(2)	3480(1)	17(1)
N(2)	7620(1)	1842(2)	4052(1)	18(1)
N(3)	7598(1)	103(2)	3266(1)	16(1)
N(4)	7737(1)	-288(2)	2355(1)	16(1)
N(5)	6086(1)	138(2)	2616(1)	16(1)
N(6)	4659(1)	1918(2)	2773(1)	18(1)
C(1)	5129(1)	2090(2)	3282(1)	17(1)
C(2)	5004(1)	3456(2)	3679(1)	18(1)
C(3)	4261(1)	4783(2)	3692(1)	22(1)
C(4)	4449(1)	6078(3)	4088(1)	23(1)
C(5)	5366(1)	6072(2)	4466(1)	21(1)
C(6)	6101(1)	4745(2)	4461(1)	20(1)
C(7)	5917(1)	3435(2)	4066(1)	18(1)
C(8)	6591(1)	2046(2)	3912(1)	18(1)
C(9)	8111(1)	969(2)	3704(1)	17(1)
C(10)	9179(1)	1119(2)	3618(1)	17(1)
C(11)	10055(1)	1849(2)	3929(1)	20(1)
C(12)	10951(1)	1966(2)	3710(1)	21(1)
C(13)	10970(1)	1438(2)	3182(1)	21(1)
C(14)	10103(1)	728(2)	2867(1)	19(1)
C(15)	9210(1)	526(2)	3091(1)	17(1)
C(16)	8168(1)	-50(2)	2865(1)	16(1)
C(17)	6708(1)	-48(2)	2239(1)	16(1)

C(18)	6087(1)	527(2)	1747(1)	17(1)
C(19)	6356(1)	734(2)	1246(1)	18(1)
C(20)	5641(1)	1501(2)	854(1)	20(1)
C(21)	4655(1)	2034(2)	952(1)	20(1)
C(22)	4393(1)	1893(2)	1455(1)	20(1)
C(23)	5120(1)	1152(2)	1862(1)	17(1)
C(24)	5180(1)	1023(2)	2439(1)	17(1)
B(1)	6464(2)	-245(3)	3188(1)	16(1)

Table S 3. Bond lengths [\AA] and angles [$^\circ$] for **Cl-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087092)**.

Cl(1)-B(1)	1.8395(19)
Cl(2)-C(4)	1.7253(18)
Cl(3)-C(5)	1.7282(18)
Cl(4)-C(12)	1.7290(17)
Cl(5)-C(13)	1.7321(17)
Cl(6)-C(20)	1.7262(17)
Cl(7)-C(21)	1.7263(17)
N(1)-C(8)	1.368(2)
N(1)-C(1)	1.368(2)
N(1)-B(1)	1.479(2)
N(2)-C(9)	1.343(2)
N(2)-C(8)	1.344(2)
N(3)-C(9)	1.365(2)
N(3)-C(16)	1.366(2)
N(3)-B(1)	1.487(2)
N(4)-C(16)	1.340(2)
N(4)-C(17)	1.343(2)
N(5)-C(17)	1.365(2)
N(5)-C(24)	1.366(2)
N(5)-B(1)	1.487(2)
N(6)-C(1)	1.346(2)
N(6)-C(24)	1.351(2)
C(1)-C(2)	1.461(2)
C(2)-C(3)	1.388(2)
C(2)-C(7)	1.419(2)
C(3)-C(4)	1.385(2)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.410(3)
C(5)-C(6)	1.378(3)
C(6)-C(7)	1.392(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.453(2)
C(9)-C(10)	1.455(2)

C(10)-C(11)	1.392(2)
C(10)-C(15)	1.421(2)
C(11)-C(12)	1.382(2)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.407(2)
C(13)-C(14)	1.382(2)
C(14)-C(15)	1.391(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.454(2)
C(17)-C(18)	1.442(2)
C(18)-C(19)	1.387(2)
C(18)-C(23)	1.424(2)
C(19)-C(20)	1.374(2)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.411(2)
C(21)-C(22)	1.386(2)
C(22)-C(23)	1.399(2)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.463(2)
C(8)-N(1)-C(1)	113.46(14)
C(8)-N(1)-B(1)	122.38(14)
C(1)-N(1)-B(1)	122.84(14)
C(9)-N(2)-C(8)	116.56(14)
C(9)-N(3)-C(16)	113.30(14)
C(9)-N(3)-B(1)	122.41(14)
C(16)-N(3)-B(1)	122.84(14)
C(16)-N(4)-C(17)	116.22(14)
C(17)-N(5)-C(24)	113.65(13)
C(17)-N(5)-B(1)	122.01(14)
C(24)-N(5)-B(1)	123.17(14)
C(1)-N(6)-C(24)	117.10(14)
N(6)-C(1)-N(1)	122.66(15)
N(6)-C(1)-C(2)	130.32(15)
N(1)-C(1)-C(2)	105.26(14)
C(3)-C(2)-C(7)	120.26(16)

C(3)-C(2)-C(1)	131.96(16)
C(7)-C(2)-C(1)	107.20(14)
C(4)-C(3)-C(2)	117.96(16)
C(4)-C(3)-H(3A)	121.0
C(2)-C(3)-H(3A)	121.0
C(3)-C(4)-C(5)	121.59(17)
C(3)-C(4)-Cl(2)	118.73(14)
C(5)-C(4)-Cl(2)	119.59(14)
C(6)-C(5)-C(4)	120.93(16)
C(6)-C(5)-Cl(3)	118.66(14)
C(4)-C(5)-Cl(3)	120.30(14)
C(5)-C(6)-C(7)	117.84(16)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	121.39(16)
C(6)-C(7)-C(8)	130.57(16)
C(2)-C(7)-C(8)	107.47(14)
N(2)-C(8)-N(1)	122.99(15)
N(2)-C(8)-C(7)	129.48(15)
N(1)-C(8)-C(7)	105.57(14)
N(2)-C(9)-N(3)	122.88(15)
N(2)-C(9)-C(10)	129.66(15)
N(3)-C(9)-C(10)	105.50(13)
C(11)-C(10)-C(15)	120.65(15)
C(11)-C(10)-C(9)	131.75(15)
C(15)-C(10)-C(9)	107.29(14)
C(12)-C(11)-C(10)	117.97(15)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.28(16)
C(11)-C(12)-Cl(4)	118.68(13)
C(13)-C(12)-Cl(4)	120.05(13)
C(14)-C(13)-C(12)	121.29(16)
C(14)-C(13)-Cl(5)	118.69(13)
C(12)-C(13)-Cl(5)	120.03(13)
C(13)-C(14)-C(15)	117.94(15)

C(13)-C(14)-H(14A)	121.0
C(15)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	120.76(15)
C(14)-C(15)-C(16)	131.76(15)
C(10)-C(15)-C(16)	107.11(14)
N(4)-C(16)-N(3)	122.81(15)
N(4)-C(16)-C(15)	129.77(15)
N(3)-C(16)-C(15)	105.78(14)
N(4)-C(17)-N(5)	123.49(14)
N(4)-C(17)-C(18)	129.14(15)
N(5)-C(17)-C(18)	105.49(14)
C(19)-C(18)-C(23)	121.52(15)
C(19)-C(18)-C(17)	129.85(15)
C(23)-C(18)-C(17)	108.07(14)
C(20)-C(19)-C(18)	117.93(16)
C(20)-C(19)-H(19A)	121.0
C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.44(15)
C(19)-C(20)-Cl(6)	117.32(13)
C(21)-C(20)-Cl(6)	121.22(13)
C(22)-C(21)-C(20)	121.01(15)
C(22)-C(21)-Cl(7)	119.87(14)
C(20)-C(21)-Cl(7)	119.10(13)
C(21)-C(22)-C(23)	118.25(16)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	119.70(15)
C(22)-C(23)-C(24)	133.44(16)
C(18)-C(23)-C(24)	106.45(14)
N(6)-C(24)-N(5)	121.93(14)
N(6)-C(24)-C(23)	130.77(15)
N(5)-C(24)-C(23)	105.32(14)
N(1)-B(1)-N(5)	105.02(14)
N(1)-B(1)-N(3)	105.33(14)
N(5)-B(1)-N(3)	105.13(13)
N(1)-B(1)-Cl(1)	113.68(12)

N(5)-B(1)-Cl(1) 113.07(12)

N(3)-B(1)-Cl(1) 113.74(12)

Symmetry transformations used to generate equivalent atoms:

Table S 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087092)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	29(1)	17(1)	23(1)	4(1)	8(1)	-3(1)
Cl(2)	27(1)	44(1)	58(1)	-23(1)	3(1)	13(1)
Cl(3)	33(1)	26(1)	29(1)	-10(1)	10(1)	-2(1)
Cl(4)	19(1)	52(1)	26(1)	-8(1)	-1(1)	-8(1)
Cl(5)	22(1)	58(1)	31(1)	-10(1)	10(1)	-10(1)
Cl(6)	31(1)	60(1)	15(1)	10(1)	4(1)	6(1)
Cl(7)	24(1)	42(1)	20(1)	5(1)	-5(1)	5(1)
N(1)	18(1)	18(1)	15(1)	1(1)	4(1)	-1(1)
N(2)	21(1)	20(1)	13(1)	2(1)	3(1)	1(1)
N(3)	19(1)	16(1)	13(1)	2(1)	2(1)	1(1)
N(4)	19(1)	14(1)	15(1)	0(1)	2(1)	0(1)
N(5)	17(1)	15(1)	15(1)	0(1)	3(1)	-2(1)
N(6)	16(1)	20(1)	18(1)	0(1)	5(1)	-4(1)
C(1)	16(1)	17(1)	19(1)	2(1)	6(1)	-3(1)
C(2)	18(1)	20(1)	18(1)	1(1)	8(1)	-4(1)
C(3)	16(1)	26(1)	25(1)	-1(1)	7(1)	-3(1)
C(4)	21(1)	24(1)	28(1)	-2(1)	11(1)	2(1)
C(5)	26(1)	21(1)	19(1)	-3(1)	11(1)	-5(1)
C(6)	22(1)	22(1)	16(1)	1(1)	6(1)	-4(1)
C(7)	20(1)	18(1)	16(1)	2(1)	8(1)	-2(1)
C(8)	21(1)	19(1)	13(1)	2(1)	4(1)	-2(1)
C(9)	21(1)	16(1)	13(1)	3(1)	1(1)	1(1)
C(10)	19(1)	16(1)	15(1)	3(1)	1(1)	3(1)
C(11)	21(1)	22(1)	15(1)	0(1)	0(1)	2(1)
C(12)	18(1)	24(1)	21(1)	-1(1)	-2(1)	-1(1)
C(13)	18(1)	23(1)	23(1)	1(1)	6(1)	0(1)
C(14)	21(1)	20(1)	17(1)	1(1)	2(1)	4(1)
C(15)	18(1)	16(1)	16(1)	2(1)	1(1)	3(1)
C(16)	18(1)	13(1)	17(1)	2(1)	4(1)	2(1)
C(17)	21(1)	12(1)	15(1)	-1(1)	4(1)	-2(1)

C(18)	18(1)	15(1)	17(1)	-2(1)	1(1)	-4(1)
C(19)	18(1)	20(1)	16(1)	-2(1)	2(1)	-3(1)
C(20)	23(1)	25(1)	13(1)	0(1)	1(1)	-4(1)
C(21)	20(1)	21(1)	18(1)	1(1)	-4(1)	-2(1)
C(22)	17(1)	21(1)	20(1)	-2(1)	1(1)	-2(1)
C(23)	19(1)	17(1)	16(1)	-2(1)	2(1)	-4(1)
C(24)	15(1)	16(1)	18(1)	0(1)	2(1)	-3(1)
B(1)	20(1)	15(1)	14(1)	1(1)	3(1)	-2(1)

Table S 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **Cl-Cl₆BsubPc** (**Toluene:Heptane**; **CCDC deposit 2087092**).

	x	y	z	U(eq)
H(3A)	3642	4802	3438	26
H(6A)	6714	4725	4720	23
H(11A)	10038	2253	4281	24
H(14A)	10116	389	2509	23
H(19A)	7014	358	1176	22
H(22A)	3736	2289	1523	23

Table S 6. Torsion angles [°] for **Cl-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087092)**.

C(24)-N(6)-C(1)-N(1)	-8.6(2)
C(24)-N(6)-C(1)-C(2)	153.94(17)
C(8)-N(1)-C(1)-N(6)	155.67(15)
B(1)-N(1)-C(1)-N(6)	-11.5(2)
C(8)-N(1)-C(1)-C(2)	-10.62(18)
B(1)-N(1)-C(1)-C(2)	-177.75(14)
N(6)-C(1)-C(2)-C(3)	12.9(3)
N(1)-C(1)-C(2)-C(3)	177.74(17)
N(6)-C(1)-C(2)-C(7)	-158.17(16)
N(1)-C(1)-C(2)-C(7)	6.66(17)
C(7)-C(2)-C(3)-C(4)	0.8(2)
C(1)-C(2)-C(3)-C(4)	-169.30(17)
C(2)-C(3)-C(4)-C(5)	0.4(3)
C(2)-C(3)-C(4)-Cl(2)	176.82(13)
C(3)-C(4)-C(5)-C(6)	-1.4(3)
Cl(2)-C(4)-C(5)-C(6)	-177.87(13)
C(3)-C(4)-C(5)-Cl(3)	174.70(14)
Cl(2)-C(4)-C(5)-Cl(3)	-1.7(2)
C(4)-C(5)-C(6)-C(7)	1.2(2)
Cl(3)-C(5)-C(6)-C(7)	-174.97(12)
C(5)-C(6)-C(7)-C(2)	0.0(2)
C(5)-C(6)-C(7)-C(8)	170.19(16)
C(3)-C(2)-C(7)-C(6)	-1.0(2)
C(1)-C(2)-C(7)-C(6)	171.31(14)
C(3)-C(2)-C(7)-C(8)	-173.24(15)
C(1)-C(2)-C(7)-C(8)	-0.92(18)
C(9)-N(2)-C(8)-N(1)	8.9(2)
C(9)-N(2)-C(8)-C(7)	-152.76(17)
C(1)-N(1)-C(8)-N(2)	-155.33(15)
B(1)-N(1)-C(8)-N(2)	11.9(2)
C(1)-N(1)-C(8)-C(7)	10.08(18)
B(1)-N(1)-C(8)-C(7)	177.28(14)
C(6)-C(7)-C(8)-N(2)	-12.3(3)

C(2)-C(7)-C(8)-N(2)	158.93(16)
C(6)-C(7)-C(8)-N(1)	-176.44(16)
C(2)-C(7)-C(8)-N(1)	-5.18(18)
C(8)-N(2)-C(9)-N(3)	-8.9(2)
C(8)-N(2)-C(9)-C(10)	152.79(17)
C(16)-N(3)-C(9)-N(2)	154.83(15)
B(1)-N(3)-C(9)-N(2)	-11.8(2)
C(16)-N(3)-C(9)-C(10)	-10.64(18)
B(1)-N(3)-C(9)-C(10)	-177.26(14)
N(2)-C(9)-C(10)-C(11)	16.8(3)
N(3)-C(9)-C(10)-C(11)	-179.08(17)
N(2)-C(9)-C(10)-C(15)	-156.62(17)
N(3)-C(9)-C(10)-C(15)	7.48(18)
C(15)-C(10)-C(11)-C(12)	-0.3(2)
C(9)-C(10)-C(11)-C(12)	-173.05(17)
C(10)-C(11)-C(12)-C(13)	2.7(3)
C(10)-C(11)-C(12)-Cl(4)	-177.42(13)
C(11)-C(12)-C(13)-C(14)	-2.1(3)
Cl(4)-C(12)-C(13)-C(14)	177.99(14)
C(11)-C(12)-C(13)-Cl(5)	178.34(14)
Cl(4)-C(12)-C(13)-Cl(5)	-1.6(2)
C(12)-C(13)-C(14)-C(15)	-0.9(3)
Cl(5)-C(13)-C(14)-C(15)	178.67(13)
C(13)-C(14)-C(15)-C(10)	3.2(2)
C(13)-C(14)-C(15)-C(16)	175.30(17)
C(11)-C(10)-C(15)-C(14)	-2.6(3)
C(9)-C(10)-C(15)-C(14)	171.67(15)
C(11)-C(10)-C(15)-C(16)	-176.48(15)
C(9)-C(10)-C(15)-C(16)	-2.17(18)
C(17)-N(4)-C(16)-N(3)	11.6(2)
C(17)-N(4)-C(16)-C(15)	-151.65(17)
C(9)-N(3)-C(16)-N(4)	-157.39(15)
B(1)-N(3)-C(16)-N(4)	9.2(2)
C(9)-N(3)-C(16)-C(15)	9.32(18)
B(1)-N(3)-C(16)-C(15)	175.88(15)
C(14)-C(15)-C(16)-N(4)	-11.4(3)

C(10)-C(15)-C(16)-N(4)	161.47(17)
C(14)-C(15)-C(16)-N(3)	-176.85(18)
C(10)-C(15)-C(16)-N(3)	-3.97(18)
C(16)-N(4)-C(17)-N(5)	-10.5(2)
C(16)-N(4)-C(17)-C(18)	151.60(17)
C(24)-N(5)-C(17)-N(4)	156.43(15)
B(1)-N(5)-C(17)-N(4)	-11.6(2)
C(24)-N(5)-C(17)-C(18)	-9.21(18)
B(1)-N(5)-C(17)-C(18)	-177.20(14)
N(4)-C(17)-C(18)-C(19)	10.4(3)
N(5)-C(17)-C(18)-C(19)	174.90(17)
N(4)-C(17)-C(18)-C(23)	-160.90(16)
N(5)-C(17)-C(18)-C(23)	3.64(18)
C(23)-C(18)-C(19)-C(20)	-2.5(2)
C(17)-C(18)-C(19)-C(20)	-172.79(17)
C(18)-C(19)-C(20)-C(21)	-1.2(3)
C(18)-C(19)-C(20)-Cl(6)	177.08(13)
C(19)-C(20)-C(21)-C(22)	3.6(3)
Cl(6)-C(20)-C(21)-C(22)	-174.62(14)
C(19)-C(20)-C(21)-Cl(7)	-178.03(14)
Cl(6)-C(20)-C(21)-Cl(7)	3.8(2)
C(20)-C(21)-C(22)-C(23)	-2.1(3)
Cl(7)-C(21)-C(22)-C(23)	179.56(13)
C(21)-C(22)-C(23)-C(18)	-1.6(2)
C(21)-C(22)-C(23)-C(24)	169.95(17)
C(19)-C(18)-C(23)-C(22)	4.0(2)
C(17)-C(18)-C(23)-C(22)	176.14(15)
C(19)-C(18)-C(23)-C(24)	-169.60(15)
C(17)-C(18)-C(23)-C(24)	2.53(18)
C(1)-N(6)-C(24)-N(5)	7.8(2)
C(1)-N(6)-C(24)-C(23)	-153.73(17)
C(17)-N(5)-C(24)-N(6)	-154.85(15)
B(1)-N(5)-C(24)-N(6)	13.0(2)
C(17)-N(5)-C(24)-C(23)	10.76(18)
B(1)-N(5)-C(24)-C(23)	178.59(14)
C(22)-C(23)-C(24)-N(6)	-16.2(3)

C(18)-C(23)-C(24)-N(6)	156.10(17)
C(22)-C(23)-C(24)-N(5)	179.92(18)
C(18)-C(23)-C(24)-N(5)	-7.73(18)
C(8)-N(1)-B(1)-N(5)	-138.63(15)
C(1)-N(1)-B(1)-N(5)	27.4(2)
C(8)-N(1)-B(1)-N(3)	-27.9(2)
C(1)-N(1)-B(1)-N(3)	138.09(15)
C(8)-N(1)-B(1)-Cl(1)	97.26(16)
C(1)-N(1)-B(1)-Cl(1)	-96.74(16)
C(17)-N(5)-B(1)-N(1)	138.60(15)
C(24)-N(5)-B(1)-N(1)	-28.2(2)
C(17)-N(5)-B(1)-N(3)	27.7(2)
C(24)-N(5)-B(1)-N(3)	-139.09(15)
C(17)-N(5)-B(1)-Cl(1)	-96.91(16)
C(24)-N(5)-B(1)-Cl(1)	96.26(17)
C(9)-N(3)-B(1)-N(1)	27.9(2)
C(16)-N(3)-B(1)-N(1)	-137.42(15)
C(9)-N(3)-B(1)-N(5)	138.57(15)
C(16)-N(3)-B(1)-N(5)	-26.8(2)
C(9)-N(3)-B(1)-Cl(1)	-97.20(17)
C(16)-N(3)-B(1)-Cl(1)	97.44(16)

Symmetry transformations used to generate equivalent atoms:

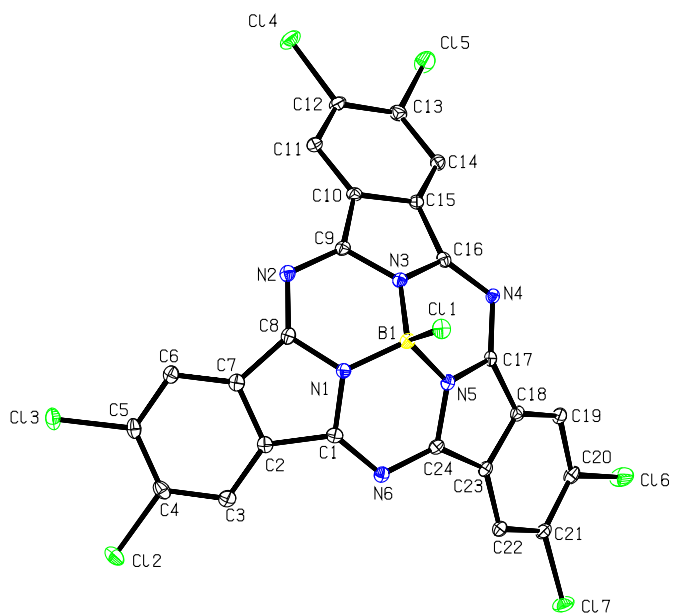


Figure S7: Anisotropic displacement ellipsoid of Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100).

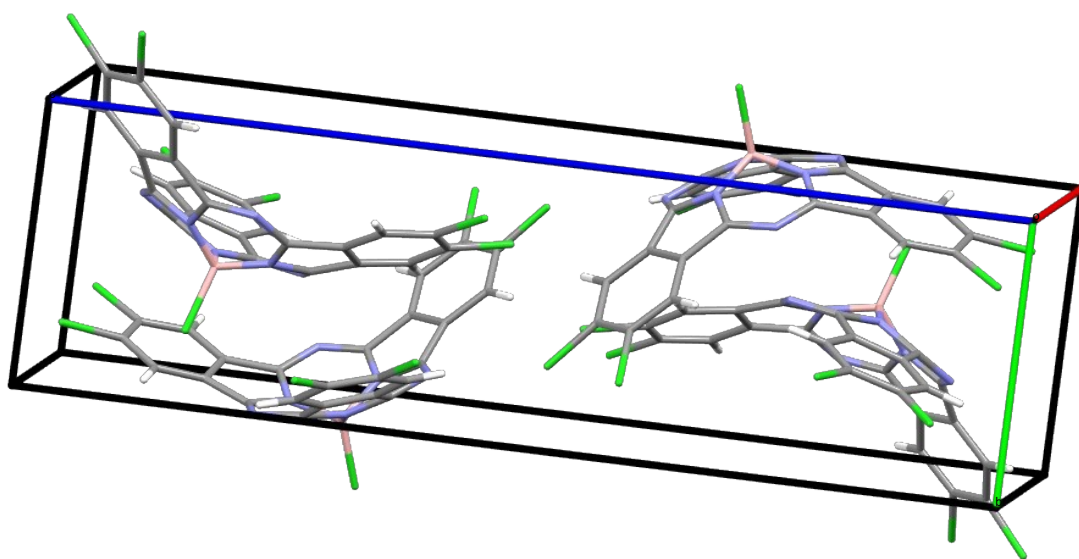


Figure S8: Populated unit cell of Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100).

Table S 7. Crystal data and structure refinement for **Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100)**.

Identification code	d19138_a	
Empirical formula	C ₂₄ H ₆ B Cl ₇ N ₆	
Formula weight	637.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 13.0845(8) Å	α = 90°.
	b = 7.4155(4) Å	β = 99.476(2)°.
	c = 25.4585(16) Å	γ = 90°.
Volume	2436.5(3) Å ³	
Z	4	
Density (calculated)	1.737 Mg/m ³	
Absorption coefficient	0.845 mm ⁻¹	
F(000)	1264	
Crystal size	0.240 x 0.070 x 0.020 mm ³	
Theta range for data collection	1.622 to 27.516°.	
Index ranges	-16 ≤ h ≤ 17, -9 ≤ k ≤ 9, -33 ≤ l ≤ 33	
Reflections collected	34990	
Independent reflections	5610 [R(int) = 0.0647]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6945	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5610 / 0 / 343	
Goodness-of-fit on F ²	1.007	
Final R indices [I > 2σ(I)]	R1 = 0.0370, wR2 = 0.0707	
R indices (all data)	R1 = 0.0688, wR2 = 0.0811	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.342 and -0.333 e.Å ⁻³	

Table S 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6126(1)	-2521(1)	3389(1)	22(1)
Cl(2)	3568(1)	7804(1)	4092(1)	43(1)
Cl(3)	5625(1)	7812(1)	4920(1)	28(1)
Cl(4)	12062(1)	2783(1)	4100(1)	32(1)
Cl(5)	12098(1)	1657(1)	2915(1)	36(1)
Cl(6)	6010(1)	1843(1)	243(1)	35(1)
Cl(7)	3779(1)	2926(1)	436(1)	29(1)
N(1)	6030(1)	1210(2)	3480(1)	15(1)
N(2)	7620(1)	1841(3)	4051(1)	18(1)
N(3)	7598(1)	101(2)	3267(1)	15(1)
N(4)	7738(1)	-289(2)	2354(1)	15(1)
N(5)	6091(1)	134(2)	2617(1)	15(1)
N(6)	4658(1)	1916(2)	2773(1)	17(1)
C(1)	5126(2)	2089(3)	3282(1)	16(1)
C(2)	5001(2)	3456(3)	3679(1)	16(1)
C(3)	4259(2)	4785(3)	3693(1)	20(1)
C(4)	4447(2)	6075(3)	4089(1)	22(1)
C(5)	5365(2)	6071(3)	4466(1)	20(1)
C(6)	6100(2)	4743(3)	4460(1)	19(1)
C(7)	5918(2)	3437(3)	4067(1)	17(1)
C(8)	6589(2)	2042(3)	3912(1)	16(1)
C(9)	8108(2)	973(3)	3705(1)	16(1)
C(10)	9176(2)	1119(3)	3617(1)	16(1)
C(11)	10054(2)	1846(3)	3930(1)	18(1)
C(12)	10950(2)	1968(3)	3710(1)	20(1)
C(13)	10971(2)	1439(3)	3183(1)	21(1)
C(14)	10102(2)	732(3)	2867(1)	18(1)
C(15)	9212(2)	527(3)	3091(1)	16(1)
C(16)	8169(2)	-50(3)	2864(1)	16(1)
C(17)	6703(2)	-47(3)	2240(1)	14(1)

C(18)	6082(2)	527(3)	1745(1)	16(1)
C(19)	6357(2)	733(3)	1247(1)	17(1)
C(20)	5638(2)	1503(3)	855(1)	20(1)
C(21)	4656(2)	2031(3)	954(1)	19(1)
C(22)	4392(2)	1888(3)	1456(1)	18(1)
C(23)	5120(2)	1150(3)	1863(1)	16(1)
C(24)	5179(2)	1026(3)	2440(1)	16(1)
B(1)	6460(2)	-243(3)	3188(1)	16(1)

Table S 9. Bond lengths [\AA] and angles [$^\circ$] for **Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100)**.

Cl(1)-B(1)	1.838(3)
Cl(2)-C(4)	1.724(2)
Cl(3)-C(5)	1.728(2)
Cl(4)-C(12)	1.729(2)
Cl(5)-C(13)	1.732(2)
Cl(6)-C(20)	1.725(2)
Cl(7)-C(21)	1.731(2)
N(1)-C(8)	1.363(3)
N(1)-C(1)	1.372(3)
N(1)-B(1)	1.473(3)
N(2)-C(9)	1.334(3)
N(2)-C(8)	1.345(3)
N(3)-C(9)	1.366(3)
N(3)-C(16)	1.369(3)
N(3)-B(1)	1.491(3)
N(4)-C(16)	1.339(3)
N(4)-C(17)	1.349(3)
N(5)-C(17)	1.355(3)
N(5)-C(24)	1.373(3)
N(5)-B(1)	1.480(3)
N(6)-C(1)	1.345(3)
N(6)-C(24)	1.346(3)
C(1)-C(2)	1.461(3)
C(2)-C(3)	1.388(3)
C(2)-C(7)	1.424(3)
C(3)-C(4)	1.381(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.409(3)
C(5)-C(6)	1.378(3)
C(6)-C(7)	1.384(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.453(3)

C(9)-C(10)	1.455(3)
C(10)-C(11)	1.394(3)
C(10)-C(15)	1.418(3)
C(11)-C(12)	1.384(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.402(3)
C(13)-C(14)	1.384(3)
C(14)-C(15)	1.386(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.455(3)
C(17)-C(18)	1.445(3)
C(18)-C(19)	1.382(3)
C(18)-C(23)	1.419(3)
C(19)-C(20)	1.379(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.406(3)
C(21)-C(22)	1.382(3)
C(22)-C(23)	1.398(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.460(3)
C(8)-N(1)-C(1)	113.41(19)
C(8)-N(1)-B(1)	122.68(19)
C(1)-N(1)-B(1)	122.60(19)
C(9)-N(2)-C(8)	116.66(19)
C(9)-N(3)-C(16)	113.40(19)
C(9)-N(3)-B(1)	122.3(2)
C(16)-N(3)-B(1)	122.79(19)
C(16)-N(4)-C(17)	116.13(19)
C(17)-N(5)-C(24)	113.38(19)
C(17)-N(5)-B(1)	122.80(19)
C(24)-N(5)-B(1)	122.65(19)
C(1)-N(6)-C(24)	117.11(19)
N(6)-C(1)-N(1)	122.6(2)
N(6)-C(1)-C(2)	130.4(2)
N(1)-C(1)-C(2)	105.25(18)

C(3)-C(2)-C(7)	120.1(2)
C(3)-C(2)-C(1)	132.1(2)
C(7)-C(2)-C(1)	107.21(19)
C(4)-C(3)-C(2)	118.0(2)
C(4)-C(3)-H(3A)	121.0
C(2)-C(3)-H(3A)	121.0
C(3)-C(4)-C(5)	121.7(2)
C(3)-C(4)-Cl(2)	118.68(19)
C(5)-C(4)-Cl(2)	119.51(19)
C(6)-C(5)-C(4)	120.8(2)
C(6)-C(5)-Cl(3)	118.71(18)
C(4)-C(5)-Cl(3)	120.39(18)
C(5)-C(6)-C(7)	118.1(2)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	121.3(2)
C(6)-C(7)-C(8)	130.9(2)
C(2)-C(7)-C(8)	107.2(2)
N(2)-C(8)-N(1)	122.9(2)
N(2)-C(8)-C(7)	129.2(2)
N(1)-C(8)-C(7)	105.90(18)
N(2)-C(9)-N(3)	123.0(2)
N(2)-C(9)-C(10)	130.0(2)
N(3)-C(9)-C(10)	105.1(2)
C(11)-C(10)-C(15)	120.5(2)
C(11)-C(10)-C(9)	131.5(2)
C(15)-C(10)-C(9)	107.77(19)
C(12)-C(11)-C(10)	117.9(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)-Cl(4)	118.61(18)
C(13)-C(12)-Cl(4)	119.99(18)
C(14)-C(13)-C(12)	121.2(2)
C(14)-C(13)-Cl(5)	118.60(19)
C(12)-C(13)-Cl(5)	120.24(17)

C(13)-C(14)-C(15)	118.0(2)
C(13)-C(14)-H(14A)	121.0
C(15)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	121.0(2)
C(14)-C(15)-C(16)	131.7(2)
C(10)-C(15)-C(16)	106.9(2)
N(4)-C(16)-N(3)	122.8(2)
N(4)-C(16)-C(15)	129.9(2)
N(3)-C(16)-C(15)	105.73(19)
N(4)-C(17)-N(5)	123.28(19)
N(4)-C(17)-C(18)	128.9(2)
N(5)-C(17)-C(18)	105.99(19)
C(19)-C(18)-C(23)	122.1(2)
C(19)-C(18)-C(17)	129.6(2)
C(23)-C(18)-C(17)	107.6(2)
C(20)-C(19)-C(18)	117.5(2)
C(20)-C(19)-H(19A)	121.3
C(18)-C(19)-H(19A)	121.3
C(19)-C(20)-C(21)	121.3(2)
C(19)-C(20)-Cl(6)	117.08(18)
C(21)-C(20)-Cl(6)	121.61(18)
C(22)-C(21)-C(20)	121.4(2)
C(22)-C(21)-Cl(7)	119.88(18)
C(20)-C(21)-Cl(7)	118.75(18)
C(21)-C(22)-C(23)	118.2(2)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	119.4(2)
C(22)-C(23)-C(24)	133.4(2)
C(18)-C(23)-C(24)	106.84(19)
N(6)-C(24)-N(5)	122.1(2)
N(6)-C(24)-C(23)	130.8(2)
N(5)-C(24)-C(23)	105.14(19)
N(1)-B(1)-N(5)	105.54(19)
N(1)-B(1)-N(3)	105.21(19)
N(5)-B(1)-N(3)	104.90(19)

N(1)-B(1)-Cl(1)	113.78(17)
N(5)-B(1)-Cl(1)	113.13(16)
N(3)-B(1)-Cl(1)	113.44(16)

Symmetry transformations used to generate equivalent atoms:

Table S 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	28(1)	17(1)	23(1)	4(1)	7(1)	-3(1)
Cl(2)	27(1)	44(1)	58(1)	-23(1)	2(1)	13(1)
Cl(3)	32(1)	26(1)	28(1)	-10(1)	10(1)	-2(1)
Cl(4)	19(1)	51(1)	25(1)	-9(1)	-1(1)	-8(1)
Cl(5)	21(1)	57(1)	31(1)	-11(1)	10(1)	-10(1)
Cl(6)	30(1)	59(1)	15(1)	10(1)	4(1)	6(1)
Cl(7)	24(1)	42(1)	19(1)	5(1)	-5(1)	5(1)
N(1)	16(1)	16(1)	14(1)	1(1)	3(1)	0(1)
N(2)	21(1)	20(1)	13(1)	2(1)	4(1)	0(1)
N(3)	18(1)	14(1)	13(1)	2(1)	1(1)	0(1)
N(4)	17(1)	14(1)	13(1)	0(1)	2(1)	0(1)
N(5)	17(1)	14(1)	14(1)	0(1)	3(1)	-3(1)
N(6)	15(1)	18(1)	18(1)	-1(1)	4(1)	-4(1)
C(1)	13(1)	18(1)	19(1)	2(1)	6(1)	-3(1)
C(2)	16(1)	18(1)	17(1)	1(1)	8(1)	-4(1)
C(3)	15(1)	25(1)	22(1)	-1(1)	6(1)	-5(1)
C(4)	20(1)	22(1)	28(1)	-1(1)	12(1)	0(1)
C(5)	25(1)	19(1)	18(1)	-3(1)	12(1)	-5(1)
C(6)	20(1)	22(1)	16(1)	0(1)	7(1)	-3(1)
C(7)	20(1)	19(1)	15(1)	3(1)	7(1)	-2(1)
C(8)	21(1)	18(1)	11(1)	2(1)	4(1)	-2(1)
C(9)	19(1)	14(1)	13(1)	3(1)	0(1)	1(1)
C(10)	16(1)	17(1)	15(1)	3(1)	1(1)	3(1)
C(11)	19(1)	20(1)	16(1)	0(1)	0(1)	2(1)
C(12)	16(1)	23(1)	19(1)	-1(1)	-3(1)	-1(1)
C(13)	16(1)	23(1)	24(1)	-1(1)	5(1)	0(1)
C(14)	21(1)	18(1)	14(1)	1(1)	2(1)	3(1)
C(15)	18(1)	15(1)	14(1)	1(1)	1(1)	3(1)
C(16)	19(1)	12(1)	17(1)	1(1)	4(1)	1(1)
C(17)	17(1)	12(1)	14(1)	-2(1)	3(1)	-1(1)

C(18)	17(1)	14(1)	17(1)	-2(1)	1(1)	-2(1)
C(19)	18(1)	19(1)	16(1)	-2(1)	3(1)	-2(1)
C(20)	23(1)	24(1)	12(1)	1(1)	2(1)	-5(1)
C(21)	20(1)	19(1)	17(1)	-1(1)	-3(1)	-2(1)
C(22)	16(1)	17(1)	21(1)	-4(1)	1(1)	-3(1)
C(23)	15(1)	14(1)	16(1)	-1(1)	2(1)	-4(1)
C(24)	14(1)	16(1)	18(1)	0(1)	2(1)	-4(1)
B(1)	18(1)	16(1)	14(1)	2(1)	2(1)	-2(1)

Table S 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **Cl-Cl₆BsubPc** (**Chlorobenzene:Heptane; CCDC deposit 2087100**).

	x	y	z	U(eq)
H(3A)	3640	4806	3439	24
H(6A)	6713	4724	4718	23
H(11A)	10037	2244	4283	22
H(14A)	10114	397	2508	21
H(19A)	7016	358	1178	21
H(22A)	3735	2280	1523	22

Table S 12. Torsion angles [°] for Cl-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087100).

C(24)-N(6)-C(1)-N(1)	-8.6(3)
C(24)-N(6)-C(1)-C(2)	153.8(2)
C(8)-N(1)-C(1)-N(6)	155.6(2)
B(1)-N(1)-C(1)-N(6)	-11.6(3)
C(8)-N(1)-C(1)-C(2)	-10.5(2)
B(1)-N(1)-C(1)-C(2)	-177.8(2)
N(6)-C(1)-C(2)-C(3)	13.0(4)
N(1)-C(1)-C(2)-C(3)	177.7(2)
N(6)-C(1)-C(2)-C(7)	-158.0(2)
N(1)-C(1)-C(2)-C(7)	6.7(2)
C(7)-C(2)-C(3)-C(4)	0.7(3)
C(1)-C(2)-C(3)-C(4)	-169.4(2)
C(2)-C(3)-C(4)-C(5)	0.6(4)
C(2)-C(3)-C(4)-Cl(2)	176.61(18)
C(3)-C(4)-C(5)-C(6)	-1.6(4)
Cl(2)-C(4)-C(5)-C(6)	-177.57(19)
C(3)-C(4)-C(5)-Cl(3)	174.51(19)
Cl(2)-C(4)-C(5)-Cl(3)	-1.5(3)
C(4)-C(5)-C(6)-C(7)	1.2(3)
Cl(3)-C(5)-C(6)-C(7)	-174.90(18)
C(5)-C(6)-C(7)-C(2)	0.0(3)
C(5)-C(6)-C(7)-C(8)	170.3(2)
C(3)-C(2)-C(7)-C(6)	-1.0(3)
C(1)-C(2)-C(7)-C(6)	171.3(2)
C(3)-C(2)-C(7)-C(8)	-173.3(2)
C(1)-C(2)-C(7)-C(8)	-1.0(3)
C(9)-N(2)-C(8)-N(1)	8.8(3)
C(9)-N(2)-C(8)-C(7)	-152.7(2)
C(1)-N(1)-C(8)-N(2)	-155.2(2)
B(1)-N(1)-C(8)-N(2)	12.0(3)
C(1)-N(1)-C(8)-C(7)	9.9(3)
B(1)-N(1)-C(8)-C(7)	177.2(2)
C(6)-C(7)-C(8)-N(2)	-12.5(4)

C(2)-C(7)-C(8)-N(2)	158.9(2)
C(6)-C(7)-C(8)-N(1)	-176.4(2)
C(2)-C(7)-C(8)-N(1)	-5.0(2)
C(8)-N(2)-C(9)-N(3)	-8.9(3)
C(8)-N(2)-C(9)-C(10)	152.9(2)
C(16)-N(3)-C(9)-N(2)	154.7(2)
B(1)-N(3)-C(9)-N(2)	-11.4(3)
C(16)-N(3)-C(9)-C(10)	-10.9(2)
B(1)-N(3)-C(9)-C(10)	-177.04(19)
N(2)-C(9)-C(10)-C(11)	17.1(4)
N(3)-C(9)-C(10)-C(11)	-178.7(2)
N(2)-C(9)-C(10)-C(15)	-156.6(2)
N(3)-C(9)-C(10)-C(15)	7.6(2)
C(15)-C(10)-C(11)-C(12)	0.1(3)
C(9)-C(10)-C(11)-C(12)	-172.9(2)
C(10)-C(11)-C(12)-C(13)	2.2(3)
C(10)-C(11)-C(12)-Cl(4)	-177.51(17)
C(11)-C(12)-C(13)-C(14)	-1.6(4)
Cl(4)-C(12)-C(13)-C(14)	178.02(18)
C(11)-C(12)-C(13)-Cl(5)	178.55(19)
Cl(4)-C(12)-C(13)-Cl(5)	-1.8(3)
C(12)-C(13)-C(14)-C(15)	-1.3(3)
Cl(5)-C(13)-C(14)-C(15)	178.55(17)
C(13)-C(14)-C(15)-C(10)	3.5(3)
C(13)-C(14)-C(15)-C(16)	175.4(2)
C(11)-C(10)-C(15)-C(14)	-3.0(3)
C(9)-C(10)-C(15)-C(14)	171.5(2)
C(11)-C(10)-C(15)-C(16)	-176.7(2)
C(9)-C(10)-C(15)-C(16)	-2.2(2)
C(17)-N(4)-C(16)-N(3)	11.7(3)
C(17)-N(4)-C(16)-C(15)	-151.6(2)
C(9)-N(3)-C(16)-N(4)	-157.2(2)
B(1)-N(3)-C(16)-N(4)	8.9(3)
C(9)-N(3)-C(16)-C(15)	9.6(2)
B(1)-N(3)-C(16)-C(15)	175.68(19)
C(14)-C(15)-C(16)-N(4)	-11.3(4)

C(10)-C(15)-C(16)-N(4)	161.4(2)
C(14)-C(15)-C(16)-N(3)	-176.8(2)
C(10)-C(15)-C(16)-N(3)	-4.1(2)
C(16)-N(4)-C(17)-N(5)	-10.6(3)
C(16)-N(4)-C(17)-C(18)	151.7(2)
C(24)-N(5)-C(17)-N(4)	156.5(2)
B(1)-N(5)-C(17)-N(4)	-11.4(3)
C(24)-N(5)-C(17)-C(18)	-9.3(2)
B(1)-N(5)-C(17)-C(18)	-177.20(19)
N(4)-C(17)-C(18)-C(19)	10.1(4)
N(5)-C(17)-C(18)-C(19)	174.7(2)
N(4)-C(17)-C(18)-C(23)	-160.9(2)
N(5)-C(17)-C(18)-C(23)	3.7(2)
C(23)-C(18)-C(19)-C(20)	-2.8(3)
C(17)-C(18)-C(19)-C(20)	-172.7(2)
C(18)-C(19)-C(20)-C(21)	-1.1(3)
C(18)-C(19)-C(20)-Cl(6)	177.26(18)
C(19)-C(20)-C(21)-C(22)	3.5(4)
Cl(6)-C(20)-C(21)-C(22)	-174.76(18)
C(19)-C(20)-C(21)-Cl(7)	-178.02(18)
Cl(6)-C(20)-C(21)-Cl(7)	3.7(3)
C(20)-C(21)-C(22)-C(23)	-1.9(3)
Cl(7)-C(21)-C(22)-C(23)	179.67(16)
C(21)-C(22)-C(23)-C(18)	-1.9(3)
C(21)-C(22)-C(23)-C(24)	169.7(2)
C(19)-C(18)-C(23)-C(22)	4.4(3)
C(17)-C(18)-C(23)-C(22)	176.23(19)
C(19)-C(18)-C(23)-C(24)	-169.3(2)
C(17)-C(18)-C(23)-C(24)	2.5(2)
C(1)-N(6)-C(24)-N(5)	7.9(3)
C(1)-N(6)-C(24)-C(23)	-153.9(2)
C(17)-N(5)-C(24)-N(6)	-155.0(2)
B(1)-N(5)-C(24)-N(6)	12.9(3)
C(17)-N(5)-C(24)-C(23)	10.8(2)
B(1)-N(5)-C(24)-C(23)	178.73(19)
C(22)-C(23)-C(24)-N(6)	-16.1(4)

C(18)-C(23)-C(24)-N(6)	156.3(2)
C(22)-C(23)-C(24)-N(5)	179.8(2)
C(18)-C(23)-C(24)-N(5)	-7.8(2)
C(8)-N(1)-B(1)-N(5)	-138.3(2)
C(1)-N(1)-B(1)-N(5)	27.7(3)
C(8)-N(1)-B(1)-N(3)	-27.7(3)
C(1)-N(1)-B(1)-N(3)	138.4(2)
C(8)-N(1)-B(1)-Cl(1)	97.1(2)
C(1)-N(1)-B(1)-Cl(1)	-96.9(2)
C(17)-N(5)-B(1)-N(1)	138.4(2)
C(24)-N(5)-B(1)-N(1)	-28.4(3)
C(17)-N(5)-B(1)-N(3)	27.5(3)
C(24)-N(5)-B(1)-N(3)	-139.3(2)
C(17)-N(5)-B(1)-Cl(1)	-96.6(2)
C(24)-N(5)-B(1)-Cl(1)	96.6(2)
C(9)-N(3)-B(1)-N(1)	27.5(3)
C(16)-N(3)-B(1)-N(1)	-137.4(2)
C(9)-N(3)-B(1)-N(5)	138.5(2)
C(16)-N(3)-B(1)-N(5)	-26.3(3)
C(9)-N(3)-B(1)-Cl(1)	-97.5(2)
C(16)-N(3)-B(1)-Cl(1)	97.6(2)

Symmetry transformations used to generate equivalent atoms:

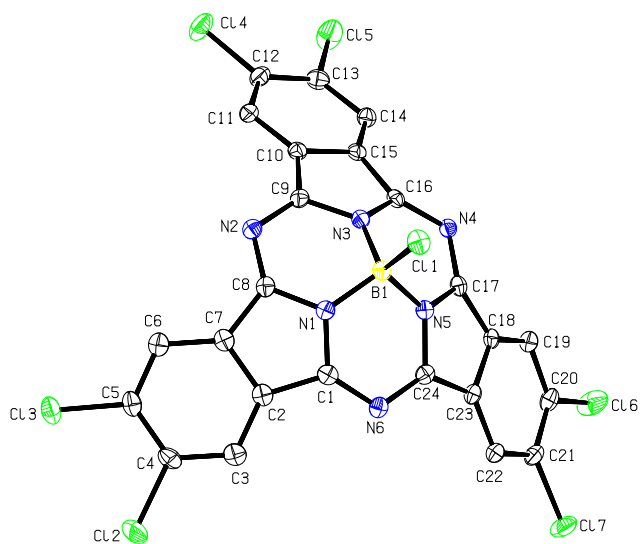


Figure S9: Anisotropic displacement ellipsoid plot of Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096).

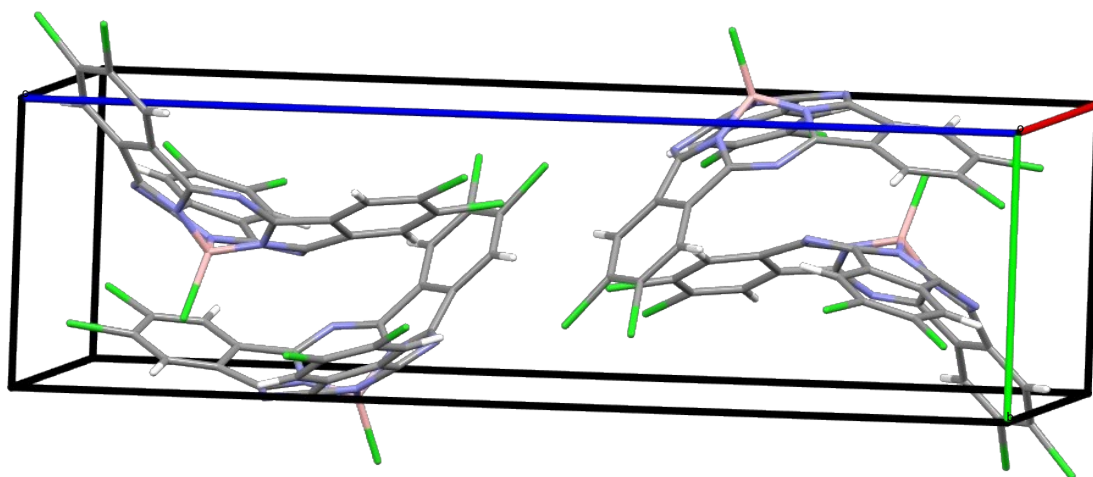


Figure S10: Populated unit cell of Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096).

Table S 13. Crystal data and structure refinement for **Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096)**.

Identification code	d19197_a	
Empirical formula	C ₂₄ H ₆ B Cl ₇ N ₆	
Formula weight	637.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 13.0941(8) Å	α = 90°.
	b = 7.4220(4) Å	β = 99.487(2)°.
	c = 25.4950(17) Å	γ = 90°.
Volume	2443.8(3) Å ³	
Z	4	
Density (calculated)	1.732 Mg/m ³	
Absorption coefficient	0.843 mm ⁻¹	
F(000)	1264	
Crystal size	0.280 x 0.050 x 0.040 mm ³	
Theta range for data collection	1.620 to 27.587°.	
Index ranges	-17 ≤ h ≤ 16, -9 ≤ k ≤ 7, -33 ≤ l ≤ 33	
Reflections collected	48146	
Independent reflections	5655 [R(int) = 0.0568]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6796	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5655 / 0 / 343	
Goodness-of-fit on F ²	1.037	
Final R indices [I > 2σ(I)]	R1 = 0.0341, wR2 = 0.0671	
R indices (all data)	R1 = 0.0604, wR2 = 0.0780	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.451 and -0.375 e.Å ⁻³	

Table S 14. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096)**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6127(1)	-2524(1)	3389(1)	22(1)
Cl(2)	3568(1)	7805(1)	4092(1)	43(1)
Cl(3)	5624(1)	7812(1)	4919(1)	28(1)
Cl(4)	12062(1)	2781(1)	4100(1)	32(1)
Cl(5)	12098(1)	1655(1)	2915(1)	36(1)
Cl(6)	6010(1)	1842(1)	242(1)	35(1)
Cl(7)	3778(1)	2924(1)	436(1)	29(1)
N(1)	6029(1)	1212(2)	3480(1)	15(1)
N(2)	7620(1)	1841(2)	4051(1)	17(1)
N(3)	7598(1)	100(2)	3267(1)	15(1)
N(4)	7738(1)	-289(2)	2354(1)	15(1)
N(5)	6087(1)	135(2)	2617(1)	15(1)
N(6)	4659(1)	1913(2)	2773(1)	17(1)
C(1)	5128(2)	2086(3)	3282(1)	17(1)
C(2)	5005(2)	3454(3)	3678(1)	17(1)
C(3)	4261(2)	4783(3)	3694(1)	21(1)
C(4)	4447(2)	6078(3)	4088(1)	22(1)
C(5)	5364(2)	6068(3)	4466(1)	20(1)
C(6)	6099(2)	4745(3)	4461(1)	19(1)
C(7)	5918(2)	3433(3)	4066(1)	17(1)
C(8)	6590(2)	2046(3)	3911(1)	16(1)
C(9)	8111(2)	967(3)	3705(1)	16(1)
C(10)	9179(2)	1125(3)	3618(1)	16(1)
C(11)	10053(2)	1842(3)	3929(1)	19(1)
C(12)	10951(2)	1961(3)	3710(1)	21(1)
C(13)	10971(2)	1432(3)	3182(1)	21(1)
C(14)	10103(2)	727(3)	2866(1)	18(1)
C(15)	9210(2)	524(3)	3091(1)	16(1)
C(16)	8168(2)	-52(3)	2864(1)	15(1)
C(17)	6706(2)	-51(3)	2238(1)	15(1)

C(18)	6085(2)	525(3)	1747(1)	15(1)
C(19)	6354(2)	731(3)	1246(1)	18(1)
C(20)	5639(2)	1495(3)	854(1)	20(1)
C(21)	4655(2)	2034(3)	952(1)	19(1)
C(22)	4391(2)	1884(3)	1456(1)	18(1)
C(23)	5119(2)	1151(3)	1861(1)	16(1)
C(24)	5180(2)	1020(3)	2440(1)	16(1)
B(1)	6463(2)	-248(3)	3188(1)	15(1)

Table S 15. Bond lengths [Å] and angles [°] for **Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096)**.

Cl(1)-B(1)	1.840(2)
Cl(2)-C(4)	1.724(2)
Cl(3)-C(5)	1.731(2)
Cl(4)-C(12)	1.731(2)
Cl(5)-C(13)	1.732(2)
Cl(6)-C(20)	1.728(2)
Cl(7)-C(21)	1.727(2)
N(1)-C(8)	1.366(3)
N(1)-C(1)	1.369(3)
N(1)-B(1)	1.481(3)
N(2)-C(9)	1.343(3)
N(2)-C(8)	1.345(3)
N(3)-C(9)	1.366(3)
N(3)-C(16)	1.370(3)
N(3)-B(1)	1.488(3)
N(4)-C(16)	1.343(3)
N(4)-C(17)	1.346(3)
N(5)-C(17)	1.365(3)
N(5)-C(24)	1.368(3)
N(5)-B(1)	1.484(3)
N(6)-C(1)	1.346(3)
N(6)-C(24)	1.349(3)
C(1)-C(2)	1.460(3)
C(2)-C(3)	1.391(3)
C(2)-C(7)	1.421(3)
C(3)-C(4)	1.382(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.411(3)
C(5)-C(6)	1.377(3)
C(6)-C(7)	1.392(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.451(3)

C(9)-C(10)	1.456(3)
C(10)-C(11)	1.386(3)
C(10)-C(15)	1.424(3)
C(11)-C(12)	1.384(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.408(3)
C(13)-C(14)	1.383(3)
C(14)-C(15)	1.391(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.455(3)
C(17)-C(18)	1.441(3)
C(18)-C(19)	1.389(3)
C(18)-C(23)	1.421(3)
C(19)-C(20)	1.375(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.410(3)
C(21)-C(22)	1.390(3)
C(22)-C(23)	1.395(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.467(3)
C(8)-N(1)-C(1)	113.53(17)
C(8)-N(1)-B(1)	122.46(18)
C(1)-N(1)-B(1)	122.70(18)
C(9)-N(2)-C(8)	116.65(18)
C(9)-N(3)-C(16)	113.26(17)
C(9)-N(3)-B(1)	122.59(17)
C(16)-N(3)-B(1)	122.67(18)
C(16)-N(4)-C(17)	116.14(17)
C(17)-N(5)-C(24)	113.51(17)
C(17)-N(5)-B(1)	122.27(17)
C(24)-N(5)-B(1)	123.07(17)
C(1)-N(6)-C(24)	117.19(18)
N(6)-C(1)-N(1)	122.60(19)
N(6)-C(1)-C(2)	130.4(2)
N(1)-C(1)-C(2)	105.11(18)

C(3)-C(2)-C(7)	120.1(2)
C(3)-C(2)-C(1)	132.1(2)
C(7)-C(2)-C(1)	107.35(18)
C(4)-C(3)-C(2)	118.2(2)
C(4)-C(3)-H(3A)	120.9
C(2)-C(3)-H(3A)	120.9
C(3)-C(4)-C(5)	121.4(2)
C(3)-C(4)-Cl(2)	118.92(18)
C(5)-C(4)-Cl(2)	119.58(17)
C(6)-C(5)-C(4)	121.0(2)
C(6)-C(5)-Cl(3)	118.60(18)
C(4)-C(5)-Cl(3)	120.27(17)
C(5)-C(6)-C(7)	118.0(2)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	121.3(2)
C(6)-C(7)-C(8)	130.9(2)
C(2)-C(7)-C(8)	107.28(18)
N(2)-C(8)-N(1)	123.02(18)
N(2)-C(8)-C(7)	129.4(2)
N(1)-C(8)-C(7)	105.70(18)
N(2)-C(9)-N(3)	122.71(19)
N(2)-C(9)-C(10)	129.60(19)
N(3)-C(9)-C(10)	105.65(17)
C(11)-C(10)-C(15)	120.66(19)
C(11)-C(10)-C(9)	131.88(19)
C(15)-C(10)-C(9)	107.22(18)
C(12)-C(11)-C(10)	118.1(2)
C(12)-C(11)-H(11A)	120.9
C(10)-C(11)-H(11A)	120.9
C(11)-C(12)-C(13)	121.2(2)
C(11)-C(12)-Cl(4)	118.79(17)
C(13)-C(12)-Cl(4)	120.00(16)
C(14)-C(13)-C(12)	121.24(19)
C(14)-C(13)-Cl(5)	118.66(17)
C(12)-C(13)-Cl(5)	120.10(17)

C(13)-C(14)-C(15)	117.90(19)
C(13)-C(14)-H(14A)	121.0
C(15)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	120.73(19)
C(14)-C(15)-C(16)	131.71(19)
C(10)-C(15)-C(16)	107.17(18)
N(4)-C(16)-N(3)	122.89(19)
N(4)-C(16)-C(15)	129.75(18)
N(3)-C(16)-C(15)	105.72(17)
N(4)-C(17)-N(5)	123.36(18)
N(4)-C(17)-C(18)	129.15(18)
N(5)-C(17)-C(18)	105.57(17)
C(19)-C(18)-C(23)	121.4(2)
C(19)-C(18)-C(17)	129.72(19)
C(23)-C(18)-C(17)	108.27(18)
C(20)-C(19)-C(18)	118.0(2)
C(20)-C(19)-H(19A)	121.0
C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.39(19)
C(19)-C(20)-Cl(6)	117.32(17)
C(21)-C(20)-Cl(6)	121.25(17)
C(22)-C(21)-C(20)	120.99(19)
C(22)-C(21)-Cl(7)	119.92(17)
C(20)-C(21)-Cl(7)	119.08(16)
C(21)-C(22)-C(23)	118.2(2)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	119.91(19)
C(22)-C(23)-C(24)	133.4(2)
C(18)-C(23)-C(24)	106.34(18)
N(6)-C(24)-N(5)	121.97(19)
N(6)-C(24)-C(23)	130.71(19)
N(5)-C(24)-C(23)	105.32(17)
N(1)-B(1)-N(5)	105.12(17)
N(1)-B(1)-N(3)	105.19(18)
N(5)-B(1)-N(3)	105.19(16)

N(1)-B(1)-Cl(1)	113.66(15)
N(5)-B(1)-Cl(1)	113.16(16)
N(3)-B(1)-Cl(1)	113.65(16)

Symmetry transformations used to generate equivalent atoms:

Table S 16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	28(1)	17(1)	23(1)	4(1)	8(1)	-4(1)
Cl(2)	27(1)	43(1)	58(1)	-22(1)	3(1)	13(1)
Cl(3)	32(1)	26(1)	29(1)	-10(1)	10(1)	-2(1)
Cl(4)	19(1)	51(1)	25(1)	-9(1)	0(1)	-8(1)
Cl(5)	22(1)	57(1)	31(1)	-11(1)	11(1)	-10(1)
Cl(6)	30(1)	59(1)	15(1)	10(1)	5(1)	6(1)
Cl(7)	24(1)	41(1)	20(1)	5(1)	-4(1)	5(1)
N(1)	16(1)	16(1)	14(1)	1(1)	4(1)	-1(1)
N(2)	20(1)	18(1)	13(1)	2(1)	3(1)	0(1)
N(3)	18(1)	14(1)	14(1)	1(1)	3(1)	1(1)
N(4)	17(1)	14(1)	14(1)	0(1)	2(1)	0(1)
N(5)	16(1)	14(1)	15(1)	0(1)	4(1)	-2(1)
N(6)	15(1)	18(1)	17(1)	-1(1)	4(1)	-4(1)
C(1)	15(1)	15(1)	20(1)	2(1)	6(1)	-3(1)
C(2)	17(1)	19(1)	18(1)	1(1)	9(1)	-4(1)
C(3)	16(1)	24(1)	24(1)	0(1)	9(1)	-3(1)
C(4)	17(1)	23(1)	28(1)	-1(1)	12(1)	2(1)
C(5)	23(1)	21(1)	20(1)	-4(1)	12(1)	-5(1)
C(6)	21(1)	22(1)	16(1)	1(1)	8(1)	-4(1)
C(7)	20(1)	18(1)	16(1)	2(1)	8(1)	-2(1)
C(8)	20(1)	16(1)	13(1)	2(1)	4(1)	-2(1)
C(9)	20(1)	14(1)	12(1)	3(1)	1(1)	1(1)
C(10)	19(1)	15(1)	15(1)	2(1)	2(1)	3(1)
C(11)	19(1)	21(1)	15(1)	-1(1)	0(1)	3(1)
C(12)	18(1)	22(1)	20(1)	-1(1)	-2(1)	-1(1)
C(13)	18(1)	23(1)	23(1)	1(1)	6(1)	2(1)
C(14)	20(1)	19(1)	15(1)	-1(1)	3(1)	2(1)
C(15)	18(1)	12(1)	16(1)	2(1)	2(1)	3(1)
C(16)	19(1)	11(1)	16(1)	1(1)	4(1)	2(1)
C(17)	19(1)	11(1)	15(1)	-1(1)	5(1)	-3(1)

C(18)	17(1)	12(1)	16(1)	-3(1)	2(1)	-3(1)
C(19)	18(1)	18(1)	17(1)	-1(1)	3(1)	-2(1)
C(20)	22(1)	24(1)	13(1)	-1(1)	2(1)	-4(1)
C(21)	20(1)	20(1)	17(1)	1(1)	-3(1)	-3(1)
C(22)	16(1)	19(1)	20(1)	-3(1)	0(1)	-1(1)
C(23)	16(1)	16(1)	16(1)	-2(1)	1(1)	-3(1)
C(24)	15(1)	15(1)	19(1)	1(1)	2(1)	-4(1)
B(1)	18(1)	13(1)	16(1)	2(1)	4(1)	-2(1)

Table S 17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096)**.

	x	y	z	U(eq)
H(3A)	3642	4800	3440	25
H(6A)	6712	4728	4719	23
H(11A)	10036	2240	4281	23
H(14A)	10116	391	2508	22
H(19A)	7013	356	1177	21
H(22A)	3733	2270	1523	22

Table S 18. Torsion angles [°] for Cl-Cl₆BsubPc (DiChlorobenzene:Heptane; CCDC deposit 2087096).

C(24)-N(6)-C(1)-N(1)	-8.4(3)
C(24)-N(6)-C(1)-C(2)	153.7(2)
C(8)-N(1)-C(1)-N(6)	155.51(19)
B(1)-N(1)-C(1)-N(6)	-11.7(3)
C(8)-N(1)-C(1)-C(2)	-10.4(2)
B(1)-N(1)-C(1)-C(2)	-177.63(18)
N(6)-C(1)-C(2)-C(3)	13.5(4)
N(1)-C(1)-C(2)-C(3)	177.9(2)
N(6)-C(1)-C(2)-C(7)	-158.0(2)
N(1)-C(1)-C(2)-C(7)	6.4(2)
C(7)-C(2)-C(3)-C(4)	1.1(3)
C(1)-C(2)-C(3)-C(4)	-169.5(2)
C(2)-C(3)-C(4)-C(5)	0.0(3)
C(2)-C(3)-C(4)-Cl(2)	176.51(16)
C(3)-C(4)-C(5)-C(6)	-1.1(3)
Cl(2)-C(4)-C(5)-C(6)	-177.56(17)
C(3)-C(4)-C(5)-Cl(3)	174.57(17)
Cl(2)-C(4)-C(5)-Cl(3)	-1.9(3)
C(4)-C(5)-C(6)-C(7)	1.0(3)
Cl(3)-C(5)-C(6)-C(7)	-174.77(15)
C(5)-C(6)-C(7)-C(2)	0.2(3)
C(5)-C(6)-C(7)-C(8)	170.2(2)
C(3)-C(2)-C(7)-C(6)	-1.2(3)
C(1)-C(2)-C(7)-C(6)	171.47(18)
C(3)-C(2)-C(7)-C(8)	-173.37(18)
C(1)-C(2)-C(7)-C(8)	-0.7(2)
C(9)-N(2)-C(8)-N(1)	9.0(3)
C(9)-N(2)-C(8)-C(7)	-153.0(2)
C(1)-N(1)-C(8)-N(2)	-155.48(19)
B(1)-N(1)-C(8)-N(2)	11.7(3)
C(1)-N(1)-C(8)-C(7)	10.1(2)
B(1)-N(1)-C(8)-C(7)	177.31(18)
C(6)-C(7)-C(8)-N(2)	-12.1(4)

C(2)-C(7)-C(8)-N(2)	159.0(2)
C(6)-C(7)-C(8)-N(1)	-176.4(2)
C(2)-C(7)-C(8)-N(1)	-5.4(2)
C(8)-N(2)-C(9)-N(3)	-8.9(3)
C(8)-N(2)-C(9)-C(10)	152.5(2)
C(16)-N(3)-C(9)-N(2)	154.70(19)
B(1)-N(3)-C(9)-N(2)	-11.8(3)
C(16)-N(3)-C(9)-C(10)	-10.5(2)
B(1)-N(3)-C(9)-C(10)	-176.97(18)
N(2)-C(9)-C(10)-C(11)	17.7(4)
N(3)-C(9)-C(10)-C(11)	-178.5(2)
N(2)-C(9)-C(10)-C(15)	-156.6(2)
N(3)-C(9)-C(10)-C(15)	7.2(2)
C(15)-C(10)-C(11)-C(12)	0.2(3)
C(9)-C(10)-C(11)-C(12)	-173.4(2)
C(10)-C(11)-C(12)-C(13)	2.3(3)
C(10)-C(11)-C(12)-Cl(4)	-177.81(17)
C(11)-C(12)-C(13)-C(14)	-1.9(4)
Cl(4)-C(12)-C(13)-C(14)	178.23(18)
C(11)-C(12)-C(13)-Cl(5)	178.23(18)
Cl(4)-C(12)-C(13)-Cl(5)	-1.7(3)
C(12)-C(13)-C(14)-C(15)	-1.1(3)
Cl(5)-C(13)-C(14)-C(15)	178.77(17)
C(13)-C(14)-C(15)-C(10)	3.6(3)
C(13)-C(14)-C(15)-C(16)	175.5(2)
C(11)-C(10)-C(15)-C(14)	-3.2(3)
C(9)-C(10)-C(15)-C(14)	171.83(19)
C(11)-C(10)-C(15)-C(16)	-176.88(19)
C(9)-C(10)-C(15)-C(16)	-1.8(2)
C(17)-N(4)-C(16)-N(3)	11.5(3)
C(17)-N(4)-C(16)-C(15)	-151.7(2)
C(9)-N(3)-C(16)-N(4)	-157.33(19)
B(1)-N(3)-C(16)-N(4)	9.1(3)
C(9)-N(3)-C(16)-C(15)	9.4(2)
B(1)-N(3)-C(16)-C(15)	175.83(18)
C(14)-C(15)-C(16)-N(4)	-11.5(4)

C(10)-C(15)-C(16)-N(4)	161.2(2)
C(14)-C(15)-C(16)-N(3)	-176.9(2)
C(10)-C(15)-C(16)-N(3)	-4.2(2)
C(16)-N(4)-C(17)-N(5)	-10.3(3)
C(16)-N(4)-C(17)-C(18)	151.6(2)
C(24)-N(5)-C(17)-N(4)	156.41(19)
B(1)-N(5)-C(17)-N(4)	-11.7(3)
C(24)-N(5)-C(17)-C(18)	-9.1(2)
B(1)-N(5)-C(17)-C(18)	-177.21(18)
N(4)-C(17)-C(18)-C(19)	10.5(4)
N(5)-C(17)-C(18)-C(19)	174.9(2)
N(4)-C(17)-C(18)-C(23)	-160.7(2)
N(5)-C(17)-C(18)-C(23)	3.6(2)
C(23)-C(18)-C(19)-C(20)	-2.7(3)
C(17)-C(18)-C(19)-C(20)	-173.0(2)
C(18)-C(19)-C(20)-C(21)	-0.8(3)
C(18)-C(19)-C(20)-Cl(6)	176.94(17)
C(19)-C(20)-C(21)-C(22)	2.9(3)
Cl(6)-C(20)-C(21)-C(22)	-174.81(17)
C(19)-C(20)-C(21)-Cl(7)	-178.10(17)
Cl(6)-C(20)-C(21)-Cl(7)	4.2(3)
C(20)-C(21)-C(22)-C(23)	-1.3(3)
Cl(7)-C(21)-C(22)-C(23)	179.73(16)
C(21)-C(22)-C(23)-C(18)	-2.2(3)
C(21)-C(22)-C(23)-C(24)	169.8(2)
C(19)-C(18)-C(23)-C(22)	4.3(3)
C(17)-C(18)-C(23)-C(22)	176.42(19)
C(19)-C(18)-C(23)-C(24)	-169.68(19)
C(17)-C(18)-C(23)-C(24)	2.4(2)
C(1)-N(6)-C(24)-N(5)	7.7(3)
C(1)-N(6)-C(24)-C(23)	-153.7(2)
C(17)-N(5)-C(24)-N(6)	-154.93(19)
B(1)-N(5)-C(24)-N(6)	13.1(3)
C(17)-N(5)-C(24)-C(23)	10.6(2)
B(1)-N(5)-C(24)-C(23)	178.59(18)
C(22)-C(23)-C(24)-N(6)	-16.7(4)

C(18)-C(23)-C(24)-N(6)	156.2(2)
C(22)-C(23)-C(24)-N(5)	179.6(2)
C(18)-C(23)-C(24)-N(5)	-7.6(2)
C(8)-N(1)-B(1)-N(5)	-138.47(18)
C(1)-N(1)-B(1)-N(5)	27.6(3)
C(8)-N(1)-B(1)-N(3)	-27.7(3)
C(1)-N(1)-B(1)-N(3)	138.35(18)
C(8)-N(1)-B(1)-Cl(1)	97.3(2)
C(1)-N(1)-B(1)-Cl(1)	-96.7(2)
C(17)-N(5)-B(1)-N(1)	138.61(19)
C(24)-N(5)-B(1)-N(1)	-28.4(3)
C(17)-N(5)-B(1)-N(3)	27.8(3)
C(24)-N(5)-B(1)-N(3)	-139.15(19)
C(17)-N(5)-B(1)-Cl(1)	-96.8(2)
C(24)-N(5)-B(1)-Cl(1)	96.2(2)
C(9)-N(3)-B(1)-N(1)	27.8(3)
C(16)-N(3)-B(1)-N(1)	-137.43(19)
C(9)-N(3)-B(1)-N(5)	138.51(19)
C(16)-N(3)-B(1)-N(5)	-26.7(3)
C(9)-N(3)-B(1)-Cl(1)	-97.2(2)
C(16)-N(3)-B(1)-Cl(1)	97.6(2)

Symmetry transformations used to generate equivalent atoms:

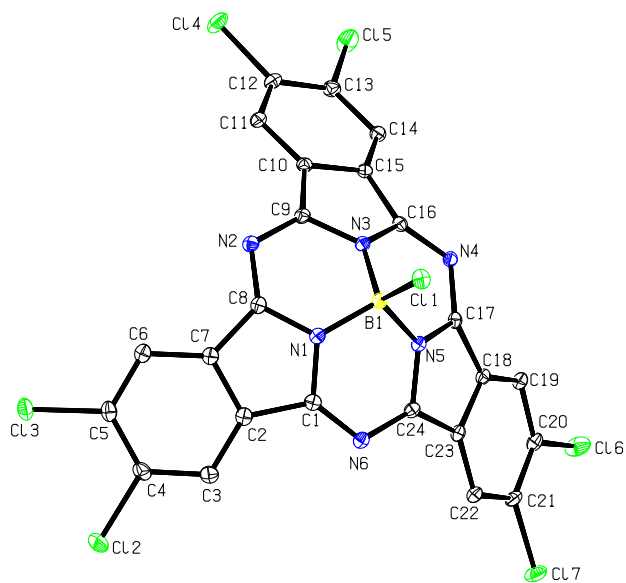


Figure S11: Anisotropic displacement ellipsoid of Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097).

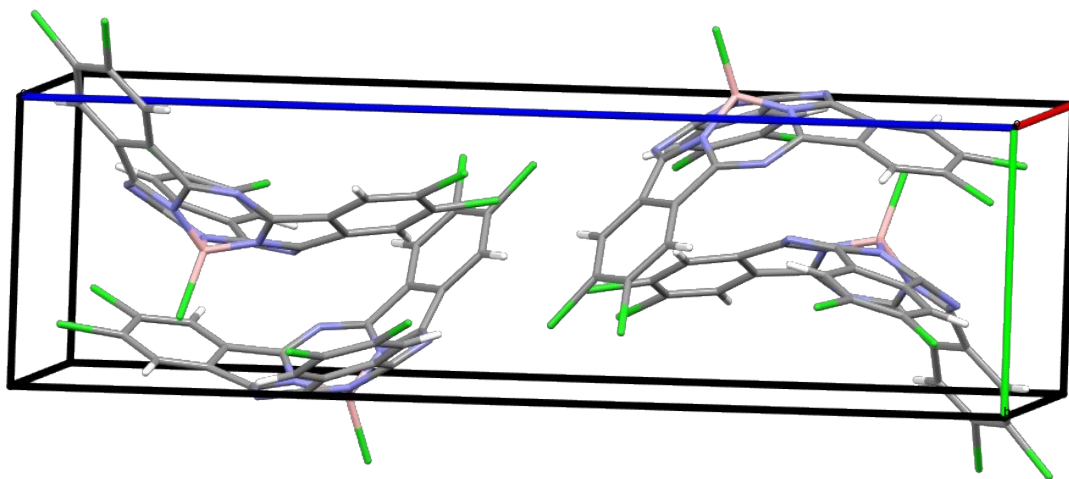


Figure S12: Populated unit cell of Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097).

Table S 19. Crystal data and structure refinement for **Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097)**.

Identification code	d19196_a	
Empirical formula	C ₂₄ H ₆ B Cl ₇ N ₆	
Formula weight	637.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 13.0807(7) Å	α = 90°.
	b = 7.4178(3) Å	β = 99.502(2)°.
	c = 25.4738(13) Å	γ = 90°.
Volume	2437.8(2) Å ³	
Z	4	
Density (calculated)	1.736 Mg/m ³	
Absorption coefficient	0.845 mm ⁻¹	
F(000)	1264	
Crystal size	0.150 x 0.100 x 0.100 mm ³	
Theta range for data collection	1.621 to 27.697°.	
Index ranges	-17<=h<=17, -9<=k<=9, -33<=l<=33	
Reflections collected	33605	
Independent reflections	5672 [R(int) = 0.0225]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7196	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5672 / 0 / 343	
Goodness-of-fit on F ²	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0263, wR2 = 0.0654	
R indices (all data)	R1 = 0.0323, wR2 = 0.0690	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.383 and -0.352 e.Å ⁻³	

Table S 20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6127(1)	-2522(1)	3389(1)	23(1)
Cl(2)	3568(1)	7805(1)	4092(1)	44(1)
Cl(3)	5624(1)	7811(1)	4920(1)	29(1)
Cl(4)	12062(1)	2782(1)	4099(1)	32(1)
Cl(5)	12099(1)	1657(1)	2915(1)	36(1)
Cl(6)	6011(1)	1843(1)	242(1)	35(1)
Cl(7)	3779(1)	2925(1)	436(1)	30(1)
N(1)	6029(1)	1212(2)	3480(1)	16(1)
N(2)	7620(1)	1841(2)	4051(1)	18(1)
N(3)	7599(1)	101(2)	3267(1)	16(1)
N(4)	7738(1)	-288(2)	2354(1)	16(1)
N(5)	6087(1)	138(2)	2616(1)	16(1)
N(6)	4658(1)	1913(2)	2773(1)	18(1)
C(1)	5129(1)	2089(2)	3282(1)	17(1)
C(2)	5003(1)	3458(2)	3678(1)	18(1)
C(3)	4260(1)	4785(2)	3693(1)	21(1)
C(4)	4450(1)	6078(2)	4089(1)	23(1)
C(5)	5366(1)	6074(2)	4466(1)	22(1)
C(6)	6103(1)	4744(2)	4462(1)	20(1)
C(7)	5918(1)	3433(2)	4067(1)	18(1)
C(8)	6592(1)	2043(2)	3912(1)	17(1)
C(9)	8112(1)	968(2)	3705(1)	17(1)
C(10)	9180(1)	1120(2)	3618(1)	17(1)
C(11)	10055(1)	1847(2)	3930(1)	20(1)
C(12)	10952(1)	1967(2)	3711(1)	21(1)
C(13)	10973(1)	1438(2)	3182(1)	21(1)
C(14)	10102(1)	729(2)	2865(1)	19(1)
C(15)	9210(1)	527(2)	3091(1)	17(1)
C(16)	8171(1)	-51(2)	2865(1)	16(1)
C(17)	6707(1)	-49(2)	2239(1)	16(1)

C(18)	6084(1)	526(2)	1747(1)	17(1)
C(19)	6357(1)	731(2)	1246(1)	18(1)
C(20)	5640(1)	1500(2)	853(1)	20(1)
C(21)	4655(1)	2034(2)	952(1)	20(1)
C(22)	4392(1)	1889(2)	1456(1)	19(1)
C(23)	5119(1)	1155(2)	1862(1)	17(1)
C(24)	5180(1)	1022(2)	2439(1)	17(1)
B(1)	6464(1)	-244(2)	3188(1)	16(1)

Table S 21. Bond lengths [Å] and angles [°] for **Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097)**.

Cl(1)-B(1)	1.8403(16)
Cl(2)-C(4)	1.7242(16)
Cl(3)-C(5)	1.7268(15)
Cl(4)-C(12)	1.7259(15)
Cl(5)-C(13)	1.7288(15)
Cl(6)-C(20)	1.7244(15)
Cl(7)-C(21)	1.7259(15)
N(1)-C(8)	1.3654(18)
N(1)-C(1)	1.3674(18)
N(1)-B(1)	1.479(2)
N(2)-C(9)	1.3416(18)
N(2)-C(8)	1.3423(19)
N(3)-C(9)	1.3652(18)
N(3)-C(16)	1.3679(17)
N(3)-B(1)	1.4866(19)
N(4)-C(16)	1.3429(18)
N(4)-C(17)	1.3428(18)
N(5)-C(17)	1.3630(17)
N(5)-C(24)	1.3655(18)
N(5)-B(1)	1.4849(19)
N(6)-C(1)	1.3460(18)
N(6)-C(24)	1.3477(18)
C(1)-C(2)	1.460(2)
C(2)-C(3)	1.389(2)
C(2)-C(7)	1.422(2)
C(3)-C(4)	1.385(2)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.407(2)
C(5)-C(6)	1.380(2)
C(6)-C(7)	1.391(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.453(2)

C(9)-C(10)	1.4535(19)
C(10)-C(11)	1.390(2)
C(10)-C(15)	1.4202(19)
C(11)-C(12)	1.382(2)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.408(2)
C(13)-C(14)	1.386(2)
C(14)-C(15)	1.3904(19)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.4505(19)
C(17)-C(18)	1.4426(19)
C(18)-C(19)	1.3883(19)
C(18)-C(23)	1.4210(19)
C(19)-C(20)	1.378(2)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.410(2)
C(21)-C(22)	1.386(2)
C(22)-C(23)	1.395(2)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.4642(19)

C(8)-N(1)-C(1)	113.58(12)
C(8)-N(1)-B(1)	122.34(12)
C(1)-N(1)-B(1)	122.74(12)
C(9)-N(2)-C(8)	116.68(12)
C(9)-N(3)-C(16)	113.20(12)
C(9)-N(3)-B(1)	122.51(12)
C(16)-N(3)-B(1)	122.82(12)
C(16)-N(4)-C(17)	116.25(12)
C(17)-N(5)-C(24)	113.68(12)
C(17)-N(5)-B(1)	122.11(12)
C(24)-N(5)-B(1)	123.04(12)
C(1)-N(6)-C(24)	117.10(12)
N(6)-C(1)-N(1)	122.62(13)
N(6)-C(1)-C(2)	130.35(13)
N(1)-C(1)-C(2)	105.26(12)

C(3)-C(2)-C(7)	120.15(14)
C(3)-C(2)-C(1)	132.15(14)
C(7)-C(2)-C(1)	107.18(12)
C(4)-C(3)-C(2)	117.99(14)
C(4)-C(3)-H(3A)	121.0
C(2)-C(3)-H(3A)	121.0
C(3)-C(4)-C(5)	121.71(14)
C(3)-C(4)-Cl(2)	118.61(12)
C(5)-C(4)-Cl(2)	119.57(12)
C(6)-C(5)-C(4)	120.90(14)
C(6)-C(5)-Cl(3)	118.62(12)
C(4)-C(5)-Cl(3)	120.38(12)
C(5)-C(6)-C(7)	117.86(14)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	121.37(14)
C(6)-C(7)-C(8)	130.70(14)
C(2)-C(7)-C(8)	107.33(12)
N(2)-C(8)-N(1)	123.08(13)
N(2)-C(8)-C(7)	129.33(13)
N(1)-C(8)-C(7)	105.62(12)
N(2)-C(9)-N(3)	122.72(13)
N(2)-C(9)-C(10)	129.77(13)
N(3)-C(9)-C(10)	105.51(12)
C(11)-C(10)-C(15)	120.71(13)
C(11)-C(10)-C(9)	131.68(13)
C(15)-C(10)-C(9)	107.33(12)
C(12)-C(11)-C(10)	117.99(13)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.30(13)
C(11)-C(12)-Cl(4)	118.75(11)
C(13)-C(12)-Cl(4)	119.95(11)
C(14)-C(13)-C(12)	121.20(13)
C(14)-C(13)-Cl(5)	118.63(11)
C(12)-C(13)-Cl(5)	120.17(12)

C(13)-C(14)-C(15)	117.78(13)
C(13)-C(14)-H(14A)	121.1
C(15)-C(14)-H(14A)	121.1
C(14)-C(15)-C(10)	120.92(13)
C(14)-C(15)-C(16)	131.56(13)
C(10)-C(15)-C(16)	107.16(12)
N(4)-C(16)-N(3)	122.67(12)
N(4)-C(16)-C(15)	129.85(12)
N(3)-C(16)-C(15)	105.81(12)
N(4)-C(17)-N(5)	123.51(12)
N(4)-C(17)-C(18)	129.15(12)
N(5)-C(17)-C(18)	105.45(12)
C(19)-C(18)-C(23)	121.67(13)
C(19)-C(18)-C(17)	129.56(13)
C(23)-C(18)-C(17)	108.17(12)
C(20)-C(19)-C(18)	117.74(13)
C(20)-C(19)-H(19A)	121.1
C(18)-C(19)-H(19A)	121.1
C(19)-C(20)-C(21)	121.27(13)
C(19)-C(20)-Cl(6)	117.24(11)
C(21)-C(20)-Cl(6)	121.46(11)
C(22)-C(21)-C(20)	121.18(13)
C(22)-C(21)-Cl(7)	119.94(12)
C(20)-C(21)-Cl(7)	118.87(11)
C(21)-C(22)-C(23)	118.24(13)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	119.74(13)
C(22)-C(23)-C(24)	133.55(13)
C(18)-C(23)-C(24)	106.36(12)
N(6)-C(24)-N(5)	122.04(12)
N(6)-C(24)-C(23)	130.65(13)
N(5)-C(24)-C(23)	105.34(12)
N(1)-B(1)-N(5)	105.14(12)
N(1)-B(1)-N(3)	105.33(12)
N(5)-B(1)-N(3)	105.21(11)

N(1)-B(1)-Cl(1)	113.63(10)
N(5)-B(1)-Cl(1)	113.08(10)
N(3)-B(1)-Cl(1)	113.61(11)

Symmetry transformations used to generate equivalent atoms:

Table S 22. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **Cl-Cl₆BsubPc** (**Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	28(1)	18(1)	23(1)	4(1)	8(1)	-3(1)
Cl(2)	26(1)	45(1)	58(1)	-23(1)	2(1)	13(1)
Cl(3)	32(1)	27(1)	29(1)	-10(1)	9(1)	-2(1)
Cl(4)	18(1)	52(1)	25(1)	-9(1)	-1(1)	-8(1)
Cl(5)	21(1)	58(1)	31(1)	-11(1)	10(1)	-10(1)
Cl(6)	30(1)	60(1)	15(1)	10(1)	4(1)	6(1)
Cl(7)	24(1)	42(1)	20(1)	5(1)	-5(1)	5(1)
N(1)	17(1)	18(1)	15(1)	1(1)	4(1)	-1(1)
N(2)	20(1)	21(1)	14(1)	2(1)	3(1)	1(1)
N(3)	18(1)	16(1)	13(1)	1(1)	2(1)	1(1)
N(4)	17(1)	15(1)	15(1)	0(1)	2(1)	0(1)
N(5)	16(1)	16(1)	15(1)	0(1)	3(1)	-2(1)
N(6)	16(1)	20(1)	18(1)	0(1)	4(1)	-4(1)
C(1)	16(1)	18(1)	19(1)	2(1)	6(1)	-3(1)
C(2)	18(1)	21(1)	18(1)	1(1)	8(1)	-4(1)
C(3)	15(1)	25(1)	25(1)	-1(1)	8(1)	-2(1)
C(4)	18(1)	26(1)	29(1)	-3(1)	11(1)	1(1)
C(5)	25(1)	22(1)	20(1)	-3(1)	11(1)	-4(1)
C(6)	21(1)	23(1)	16(1)	0(1)	7(1)	-4(1)
C(7)	19(1)	20(1)	16(1)	2(1)	7(1)	-2(1)
C(8)	21(1)	19(1)	13(1)	2(1)	5(1)	-2(1)
C(9)	20(1)	17(1)	14(1)	3(1)	1(1)	0(1)
C(10)	18(1)	18(1)	15(1)	2(1)	2(1)	3(1)
C(11)	20(1)	23(1)	16(1)	0(1)	-1(1)	2(1)
C(12)	17(1)	25(1)	20(1)	0(1)	-2(1)	-1(1)
C(13)	17(1)	25(1)	23(1)	0(1)	5(1)	1(1)
C(14)	19(1)	20(1)	16(1)	0(1)	2(1)	2(1)
C(15)	18(1)	16(1)	16(1)	1(1)	1(1)	3(1)
C(16)	18(1)	14(1)	17(1)	1(1)	4(1)	1(1)
C(17)	20(1)	14(1)	15(1)	-1(1)	4(1)	-2(1)

C(18)	17(1)	16(1)	16(1)	-1(1)	1(1)	-3(1)
C(19)	18(1)	21(1)	16(1)	-2(1)	2(1)	-3(1)
C(20)	22(1)	25(1)	13(1)	0(1)	2(1)	-4(1)
C(21)	19(1)	22(1)	18(1)	1(1)	-4(1)	-2(1)
C(22)	16(1)	21(1)	20(1)	-2(1)	0(1)	-2(1)
C(23)	18(1)	17(1)	17(1)	-1(1)	2(1)	-4(1)
C(24)	15(1)	18(1)	18(1)	1(1)	2(1)	-3(1)
B(1)	18(1)	16(1)	15(1)	2(1)	3(1)	-2(1)

Table S 23. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097)**.

	x	y	z	U(eq)
H(3A)	3640	4804	3439	26
H(6A)	6716	4725	4720	23
H(11A)	10038	2248	4282	24
H(14A)	10113	393	2507	22
H(19A)	7016	354	1177	22
H(22A)	3734	2280	1523	23

Table S 24. Torsion angles [°] for Cl-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087097).

C(24)-N(6)-C(1)-N(1)	-8.8(2)
C(24)-N(6)-C(1)-C(2)	153.75(14)
C(8)-N(1)-C(1)-N(6)	155.77(13)
B(1)-N(1)-C(1)-N(6)	-11.3(2)
C(8)-N(1)-C(1)-C(2)	-10.52(15)
B(1)-N(1)-C(1)-C(2)	-177.60(12)
N(6)-C(1)-C(2)-C(3)	13.1(3)
N(1)-C(1)-C(2)-C(3)	177.91(15)
N(6)-C(1)-C(2)-C(7)	-158.35(14)
N(1)-C(1)-C(2)-C(7)	6.47(15)
C(7)-C(2)-C(3)-C(4)	1.1(2)
C(1)-C(2)-C(3)-C(4)	-169.46(15)
C(2)-C(3)-C(4)-C(5)	0.3(2)
C(2)-C(3)-C(4)-Cl(2)	176.55(11)
C(3)-C(4)-C(5)-C(6)	-1.5(2)
Cl(2)-C(4)-C(5)-C(6)	-177.72(11)
C(3)-C(4)-C(5)-Cl(3)	174.68(12)
Cl(2)-C(4)-C(5)-Cl(3)	-1.49(18)
C(4)-C(5)-C(6)-C(7)	1.2(2)
Cl(3)-C(5)-C(6)-C(7)	-175.07(11)
C(5)-C(6)-C(7)-C(2)	0.2(2)
C(5)-C(6)-C(7)-C(8)	170.12(14)
C(3)-C(2)-C(7)-C(6)	-1.4(2)
C(1)-C(2)-C(7)-C(6)	171.29(13)
C(3)-C(2)-C(7)-C(8)	-173.39(13)
C(1)-C(2)-C(7)-C(8)	-0.72(15)
C(9)-N(2)-C(8)-N(1)	8.8(2)
C(9)-N(2)-C(8)-C(7)	-152.87(14)
C(1)-N(1)-C(8)-N(2)	-155.23(13)
B(1)-N(1)-C(8)-N(2)	11.9(2)
C(1)-N(1)-C(8)-C(7)	10.11(15)
B(1)-N(1)-C(8)-C(7)	177.24(12)

C(6)-C(7)-C(8)-N(2)	-12.2(3)
C(2)-C(7)-C(8)-N(2)	158.77(14)
C(6)-C(7)-C(8)-N(1)	-176.31(14)
C(2)-C(7)-C(8)-N(1)	-5.32(15)
C(8)-N(2)-C(9)-N(3)	-8.8(2)
C(8)-N(2)-C(9)-C(10)	152.67(14)
C(16)-N(3)-C(9)-N(2)	154.77(13)
B(1)-N(3)-C(9)-N(2)	-11.7(2)
C(16)-N(3)-C(9)-C(10)	-10.54(16)
B(1)-N(3)-C(9)-C(10)	-177.02(12)
N(2)-C(9)-C(10)-C(11)	17.2(3)
N(3)-C(9)-C(10)-C(11)	-178.88(15)
N(2)-C(9)-C(10)-C(15)	-156.44(14)
N(3)-C(9)-C(10)-C(15)	7.45(15)
C(15)-C(10)-C(11)-C(12)	-0.2(2)
C(9)-C(10)-C(11)-C(12)	-173.15(15)
C(10)-C(11)-C(12)-C(13)	2.4(2)
C(10)-C(11)-C(12)-Cl(4)	-177.48(11)
C(11)-C(12)-C(13)-C(14)	-1.8(2)
Cl(4)-C(12)-C(13)-C(14)	178.10(12)
C(11)-C(12)-C(13)-Cl(5)	178.40(12)
Cl(4)-C(12)-C(13)-Cl(5)	-1.67(19)
C(12)-C(13)-C(14)-C(15)	-1.1(2)
Cl(5)-C(13)-C(14)-C(15)	178.63(12)
C(13)-C(14)-C(15)-C(10)	3.4(2)
C(13)-C(14)-C(15)-C(16)	175.57(15)
C(11)-C(10)-C(15)-C(14)	-2.8(2)
C(9)-C(10)-C(15)-C(14)	171.70(13)
C(11)-C(10)-C(15)-C(16)	-176.68(13)
C(9)-C(10)-C(15)-C(16)	-2.17(15)
C(17)-N(4)-C(16)-N(3)	11.5(2)
C(17)-N(4)-C(16)-C(15)	-151.53(15)
C(9)-N(3)-C(16)-N(4)	-157.31(13)
B(1)-N(3)-C(16)-N(4)	9.1(2)
C(9)-N(3)-C(16)-C(15)	9.23(16)
B(1)-N(3)-C(16)-C(15)	175.66(12)

C(14)-C(15)-C(16)-N(4)	-11.7(3)
C(10)-C(15)-C(16)-N(4)	161.30(14)
C(14)-C(15)-C(16)-N(3)	-176.88(15)
C(10)-C(15)-C(16)-N(3)	-3.91(15)
C(16)-N(4)-C(17)-N(5)	-10.3(2)
C(16)-N(4)-C(17)-C(18)	151.68(15)
C(24)-N(5)-C(17)-N(4)	156.38(13)
B(1)-N(5)-C(17)-N(4)	-11.6(2)
C(24)-N(5)-C(17)-C(18)	-9.21(16)
B(1)-N(5)-C(17)-C(18)	-177.22(12)
N(4)-C(17)-C(18)-C(19)	10.4(3)
N(5)-C(17)-C(18)-C(19)	174.87(15)
N(4)-C(17)-C(18)-C(23)	-160.70(14)
N(5)-C(17)-C(18)-C(23)	3.79(15)
C(23)-C(18)-C(19)-C(20)	-2.7(2)
C(17)-C(18)-C(19)-C(20)	-172.77(15)
C(18)-C(19)-C(20)-C(21)	-1.1(2)
C(18)-C(19)-C(20)-Cl(6)	177.04(11)
C(19)-C(20)-C(21)-C(22)	3.4(2)
Cl(6)-C(20)-C(21)-C(22)	-174.68(12)
C(19)-C(20)-C(21)-Cl(7)	-178.04(12)
Cl(6)-C(20)-C(21)-Cl(7)	3.91(19)
C(20)-C(21)-C(22)-C(23)	-1.7(2)
Cl(7)-C(21)-C(22)-C(23)	179.74(11)
C(21)-C(22)-C(23)-C(18)	-2.1(2)
C(21)-C(22)-C(23)-C(24)	170.01(15)
C(19)-C(18)-C(23)-C(22)	4.4(2)
C(17)-C(18)-C(23)-C(22)	176.32(13)
C(19)-C(18)-C(23)-C(24)	-169.63(13)
C(17)-C(18)-C(23)-C(24)	2.30(16)
C(1)-N(6)-C(24)-N(5)	8.0(2)
C(1)-N(6)-C(24)-C(23)	-153.60(15)
C(17)-N(5)-C(24)-N(6)	-154.98(13)
B(1)-N(5)-C(24)-N(6)	12.9(2)
C(17)-N(5)-C(24)-C(23)	10.63(16)
B(1)-N(5)-C(24)-C(23)	178.51(12)

C(22)-C(23)-C(24)-N(6)	-16.5(3)
C(18)-C(23)-C(24)-N(6)	156.38(14)
C(22)-C(23)-C(24)-N(5)	179.67(15)
C(18)-C(23)-C(24)-N(5)	-7.50(15)
C(8)-N(1)-B(1)-N(5)	-138.60(13)
C(1)-N(1)-B(1)-N(5)	27.35(17)
C(8)-N(1)-B(1)-N(3)	-27.75(17)
C(1)-N(1)-B(1)-N(3)	138.20(13)
C(8)-N(1)-B(1)-Cl(1)	97.23(14)
C(1)-N(1)-B(1)-Cl(1)	-96.82(14)
C(17)-N(5)-B(1)-N(1)	138.64(13)
C(24)-N(5)-B(1)-N(1)	-28.24(17)
C(17)-N(5)-B(1)-N(3)	27.70(18)
C(24)-N(5)-B(1)-N(3)	-139.18(13)
C(17)-N(5)-B(1)-Cl(1)	-96.84(14)
C(24)-N(5)-B(1)-Cl(1)	96.28(14)
C(9)-N(3)-B(1)-N(1)	27.74(17)
C(16)-N(3)-B(1)-N(1)	-137.45(13)
C(9)-N(3)-B(1)-N(5)	138.54(13)
C(16)-N(3)-B(1)-N(5)	-26.65(18)
C(9)-N(3)-B(1)-Cl(1)	-97.25(14)
C(16)-N(3)-B(1)-Cl(1)	97.56(14)

Symmetry transformations used to generate equivalent atoms:

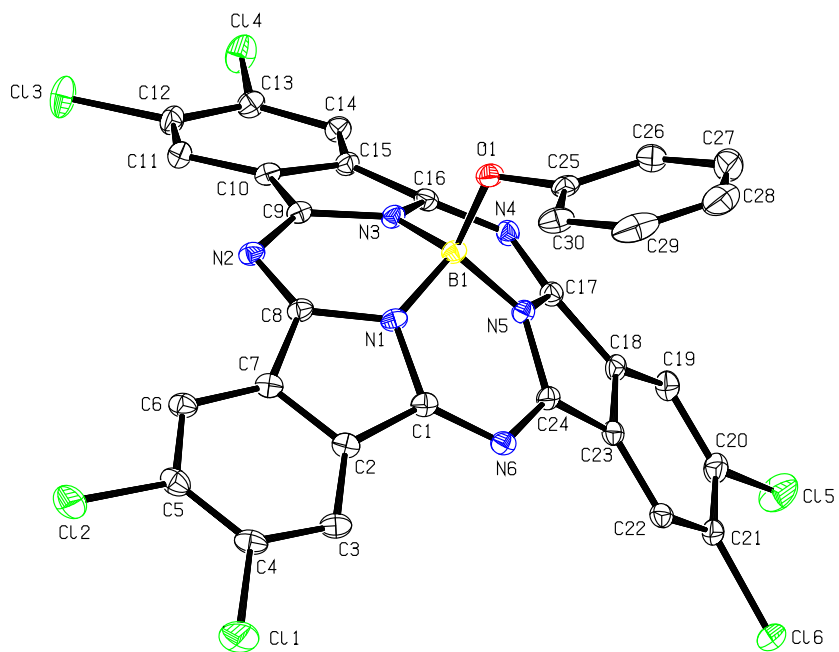


Figure S13: Anisotropic displacement ellipsoid plot of **PhO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit **2087093**).

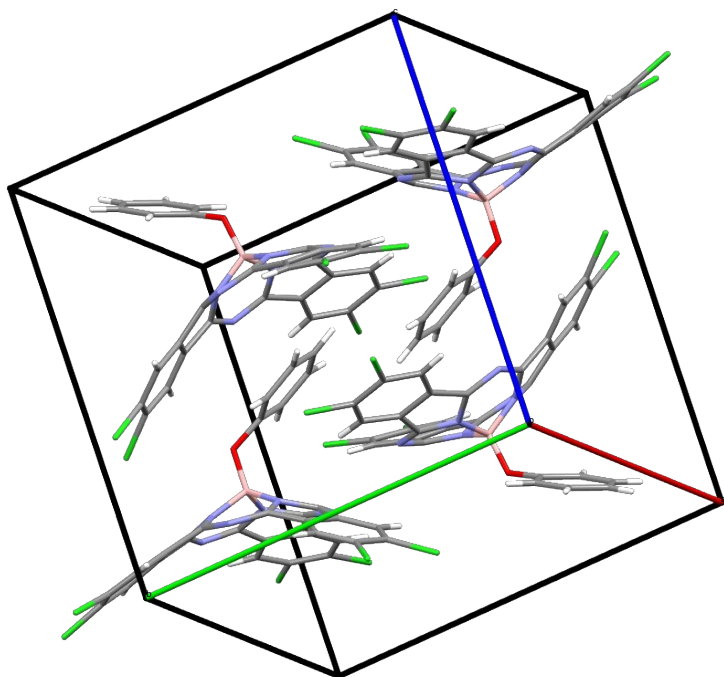


Figure S14: Populated unit Cell of **PhO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087093).

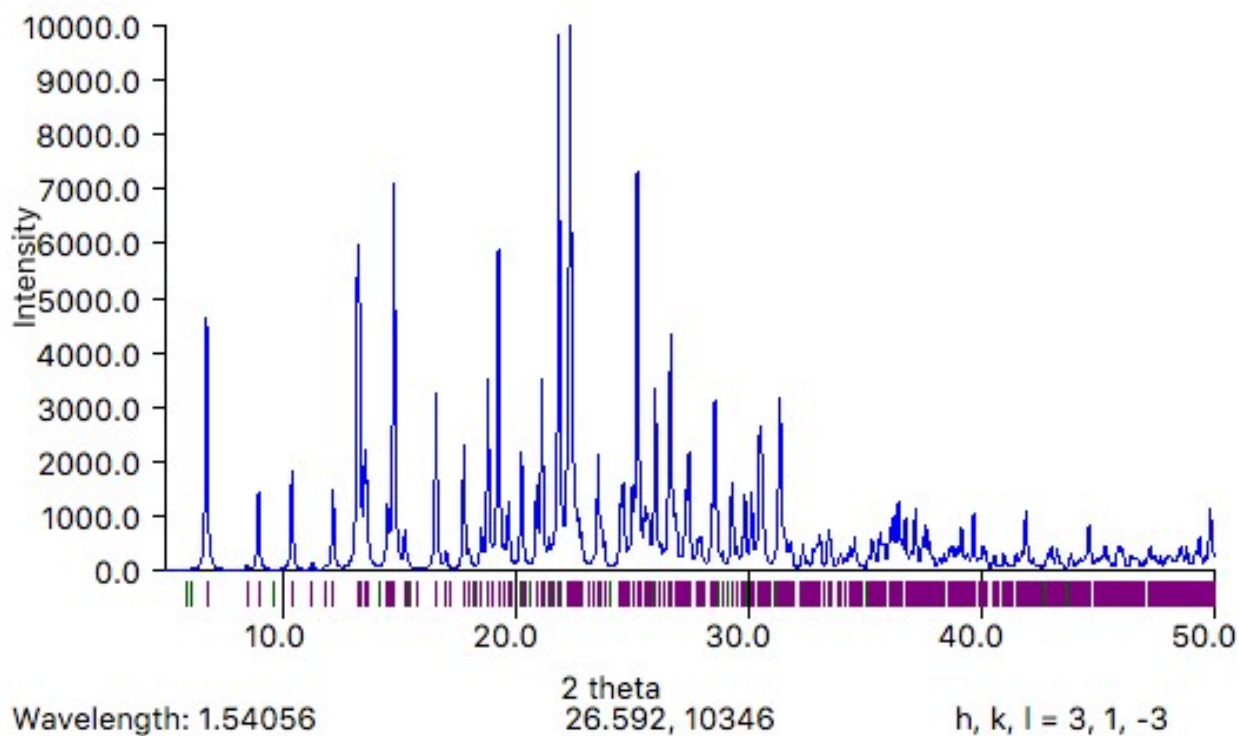


Figure S15: Powder x-ray diffraction of **PhO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087093).

Table S 25. Crystal data and structure refinement for **PhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087093)**.

Identification code	d19152_a	
Empirical formula	C ₃₀ H ₁₁ B Cl ₆ N ₆ O	
Formula weight	694.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 13.1387(10) Å	α = 90°.
	b = 14.9262(10) Å	β = 96.620(2)°.
	c = 14.6051(11) Å	γ = 90°.
Volume	2845.1(4) Å ³	
Z	4	
Density (calculated)	1.622 Mg/m ³	
Absorption coefficient	0.643 mm ⁻¹	
F(000)	1392	
Crystal size	0.150 x 0.130 x 0.120 mm ³	
Theta range for data collection	1.560 to 27.591°.	
Index ranges	-17<=h<=17, -18<=k<=19, -17<=l<=18	
Reflections collected	35148	
Independent reflections	6539 [R(int) = 0.0704]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7022	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6539 / 0 / 397	
Goodness-of-fit on F ²	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0811	
R indices (all data)	R1 = 0.0934, wR2 = 0.1011	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.480 and -0.477 e.Å ⁻³	

Table S 26. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087093)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	9475(1)	6747(1)	6936(1)	50(1)
Cl(2)	9091(1)	4693(1)	7291(1)	44(1)
Cl(3)	1849(1)	2147(1)	5613(1)	40(1)
Cl(4)	-138(1)	3345(1)	5320(1)	37(1)
Cl(5)	1101(1)	9905(1)	4091(1)	49(1)
Cl(6)	3358(1)	10665(1)	4343(1)	34(1)
O(1)	3591(1)	6737(1)	8579(1)	25(1)
N(1)	4868(2)	6474(1)	7461(1)	20(1)
N(2)	4655(2)	4898(1)	7286(1)	22(1)
N(3)	3213(2)	5868(1)	7210(1)	20(1)
N(4)	1875(2)	6753(1)	6438(1)	22(1)
N(5)	3470(2)	7416(1)	7009(1)	18(1)
N(6)	5169(2)	7911(1)	6844(1)	21(1)
C(1)	5505(2)	7116(2)	7180(2)	21(1)
C(2)	6489(2)	6670(2)	7143(2)	23(1)
C(3)	7455(2)	6977(2)	6988(2)	28(1)
C(4)	8254(2)	6369(2)	7046(2)	30(1)
C(5)	8088(2)	5451(2)	7206(2)	29(1)
C(6)	7124(2)	5132(2)	7304(2)	26(1)
C(7)	6326(2)	5742(2)	7296(2)	23(1)
C(8)	5252(2)	5628(2)	7409(2)	22(1)
C(9)	3638(2)	5044(2)	7130(2)	21(1)
C(10)	2820(2)	4486(2)	6682(2)	22(1)
C(11)	2797(2)	3593(2)	6410(2)	24(1)
C(12)	1890(2)	3255(2)	5968(2)	27(1)
C(13)	1012(2)	3795(2)	5802(2)	26(1)
C(14)	1047(2)	4698(2)	6010(2)	23(1)
C(15)	1952(2)	5048(2)	6458(2)	21(1)
C(16)	2261(2)	5958(2)	6736(2)	20(1)
C(17)	2520(2)	7459(2)	6522(2)	21(1)

C(18)	2512(2)	8275(2)	5977(2)	21(1)
C(19)	1756(2)	8674(2)	5362(2)	26(1)
C(20)	2024(2)	9416(2)	4876(2)	28(1)
C(21)	3026(2)	9754(2)	4992(2)	25(1)
C(22)	3783(2)	9360(2)	5591(2)	22(1)
C(23)	3527(2)	8619(2)	6089(2)	21(1)
C(24)	4145(2)	8021(2)	6710(2)	20(1)
C(25)	3799(2)	7523(2)	9051(2)	24(1)
C(26)	2994(2)	8112(2)	9137(2)	35(1)
C(27)	3169(3)	8891(2)	9632(2)	52(1)
C(28)	4132(4)	9094(2)	10042(2)	56(1)
C(29)	4934(3)	8514(2)	9957(2)	49(1)
C(30)	4770(2)	7712(2)	9465(2)	33(1)
B(1)	3789(2)	6651(2)	7639(2)	20(1)

Table S 27. Bond lengths [\AA] and angles [$^\circ$] for **PhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087093)**.

Cl(1)-C(4)	1.726(3)
Cl(2)-C(5)	1.730(3)
Cl(3)-C(12)	1.733(2)
Cl(4)-C(13)	1.728(3)
Cl(5)-C(20)	1.731(3)
Cl(6)-C(21)	1.741(3)
O(1)-C(25)	1.372(3)
O(1)-B(1)	1.433(3)
N(1)-C(8)	1.364(3)
N(1)-C(1)	1.367(3)
N(1)-B(1)	1.494(3)
N(2)-C(8)	1.342(3)
N(2)-C(9)	1.347(3)
N(3)-C(9)	1.361(3)
N(3)-C(16)	1.364(3)
N(3)-B(1)	1.491(3)
N(4)-C(16)	1.343(3)
N(4)-C(17)	1.348(3)
N(5)-C(17)	1.365(3)
N(5)-C(24)	1.372(3)
N(5)-B(1)	1.495(3)
N(6)-C(1)	1.339(3)
N(6)-C(24)	1.347(3)
C(1)-C(2)	1.461(3)
C(2)-C(3)	1.393(3)
C(2)-C(7)	1.423(3)
C(3)-C(4)	1.382(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.412(4)
C(5)-C(6)	1.376(4)
C(6)-C(7)	1.387(3)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.451(3)
C(9)-C(10)	1.454(3)
C(10)-C(11)	1.391(3)
C(10)-C(15)	1.423(3)
C(11)-C(12)	1.383(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.405(4)
C(13)-C(14)	1.380(3)
C(14)-C(15)	1.391(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.462(3)
C(17)-C(18)	1.455(3)
C(18)-C(19)	1.392(3)
C(18)-C(23)	1.421(3)
C(19)-C(20)	1.383(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.402(4)
C(21)-C(22)	1.378(4)
C(22)-C(23)	1.387(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.452(3)
C(25)-C(30)	1.377(4)
C(25)-C(26)	1.391(4)
C(26)-C(27)	1.374(4)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.369(5)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.380(5)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.400(4)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
C(25)-O(1)-B(1)	120.69(19)
C(8)-N(1)-C(1)	113.0(2)
C(8)-N(1)-B(1)	122.5(2)

C(1)-N(1)-B(1)	123.6(2)
C(8)-N(2)-C(9)	116.4(2)
C(9)-N(3)-C(16)	114.0(2)
C(9)-N(3)-B(1)	123.4(2)
C(16)-N(3)-B(1)	121.8(2)
C(16)-N(4)-C(17)	116.8(2)
C(17)-N(5)-C(24)	112.9(2)
C(17)-N(5)-B(1)	122.1(2)
C(24)-N(5)-B(1)	123.6(2)
C(1)-N(6)-C(24)	116.3(2)
N(6)-C(1)-N(1)	123.0(2)
N(6)-C(1)-C(2)	130.3(2)
N(1)-C(1)-C(2)	105.4(2)
C(3)-C(2)-C(7)	120.1(2)
C(3)-C(2)-C(1)	133.1(2)
C(7)-C(2)-C(1)	106.8(2)
C(4)-C(3)-C(2)	118.3(2)
C(4)-C(3)-H(3A)	120.9
C(2)-C(3)-H(3A)	120.9
C(3)-C(4)-C(5)	121.1(2)
C(3)-C(4)-Cl(1)	119.2(2)
C(5)-C(4)-Cl(1)	119.7(2)
C(6)-C(5)-C(4)	121.0(2)
C(6)-C(5)-Cl(2)	118.0(2)
C(4)-C(5)-Cl(2)	121.0(2)
C(5)-C(6)-C(7)	118.4(2)
C(5)-C(6)-H(6A)	120.8
C(7)-C(6)-H(6A)	120.8
C(6)-C(7)-C(2)	120.9(2)
C(6)-C(7)-C(8)	131.8(2)
C(2)-C(7)-C(8)	107.3(2)
N(2)-C(8)-N(1)	123.0(2)
N(2)-C(8)-C(7)	129.9(2)
N(1)-C(8)-C(7)	105.6(2)
N(2)-C(9)-N(3)	122.7(2)
N(2)-C(9)-C(10)	130.6(2)

N(3)-C(9)-C(10)	105.4(2)
C(11)-C(10)-C(15)	120.5(2)
C(11)-C(10)-C(9)	131.9(2)
C(15)-C(10)-C(9)	107.3(2)
C(12)-C(11)-C(10)	118.2(2)
C(12)-C(11)-H(11A)	120.9
C(10)-C(11)-H(11A)	120.9
C(11)-C(12)-C(13)	121.2(2)
C(11)-C(12)-Cl(3)	118.9(2)
C(13)-C(12)-Cl(3)	120.0(2)
C(14)-C(13)-C(12)	121.1(2)
C(14)-C(13)-Cl(4)	118.3(2)
C(12)-C(13)-Cl(4)	120.59(19)
C(13)-C(14)-C(15)	118.3(2)
C(13)-C(14)-H(14A)	120.8
C(15)-C(14)-H(14A)	120.8
C(14)-C(15)-C(10)	120.4(2)
C(14)-C(15)-C(16)	132.4(2)
C(10)-C(15)-C(16)	107.1(2)
N(4)-C(16)-N(3)	122.8(2)
N(4)-C(16)-C(15)	130.5(2)
N(3)-C(16)-C(15)	104.9(2)
N(4)-C(17)-N(5)	122.6(2)
N(4)-C(17)-C(18)	129.8(2)
N(5)-C(17)-C(18)	105.8(2)
C(19)-C(18)-C(23)	120.6(2)
C(19)-C(18)-C(17)	132.1(2)
C(23)-C(18)-C(17)	107.0(2)
C(20)-C(19)-C(18)	118.0(2)
C(20)-C(19)-H(19A)	121.0
C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.1(2)
C(19)-C(20)-Cl(5)	118.6(2)
C(21)-C(20)-Cl(5)	120.3(2)
C(22)-C(21)-C(20)	121.5(2)
C(22)-C(21)-Cl(6)	118.1(2)

C(20)-C(21)-Cl(6)	120.4(2)
C(21)-C(22)-C(23)	118.2(2)
C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	120.6(2)
C(22)-C(23)-C(24)	131.8(2)
C(18)-C(23)-C(24)	107.4(2)
N(6)-C(24)-N(5)	123.0(2)
N(6)-C(24)-C(23)	130.0(2)
N(5)-C(24)-C(23)	105.5(2)
O(1)-C(25)-C(30)	121.0(2)
O(1)-C(25)-C(26)	118.5(2)
C(30)-C(25)-C(26)	120.4(3)
C(27)-C(26)-C(25)	120.0(3)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(28)-C(27)-C(26)	120.4(3)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
C(27)-C(28)-C(29)	119.9(3)
C(27)-C(28)-H(28A)	120.0
C(29)-C(28)-H(28A)	120.0
C(28)-C(29)-C(30)	120.6(3)
C(28)-C(29)-H(29A)	119.7
C(30)-C(29)-H(29A)	119.7
C(25)-C(30)-C(29)	118.7(3)
C(25)-C(30)-H(30A)	120.7
C(29)-C(30)-H(30A)	120.7
O(1)-B(1)-N(3)	109.5(2)
O(1)-B(1)-N(1)	117.6(2)
N(3)-B(1)-N(1)	103.5(2)
O(1)-B(1)-N(5)	116.9(2)
N(3)-B(1)-N(5)	104.4(2)
N(1)-B(1)-N(5)	103.5(2)

Symmetry transformations used to generate equivalent atoms:

Table S 28. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087093)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	21(1)	57(1)	75(1)	10(1)	15(1)	-6(1)
Cl(2)	24(1)	51(1)	57(1)	5(1)	11(1)	10(1)
Cl(3)	51(1)	21(1)	45(1)	-11(1)	-8(1)	2(1)
Cl(4)	32(1)	28(1)	49(1)	-7(1)	-10(1)	-8(1)
Cl(5)	41(1)	47(1)	56(1)	22(1)	-10(1)	4(1)
Cl(6)	43(1)	26(1)	34(1)	10(1)	10(1)	3(1)
O(1)	31(1)	23(1)	21(1)	0(1)	7(1)	-5(1)
N(1)	19(1)	22(1)	20(1)	1(1)	1(1)	-5(1)
N(2)	19(1)	23(1)	22(1)	5(1)	1(1)	0(1)
N(3)	17(1)	17(1)	24(1)	1(1)	2(1)	-3(1)
N(4)	18(1)	20(1)	28(1)	-2(1)	4(1)	0(1)
N(5)	18(1)	17(1)	19(1)	-2(1)	1(1)	-3(1)
N(6)	20(1)	21(1)	22(1)	-4(1)	3(1)	-5(1)
C(1)	20(1)	23(1)	20(1)	-2(1)	0(1)	-6(1)
C(2)	19(1)	28(1)	20(1)	-1(1)	0(1)	-2(1)
C(3)	23(1)	34(2)	26(2)	2(1)	2(1)	-7(1)
C(4)	19(1)	41(2)	30(2)	2(1)	6(1)	-4(1)
C(5)	22(1)	39(2)	27(2)	1(1)	3(1)	4(1)
C(6)	24(1)	31(2)	21(1)	4(1)	3(1)	1(1)
C(7)	21(1)	28(1)	19(1)	1(1)	1(1)	-2(1)
C(8)	22(1)	23(1)	19(1)	4(1)	1(1)	0(1)
C(9)	22(1)	20(1)	20(1)	2(1)	3(1)	-3(1)
C(10)	21(1)	22(1)	22(1)	3(1)	3(1)	-3(1)
C(11)	25(1)	20(1)	26(2)	1(1)	2(1)	1(1)
C(12)	34(2)	18(1)	27(2)	-2(1)	2(1)	-1(1)
C(13)	27(1)	24(1)	25(2)	-1(1)	0(1)	-4(1)
C(14)	21(1)	23(1)	25(1)	1(1)	1(1)	-1(1)
C(15)	21(1)	19(1)	24(1)	1(1)	3(1)	-3(1)
C(16)	18(1)	22(1)	21(1)	-2(1)	5(1)	-2(1)

C(17)	20(1)	20(1)	22(1)	-1(1)	2(1)	0(1)
C(18)	27(1)	16(1)	20(1)	-5(1)	2(1)	0(1)
C(19)	23(1)	23(1)	31(2)	-4(1)	1(1)	1(1)
C(20)	31(2)	24(1)	28(2)	1(1)	1(1)	6(1)
C(21)	34(2)	18(1)	25(1)	-1(1)	8(1)	2(1)
C(22)	24(1)	20(1)	23(1)	-5(1)	6(1)	-3(1)
C(23)	24(1)	18(1)	21(1)	-5(1)	4(1)	-1(1)
C(24)	25(1)	17(1)	18(1)	-4(1)	3(1)	-5(1)
C(25)	35(2)	23(1)	15(1)	3(1)	5(1)	-5(1)
C(26)	43(2)	34(2)	28(2)	4(1)	11(1)	3(1)
C(27)	86(3)	34(2)	41(2)	3(2)	30(2)	11(2)
C(28)	109(3)	34(2)	28(2)	-7(2)	25(2)	-17(2)
C(29)	67(2)	54(2)	24(2)	3(2)	-4(2)	-35(2)
C(30)	36(2)	38(2)	23(2)	6(1)	1(1)	-9(1)
B(1)	22(1)	20(1)	19(2)	0(1)	2(1)	-3(1)

Table S 29. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087093).

	x	y	z	U(eq)
H(3A)	7563	7588	6845	33
H(6A)	7007	4509	7376	31
H(11A)	3387	3225	6525	29
H(14A)	467	5070	5852	28
H(19A)	1078	8443	5280	31
H(22A)	4462	9590	5661	27
H(26A)	2325	7975	8854	42
H(27A)	2618	9291	9691	62
H(28A)	4247	9632	10384	67
H(29A)	5602	8661	10235	59
H(30A)	5319	7306	9417	39

Table S 30. Torsion angles [°] for **PhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087093)**.

C(24)-N(6)-C(1)-N(1)	-6.1(3)
C(24)-N(6)-C(1)-C(2)	158.6(2)
C(8)-N(1)-C(1)-N(6)	154.2(2)
B(1)-N(1)-C(1)-N(6)	-15.2(4)
C(8)-N(1)-C(1)-C(2)	-13.8(3)
B(1)-N(1)-C(1)-C(2)	176.8(2)
N(6)-C(1)-C(2)-C(3)	19.8(5)
N(1)-C(1)-C(2)-C(3)	-173.4(3)
N(6)-C(1)-C(2)-C(7)	-159.4(2)
N(1)-C(1)-C(2)-C(7)	7.4(3)
C(7)-C(2)-C(3)-C(4)	-4.1(4)
C(1)-C(2)-C(3)-C(4)	176.7(3)
C(2)-C(3)-C(4)-C(5)	3.6(4)
C(2)-C(3)-C(4)-Cl(1)	-175.5(2)
C(3)-C(4)-C(5)-C(6)	0.4(4)
Cl(1)-C(4)-C(5)-C(6)	179.5(2)
C(3)-C(4)-C(5)-Cl(2)	-179.4(2)
Cl(1)-C(4)-C(5)-Cl(2)	-0.2(3)
C(4)-C(5)-C(6)-C(7)	-3.7(4)
Cl(2)-C(5)-C(6)-C(7)	176.0(2)
C(5)-C(6)-C(7)-C(2)	3.1(4)
C(5)-C(6)-C(7)-C(8)	-177.8(3)
C(3)-C(2)-C(7)-C(6)	0.8(4)
C(1)-C(2)-C(7)-C(6)	-179.8(2)
C(3)-C(2)-C(7)-C(8)	-178.5(2)
C(1)-C(2)-C(7)-C(8)	0.9(3)
C(9)-N(2)-C(8)-N(1)	5.8(3)
C(9)-N(2)-C(8)-C(7)	-157.8(2)
C(1)-N(1)-C(8)-N(2)	-152.6(2)
B(1)-N(1)-C(8)-N(2)	16.9(4)
C(1)-N(1)-C(8)-C(7)	14.4(3)
B(1)-N(1)-C(8)-C(7)	-176.1(2)
C(6)-C(7)-C(8)-N(2)	-22.3(5)

C(2)-C(7)-C(8)-N(2)	156.9(3)
C(6)-C(7)-C(8)-N(1)	171.9(3)
C(2)-C(7)-C(8)-N(1)	-8.8(3)
C(8)-N(2)-C(9)-N(3)	-8.4(3)
C(8)-N(2)-C(9)-C(10)	157.0(2)
C(16)-N(3)-C(9)-N(2)	158.5(2)
B(1)-N(3)-C(9)-N(2)	-11.6(4)
C(16)-N(3)-C(9)-C(10)	-10.1(3)
B(1)-N(3)-C(9)-C(10)	179.8(2)
N(2)-C(9)-C(10)-C(11)	11.8(5)
N(3)-C(9)-C(10)-C(11)	179.1(3)
N(2)-C(9)-C(10)-C(15)	-163.1(2)
N(3)-C(9)-C(10)-C(15)	4.1(3)
C(15)-C(10)-C(11)-C(12)	-3.8(4)
C(9)-C(10)-C(11)-C(12)	-178.2(3)
C(10)-C(11)-C(12)-C(13)	-0.4(4)
C(10)-C(11)-C(12)-Cl(3)	179.3(2)
C(11)-C(12)-C(13)-C(14)	5.0(4)
Cl(3)-C(12)-C(13)-C(14)	-174.7(2)
C(11)-C(12)-C(13)-Cl(4)	-175.6(2)
Cl(3)-C(12)-C(13)-Cl(4)	4.7(3)
C(12)-C(13)-C(14)-C(15)	-5.1(4)
Cl(4)-C(13)-C(14)-C(15)	175.5(2)
C(13)-C(14)-C(15)-C(10)	0.8(4)
C(13)-C(14)-C(15)-C(16)	176.8(3)
C(11)-C(10)-C(15)-C(14)	3.7(4)
C(9)-C(10)-C(15)-C(14)	179.3(2)
C(11)-C(10)-C(15)-C(16)	-173.2(2)
C(9)-C(10)-C(15)-C(16)	2.5(3)
C(17)-N(4)-C(16)-N(3)	8.3(4)
C(17)-N(4)-C(16)-C(15)	-153.9(3)
C(9)-N(3)-C(16)-N(4)	-154.5(2)
B(1)-N(3)-C(16)-N(4)	15.8(4)
C(9)-N(3)-C(16)-C(15)	11.5(3)
B(1)-N(3)-C(16)-C(15)	-178.2(2)
C(14)-C(15)-C(16)-N(4)	-19.9(5)

C(10)-C(15)-C(16)-N(4)	156.4(3)
C(14)-C(15)-C(16)-N(3)	175.5(3)
C(10)-C(15)-C(16)-N(3)	-8.1(3)
C(16)-N(4)-C(17)-N(5)	-9.9(4)
C(16)-N(4)-C(17)-C(18)	152.4(3)
C(24)-N(5)-C(17)-N(4)	154.1(2)
B(1)-N(5)-C(17)-N(4)	-12.5(4)
C(24)-N(5)-C(17)-C(18)	-11.8(3)
B(1)-N(5)-C(17)-C(18)	-178.4(2)
N(4)-C(17)-C(18)-C(19)	16.4(5)
N(5)-C(17)-C(18)-C(19)	-179.1(3)
N(4)-C(17)-C(18)-C(23)	-157.1(3)
N(5)-C(17)-C(18)-C(23)	7.4(3)
C(23)-C(18)-C(19)-C(20)	-0.7(4)
C(17)-C(18)-C(19)-C(20)	-173.5(3)
C(18)-C(19)-C(20)-C(21)	0.4(4)
C(18)-C(19)-C(20)-Cl(5)	178.71(19)
C(19)-C(20)-C(21)-C(22)	0.3(4)
Cl(5)-C(20)-C(21)-C(22)	-178.0(2)
C(19)-C(20)-C(21)-Cl(6)	177.7(2)
Cl(5)-C(20)-C(21)-Cl(6)	-0.6(3)
C(20)-C(21)-C(22)-C(23)	-0.7(4)
Cl(6)-C(21)-C(22)-C(23)	-178.18(18)
C(21)-C(22)-C(23)-C(18)	0.4(4)
C(21)-C(22)-C(23)-C(24)	174.7(2)
C(19)-C(18)-C(23)-C(22)	0.3(4)
C(17)-C(18)-C(23)-C(22)	174.7(2)
C(19)-C(18)-C(23)-C(24)	-175.3(2)
C(17)-C(18)-C(23)-C(24)	-0.9(3)
C(1)-N(6)-C(24)-N(5)	8.6(3)
C(1)-N(6)-C(24)-C(23)	-155.7(2)
C(17)-N(5)-C(24)-N(6)	-156.3(2)
B(1)-N(5)-C(24)-N(6)	10.1(4)
C(17)-N(5)-C(24)-C(23)	11.3(3)
B(1)-N(5)-C(24)-C(23)	177.6(2)
C(22)-C(23)-C(24)-N(6)	-14.5(4)

C(18)-C(23)-C(24)-N(6)	160.4(2)
C(22)-C(23)-C(24)-N(5)	179.2(2)
C(18)-C(23)-C(24)-N(5)	-5.9(3)
B(1)-O(1)-C(25)-C(30)	-83.4(3)
B(1)-O(1)-C(25)-C(26)	99.4(3)
O(1)-C(25)-C(26)-C(27)	177.7(2)
C(30)-C(25)-C(26)-C(27)	0.5(4)
C(25)-C(26)-C(27)-C(28)	0.1(5)
C(26)-C(27)-C(28)-C(29)	0.1(5)
C(27)-C(28)-C(29)-C(30)	-0.9(5)
O(1)-C(25)-C(30)-C(29)	-178.4(2)
C(26)-C(25)-C(30)-C(29)	-1.3(4)
C(28)-C(29)-C(30)-C(25)	1.4(4)
C(25)-O(1)-B(1)-N(3)	-162.5(2)
C(25)-O(1)-B(1)-N(1)	79.8(3)
C(25)-O(1)-B(1)-N(5)	-44.2(3)
C(9)-N(3)-B(1)-O(1)	-97.4(3)
C(16)-N(3)-B(1)-O(1)	93.2(3)
C(9)-N(3)-B(1)-N(1)	28.8(3)
C(16)-N(3)-B(1)-N(1)	-140.6(2)
C(9)-N(3)-B(1)-N(5)	136.8(2)
C(16)-N(3)-B(1)-N(5)	-32.6(3)
C(8)-N(1)-B(1)-O(1)	89.7(3)
C(1)-N(1)-B(1)-O(1)	-102.0(3)
C(8)-N(1)-B(1)-N(3)	-31.1(3)
C(1)-N(1)-B(1)-N(3)	137.2(2)
C(8)-N(1)-B(1)-N(5)	-139.8(2)
C(1)-N(1)-B(1)-N(5)	28.5(3)
C(17)-N(5)-B(1)-O(1)	-90.0(3)
C(24)-N(5)-B(1)-O(1)	104.9(3)
C(17)-N(5)-B(1)-N(3)	31.1(3)
C(24)-N(5)-B(1)-N(3)	-134.1(2)
C(17)-N(5)-B(1)-N(1)	139.1(2)
C(24)-N(5)-B(1)-N(1)	-26.0(3)

Symmetry transformations used to generate equivalent atoms:

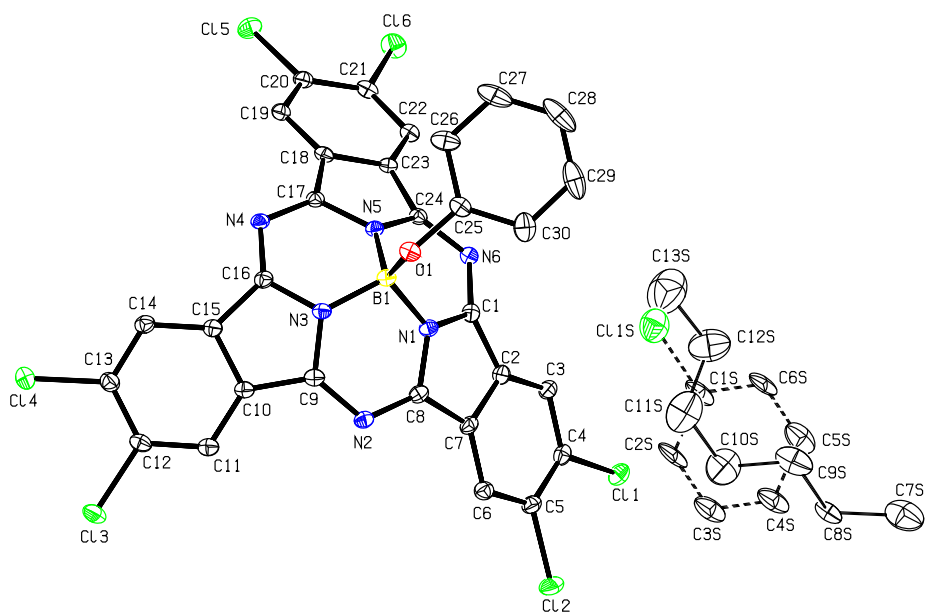


Figure S16: Anisotropic displacement ellipsoid plot of **PhO-Cl₆BsubPc** (Chlorobenzene:Heptane; CCDC deposit **2087094**).

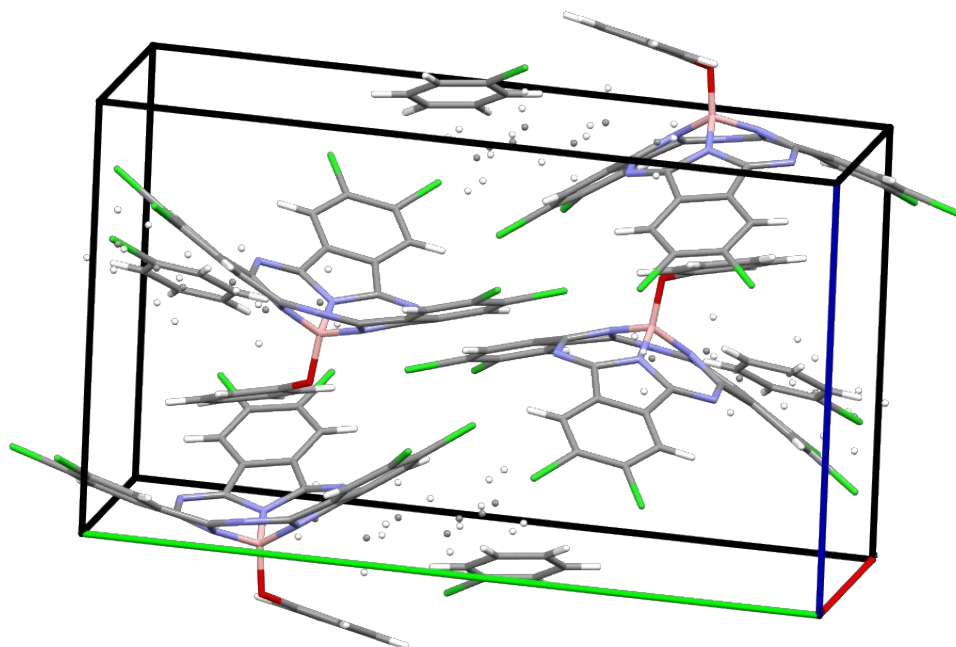


Figure S17: Populated unit cell of **PhO-Cl₆BsubPc** (Chlorobenzene:Heptane; CCDC deposit 2087094).

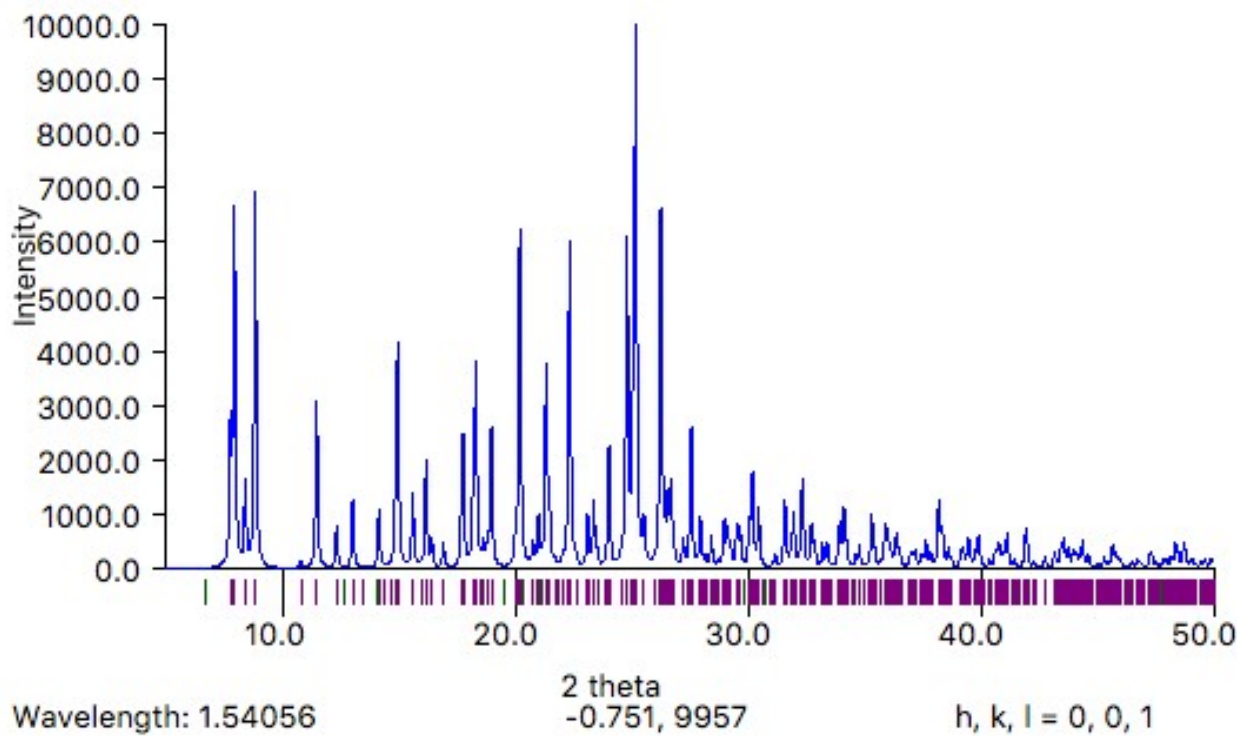


Figure S18: Powder x-ray diffraction **PhO-Cl₆BsubPc** (Chlorobenzene:Heptane; CCDC deposit 2087094).

Table S 31. Crystal data and structure refinement for **PhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087094)**.

Identification code	d19160_a	
Empirical formula	C _{36.71} H _{23.76} B Cl _{6.30} N ₆ O	
Formula weight	798.80	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 12.5724(6) Å	a = 90°.
	b = 20.9451(10) Å	b = 115.589(2)°.
	c = 14.5210(8) Å	γ = 90°.
Volume	3448.8(3) Å ³	
Z	4	
Density (calculated)	1.538 Mg/m ³	
Absorption coefficient	0.564 mm ⁻¹	
F(000)	1624	
Crystal size	0.320 x 0.100 x 0.100 mm ³	
Theta range for data collection	1.796 to 27.535°.	
Index ranges	-15 ≤ h ≤ 16, -27 ≤ k ≤ 27, -18 ≤ l ≤ 9	
Reflections collected	51213	
Independent reflections	7945 [R(int) = 0.0685]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6935	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7945 / 80 / 512	
Goodness-of-fit on F ²	1.068	
Final R indices [I > 2σ(I)]	R1 = 0.0506, wR2 = 0.1209	
R indices (all data)	R1 = 0.1119, wR2 = 0.1607	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.978 and -0.511 e.Å ⁻³	

Table S 32. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087094)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	3565(1)	9971(1)	7979(1)	34(1)
Cl(2)	1193(1)	9281(1)	7552(1)	40(1)
Cl(3)	791(1)	4576(1)	6557(1)	37(1)
Cl(4)	2860(1)	3821(1)	6414(1)	45(1)
Cl(5)	10159(1)	6085(1)	7546(1)	38(1)
Cl(6)	10382(1)	7568(1)	7878(1)	40(1)
O(1)	3293(2)	7233(1)	3597(2)	26(1)
N(1)	3419(2)	7664(1)	5250(2)	22(1)
N(2)	1894(2)	7074(1)	5419(2)	24(1)
N(3)	3259(2)	6553(1)	4936(2)	21(1)
N(4)	5028(2)	5963(1)	5346(2)	22(1)
N(5)	5034(2)	7094(1)	5268(2)	21(1)
N(6)	5331(2)	8138(1)	5973(2)	23(1)
C(1)	4182(3)	8147(2)	5760(2)	23(1)
C(2)	3559(3)	8531(2)	6204(3)	25(1)
C(3)	3891(3)	9078(2)	6804(3)	25(1)
C(4)	3148(3)	9299(2)	7208(3)	26(1)
C(5)	2096(3)	8986(2)	7027(3)	27(1)
C(6)	1768(3)	8431(2)	6455(3)	26(1)
C(7)	2503(3)	8205(2)	6038(2)	24(1)
C(8)	2481(3)	7621(2)	5487(2)	23(1)
C(9)	2348(3)	6538(2)	5208(2)	23(1)
C(10)	2232(3)	5880(2)	5457(2)	23(1)
C(11)	1489(3)	5587(2)	5808(3)	26(1)
C(12)	1688(3)	4950(2)	6095(3)	27(1)
C(13)	2618(3)	4614(2)	6033(3)	28(1)
C(14)	3373(3)	4898(2)	5694(3)	26(1)
C(15)	3183(3)	5537(2)	5408(2)	23(1)
C(16)	3883(3)	5993(2)	5154(2)	22(1)
C(17)	5600(3)	6520(2)	5464(2)	21(1)

C(18)	6851(3)	6667(2)	6024(2)	22(1)
C(19)	7848(3)	6278(2)	6438(3)	25(1)
C(20)	8923(3)	6565(2)	7013(3)	26(1)
C(21)	9017(3)	7229(2)	7193(3)	26(1)
C(22)	8029(3)	7616(2)	6813(2)	24(1)
C(23)	6939(3)	7334(2)	6219(2)	22(1)
C(24)	5743(3)	7591(2)	5772(2)	21(1)
C(25)	3879(3)	7678(2)	3285(2)	26(1)
C(26)	4867(3)	7489(2)	3159(3)	38(1)
C(27)	5485(4)	7929(3)	2879(3)	54(1)
C(28)	5116(5)	8554(3)	2706(3)	63(2)
C(29)	4129(5)	8737(2)	2811(3)	59(1)
C(30)	3484(4)	8299(2)	3097(3)	41(1)
B(1)	3722(3)	7151(2)	4679(3)	23(1)
Cl(1S)	2915(6)	9763(3)	4147(5)	69(2)
C(1S)	2305(9)	10307(4)	4680(9)	53(3)
C(2S)	1467(9)	10106(4)	5002(9)	52(3)
C(3S)	953(8)	10545(5)	5406(8)	56(3)
C(4S)	1277(9)	11184(5)	5488(9)	56(3)
C(5S)	2115(9)	11385(4)	5166(9)	61(3)
C(6S)	2630(9)	10947(4)	4762(8)	47(3)
C(7S)	1116(8)	12474(3)	5331(6)	80(3)
C(8S)	1285(4)	11756(2)	5620(4)	32(1)
C(9S)	1593(7)	11317(4)	5023(6)	64(2)
C(10S)	1583(9)	10648(4)	5271(6)	84(3)
C(11S)	1941(7)	10159(5)	4667(7)	84(3)
C(12S)	3120(9)	10387(5)	4674(8)	95(3)
C(13S)	3536(17)	9880(7)	4163(12)	135(6)

Table S 33. Bond lengths [\AA] and angles [$^\circ$] for **PhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087094)**.

Cl(1)-C(4)	1.733(3)
Cl(2)-C(5)	1.733(3)
Cl(3)-C(12)	1.730(3)
Cl(4)-C(13)	1.734(4)
Cl(5)-C(20)	1.727(3)
Cl(6)-C(21)	1.721(3)
O(1)-C(25)	1.379(4)
O(1)-B(1)	1.434(4)
N(1)-C(8)	1.366(4)
N(1)-C(1)	1.371(4)
N(1)-B(1)	1.504(4)
N(2)-C(8)	1.343(4)
N(2)-C(9)	1.352(4)
N(3)-C(9)	1.363(4)
N(3)-C(16)	1.370(4)
N(3)-B(1)	1.494(5)
N(4)-C(17)	1.342(4)
N(4)-C(16)	1.344(4)
N(5)-C(24)	1.360(4)
N(5)-C(17)	1.362(4)
N(5)-B(1)	1.500(4)
N(6)-C(24)	1.340(4)
N(6)-C(1)	1.341(4)
C(1)-C(2)	1.454(5)
C(2)-C(3)	1.390(5)
C(2)-C(7)	1.417(5)
C(3)-C(4)	1.380(5)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.395(5)
C(5)-C(6)	1.384(5)
C(6)-C(7)	1.389(5)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.455(5)
C(9)-C(10)	1.448(5)
C(10)-C(11)	1.386(5)
C(10)-C(15)	1.422(5)
C(11)-C(12)	1.387(5)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.400(5)
C(13)-C(14)	1.379(5)
C(14)-C(15)	1.391(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.452(5)
C(17)-C(18)	1.459(4)
C(18)-C(19)	1.395(5)
C(18)-C(23)	1.421(5)
C(19)-C(20)	1.381(5)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.411(5)
C(21)-C(22)	1.383(5)
C(22)-C(23)	1.396(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.458(4)
C(25)-C(30)	1.376(5)
C(25)-C(26)	1.389(5)
C(26)-C(27)	1.376(6)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.377(8)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.368(8)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.400(6)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
Cl(1S)-C(1S)	1.732(11)
C(1S)-C(2S)	1.3900
C(1S)-C(6S)	1.3900
C(2S)-C(3S)	1.3900

C(2S)-H(2SA)	0.9500
C(3S)-C(4S)	1.3900
C(3S)-H(3SA)	0.9500
C(4S)-C(5S)	1.3900
C(4S)-H(4SA)	0.9500
C(5S)-C(6S)	1.3900
C(5S)-H(5SA)	0.9500
C(6S)-H(6SA)	0.9500
C(7S)-C(8S)	1.551(7)
C(7S)-H(7SA)	0.9800
C(7S)-H(7SB)	0.9800
C(7S)-H(7SC)	0.9800
C(8S)-C(9S)	1.427(9)
C(8S)-H(8SA)	0.9900
C(8S)-H(8SB)	0.9900
C(9S)-C(10S)	1.450(12)
C(9S)-H(9SA)	0.9900
C(9S)-H(9SB)	0.9900
C(10S)-C(11S)	1.536(8)
C(10S)-H(10A)	0.9900
C(10S)-H(10B)	0.9900
C(11S)-C(12S)	1.553(8)
C(11S)-H(11B)	0.9900
C(11S)-H(11C)	0.9900
C(12S)-C(13S)	1.511(9)
C(12S)-H(12A)	0.9900
C(12S)-H(12B)	0.9900
C(13S)-H(13A)	0.9800
C(13S)-H(13B)	0.9800
C(13S)-H(13C)	0.9800
C(25)-O(1)-B(1)	116.1(3)
C(8)-N(1)-C(1)	113.0(3)
C(8)-N(1)-B(1)	122.9(3)
C(1)-N(1)-B(1)	122.7(3)
C(8)-N(2)-C(9)	116.9(3)

C(9)-N(3)-C(16)	112.5(3)
C(9)-N(3)-B(1)	123.9(3)
C(16)-N(3)-B(1)	121.9(3)
C(17)-N(4)-C(16)	116.9(3)
C(24)-N(5)-C(17)	113.7(3)
C(24)-N(5)-B(1)	123.3(3)
C(17)-N(5)-B(1)	122.4(3)
C(24)-N(6)-C(1)	116.2(3)
N(6)-C(1)-N(1)	123.1(3)
N(6)-C(1)-C(2)	129.8(3)
N(1)-C(1)-C(2)	105.2(3)
C(3)-C(2)-C(7)	120.7(3)
C(3)-C(2)-C(1)	131.3(3)
C(7)-C(2)-C(1)	107.6(3)
C(4)-C(3)-C(2)	117.9(3)
C(4)-C(3)-H(3A)	121.1
C(2)-C(3)-H(3A)	121.1
C(3)-C(4)-C(5)	121.5(3)
C(3)-C(4)-Cl(1)	118.4(3)
C(5)-C(4)-Cl(1)	120.1(3)
C(6)-C(5)-C(4)	121.4(3)
C(6)-C(5)-Cl(2)	118.8(3)
C(4)-C(5)-Cl(2)	119.8(3)
C(5)-C(6)-C(7)	117.8(3)
C(5)-C(6)-H(6A)	121.1
C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.7(3)
C(6)-C(7)-C(8)	131.9(3)
C(2)-C(7)-C(8)	107.1(3)
N(2)-C(8)-N(1)	123.0(3)
N(2)-C(8)-C(7)	129.6(3)
N(1)-C(8)-C(7)	105.6(3)
N(2)-C(9)-N(3)	122.4(3)
N(2)-C(9)-C(10)	129.4(3)
N(3)-C(9)-C(10)	106.3(3)
C(11)-C(10)-C(15)	120.5(3)

C(11)-C(10)-C(9)	132.1(3)
C(15)-C(10)-C(9)	107.0(3)
C(10)-C(11)-C(12)	118.3(3)
C(10)-C(11)-H(11A)	120.8
C(12)-C(11)-H(11A)	120.8
C(11)-C(12)-C(13)	120.8(3)
C(11)-C(12)-Cl(3)	119.3(3)
C(13)-C(12)-Cl(3)	119.9(3)
C(14)-C(13)-C(12)	121.9(3)
C(14)-C(13)-Cl(4)	118.2(3)
C(12)-C(13)-Cl(4)	119.9(3)
C(13)-C(14)-C(15)	117.7(3)
C(13)-C(14)-H(14A)	121.1
C(15)-C(14)-H(14A)	121.1
C(14)-C(15)-C(10)	120.8(3)
C(14)-C(15)-C(16)	131.7(3)
C(10)-C(15)-C(16)	107.1(3)
N(4)-C(16)-N(3)	122.9(3)
N(4)-C(16)-C(15)	129.0(3)
N(3)-C(16)-C(15)	105.8(3)
N(4)-C(17)-N(5)	122.5(3)
N(4)-C(17)-C(18)	130.1(3)
N(5)-C(17)-C(18)	105.7(3)
C(19)-C(18)-C(23)	120.7(3)
C(19)-C(18)-C(17)	132.0(3)
C(23)-C(18)-C(17)	106.9(3)
C(20)-C(19)-C(18)	118.0(3)
C(20)-C(19)-H(19A)	121.0
C(18)-C(19)-H(19A)	121.0
C(19)-C(20)-C(21)	121.5(3)
C(19)-C(20)-Cl(5)	118.3(3)
C(21)-C(20)-Cl(5)	120.2(3)
C(22)-C(21)-C(20)	121.0(3)
C(22)-C(21)-Cl(6)	119.3(3)
C(20)-C(21)-Cl(6)	119.7(3)
C(21)-C(22)-C(23)	118.2(3)

C(21)-C(22)-H(22A)	120.9
C(23)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	120.6(3)
C(22)-C(23)-C(24)	131.9(3)
C(18)-C(23)-C(24)	107.3(3)
N(6)-C(24)-N(5)	123.1(3)
N(6)-C(24)-C(23)	129.7(3)
N(5)-C(24)-C(23)	105.5(3)
C(30)-C(25)-O(1)	120.4(3)
C(30)-C(25)-C(26)	120.6(4)
O(1)-C(25)-C(26)	119.0(3)
C(27)-C(26)-C(25)	120.0(4)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(26)-C(27)-C(28)	120.1(5)
C(26)-C(27)-H(27A)	119.9
C(28)-C(27)-H(27A)	119.9
C(29)-C(28)-C(27)	119.7(4)
C(29)-C(28)-H(28A)	120.1
C(27)-C(28)-H(28A)	120.1
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(25)-C(30)-C(29)	118.3(4)
C(25)-C(30)-H(30A)	120.9
C(29)-C(30)-H(30A)	120.9
O(1)-B(1)-N(3)	111.8(3)
O(1)-B(1)-N(5)	115.8(3)
N(3)-B(1)-N(5)	104.0(3)
O(1)-B(1)-N(1)	117.0(3)
N(3)-B(1)-N(1)	104.0(3)
N(5)-B(1)-N(1)	102.7(3)
C(2S)-C(1S)-C(6S)	120.0
C(2S)-C(1S)-Cl(1S)	119.8(3)
C(6S)-C(1S)-Cl(1S)	120.2(3)
C(3S)-C(2S)-C(1S)	120.0

C(3S)-C(2S)-H(2SA)	120.0
C(1S)-C(2S)-H(2SA)	120.0
C(4S)-C(3S)-C(2S)	120.0
C(4S)-C(3S)-H(3SA)	120.0
C(2S)-C(3S)-H(3SA)	120.0
C(5S)-C(4S)-C(3S)	120.0
C(5S)-C(4S)-H(4SA)	120.0
C(3S)-C(4S)-H(4SA)	120.0
C(4S)-C(5S)-C(6S)	120.0
C(4S)-C(5S)-H(5SA)	120.0
C(6S)-C(5S)-H(5SA)	120.0
C(5S)-C(6S)-C(1S)	120.0
C(5S)-C(6S)-H(6SA)	120.0
C(1S)-C(6S)-H(6SA)	120.0
C(8S)-C(7S)-H(7SA)	109.5
C(8S)-C(7S)-H(7SB)	109.5
H(7SA)-C(7S)-H(7SB)	109.5
C(8S)-C(7S)-H(7SC)	109.5
H(7SA)-C(7S)-H(7SC)	109.5
H(7SB)-C(7S)-H(7SC)	109.5
C(9S)-C(8S)-C(7S)	120.0(6)
C(9S)-C(8S)-H(8SA)	107.3
C(7S)-C(8S)-H(8SA)	107.3
C(9S)-C(8S)-H(8SB)	107.3
C(7S)-C(8S)-H(8SB)	107.3
H(8SA)-C(8S)-H(8SB)	106.9
C(8S)-C(9S)-C(10S)	115.9(7)
C(8S)-C(9S)-H(9SA)	108.3
C(10S)-C(9S)-H(9SA)	108.3
C(8S)-C(9S)-H(9SB)	108.3
C(10S)-C(9S)-H(9SB)	108.3
H(9SA)-C(9S)-H(9SB)	107.4
C(9S)-C(10S)-C(11S)	117.8(8)
C(9S)-C(10S)-H(10A)	107.9
C(11S)-C(10S)-H(10A)	107.9
C(9S)-C(10S)-H(10B)	107.9

C(11S)-C(10S)-H(10B)	107.9
H(10A)-C(10S)-H(10B)	107.2
C(10S)-C(11S)-C(12S)	107.8(7)
C(10S)-C(11S)-H(11B)	110.1
C(12S)-C(11S)-H(11B)	110.1
C(10S)-C(11S)-H(11C)	110.1
C(12S)-C(11S)-H(11C)	110.1
H(11B)-C(11S)-H(11C)	108.5
C(13S)-C(12S)-C(11S)	108.2(10)
C(13S)-C(12S)-H(12A)	110.1
C(11S)-C(12S)-H(12A)	110.1
C(13S)-C(12S)-H(12B)	110.1
C(11S)-C(12S)-H(12B)	110.1
H(12A)-C(12S)-H(12B)	108.4
C(12S)-C(13S)-H(13A)	109.5
C(12S)-C(13S)-H(13B)	109.5
H(13A)-C(13S)-H(13B)	109.5
C(12S)-C(13S)-H(13C)	109.5
H(13A)-C(13S)-H(13C)	109.5
H(13B)-C(13S)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S 34. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087094)**. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	39(1)	28(1)	36(1)	-8(1)	18(1)	3(1)
Cl(2)	43(1)	40(1)	48(1)	-8(1)	31(1)	4(1)
Cl(3)	35(1)	40(1)	45(1)	2(1)	26(1)	-7(1)
Cl(4)	49(1)	29(1)	69(1)	10(1)	37(1)	2(1)
Cl(5)	24(1)	42(1)	47(1)	4(1)	14(1)	8(1)
Cl(6)	25(1)	45(1)	40(1)	-2(1)	6(1)	-8(1)
O(1)	24(1)	31(1)	19(1)	-3(1)	8(1)	-4(1)
N(1)	21(1)	25(1)	20(1)	-2(1)	9(1)	1(1)
N(2)	20(1)	27(2)	23(1)	0(1)	9(1)	3(1)
N(3)	18(1)	25(1)	22(1)	-4(1)	10(1)	-2(1)
N(4)	24(1)	23(1)	24(1)	-4(1)	15(1)	-1(1)
N(5)	20(1)	22(1)	21(1)	-2(1)	11(1)	0(1)
N(6)	24(2)	23(1)	25(1)	1(1)	13(1)	1(1)
C(1)	27(2)	22(2)	18(2)	0(1)	9(1)	0(1)
C(2)	25(2)	23(2)	24(2)	2(1)	10(1)	2(1)
C(3)	28(2)	24(2)	25(2)	1(1)	12(2)	5(1)
C(4)	33(2)	22(2)	22(2)	1(1)	10(2)	5(1)
C(5)	30(2)	28(2)	25(2)	2(1)	15(2)	7(1)
C(6)	27(2)	29(2)	25(2)	2(1)	12(2)	3(1)
C(7)	22(2)	24(2)	22(2)	3(1)	8(1)	7(1)
C(8)	19(2)	27(2)	21(2)	-1(1)	6(1)	3(1)
C(9)	18(2)	30(2)	19(2)	-3(1)	6(1)	-1(1)
C(10)	20(2)	27(2)	22(2)	-4(1)	10(1)	-2(1)
C(11)	23(2)	31(2)	26(2)	-4(2)	12(1)	-2(1)
C(12)	24(2)	33(2)	25(2)	-4(2)	12(2)	-7(2)
C(13)	30(2)	27(2)	31(2)	-2(2)	15(2)	-4(1)
C(14)	24(2)	27(2)	28(2)	-6(1)	12(2)	-2(1)
C(15)	22(2)	24(2)	22(2)	-7(1)	10(1)	-5(1)
C(16)	25(2)	23(2)	21(2)	-4(1)	11(1)	-1(1)

C(17)	24(2)	23(2)	20(2)	-2(1)	13(1)	-1(1)
C(18)	22(2)	27(2)	20(2)	-2(1)	12(1)	-4(1)
C(19)	27(2)	25(2)	28(2)	-1(1)	17(2)	-1(1)
C(20)	24(2)	31(2)	26(2)	3(1)	14(2)	1(1)
C(21)	23(2)	35(2)	22(2)	1(1)	10(1)	-6(1)
C(22)	24(2)	26(2)	23(2)	-1(1)	11(1)	-3(1)
C(23)	24(2)	25(2)	24(2)	0(1)	16(1)	1(1)
C(24)	23(2)	22(2)	19(2)	-3(1)	11(1)	-3(1)
C(25)	26(2)	34(2)	14(2)	-1(1)	6(1)	-5(1)
C(26)	36(2)	60(3)	22(2)	-10(2)	16(2)	-8(2)
C(27)	52(3)	89(4)	30(2)	-11(2)	26(2)	-26(3)
C(28)	73(4)	86(4)	26(2)	5(2)	17(2)	-44(3)
C(29)	81(4)	44(3)	31(2)	13(2)	5(2)	-18(2)
C(30)	43(2)	38(2)	29(2)	6(2)	3(2)	0(2)
B(1)	21(2)	25(2)	22(2)	-1(2)	10(2)	0(2)
Cl(1S)	74(4)	67(3)	58(3)	13(2)	21(3)	11(3)
C(1S)	43(5)	74(6)	42(4)	32(4)	19(4)	-6(4)
C(2S)	41(5)	77(6)	41(5)	33(4)	20(4)	-10(4)
C(3S)	42(5)	84(6)	43(5)	27(5)	18(4)	-6(5)
C(4S)	40(5)	87(6)	41(5)	28(5)	18(4)	-5(5)
C(5S)	46(5)	81(6)	43(5)	28(5)	8(4)	-8(5)
C(6S)	38(5)	72(6)	35(5)	31(4)	20(4)	-3(4)
C(7S)	93(6)	100(5)	63(5)	-28(4)	47(5)	-32(5)
C(8S)	29(3)	49(3)	13(2)	-12(2)	5(2)	-26(2)
C(9S)	54(5)	96(5)	40(4)	-20(4)	18(4)	-35(4)
C(10S)	110(8)	96(5)	44(4)	16(4)	32(5)	24(6)
C(11S)	68(5)	93(6)	50(5)	-5(5)	-13(4)	14(5)
C(12S)	94(7)	120(8)	79(6)	-21(6)	45(6)	2(6)
C(13S)	188(17)	111(11)	117(11)	-1(9)	78(13)	31(11)

Table S 35. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc** (**Chlorobenzene:Heptane; CCDC deposit 2087094**).

	x	y	z	U(eq)
H(3A)	4606	9293	6931	30
H(6A)	1063	8213	6350	32
H(11A)	860	5816	5851	31
H(14A)	4001	4665	5656	31
H(19A)	7790	5830	6327	30
H(22A)	8090	8061	6954	29
H(26A)	5115	7056	3266	46
H(27A)	6169	7800	2805	65
H(28A)	5544	8858	2515	76
H(29A)	3876	9169	2688	71
H(30A)	2793	8426	3159	50
H(2SA)	1245	9669	4946	62
H(3SA)	380	10407	5626	67
H(4SA)	926	11484	5764	67
H(5SA)	2337	11822	5222	73
H(6SA)	3203	11084	4542	56
H(7SA)	908	12705	5816	121
H(7SB)	1850	12647	5353	121
H(7SC)	482	12522	4640	121
H(8SA)	1902	11726	6331	38
H(8SB)	542	11602	5623	38
H(9SA)	2392	11427	5098	77
H(9SB)	1040	11379	4296	77
H(10A)	777	10539	5180	100
H(10B)	2117	10592	6004	100
H(11B)	1322	10130	3956	101
H(11C)	2043	9732	4986	101
H(12A)	3000	10796	4302	114
H(12B)	3718	10453	5385	114

H(13A)	4281	10015	4160	202
H(13B)	3656	9478	4538	202
H(13C)	2941	9819	3459	202

Table S 36. Torsion angles [°] for **PhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087094)**.

C(24)-N(6)-C(1)-N(1)	-7.9(4)
C(24)-N(6)-C(1)-C(2)	154.0(3)
C(8)-N(1)-C(1)-N(6)	153.2(3)
B(1)-N(1)-C(1)-N(6)	-14.1(5)
C(8)-N(1)-C(1)-C(2)	-12.4(4)
B(1)-N(1)-C(1)-C(2)	-179.7(3)
N(6)-C(1)-C(2)-C(3)	15.3(6)
N(1)-C(1)-C(2)-C(3)	179.7(3)
N(6)-C(1)-C(2)-C(7)	-157.1(3)
N(1)-C(1)-C(2)-C(7)	7.2(3)
C(7)-C(2)-C(3)-C(4)	-1.5(5)
C(1)-C(2)-C(3)-C(4)	-173.1(3)
C(2)-C(3)-C(4)-C(5)	0.1(5)
C(2)-C(3)-C(4)-Cl(1)	178.7(2)
C(3)-C(4)-C(5)-C(6)	1.6(5)
Cl(1)-C(4)-C(5)-C(6)	-176.9(3)
C(3)-C(4)-C(5)-Cl(2)	180.0(3)
Cl(1)-C(4)-C(5)-Cl(2)	1.5(4)
C(4)-C(5)-C(6)-C(7)	-1.9(5)
Cl(2)-C(5)-C(6)-C(7)	179.7(3)
C(5)-C(6)-C(7)-C(2)	0.5(5)
C(5)-C(6)-C(7)-C(8)	173.8(3)
C(3)-C(2)-C(7)-C(6)	1.2(5)
C(1)-C(2)-C(7)-C(6)	174.6(3)
C(3)-C(2)-C(7)-C(8)	-173.6(3)
C(1)-C(2)-C(7)-C(8)	-0.2(4)
C(9)-N(2)-C(8)-N(1)	7.1(5)
C(9)-N(2)-C(8)-C(7)	-155.2(3)
C(1)-N(1)-C(8)-N(2)	-153.5(3)
B(1)-N(1)-C(8)-N(2)	13.8(5)
C(1)-N(1)-C(8)-C(7)	12.4(4)
B(1)-N(1)-C(8)-C(7)	179.6(3)
C(6)-C(7)-C(8)-N(2)	-16.4(6)

C(2)-C(7)-C(8)-N(2)	157.6(3)
C(6)-C(7)-C(8)-N(1)	179.0(3)
C(2)-C(7)-C(8)-N(1)	-7.0(4)
C(8)-N(2)-C(9)-N(3)	-8.9(5)
C(8)-N(2)-C(9)-C(10)	153.7(3)
C(16)-N(3)-C(9)-N(2)	155.2(3)
B(1)-N(3)-C(9)-N(2)	-10.3(5)
C(16)-N(3)-C(9)-C(10)	-10.8(4)
B(1)-N(3)-C(9)-C(10)	-176.3(3)
N(2)-C(9)-C(10)-C(11)	13.0(6)
N(3)-C(9)-C(10)-C(11)	177.7(3)
N(2)-C(9)-C(10)-C(15)	-159.3(3)
N(3)-C(9)-C(10)-C(15)	5.4(3)
C(15)-C(10)-C(11)-C(12)	-0.9(5)
C(9)-C(10)-C(11)-C(12)	-172.4(3)
C(10)-C(11)-C(12)-C(13)	0.2(5)
C(10)-C(11)-C(12)-Cl(3)	178.9(3)
C(11)-C(12)-C(13)-C(14)	0.3(5)
Cl(3)-C(12)-C(13)-C(14)	-178.4(3)
C(11)-C(12)-C(13)-Cl(4)	179.1(3)
Cl(3)-C(12)-C(13)-Cl(4)	0.4(4)
C(12)-C(13)-C(14)-C(15)	-0.1(5)
Cl(4)-C(13)-C(14)-C(15)	-178.9(3)
C(13)-C(14)-C(15)-C(10)	-0.6(5)
C(13)-C(14)-C(15)-C(16)	170.6(3)
C(11)-C(10)-C(15)-C(14)	1.2(5)
C(9)-C(10)-C(15)-C(14)	174.6(3)
C(11)-C(10)-C(15)-C(16)	-172.0(3)
C(9)-C(10)-C(15)-C(16)	1.3(4)
C(17)-N(4)-C(16)-N(3)	9.4(4)
C(17)-N(4)-C(16)-C(15)	-151.0(3)
C(9)-N(3)-C(16)-N(4)	-152.7(3)
B(1)-N(3)-C(16)-N(4)	13.2(5)
C(9)-N(3)-C(16)-C(15)	11.6(4)
B(1)-N(3)-C(16)-C(15)	177.4(3)
C(14)-C(15)-C(16)-N(4)	-16.7(6)

C(10)-C(15)-C(16)-N(4)	155.4(3)
C(14)-C(15)-C(16)-N(3)	-179.7(3)
C(10)-C(15)-C(16)-N(3)	-7.5(3)
C(16)-N(4)-C(17)-N(5)	-8.6(4)
C(16)-N(4)-C(17)-C(18)	154.4(3)
C(24)-N(5)-C(17)-N(4)	156.6(3)
B(1)-N(5)-C(17)-N(4)	-14.8(5)
C(24)-N(5)-C(17)-C(18)	-10.0(3)
B(1)-N(5)-C(17)-C(18)	178.7(3)
N(4)-C(17)-C(18)-C(19)	13.9(6)
N(5)-C(17)-C(18)-C(19)	179.0(3)
N(4)-C(17)-C(18)-C(23)	-159.3(3)
N(5)-C(17)-C(18)-C(23)	5.9(3)
C(23)-C(18)-C(19)-C(20)	-2.0(5)
C(17)-C(18)-C(19)-C(20)	-174.3(3)
C(18)-C(19)-C(20)-C(21)	0.8(5)
C(18)-C(19)-C(20)-Cl(5)	178.9(2)
C(19)-C(20)-C(21)-C(22)	1.2(5)
Cl(5)-C(20)-C(21)-C(22)	-176.8(3)
C(19)-C(20)-C(21)-Cl(6)	-177.8(3)
Cl(5)-C(20)-C(21)-Cl(6)	4.2(4)
C(20)-C(21)-C(22)-C(23)	-2.1(5)
Cl(6)-C(21)-C(22)-C(23)	176.9(2)
C(21)-C(22)-C(23)-C(18)	0.9(5)
C(21)-C(22)-C(23)-C(24)	175.1(3)
C(19)-C(18)-C(23)-C(22)	1.1(5)
C(17)-C(18)-C(23)-C(22)	175.2(3)
C(19)-C(18)-C(23)-C(24)	-174.4(3)
C(17)-C(18)-C(23)-C(24)	-0.3(3)
C(1)-N(6)-C(24)-N(5)	7.8(4)
C(1)-N(6)-C(24)-C(23)	-155.3(3)
C(17)-N(5)-C(24)-N(6)	-156.8(3)
B(1)-N(5)-C(24)-N(6)	14.4(5)
C(17)-N(5)-C(24)-C(23)	9.8(3)
B(1)-N(5)-C(24)-C(23)	-178.9(3)
C(22)-C(23)-C(24)-N(6)	-14.8(6)

C(18)-C(23)-C(24)-N(6)	160.0(3)
C(22)-C(23)-C(24)-N(5)	179.8(3)
C(18)-C(23)-C(24)-N(5)	-5.4(3)
B(1)-O(1)-C(25)-C(30)	-93.1(4)
B(1)-O(1)-C(25)-C(26)	87.3(4)
C(30)-C(25)-C(26)-C(27)	2.4(5)
O(1)-C(25)-C(26)-C(27)	-178.0(3)
C(25)-C(26)-C(27)-C(28)	-1.1(6)
C(26)-C(27)-C(28)-C(29)	-0.2(7)
C(27)-C(28)-C(29)-C(30)	0.3(7)
O(1)-C(25)-C(30)-C(29)	178.2(3)
C(26)-C(25)-C(30)-C(29)	-2.2(5)
C(28)-C(29)-C(30)-C(25)	0.9(6)
C(25)-O(1)-B(1)-N(3)	-165.0(3)
C(25)-O(1)-B(1)-N(5)	-46.1(4)
C(25)-O(1)-B(1)-N(1)	75.3(4)
C(9)-N(3)-B(1)-O(1)	-101.0(3)
C(16)-N(3)-B(1)-O(1)	94.8(4)
C(9)-N(3)-B(1)-N(5)	133.4(3)
C(16)-N(3)-B(1)-N(5)	-30.9(4)
C(9)-N(3)-B(1)-N(1)	26.1(4)
C(16)-N(3)-B(1)-N(1)	-138.1(3)
C(24)-N(5)-B(1)-O(1)	98.2(4)
C(17)-N(5)-B(1)-O(1)	-91.3(4)
C(24)-N(5)-B(1)-N(3)	-138.7(3)
C(17)-N(5)-B(1)-N(3)	31.8(4)
C(24)-N(5)-B(1)-N(1)	-30.5(4)
C(17)-N(5)-B(1)-N(1)	140.0(3)
C(8)-N(1)-B(1)-O(1)	96.2(4)
C(1)-N(1)-B(1)-O(1)	-97.8(4)
C(8)-N(1)-B(1)-N(3)	-27.7(4)
C(1)-N(1)-B(1)-N(3)	138.4(3)
C(8)-N(1)-B(1)-N(5)	-135.8(3)
C(1)-N(1)-B(1)-N(5)	30.2(4)
C(6S)-C(1S)-C(2S)-C(3S)	0.0
Cl(1S)-C(1S)-C(2S)-C(3S)	-178.3(9)

C(1S)-C(2S)-C(3S)-C(4S)	0.0
C(2S)-C(3S)-C(4S)-C(5S)	0.0
C(3S)-C(4S)-C(5S)-C(6S)	0.0
C(4S)-C(5S)-C(6S)-C(1S)	0.0
C(2S)-C(1S)-C(6S)-C(5S)	0.0
Cl(1S)-C(1S)-C(6S)-C(5S)	178.3(9)
C(7S)-C(8S)-C(9S)-C(10S)	-172.4(7)
C(8S)-C(9S)-C(10S)-C(11S)	-178.4(7)
C(9S)-C(10S)-C(11S)-C(12S)	49.3(11)
C(10S)-C(11S)-C(12S)-C(13S)	175.0(9)

Symmetry transformations used to generate equivalent atoms:

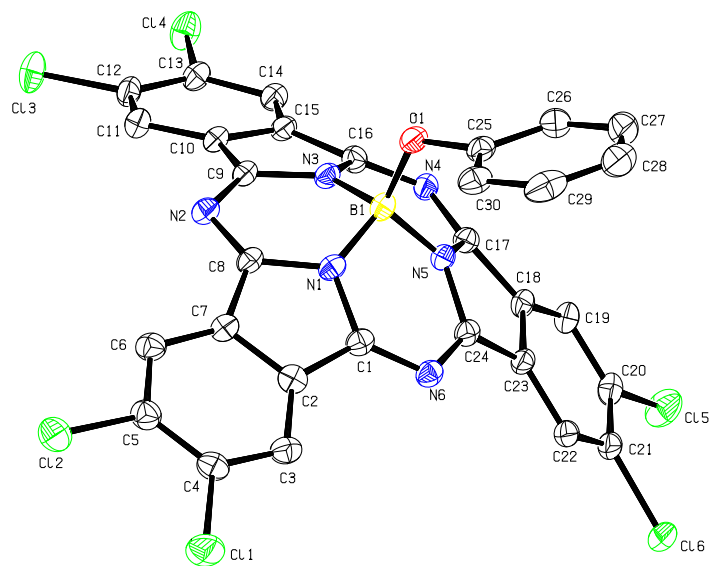


Figure S19: Anisotropic displacement ellipsoid plot of **PhO-Cl₆BsubPc** (Dichlorobenzene: Pentane; CCDC deposit 2087095).

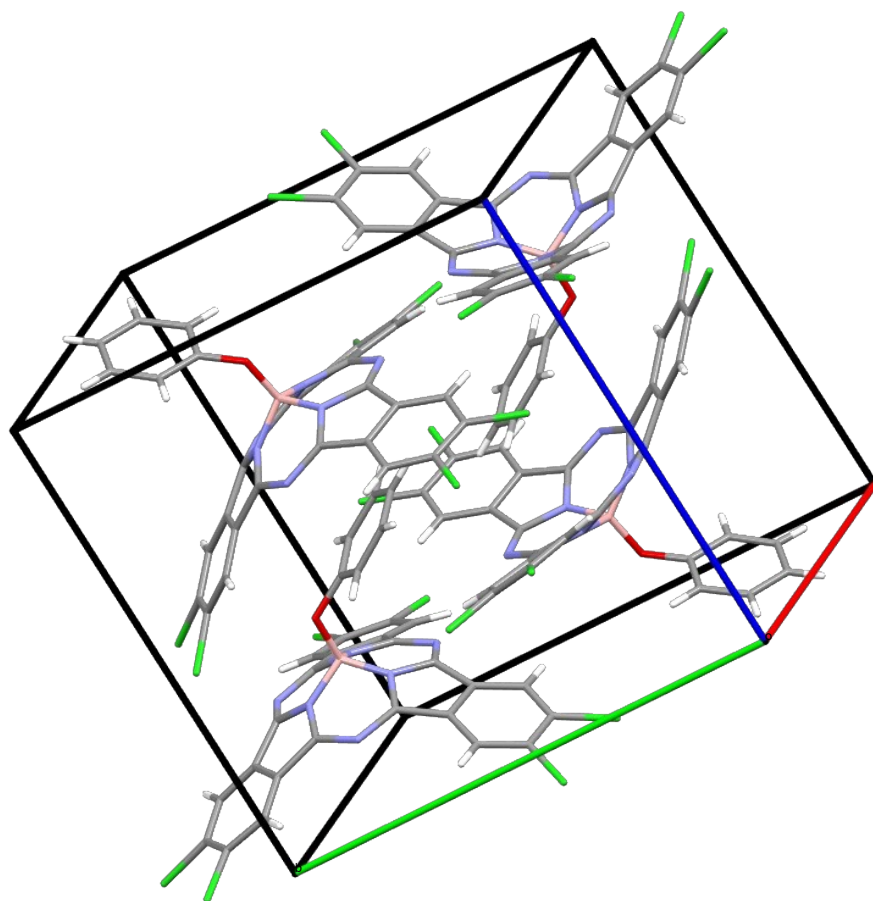


Figure S20: Populated unit cell of PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095).

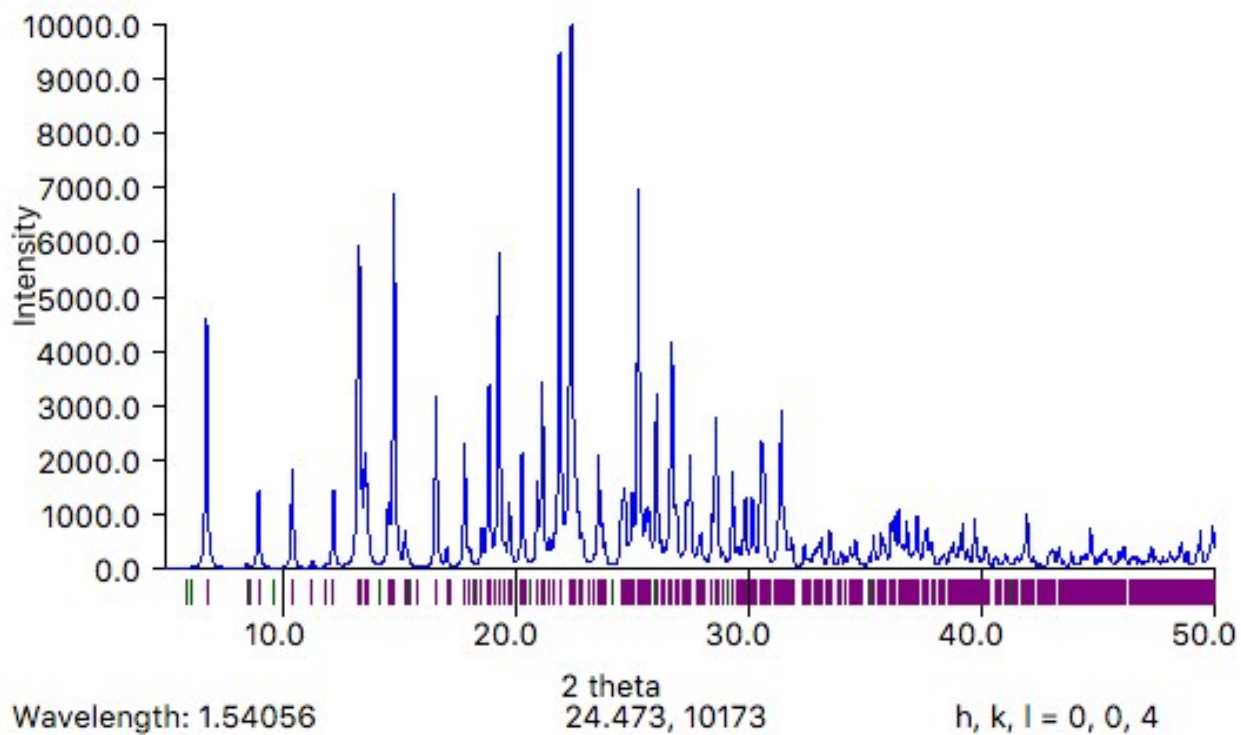


Figure S 21: Powder x-ray diffraction **PhO-Cl₆BsubPc** (Dichlorobenzene:Pentane; CCDC deposit 2087095).

Table S 37. Crystal data and structure refinement for **PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095)**.

Identification code	d2026	
Empirical formula	C ₃₀ H ₁₁ B Cl ₆ N ₆ O	
Formula weight	694.96	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 13.1340(6) Å	α = 90°.
	b = 14.9016(6) Å	β = 96.515(3)°.
	c = 14.5799(7) Å	γ = 90°.
Volume	2835.1(2) Å ³	
Z	4	
Density (calculated)	1.628 Mg/m ³	
Absorption coefficient	5.859 mm ⁻¹	
F(000)	1392	
Crystal size	0.290 x 0.240 x 0.010 mm ³	
Theta range for data collection	3.387 to 65.118°.	
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -17 ≤ l ≤ 16	
Reflections collected	37982	
Independent reflections	4780 [R(int) = 0.1239]	
Completeness to theta = 65.118°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7526 and 0.5026	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4780 / 0 / 398	
Goodness-of-fit on F ²	1.042	
Final R indices [I > 2σ(I)]	R1 = 0.0550, wR2 = 0.1289	
R indices (all data)	R1 = 0.0806, wR2 = 0.1437	
Extinction coefficient	0.0035(3)	
Largest diff. peak and hole	0.679 and -0.427 e.Å ⁻³	

Table S 38. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	9471(1)	6746(1)	6932(1)	65(1)
Cl(2)	9088(1)	4692(1)	7285(1)	58(1)
Cl(3)	1846(1)	2143(1)	5613(1)	54(1)
Cl(4)	-138(1)	3344(1)	5319(1)	52(1)
Cl(5)	1102(1)	9909(1)	4090(1)	62(1)
Cl(6)	3359(1)	10668(1)	4341(1)	47(1)
O(1)	3590(2)	6737(1)	8581(2)	38(1)
N(1)	4865(2)	6474(2)	7461(2)	32(1)
N(2)	4650(2)	4895(2)	7283(2)	35(1)
N(3)	3213(2)	5865(2)	7208(2)	32(1)
N(4)	1874(2)	6754(2)	6436(2)	33(1)
N(5)	3469(2)	7416(2)	7007(2)	32(1)
N(6)	5167(2)	7913(2)	6846(2)	34(1)
C(1)	5510(3)	7117(2)	7175(2)	35(1)
C(2)	6494(3)	6666(2)	7146(2)	38(1)
C(3)	7455(3)	6975(2)	6984(3)	42(1)
C(4)	8258(3)	6367(3)	7049(3)	43(1)
C(5)	8090(3)	5452(3)	7204(3)	44(1)
C(6)	7124(3)	5134(2)	7304(2)	40(1)
C(7)	6326(3)	5741(2)	7293(2)	34(1)
C(8)	5250(3)	5626(2)	7410(2)	33(1)
C(9)	3640(3)	5038(2)	7128(2)	32(1)
C(10)	2816(3)	4487(2)	6679(2)	33(1)
C(11)	2792(3)	3589(2)	6406(2)	38(1)
C(12)	1886(3)	3251(2)	5969(2)	38(1)
C(13)	1015(3)	3790(2)	5801(2)	38(1)
C(14)	1050(3)	4699(2)	6014(2)	36(1)
C(15)	1952(3)	5044(2)	6457(2)	33(1)
C(16)	2258(3)	5956(2)	6734(2)	34(1)
C(17)	2517(3)	7460(2)	6522(2)	32(1)

C(18)	2510(3)	8274(2)	5976(2)	32(1)
C(19)	1760(3)	8677(2)	5362(2)	38(1)
C(20)	2026(3)	9420(2)	4871(2)	40(1)
C(21)	3023(3)	9755(2)	4989(2)	37(1)
C(22)	3787(3)	9369(2)	5588(2)	35(1)
C(23)	3524(3)	8623(2)	6091(2)	32(1)
C(24)	4142(3)	8027(2)	6712(2)	32(1)
C(25)	3796(3)	7524(2)	9050(2)	38(1)
C(26)	2989(3)	8113(3)	9132(3)	49(1)
C(27)	3168(4)	8886(3)	9632(3)	64(1)
C(28)	4125(5)	9091(3)	10035(3)	71(2)
C(29)	4936(4)	8518(3)	9961(3)	62(1)
C(30)	4767(3)	7712(3)	9463(3)	46(1)
B(1)	3788(3)	6653(2)	7637(3)	34(1)

Table S 39. Bond lengths [\AA] and angles [$^\circ$] for **PhO-Cl₆BsubPc (Dichlorobenzene: Pentane; CCDC deposit 2087095)**.

Cl(1)-C(4)	1.716(4)
Cl(2)-C(5)	1.725(4)
Cl(3)-C(12)	1.730(3)
Cl(4)-C(13)	1.729(4)
Cl(5)-C(20)	1.729(4)
Cl(6)-C(21)	1.741(3)
O(1)-C(25)	1.369(4)
O(1)-B(1)	1.435(5)
N(1)-C(8)	1.366(4)
N(1)-C(1)	1.374(4)
N(1)-B(1)	1.490(5)
N(2)-C(9)	1.338(4)
N(2)-C(8)	1.345(4)
N(3)-C(9)	1.364(4)
N(3)-C(16)	1.368(4)
N(3)-B(1)	1.494(5)
N(4)-C(16)	1.344(4)
N(4)-C(17)	1.346(4)
N(5)-C(17)	1.367(4)
N(5)-C(24)	1.372(4)
N(5)-B(1)	1.491(5)
N(6)-C(1)	1.339(4)
N(6)-C(24)	1.348(4)
C(1)-C(2)	1.460(5)
C(2)-C(3)	1.389(5)
C(2)-C(7)	1.416(5)
C(3)-C(4)	1.385(5)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.404(5)
C(5)-C(6)	1.378(5)
C(6)-C(7)	1.384(5)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.452(5)
C(9)-C(10)	1.454(5)
C(10)-C(11)	1.396(5)
C(10)-C(15)	1.414(5)
C(11)-C(12)	1.380(5)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.396(5)
C(13)-C(14)	1.388(5)
C(14)-C(15)	1.383(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.460(4)
C(17)-C(18)	1.451(5)
C(18)-C(19)	1.389(5)
C(18)-C(23)	1.422(5)
C(19)-C(20)	1.386(5)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.393(5)
C(21)-C(22)	1.379(5)
C(22)-C(23)	1.396(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.450(5)
C(25)-C(30)	1.377(5)
C(25)-C(26)	1.392(5)
C(26)-C(27)	1.368(6)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.360(7)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.379(7)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.408(6)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
C(25)-O(1)-B(1)	120.4(3)
C(8)-N(1)-C(1)	112.5(3)
C(8)-N(1)-B(1)	122.6(3)

C(1)-N(1)-B(1)	123.9(3)
C(9)-N(2)-C(8)	116.6(3)
C(9)-N(3)-C(16)	114.1(3)
C(9)-N(3)-B(1)	123.5(3)
C(16)-N(3)-B(1)	121.7(3)
C(16)-N(4)-C(17)	116.9(3)
C(17)-N(5)-C(24)	113.0(3)
C(17)-N(5)-B(1)	122.2(3)
C(24)-N(5)-B(1)	123.6(3)
C(1)-N(6)-C(24)	117.0(3)
N(6)-C(1)-N(1)	122.1(3)
N(6)-C(1)-C(2)	131.3(3)
N(1)-C(1)-C(2)	105.4(3)
C(3)-C(2)-C(7)	120.5(3)
C(3)-C(2)-C(1)	132.6(3)
C(7)-C(2)-C(1)	106.9(3)
C(4)-C(3)-C(2)	118.2(3)
C(4)-C(3)-H(3A)	120.9
C(2)-C(3)-H(3A)	120.9
C(3)-C(4)-C(5)	120.9(3)
C(3)-C(4)-Cl(1)	119.1(3)
C(5)-C(4)-Cl(1)	120.0(3)
C(6)-C(5)-C(4)	121.0(3)
C(6)-C(5)-Cl(2)	117.9(3)
C(4)-C(5)-Cl(2)	121.1(3)
C(5)-C(6)-C(7)	118.6(3)
C(5)-C(6)-H(6A)	120.7
C(7)-C(6)-H(6A)	120.7
C(6)-C(7)-C(2)	120.5(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)	122.8(3)
N(2)-C(8)-C(7)	129.9(3)
N(1)-C(8)-C(7)	105.6(3)
N(2)-C(9)-N(3)	122.7(3)
N(2)-C(9)-C(10)	131.3(3)

N(3)-C(9)-C(10)	104.8(3)
C(11)-C(10)-C(15)	120.4(3)
C(11)-C(10)-C(9)	131.4(3)
C(15)-C(10)-C(9)	108.0(3)
C(12)-C(11)-C(10)	118.2(3)
C(12)-C(11)-H(11A)	120.9
C(10)-C(11)-H(11A)	120.9
C(11)-C(12)-C(13)	121.1(3)
C(11)-C(12)-Cl(3)	118.8(3)
C(13)-C(12)-Cl(3)	120.0(3)
C(14)-C(13)-C(12)	121.1(3)
C(14)-C(13)-Cl(4)	118.1(3)
C(12)-C(13)-Cl(4)	120.8(3)
C(15)-C(14)-C(13)	118.2(3)
C(15)-C(14)-H(14A)	120.9
C(13)-C(14)-H(14A)	120.9
C(14)-C(15)-C(10)	120.7(3)
C(14)-C(15)-C(16)	132.1(3)
C(10)-C(15)-C(16)	107.1(3)
N(4)-C(16)-N(3)	122.6(3)
N(4)-C(16)-C(15)	130.7(3)
N(3)-C(16)-C(15)	104.8(3)
N(4)-C(17)-N(5)	122.5(3)
N(4)-C(17)-C(18)	129.6(3)
N(5)-C(17)-C(18)	105.8(3)
C(19)-C(18)-C(23)	120.3(3)
C(19)-C(18)-C(17)	132.4(3)
C(23)-C(18)-C(17)	107.0(3)
C(20)-C(19)-C(18)	118.4(3)
C(20)-C(19)-H(19A)	120.8
C(18)-C(19)-H(19A)	120.8
C(19)-C(20)-C(21)	120.8(3)
C(19)-C(20)-Cl(5)	118.5(3)
C(21)-C(20)-Cl(5)	120.7(3)
C(22)-C(21)-C(20)	122.3(3)
C(22)-C(21)-Cl(6)	117.3(3)

C(20)-C(21)-Cl(6)	120.3(3)
C(21)-C(22)-C(23)	117.4(3)
C(21)-C(22)-H(22A)	121.3
C(23)-C(22)-H(22A)	121.3
C(22)-C(23)-C(18)	120.8(3)
C(22)-C(23)-C(24)	131.4(3)
C(18)-C(23)-C(24)	107.5(3)
N(6)-C(24)-N(5)	122.7(3)
N(6)-C(24)-C(23)	130.2(3)
N(5)-C(24)-C(23)	105.5(3)
O(1)-C(25)-C(30)	121.0(3)
O(1)-C(25)-C(26)	118.3(3)
C(30)-C(25)-C(26)	120.7(4)
C(27)-C(26)-C(25)	119.4(4)
C(27)-C(26)-H(26A)	120.3
C(25)-C(26)-H(26A)	120.3
C(28)-C(27)-C(26)	120.9(5)
C(28)-C(27)-H(27A)	119.5
C(26)-C(27)-H(27A)	119.5
C(27)-C(28)-C(29)	120.7(4)
C(27)-C(28)-H(28A)	119.6
C(29)-C(28)-H(28A)	119.6
C(28)-C(29)-C(30)	119.4(4)
C(28)-C(29)-H(29A)	120.3
C(30)-C(29)-H(29A)	120.3
C(25)-C(30)-C(29)	118.9(4)
C(25)-C(30)-H(30A)	120.5
C(29)-C(30)-H(30A)	120.5
O(1)-B(1)-N(1)	117.4(3)
O(1)-B(1)-N(5)	117.1(3)
N(1)-B(1)-N(5)	103.7(3)
O(1)-B(1)-N(3)	109.3(3)
N(1)-B(1)-N(3)	103.5(3)
N(5)-B(1)-N(3)	104.3(3)

Symmetry transformations used to generate equivalent atoms:

Table S 40. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095)**. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^* U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	37(1)	69(1)	90(1)	11(1)	16(1)	-6(1)
Cl(2)	42(1)	61(1)	72(1)	5(1)	12(1)	9(1)
Cl(3)	68(1)	30(1)	61(1)	-11(1)	-8(1)	2(1)
Cl(4)	50(1)	36(1)	66(1)	-7(1)	-10(1)	-8(1)
Cl(5)	58(1)	55(1)	70(1)	22(1)	-9(1)	4(1)
Cl(6)	61(1)	34(1)	49(1)	10(1)	13(1)	2(1)
O(1)	50(2)	31(1)	33(1)	0(1)	8(1)	-6(1)
N(1)	34(2)	30(1)	33(2)	2(1)	1(1)	-6(1)
N(2)	36(2)	32(2)	36(2)	6(1)	2(1)	-1(1)
N(3)	31(2)	27(1)	37(2)	1(1)	4(1)	-4(1)
N(4)	32(2)	27(2)	40(2)	0(1)	6(1)	0(1)
N(5)	35(2)	25(1)	35(2)	-3(1)	6(1)	-4(1)
N(6)	39(2)	30(2)	33(2)	-2(1)	2(1)	-6(1)
C(1)	37(2)	34(2)	33(2)	-2(2)	1(2)	-7(2)
C(2)	36(2)	42(2)	35(2)	-2(2)	1(2)	-1(2)
C(3)	42(2)	43(2)	41(2)	1(2)	7(2)	-8(2)
C(4)	32(2)	52(2)	47(2)	-1(2)	7(2)	-3(2)
C(5)	38(2)	48(2)	45(2)	3(2)	6(2)	4(2)
C(6)	42(2)	44(2)	35(2)	5(2)	4(2)	1(2)
C(7)	34(2)	34(2)	34(2)	3(1)	-2(2)	-3(2)
C(8)	39(2)	28(2)	30(2)	4(1)	1(2)	-2(2)
C(9)	36(2)	26(2)	33(2)	4(1)	4(2)	-1(1)
C(10)	38(2)	26(2)	36(2)	5(1)	5(2)	-2(2)
C(11)	40(2)	30(2)	42(2)	1(2)	2(2)	1(2)
C(12)	50(2)	25(2)	39(2)	-2(1)	5(2)	1(2)
C(13)	42(2)	31(2)	39(2)	0(2)	0(2)	-6(2)
C(14)	38(2)	32(2)	39(2)	1(2)	5(2)	-2(2)
C(15)	38(2)	28(2)	34(2)	2(1)	6(2)	-4(2)

C(16)	32(2)	32(2)	39(2)	-4(2)	6(2)	-1(2)
C(17)	33(2)	30(2)	33(2)	-3(1)	5(2)	-4(2)
C(18)	38(2)	24(2)	34(2)	-4(1)	2(2)	-2(1)
C(19)	43(2)	28(2)	43(2)	-3(2)	2(2)	1(2)
C(20)	48(2)	31(2)	40(2)	-1(2)	0(2)	7(2)
C(21)	52(2)	27(2)	35(2)	-2(2)	11(2)	2(2)
C(22)	43(2)	29(2)	34(2)	-3(1)	9(2)	-2(2)
C(23)	43(2)	24(2)	29(2)	-1(1)	6(2)	-2(2)
C(24)	39(2)	27(2)	31(2)	-5(1)	3(2)	-6(2)
C(25)	51(2)	33(2)	29(2)	2(2)	8(2)	-5(2)
C(26)	59(3)	46(2)	42(2)	5(2)	14(2)	4(2)
C(27)	100(4)	45(2)	53(3)	-2(2)	32(3)	6(3)
C(28)	128(5)	46(3)	42(3)	-10(2)	30(3)	-13(3)
C(29)	85(4)	62(3)	35(2)	2(2)	-2(2)	-32(3)
C(30)	53(3)	48(2)	36(2)	7(2)	4(2)	-6(2)
B(1)	38(2)	27(2)	35(2)	0(2)	-1(2)	-2(2)

Table S 41. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095)**.

	x	y	z	U(eq)
H(3A)	7559	7586	6834	50
H(6A)	7009	4510	7378	49
H(11A)	3383	3221	6519	45
H(14A)	470	5072	5859	43
H(19A)	1080	8448	5282	46
H(22A)	4465	9601	5655	42
H(26A)	2320	7980	8845	58
H(27A)	2617	9285	9697	77
H(28A)	4235	9635	10372	85
H(29A)	5603	8667	10243	74
H(30A)	5315	7305	9413	55

Table S 42. Torsion angles [°] for **PhO-Cl₆BsubPc (Dichlorobenzene:Pentane; CCDC deposit 2087095)**.

C(24)-N(6)-C(1)-N(1)	-6.9(5)
C(24)-N(6)-C(1)-C(2)	159.1(3)
C(8)-N(1)-C(1)-N(6)	154.9(3)
B(1)-N(1)-C(1)-N(6)	-14.3(5)
C(8)-N(1)-C(1)-C(2)	-14.3(4)
B(1)-N(1)-C(1)-C(2)	176.6(3)
N(6)-C(1)-C(2)-C(3)	18.4(6)
N(1)-C(1)-C(2)-C(3)	-173.9(4)
N(6)-C(1)-C(2)-C(7)	-159.6(3)
N(1)-C(1)-C(2)-C(7)	8.2(4)
C(7)-C(2)-C(3)-C(4)	-5.3(5)
C(1)-C(2)-C(3)-C(4)	177.0(4)
C(2)-C(3)-C(4)-C(5)	4.7(6)
C(2)-C(3)-C(4)-Cl(1)	-175.5(3)
C(3)-C(4)-C(5)-C(6)	-0.5(6)
Cl(1)-C(4)-C(5)-C(6)	179.7(3)
C(3)-C(4)-C(5)-Cl(2)	-180.0(3)
Cl(1)-C(4)-C(5)-Cl(2)	0.2(5)
C(4)-C(5)-C(6)-C(7)	-3.1(5)
Cl(2)-C(5)-C(6)-C(7)	176.4(3)
C(5)-C(6)-C(7)-C(2)	2.4(5)
C(5)-C(6)-C(7)-C(8)	-177.6(4)
C(3)-C(2)-C(7)-C(6)	1.8(5)
C(1)-C(2)-C(7)-C(6)	-180.0(3)
C(3)-C(2)-C(7)-C(8)	-178.1(3)
C(1)-C(2)-C(7)-C(8)	0.1(4)
C(9)-N(2)-C(8)-N(1)	5.6(5)
C(9)-N(2)-C(8)-C(7)	-157.5(3)
C(1)-N(1)-C(8)-N(2)	-152.2(3)
B(1)-N(1)-C(8)-N(2)	17.0(5)
C(1)-N(1)-C(8)-C(7)	14.3(4)
B(1)-N(1)-C(8)-C(7)	-176.4(3)
C(6)-C(7)-C(8)-N(2)	-23.0(6)

C(2)-C(7)-C(8)-N(2)	156.9(3)
C(6)-C(7)-C(8)-N(1)	171.7(4)
C(2)-C(7)-C(8)-N(1)	-8.4(4)
C(8)-N(2)-C(9)-N(3)	-8.2(5)
C(8)-N(2)-C(9)-C(10)	157.0(3)
C(16)-N(3)-C(9)-N(2)	158.6(3)
B(1)-N(3)-C(9)-N(2)	-11.6(5)
C(16)-N(3)-C(9)-C(10)	-10.0(4)
B(1)-N(3)-C(9)-C(10)	179.9(3)
N(2)-C(9)-C(10)-C(11)	12.0(6)
N(3)-C(9)-C(10)-C(11)	179.1(4)
N(2)-C(9)-C(10)-C(15)	-163.0(3)
N(3)-C(9)-C(10)-C(15)	4.1(4)
C(15)-C(10)-C(11)-C(12)	-4.0(5)
C(9)-C(10)-C(11)-C(12)	-178.5(3)
C(10)-C(11)-C(12)-C(13)	0.1(5)
C(10)-C(11)-C(12)-Cl(3)	179.2(3)
C(11)-C(12)-C(13)-C(14)	4.3(6)
Cl(3)-C(12)-C(13)-C(14)	-174.9(3)
C(11)-C(12)-C(13)-Cl(4)	-175.9(3)
Cl(3)-C(12)-C(13)-Cl(4)	5.0(4)
C(12)-C(13)-C(14)-C(15)	-4.5(5)
Cl(4)-C(13)-C(14)-C(15)	175.7(3)
C(13)-C(14)-C(15)-C(10)	0.5(5)
C(13)-C(14)-C(15)-C(16)	176.6(4)
C(11)-C(10)-C(15)-C(14)	3.8(5)
C(9)-C(10)-C(15)-C(14)	179.5(3)
C(11)-C(10)-C(15)-C(16)	-173.2(3)
C(9)-C(10)-C(15)-C(16)	2.5(4)
C(17)-N(4)-C(16)-N(3)	8.0(5)
C(17)-N(4)-C(16)-C(15)	-154.0(3)
C(9)-N(3)-C(16)-N(4)	-154.5(3)
B(1)-N(3)-C(16)-N(4)	15.8(5)
C(9)-N(3)-C(16)-C(15)	11.5(4)
B(1)-N(3)-C(16)-C(15)	-178.2(3)
C(14)-C(15)-C(16)-N(4)	-20.2(6)

C(10)-C(15)-C(16)-N(4)	156.3(3)
C(14)-C(15)-C(16)-N(3)	175.4(3)
C(10)-C(15)-C(16)-N(3)	-8.1(4)
C(16)-N(4)-C(17)-N(5)	-9.5(5)
C(16)-N(4)-C(17)-C(18)	152.1(3)
C(24)-N(5)-C(17)-N(4)	154.4(3)
B(1)-N(5)-C(17)-N(4)	-12.9(5)
C(24)-N(5)-C(17)-C(18)	-11.0(4)
B(1)-N(5)-C(17)-C(18)	-178.3(3)
N(4)-C(17)-C(18)-C(19)	16.9(6)
N(5)-C(17)-C(18)-C(19)	-179.1(4)
N(4)-C(17)-C(18)-C(23)	-157.3(3)
N(5)-C(17)-C(18)-C(23)	6.7(3)
C(23)-C(18)-C(19)-C(20)	0.0(5)
C(17)-C(18)-C(19)-C(20)	-173.5(3)
C(18)-C(19)-C(20)-C(21)	0.1(5)
C(18)-C(19)-C(20)-Cl(5)	178.7(3)
C(19)-C(20)-C(21)-C(22)	0.3(5)
Cl(5)-C(20)-C(21)-C(22)	-178.3(3)
C(19)-C(20)-C(21)-Cl(6)	178.0(3)
Cl(5)-C(20)-C(21)-Cl(6)	-0.6(4)
C(20)-C(21)-C(22)-C(23)	-0.7(5)
Cl(6)-C(21)-C(22)-C(23)	-178.5(2)
C(21)-C(22)-C(23)-C(18)	0.8(5)
C(21)-C(22)-C(23)-C(24)	174.6(3)
C(19)-C(18)-C(23)-C(22)	-0.5(5)
C(17)-C(18)-C(23)-C(22)	174.5(3)
C(19)-C(18)-C(23)-C(24)	-175.6(3)
C(17)-C(18)-C(23)-C(24)	-0.5(4)
C(1)-N(6)-C(24)-N(5)	8.5(5)
C(1)-N(6)-C(24)-C(23)	-154.9(3)
C(17)-N(5)-C(24)-N(6)	-156.3(3)
B(1)-N(5)-C(24)-N(6)	10.8(5)
C(17)-N(5)-C(24)-C(23)	10.7(4)
B(1)-N(5)-C(24)-C(23)	177.8(3)
C(22)-C(23)-C(24)-N(6)	-14.6(6)

C(18)-C(23)-C(24)-N(6)	159.8(3)
C(22)-C(23)-C(24)-N(5)	179.9(3)
C(18)-C(23)-C(24)-N(5)	-5.8(3)
B(1)-O(1)-C(25)-C(30)	-83.6(4)
B(1)-O(1)-C(25)-C(26)	99.1(4)
O(1)-C(25)-C(26)-C(27)	177.2(3)
C(30)-C(25)-C(26)-C(27)	-0.1(5)
C(25)-C(26)-C(27)-C(28)	1.0(6)
C(26)-C(27)-C(28)-C(29)	-0.8(7)
C(27)-C(28)-C(29)-C(30)	-0.2(6)
O(1)-C(25)-C(30)-C(29)	-178.1(3)
C(26)-C(25)-C(30)-C(29)	-0.9(5)
C(28)-C(29)-C(30)-C(25)	1.0(6)
C(25)-O(1)-B(1)-N(1)	80.1(4)
C(25)-O(1)-B(1)-N(5)	-44.2(5)
C(25)-O(1)-B(1)-N(3)	-162.5(3)
C(8)-N(1)-B(1)-O(1)	89.5(4)
C(1)-N(1)-B(1)-O(1)	-102.4(4)
C(8)-N(1)-B(1)-N(5)	-139.7(3)
C(1)-N(1)-B(1)-N(5)	28.4(4)
C(8)-N(1)-B(1)-N(3)	-31.0(4)
C(1)-N(1)-B(1)-N(3)	137.1(3)
C(17)-N(5)-B(1)-O(1)	-89.6(4)
C(24)-N(5)-B(1)-O(1)	104.4(4)
C(17)-N(5)-B(1)-N(1)	139.4(3)
C(24)-N(5)-B(1)-N(1)	-26.6(4)
C(17)-N(5)-B(1)-N(3)	31.3(4)
C(24)-N(5)-B(1)-N(3)	-134.6(3)
C(9)-N(3)-B(1)-O(1)	-97.3(4)
C(16)-N(3)-B(1)-O(1)	93.3(4)
C(9)-N(3)-B(1)-N(1)	28.6(4)
C(16)-N(3)-B(1)-N(1)	-140.9(3)
C(9)-N(3)-B(1)-N(5)	136.8(3)
C(16)-N(3)-B(1)-N(5)	-32.7(4)

Symmetry transformations used to generate equivalent atoms:

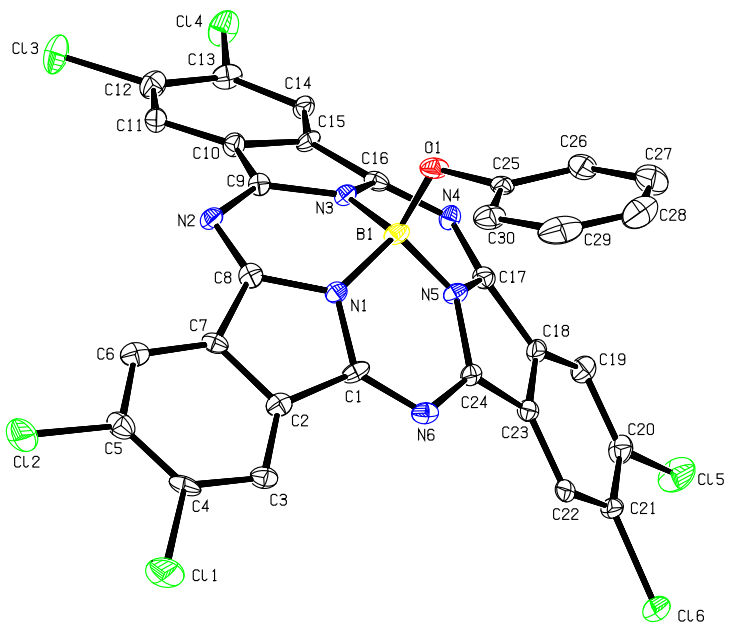


Figure S22: Anisotropic displacement ellipsoid plot of PhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098).

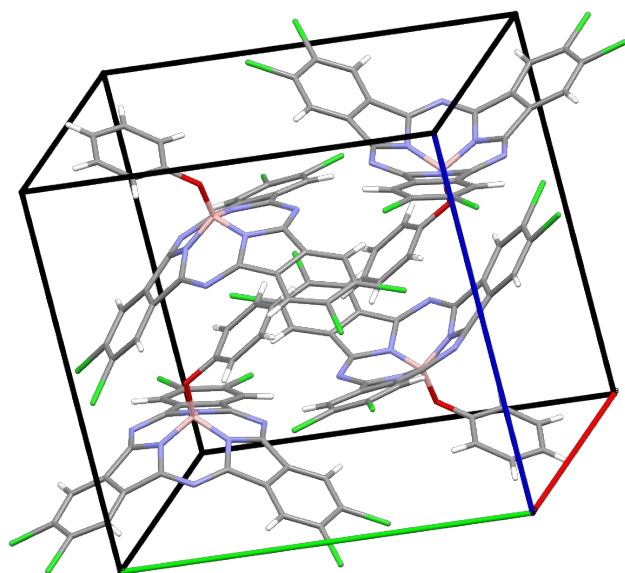


Figure S23: Populated unit cell of **PhO-Cl₆BsubPc** (Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098).

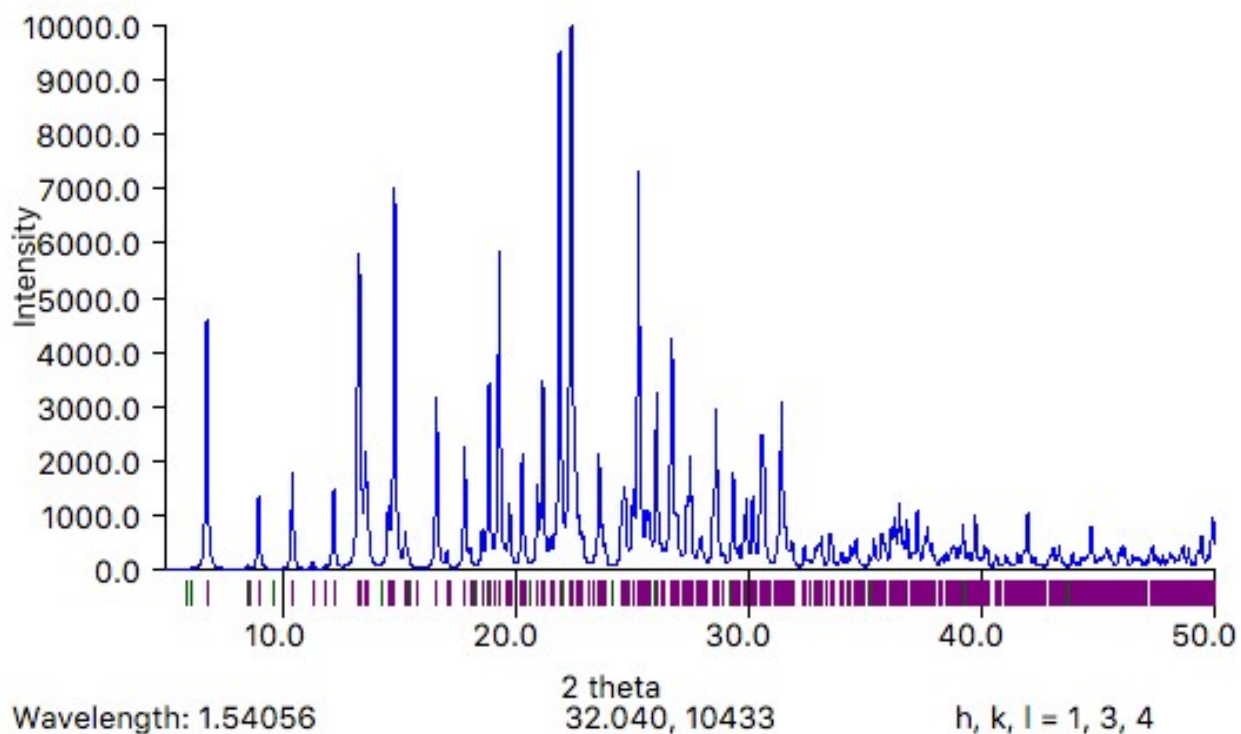


Figure S24: Powder x-ray diffraction **PhO-Cl₆BsubPc** (Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098).

Table S 43. Crystal data and structure refinement for **PhO-Cl₆BsubPc**
(**Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098**).

Identification code	d19194_a	
Empirical formula	C ₃₀ H ₁₁ B Cl ₆ N ₆ O	
Formula weight	694.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 13.118(3) Å	α = 90°.
	b = 14.899(2) Å	β = 96.581(9)°.
	c = 14.576(3) Å	γ = 90°.
Volume	2830.1(9) Å ³	
Z	4	
Density (calculated)	1.631 Mg/m ³	
Absorption coefficient	0.647 mm ⁻¹	
F(000)	1392	
Crystal size	0.160 x 0.130 x 0.030 mm ³	
Theta range for data collection	1.563 to 24.998°.	
Index ranges	-14 ≤ h ≤ 15, -17 ≤ k ≤ 17, -17 ≤ l ≤ 15	
Reflections collected	25715	
Independent reflections	4992 [R(int) = 0.2229]	
Completeness to theta = 24.998°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6619	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4992 / 0 / 397	
Goodness-of-fit on F ²	0.992	
Final R indices [I > 2σ(I)]	R1 = 0.0635, wR2 = 0.0834	
R indices (all data)	R1 = 0.1968, wR2 = 0.1200	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.442 and -0.453 e.Å ⁻³	

Table S 44. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098)**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	9472(1)	6749(1)	6934(1)	54(1)
Cl(2)	9088(1)	4694(1)	7285(1)	48(1)
Cl(3)	1846(1)	2143(1)	5613(1)	43(1)
Cl(4)	-135(1)	3345(1)	5318(1)	41(1)
Cl(5)	1101(2)	9908(1)	4090(1)	50(1)
Cl(6)	3357(1)	10668(1)	4340(1)	36(1)
O(1)	3587(3)	6734(2)	8575(2)	27(1)
N(1)	4867(4)	6482(3)	7460(3)	19(1)
N(2)	4650(4)	4894(3)	7287(3)	22(1)
N(3)	3201(4)	5871(3)	7211(3)	19(1)
N(4)	1868(4)	6756(3)	6439(3)	21(1)
N(5)	3471(4)	7420(3)	7013(3)	19(1)
N(6)	5168(4)	7912(3)	6849(3)	23(1)
C(1)	5510(5)	7115(4)	7185(4)	23(2)
C(2)	6505(5)	6667(4)	7138(4)	24(2)
C(3)	7455(5)	6982(4)	6985(4)	26(2)
C(4)	8246(5)	6372(4)	7046(4)	29(2)
C(5)	8091(5)	5460(4)	7199(4)	32(2)
C(6)	7117(5)	5134(4)	7297(3)	27(2)
C(7)	6331(5)	5745(4)	7294(4)	21(2)
C(8)	5253(5)	5631(4)	7409(4)	23(2)
C(9)	3639(5)	5046(4)	7126(4)	20(2)
C(10)	2819(5)	4478(4)	6678(4)	23(2)
C(11)	2794(5)	3589(4)	6398(4)	25(2)
C(12)	1880(5)	3245(4)	5967(4)	31(2)
C(13)	1014(5)	3791(4)	5803(4)	28(2)
C(14)	1051(5)	4693(4)	6010(4)	23(2)
C(15)	1960(5)	5046(3)	6464(4)	21(2)
C(16)	2261(5)	5949(4)	6735(4)	21(2)
C(17)	2513(5)	7460(4)	6524(4)	23(2)

C(18)	2519(5)	8282(4)	5979(4)	23(2)
C(19)	1749(5)	8677(4)	5362(4)	28(2)
C(20)	2026(5)	9423(4)	4872(4)	29(2)
C(21)	3022(5)	9759(4)	4993(4)	26(2)
C(22)	3788(5)	9366(3)	5590(4)	22(2)
C(23)	3517(5)	8622(4)	6089(4)	21(2)
C(24)	4141(5)	8029(3)	6714(4)	19(2)
C(25)	3797(5)	7525(4)	9050(4)	22(2)
C(26)	3005(6)	8109(4)	9134(4)	37(2)
C(27)	3170(7)	8886(5)	9631(5)	51(2)
C(28)	4140(8)	9082(5)	10041(5)	57(3)
C(29)	4924(7)	8503(5)	9964(4)	50(2)
C(30)	4769(6)	7710(4)	9463(4)	34(2)
B(1)	3790(6)	6653(4)	7646(5)	23(2)

Table S 45. Bond lengths [Å] and angles [°] for **PhO-Cl₆BsubPc**
(**Dichlorobenzene:Dimethoxybenzene:Pentane**; CCDC deposit 2087098).

Cl(1)-C(4)	1.730(6)
Cl(2)-C(5)	1.730(6)
Cl(3)-C(12)	1.721(6)
Cl(4)-C(13)	1.723(6)
Cl(5)-C(20)	1.726(6)
Cl(6)-C(21)	1.740(6)
O(1)-C(25)	1.379(6)
O(1)-B(1)	1.415(7)
N(1)-C(1)	1.357(7)
N(1)-C(8)	1.371(7)
N(1)-B(1)	1.490(8)
N(2)-C(9)	1.340(7)
N(2)-C(8)	1.354(7)
N(3)-C(16)	1.349(7)
N(3)-C(9)	1.367(6)
N(3)-B(1)	1.498(7)
N(4)-C(17)	1.344(7)
N(4)-C(16)	1.358(6)
N(5)-C(24)	1.368(7)
N(5)-C(17)	1.374(7)
N(5)-B(1)	1.498(7)
N(6)-C(1)	1.342(7)
N(6)-C(24)	1.351(7)
C(1)-C(2)	1.475(8)
C(2)-C(3)	1.374(8)
C(2)-C(7)	1.414(7)
C(3)-C(4)	1.374(8)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.396(8)
C(5)-C(6)	1.390(8)
C(6)-C(7)	1.375(8)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.453(8)
C(9)-C(10)	1.463(7)
C(10)-C(11)	1.385(7)
C(10)-C(15)	1.416(7)
C(11)-C(12)	1.386(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.395(8)
C(13)-C(14)	1.377(7)
C(14)-C(15)	1.398(7)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.444(7)
C(17)-C(18)	1.460(7)
C(18)-C(23)	1.395(8)
C(18)-C(19)	1.402(7)
C(19)-C(20)	1.392(7)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.391(8)
C(21)-C(22)	1.381(7)
C(22)-C(23)	1.395(7)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.453(7)
C(25)-C(26)	1.371(8)
C(25)-C(30)	1.373(8)
C(26)-C(27)	1.370(8)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.374(10)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.357(10)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.391(8)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
C(25)-O(1)-B(1)	120.3(4)
C(1)-N(1)-C(8)	112.3(5)
C(1)-N(1)-B(1)	124.7(5)

C(8)-N(1)-B(1)	122.2(5)
C(9)-N(2)-C(8)	116.0(5)
C(16)-N(3)-C(9)	113.5(5)
C(16)-N(3)-B(1)	123.2(5)
C(9)-N(3)-B(1)	122.4(5)
C(17)-N(4)-C(16)	116.7(5)
C(24)-N(5)-C(17)	112.9(5)
C(24)-N(5)-B(1)	123.9(5)
C(17)-N(5)-B(1)	121.8(5)
C(1)-N(6)-C(24)	116.9(5)
N(6)-C(1)-N(1)	122.0(6)
N(6)-C(1)-C(2)	130.1(6)
N(1)-C(1)-C(2)	106.4(5)
C(3)-C(2)-C(7)	121.6(6)
C(3)-C(2)-C(1)	132.6(6)
C(7)-C(2)-C(1)	105.8(6)
C(2)-C(3)-C(4)	117.1(6)
C(2)-C(3)-H(3A)	121.4
C(4)-C(3)-H(3A)	121.4
C(3)-C(4)-C(5)	122.1(6)
C(3)-C(4)-Cl(1)	118.9(5)
C(5)-C(4)-Cl(1)	119.0(5)
C(6)-C(5)-C(4)	120.6(6)
C(6)-C(5)-Cl(2)	117.3(5)
C(4)-C(5)-Cl(2)	122.1(5)
C(7)-C(6)-C(5)	117.7(6)
C(7)-C(6)-H(6A)	121.1
C(5)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.6(6)
C(6)-C(7)-C(8)	131.3(6)
C(2)-C(7)-C(8)	108.0(5)
N(2)-C(8)-N(1)	122.9(6)
N(2)-C(8)-C(7)	130.0(6)
N(1)-C(8)-C(7)	105.6(5)
N(2)-C(9)-N(3)	123.6(5)
N(2)-C(9)-C(10)	130.0(5)

N(3)-C(9)-C(10)	105.4(5)
C(11)-C(10)-C(15)	121.0(6)
C(11)-C(10)-C(9)	132.6(6)
C(15)-C(10)-C(9)	106.1(5)
C(10)-C(11)-C(12)	118.5(6)
C(10)-C(11)-H(11A)	120.8
C(12)-C(11)-H(11A)	120.8
C(11)-C(12)-C(13)	120.5(5)
C(11)-C(12)-Cl(3)	118.7(5)
C(13)-C(12)-Cl(3)	120.8(5)
C(14)-C(13)-C(12)	121.6(6)
C(14)-C(13)-Cl(4)	118.3(5)
C(12)-C(13)-Cl(4)	120.1(5)
C(13)-C(14)-C(15)	118.5(5)
C(13)-C(14)-H(14A)	120.7
C(15)-C(14)-H(14A)	120.7
C(14)-C(15)-C(10)	119.5(5)
C(14)-C(15)-C(16)	132.2(6)
C(10)-C(15)-C(16)	108.1(5)
N(3)-C(16)-N(4)	122.1(5)
N(3)-C(16)-C(15)	105.4(5)
N(4)-C(16)-C(15)	130.9(5)
N(4)-C(17)-N(5)	122.8(5)
N(4)-C(17)-C(18)	130.4(6)
N(5)-C(17)-C(18)	104.9(5)
C(23)-C(18)-C(19)	121.3(5)
C(23)-C(18)-C(17)	107.8(5)
C(19)-C(18)-C(17)	130.7(6)
C(20)-C(19)-C(18)	116.9(6)
C(20)-C(19)-H(19A)	121.5
C(18)-C(19)-H(19A)	121.5
C(21)-C(20)-C(19)	121.3(6)
C(21)-C(20)-Cl(5)	120.8(5)
C(19)-C(20)-Cl(5)	117.9(5)
C(22)-C(21)-C(20)	122.2(5)
C(22)-C(21)-Cl(6)	117.6(5)

C(20)-C(21)-Cl(6)	120.2(5)
C(21)-C(22)-C(23)	117.0(6)
C(21)-C(22)-H(22A)	121.5
C(23)-C(22)-H(22A)	121.5
C(18)-C(23)-C(22)	121.4(5)
C(18)-C(23)-C(24)	107.8(5)
C(22)-C(23)-C(24)	130.7(6)
N(6)-C(24)-N(5)	122.3(5)
N(6)-C(24)-C(23)	130.6(6)
N(5)-C(24)-C(23)	105.5(5)
C(26)-C(25)-C(30)	120.6(6)
C(26)-C(25)-O(1)	118.5(6)
C(30)-C(25)-O(1)	120.9(6)
C(27)-C(26)-C(25)	120.5(7)
C(27)-C(26)-H(26A)	119.7
C(25)-C(26)-H(26A)	119.7
C(26)-C(27)-C(28)	119.5(7)
C(26)-C(27)-H(27A)	120.3
C(28)-C(27)-H(27A)	120.3
C(29)-C(28)-C(27)	120.1(7)
C(29)-C(28)-H(28A)	120.0
C(27)-C(28)-H(28A)	120.0
C(28)-C(29)-C(30)	121.1(7)
C(28)-C(29)-H(29A)	119.4
C(30)-C(29)-H(29A)	119.4
C(25)-C(30)-C(29)	118.2(7)
C(25)-C(30)-H(30A)	120.9
C(29)-C(30)-H(30A)	120.9
O(1)-B(1)-N(1)	118.3(5)
O(1)-B(1)-N(3)	109.1(5)
N(1)-B(1)-N(3)	104.1(5)
O(1)-B(1)-N(5)	117.1(5)
N(1)-B(1)-N(5)	102.8(5)
N(3)-B(1)-N(5)	103.8(5)

Symmetry transformations used to generate equivalent atoms:

Table S 46. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **PhO-Cl₆BsubPc** (**Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	22(1)	65(1)	79(1)	10(1)	15(1)	-7(1)
Cl(2)	26(1)	56(1)	61(1)	5(1)	11(1)	10(1)
Cl(3)	54(1)	25(1)	46(1)	-10(1)	-9(1)	5(1)
Cl(4)	33(1)	30(1)	56(1)	-7(1)	-10(1)	-9(1)
Cl(5)	43(1)	50(1)	55(1)	22(1)	-11(1)	5(1)
Cl(6)	48(1)	27(1)	37(1)	9(1)	12(1)	2(1)
O(1)	34(3)	30(2)	18(2)	-2(2)	7(2)	-10(2)
N(1)	20(3)	19(3)	18(3)	2(2)	0(2)	0(3)
N(2)	24(4)	18(3)	25(3)	5(2)	2(3)	0(3)
N(3)	18(4)	17(3)	22(3)	3(2)	0(3)	-1(2)
N(4)	21(3)	18(3)	24(3)	-2(2)	-1(2)	-1(3)
N(5)	15(3)	18(3)	22(3)	-1(2)	-2(3)	-8(2)
N(6)	26(4)	25(3)	19(3)	-3(2)	2(3)	-10(3)
C(1)	25(5)	19(4)	22(4)	2(3)	-6(3)	-13(3)
C(2)	28(5)	25(4)	17(4)	1(3)	-2(3)	-3(3)
C(3)	23(5)	30(4)	25(4)	-1(3)	4(3)	-8(3)
C(4)	9(4)	48(5)	31(4)	4(3)	7(3)	-5(3)
C(5)	27(5)	43(5)	26(4)	3(3)	4(3)	7(4)
C(6)	32(5)	31(4)	18(4)	0(3)	-1(3)	-7(4)
C(7)	16(4)	32(4)	17(3)	2(3)	2(3)	-1(3)
C(8)	24(5)	28(4)	14(3)	4(3)	-4(3)	6(3)
C(9)	19(4)	21(4)	17(3)	0(3)	-1(3)	1(3)
C(10)	23(4)	21(4)	25(4)	1(3)	2(3)	2(3)
C(11)	28(5)	22(4)	26(4)	0(3)	5(3)	4(3)
C(12)	38(5)	25(4)	29(4)	-1(3)	0(4)	-2(4)
C(13)	26(5)	30(4)	26(4)	-3(3)	-4(3)	-13(3)
C(14)	19(4)	19(3)	31(4)	6(3)	3(3)	4(3)
C(15)	25(4)	14(3)	23(4)	-1(3)	0(3)	-9(3)
C(16)	14(4)	29(4)	19(4)	3(3)	3(3)	0(3)
C(17)	24(4)	22(4)	23(4)	-3(3)	6(3)	-2(3)

C(18)	33(5)	17(3)	22(4)	-2(3)	7(3)	2(3)
C(19)	30(5)	22(4)	33(4)	-7(3)	2(3)	-7(3)
C(20)	31(5)	28(4)	26(4)	3(3)	-3(3)	8(3)
C(21)	39(5)	19(3)	22(4)	2(3)	12(3)	0(3)
C(22)	27(4)	17(3)	21(4)	-11(3)	8(3)	-6(3)
C(23)	23(4)	19(3)	21(4)	-4(3)	5(3)	-3(3)
C(24)	26(5)	15(3)	16(3)	-5(3)	2(3)	-5(3)
C(25)	30(5)	23(4)	13(4)	0(3)	8(3)	-3(3)
C(26)	52(6)	37(4)	24(4)	0(3)	15(4)	1(4)
C(27)	70(7)	55(5)	31(5)	4(4)	21(5)	9(5)
C(28)	119(9)	33(5)	22(4)	-9(3)	17(5)	-15(5)
C(29)	73(7)	60(6)	16(4)	4(4)	-4(4)	-28(5)
C(30)	43(6)	38(4)	21(4)	3(3)	4(4)	-7(4)
B(1)	16(5)	20(4)	30(5)	3(3)	-1(4)	-7(4)

Table S 47. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **PhO-Cl₆BsubPc** (**Dichlorobenzene:Dimethoxybenzene:Pentane; CCDC deposit 2087098**).

	x	y	z	U(eq)
H(3A)	7561	7595	6843	31
H(6A)	6997	4509	7364	33
H(11A)	3389	3223	6499	30
H(14A)	472	5068	5847	28
H(19A)	1070	8445	5281	34
H(22A)	4470	9593	5657	26
H(26A)	2337	7973	8845	44
H(27A)	2618	9286	9692	61
H(28A)	4262	9624	10379	69
H(29A)	5590	8641	10257	61
H(30A)	5320	7307	9408	41

Table S 48. Torsion angles [°] for **PhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene: Pentane; CCDC deposit 2087098)**.

C(24)-N(6)-C(1)-N(1)	-6.1(8)
C(24)-N(6)-C(1)-C(2)	158.3(5)
C(8)-N(1)-C(1)-N(6)	154.4(5)
B(1)-N(1)-C(1)-N(6)	-15.7(8)
C(8)-N(1)-C(1)-C(2)	-13.2(6)
B(1)-N(1)-C(1)-C(2)	176.7(5)
N(6)-C(1)-C(2)-C(3)	20.6(10)
N(1)-C(1)-C(2)-C(3)	-173.2(6)
N(6)-C(1)-C(2)-C(7)	-159.5(5)
N(1)-C(1)-C(2)-C(7)	6.7(6)
C(7)-C(2)-C(3)-C(4)	-3.9(8)
C(1)-C(2)-C(3)-C(4)	176.0(5)
C(2)-C(3)-C(4)-C(5)	3.9(9)
C(2)-C(3)-C(4)-Cl(1)	-175.8(4)
C(3)-C(4)-C(5)-C(6)	0.0(9)
Cl(1)-C(4)-C(5)-C(6)	179.7(4)
C(3)-C(4)-C(5)-Cl(2)	-179.5(5)
Cl(1)-C(4)-C(5)-Cl(2)	0.2(7)
C(4)-C(5)-C(6)-C(7)	-3.9(8)
Cl(2)-C(5)-C(6)-C(7)	175.6(4)
C(5)-C(6)-C(7)-C(2)	3.9(8)
C(5)-C(6)-C(7)-C(8)	-177.8(6)
C(3)-C(2)-C(7)-C(6)	0.0(8)
C(1)-C(2)-C(7)-C(6)	-179.9(5)
C(3)-C(2)-C(7)-C(8)	-178.6(5)
C(1)-C(2)-C(7)-C(8)	1.4(6)
C(9)-N(2)-C(8)-N(1)	6.4(8)
C(9)-N(2)-C(8)-C(7)	-157.3(6)
C(1)-N(1)-C(8)-N(2)	-153.2(5)
B(1)-N(1)-C(8)-N(2)	17.3(8)
C(1)-N(1)-C(8)-C(7)	14.0(6)
B(1)-N(1)-C(8)-C(7)	-175.6(5)

C(6)-C(7)-C(8)-N(2)	-21.6(10)
C(2)-C(7)-C(8)-N(2)	156.9(5)
C(6)-C(7)-C(8)-N(1)	172.5(6)
C(2)-C(7)-C(8)-N(1)	-9.0(6)
C(8)-N(2)-C(9)-N(3)	-9.7(8)
C(8)-N(2)-C(9)-C(10)	157.5(6)
C(16)-N(3)-C(9)-N(2)	158.9(5)
B(1)-N(3)-C(9)-N(2)	-10.5(9)
C(16)-N(3)-C(9)-C(10)	-11.0(6)
B(1)-N(3)-C(9)-C(10)	179.6(5)
N(2)-C(9)-C(10)-C(11)	9.8(11)
N(3)-C(9)-C(10)-C(11)	178.8(6)
N(2)-C(9)-C(10)-C(15)	-164.4(6)
N(3)-C(9)-C(10)-C(15)	4.6(6)
C(15)-C(10)-C(11)-C(12)	-5.2(9)
C(9)-C(10)-C(11)-C(12)	-178.7(6)
C(10)-C(11)-C(12)-C(13)	1.5(9)
C(10)-C(11)-C(12)-Cl(3)	179.7(4)
C(11)-C(12)-C(13)-C(14)	3.9(9)
Cl(3)-C(12)-C(13)-C(14)	-174.3(4)
C(11)-C(12)-C(13)-Cl(4)	-176.8(5)
Cl(3)-C(12)-C(13)-Cl(4)	5.0(8)
C(12)-C(13)-C(14)-C(15)	-5.3(9)
Cl(4)-C(13)-C(14)-C(15)	175.4(4)
C(13)-C(14)-C(15)-C(10)	1.5(8)
C(13)-C(14)-C(15)-C(16)	176.6(6)
C(11)-C(10)-C(15)-C(14)	3.7(9)
C(9)-C(10)-C(15)-C(14)	178.8(5)
C(11)-C(10)-C(15)-C(16)	-172.4(5)
C(9)-C(10)-C(15)-C(16)	2.6(6)
C(9)-N(3)-C(16)-N(4)	-154.6(5)
B(1)-N(3)-C(16)-N(4)	14.7(9)
C(9)-N(3)-C(16)-C(15)	12.6(7)
B(1)-N(3)-C(16)-C(15)	-178.2(5)
C(17)-N(4)-C(16)-N(3)	9.4(8)
C(17)-N(4)-C(16)-C(15)	-154.1(6)

C(14)-C(15)-C(16)-N(3)	175.6(6)
C(10)-C(15)-C(16)-N(3)	-8.9(6)
C(14)-C(15)-C(16)-N(4)	-18.9(11)
C(10)-C(15)-C(16)-N(4)	156.7(6)
C(16)-N(4)-C(17)-N(5)	-10.3(8)
C(16)-N(4)-C(17)-C(18)	151.5(6)
C(24)-N(5)-C(17)-N(4)	154.3(5)
B(1)-N(5)-C(17)-N(4)	-12.7(9)
C(24)-N(5)-C(17)-C(18)	-11.4(6)
B(1)-N(5)-C(17)-C(18)	-178.4(5)
N(4)-C(17)-C(18)-C(23)	-157.0(6)
N(5)-C(17)-C(18)-C(23)	7.3(6)
N(4)-C(17)-C(18)-C(19)	16.8(11)
N(5)-C(17)-C(18)-C(19)	-179.0(6)
C(23)-C(18)-C(19)-C(20)	-0.5(8)
C(17)-C(18)-C(19)-C(20)	-173.5(6)
C(18)-C(19)-C(20)-C(21)	0.0(9)
C(18)-C(19)-C(20)-Cl(5)	178.7(4)
C(19)-C(20)-C(21)-C(22)	1.0(9)
Cl(5)-C(20)-C(21)-C(22)	-177.7(4)
C(19)-C(20)-C(21)-Cl(6)	177.6(4)
Cl(5)-C(20)-C(21)-Cl(6)	-1.0(7)
C(20)-C(21)-C(22)-C(23)	-1.4(8)
Cl(6)-C(21)-C(22)-C(23)	-178.1(4)
C(19)-C(18)-C(23)-C(22)	0.0(8)
C(17)-C(18)-C(23)-C(22)	174.5(5)
C(19)-C(18)-C(23)-C(24)	-175.5(5)
C(17)-C(18)-C(23)-C(24)	-1.1(6)
C(21)-C(22)-C(23)-C(18)	0.9(8)
C(21)-C(22)-C(23)-C(24)	175.3(5)
C(1)-N(6)-C(24)-N(5)	8.4(8)
C(1)-N(6)-C(24)-C(23)	-154.9(5)
C(17)-N(5)-C(24)-N(6)	-156.1(5)
B(1)-N(5)-C(24)-N(6)	10.6(8)
C(17)-N(5)-C(24)-C(23)	10.8(6)
B(1)-N(5)-C(24)-C(23)	177.5(5)

C(18)-C(23)-C(24)-N(6)	159.8(6)
C(22)-C(23)-C(24)-N(6)	-15.2(10)
C(18)-C(23)-C(24)-N(5)	-5.6(6)
C(22)-C(23)-C(24)-N(5)	179.4(5)
B(1)-O(1)-C(25)-C(26)	99.5(7)
B(1)-O(1)-C(25)-C(30)	-83.0(7)
C(30)-C(25)-C(26)-C(27)	-0.1(9)
O(1)-C(25)-C(26)-C(27)	177.4(5)
C(25)-C(26)-C(27)-C(28)	0.6(10)
C(26)-C(27)-C(28)-C(29)	-0.9(11)
C(27)-C(28)-C(29)-C(30)	0.8(11)
C(26)-C(25)-C(30)-C(29)	-0.1(9)
O(1)-C(25)-C(30)-C(29)	-177.5(5)
C(28)-C(29)-C(30)-C(25)	-0.3(9)
C(25)-O(1)-B(1)-N(1)	79.3(7)
C(25)-O(1)-B(1)-N(3)	-162.1(5)
C(25)-O(1)-B(1)-N(5)	-44.6(8)
C(1)-N(1)-B(1)-O(1)	-101.6(6)
C(8)-N(1)-B(1)-O(1)	89.2(6)
C(1)-N(1)-B(1)-N(3)	137.2(5)
C(8)-N(1)-B(1)-N(3)	-32.0(7)
C(1)-N(1)-B(1)-N(5)	29.2(7)
C(8)-N(1)-B(1)-N(5)	-140.0(5)
C(16)-N(3)-B(1)-O(1)	93.3(7)
C(9)-N(3)-B(1)-O(1)	-98.3(6)
C(16)-N(3)-B(1)-N(1)	-139.5(5)
C(9)-N(3)-B(1)-N(1)	28.9(7)
C(16)-N(3)-B(1)-N(5)	-32.2(8)
C(9)-N(3)-B(1)-N(5)	136.1(5)
C(24)-N(5)-B(1)-O(1)	105.1(7)
C(17)-N(5)-B(1)-O(1)	-89.4(7)
C(24)-N(5)-B(1)-N(1)	-26.4(7)
C(17)-N(5)-B(1)-N(1)	139.1(5)
C(24)-N(5)-B(1)-N(3)	-134.7(5)
C(17)-N(5)-B(1)-N(3)	30.9(8)

Symmetry transformations used to generate equivalent atoms:

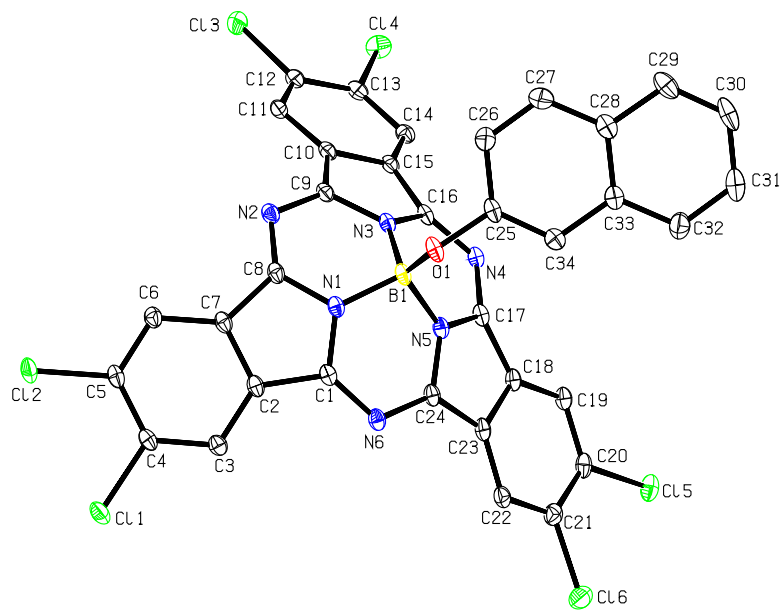


Figure S25: Anisotropic displacement plot of **NaphO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087099).

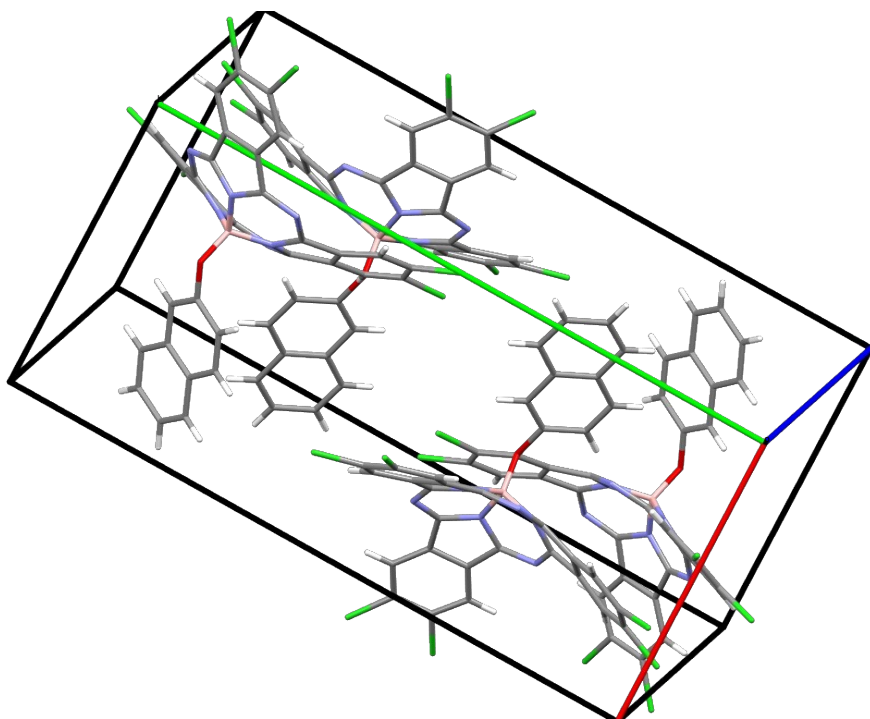


Figure S26: Populated unit cell of **NaphO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087099).

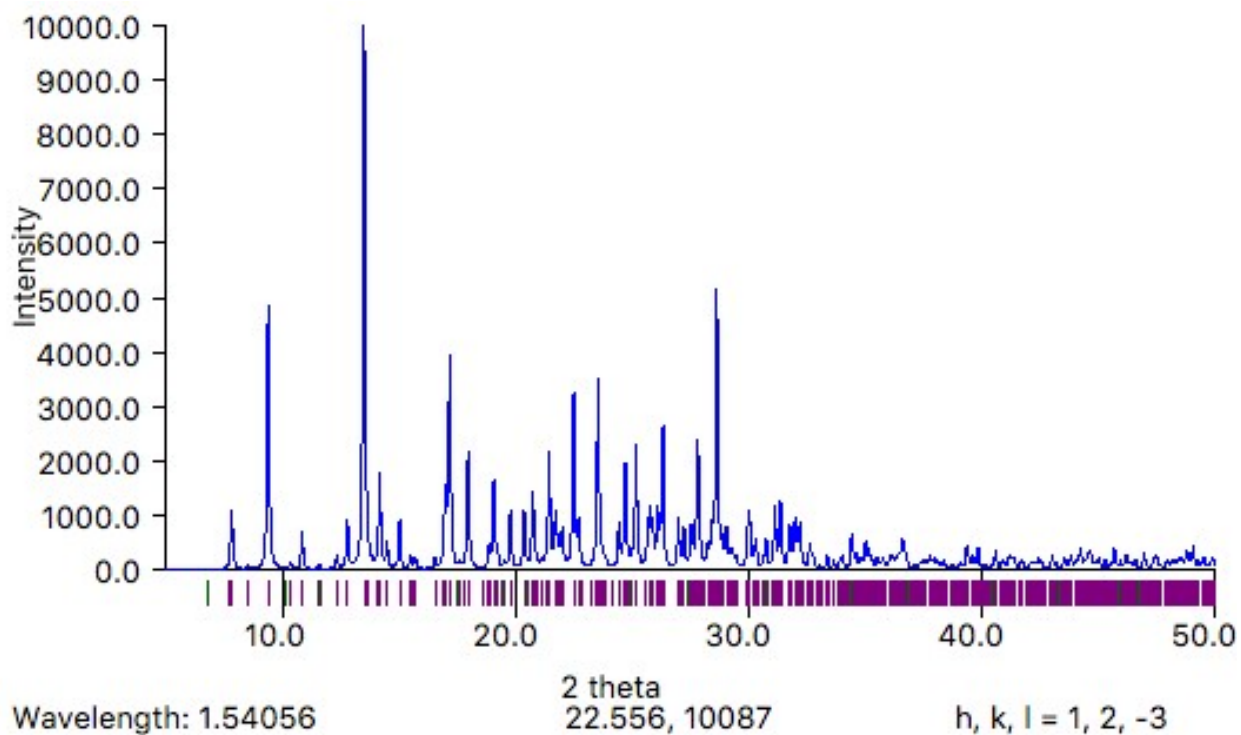


Figure S 27: Powder x-ray diffraction **NaphO-Cl₆BsubPc** (Toluene:Heptane; CCDC deposit 2087099).

Table S 49. Crystal data and structure refinement for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**.

Identification code	d19200_a	
Empirical formula	C ₃₄ H ₁₃ B Cl ₆ N ₆ O	
Formula weight	745.01	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.4162(2) Å	α = 90°.
	b = 22.7272(5) Å	β = 98.322(1)°.
	c = 13.1011(3) Å	γ = 90°.
Volume	3068.78(11) Å ³	
Z	4	
Density (calculated)	1.613 Mg/m ³	
Absorption coefficient	0.603 mm ⁻¹	
F(000)	1496	
Crystal size	0.230 x 0.170 x 0.110 mm ³	
Theta range for data collection	1.792 to 27.560°.	
Index ranges	-13<=h<=13, -29<=k<=29, -9<=l<=17	
Reflections collected	38079	
Independent reflections	7069 [R(int) = 0.0315]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6845	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7069 / 0 / 433	
Goodness-of-fit on F ²	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0814	
R indices (all data)	R1 = 0.0615, wR2 = 0.0950	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.407 and -0.415 e.Å ⁻³	

Table S 50. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	13888(1)	4561(1)	6108(1)	35(1)
Cl(2)	14027(1)	3317(1)	7174(1)	38(1)
Cl(3)	9333(1)	117(1)	3450(1)	39(1)
Cl(4)	7507(1)	337(1)	1356(1)	35(1)
Cl(5)	5754(1)	4634(1)	-1286(1)	33(1)
Cl(6)	7250(1)	5664(1)	2(1)	39(1)
O(1)	6141(1)	3407(1)	4704(1)	28(1)
N(1)	8469(2)	3449(1)	4728(1)	22(1)
N(2)	9072(2)	2458(1)	5140(1)	26(1)
N(3)	7336(2)	2671(1)	3789(1)	22(1)
N(4)	6499(2)	2836(1)	2016(1)	23(1)
N(5)	7148(2)	3634(1)	3140(1)	23(1)
N(6)	8689(2)	4347(1)	3836(1)	24(1)
C(1)	9094(2)	3962(1)	4587(2)	22(1)
C(2)	10351(2)	3920(1)	5241(2)	23(1)
C(3)	11410(2)	4299(1)	5374(2)	25(1)
C(4)	12541(2)	4105(1)	5963(2)	26(1)
C(5)	12623(2)	3543(1)	6414(2)	26(1)
C(6)	11591(2)	3155(1)	6253(2)	26(1)
C(7)	10444(2)	3348(1)	5669(2)	24(1)
C(8)	9262(2)	3036(1)	5257(2)	24(1)
C(9)	8172(2)	2286(1)	4354(2)	24(1)
C(10)	8133(2)	1751(1)	3759(2)	24(1)
C(11)	8787(2)	1219(1)	3954(2)	27(1)
C(12)	8605(2)	794(1)	3198(2)	27(1)
C(13)	7805(2)	898(1)	2251(2)	25(1)
C(14)	7194(2)	1432(1)	2032(2)	24(1)
C(15)	7352(2)	1862(1)	2794(2)	22(1)
C(16)	6927(2)	2472(1)	2806(2)	22(1)
C(17)	6666(2)	3415(1)	2188(2)	23(1)

C(18)	6698(2)	3910(1)	1477(2)	24(1)
C(19)	6233(2)	3986(1)	436(2)	25(1)
C(20)	6411(2)	4525(1)	-11(2)	27(1)
C(21)	7076(2)	4985(1)	559(2)	28(1)
C(22)	7564(2)	4913(1)	1592(2)	26(1)
C(23)	7363(2)	4376(1)	2050(2)	25(1)
C(24)	7743(2)	4164(1)	3098(2)	23(1)
C(25)	4891(2)	3225(1)	4334(2)	26(1)
C(26)	4458(2)	2691(1)	4720(2)	32(1)
C(27)	3214(2)	2504(1)	4414(2)	36(1)
C(28)	2354(2)	2840(1)	3714(2)	31(1)
C(29)	1049(2)	2655(1)	3368(2)	40(1)
C(30)	251(2)	2986(1)	2691(2)	44(1)
C(31)	682(3)	3521(1)	2325(2)	45(1)
C(32)	1920(3)	3713(1)	2639(2)	41(1)
C(33)	2779(2)	3375(1)	3332(2)	28(1)
C(34)	4088(2)	3562(1)	3668(2)	30(1)
B(1)	7180(2)	3294(1)	4122(2)	23(1)

Table S 51. Bond lengths [\AA] and angles [$^\circ$] for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**.

Cl(1)-C(4)	1.732(2)
Cl(2)-C(5)	1.725(2)
Cl(3)-C(12)	1.727(2)
Cl(4)-C(13)	1.730(2)
Cl(5)-C(20)	1.729(2)
Cl(6)-C(21)	1.728(2)
O(1)-C(25)	1.385(2)
O(1)-B(1)	1.434(3)
N(1)-C(1)	1.360(3)
N(1)-C(8)	1.370(3)
N(1)-B(1)	1.500(3)
N(2)-C(8)	1.335(3)
N(2)-C(9)	1.346(3)
N(3)-C(9)	1.372(3)
N(3)-C(16)	1.373(3)
N(3)-B(1)	1.498(3)
N(4)-C(17)	1.341(3)
N(4)-C(16)	1.350(3)
N(5)-C(24)	1.360(3)
N(5)-C(17)	1.369(3)
N(5)-B(1)	1.497(3)
N(6)-C(1)	1.339(3)
N(6)-C(24)	1.343(3)
C(1)-C(2)	1.461(3)
C(2)-C(3)	1.391(3)
C(2)-C(7)	1.415(3)
C(3)-C(4)	1.384(3)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.404(3)
C(5)-C(6)	1.384(3)
C(6)-C(7)	1.393(3)
C(6)-H(6A)	0.9300

C(7)-C(8)	1.454(3)
C(9)-C(10)	1.444(3)
C(10)-C(11)	1.392(3)
C(10)-C(15)	1.423(3)
C(11)-C(12)	1.376(3)
C(11)-H(11A)	0.9300
C(12)-C(13)	1.410(3)
C(13)-C(14)	1.381(3)
C(14)-C(15)	1.391(3)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.455(3)
C(17)-C(18)	1.464(3)
C(18)-C(19)	1.390(3)
C(18)-C(23)	1.421(3)
C(19)-C(20)	1.382(3)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.406(3)
C(21)-C(22)	1.385(3)
C(22)-C(23)	1.388(3)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.455(3)
C(25)-C(34)	1.355(3)
C(25)-C(26)	1.415(3)
C(26)-C(27)	1.367(3)
C(26)-H(26A)	0.9300
C(27)-C(28)	1.409(4)
C(27)-H(27A)	0.9300
C(28)-C(33)	1.412(3)
C(28)-C(29)	1.433(3)
C(29)-C(30)	1.354(4)
C(29)-H(29A)	0.9300
C(30)-C(31)	1.404(4)
C(30)-H(30A)	0.9300
C(31)-C(32)	1.367(4)
C(31)-H(31A)	0.9300
C(32)-C(33)	1.406(3)

C(32)-H(32A)	0.9300
C(33)-C(34)	1.435(3)
C(34)-H(34A)	0.9300
C(25)-O(1)-B(1)	120.27(16)
C(1)-N(1)-C(8)	112.95(17)
C(1)-N(1)-B(1)	122.66(18)
C(8)-N(1)-B(1)	122.27(19)
C(8)-N(2)-C(9)	116.67(19)
C(9)-N(3)-C(16)	112.56(18)
C(9)-N(3)-B(1)	122.14(17)
C(16)-N(3)-B(1)	123.50(18)
C(17)-N(4)-C(16)	116.83(18)
C(24)-N(5)-C(17)	113.22(18)
C(24)-N(5)-B(1)	122.63(17)
C(17)-N(5)-B(1)	123.67(18)
C(1)-N(6)-C(24)	116.54(19)
N(6)-C(1)-N(1)	123.64(18)
N(6)-C(1)-C(2)	129.3(2)
N(1)-C(1)-C(2)	105.70(18)
C(3)-C(2)-C(7)	120.87(19)
C(3)-C(2)-C(1)	131.3(2)
C(7)-C(2)-C(1)	107.25(18)
C(4)-C(3)-C(2)	117.9(2)
C(4)-C(3)-H(3A)	121.1
C(2)-C(3)-H(3A)	121.1
C(3)-C(4)-C(5)	121.3(2)
C(3)-C(4)-Cl(1)	118.75(18)
C(5)-C(4)-Cl(1)	119.93(16)
C(6)-C(5)-C(4)	121.2(2)
C(6)-C(5)-Cl(2)	118.21(18)
C(4)-C(5)-Cl(2)	120.58(17)
C(5)-C(6)-C(7)	117.9(2)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	120.7(2)

C(6)-C(7)-C(8)	131.6(2)
C(2)-C(7)-C(8)	107.12(18)
N(2)-C(8)-N(1)	123.23(18)
N(2)-C(8)-C(7)	128.7(2)
N(1)-C(8)-C(7)	105.71(19)
N(2)-C(9)-N(3)	123.1(2)
N(2)-C(9)-C(10)	128.3(2)
N(3)-C(9)-C(10)	106.20(17)
C(11)-C(10)-C(15)	121.3(2)
C(11)-C(10)-C(9)	131.1(2)
C(15)-C(10)-C(9)	107.29(19)
C(12)-C(11)-C(10)	117.6(2)
C(12)-C(11)-H(11A)	121.2
C(10)-C(11)-H(11A)	121.2
C(11)-C(12)-C(13)	121.2(2)
C(11)-C(12)-Cl(3)	118.49(17)
C(13)-C(12)-Cl(3)	120.25(18)
C(14)-C(13)-C(12)	121.7(2)
C(14)-C(13)-Cl(4)	118.27(17)
C(12)-C(13)-Cl(4)	119.97(18)
C(13)-C(14)-C(15)	117.76(19)
C(13)-C(14)-H(14A)	121.1
C(15)-C(14)-H(14A)	121.1
C(14)-C(15)-C(10)	120.3(2)
C(14)-C(15)-C(16)	132.31(19)
C(10)-C(15)-C(16)	107.24(18)
N(4)-C(16)-N(3)	122.77(19)
N(4)-C(16)-C(15)	130.01(19)
N(3)-C(16)-C(15)	105.62(18)
N(4)-C(17)-N(5)	122.13(19)
N(4)-C(17)-C(18)	131.30(19)
N(5)-C(17)-C(18)	105.16(18)
C(19)-C(18)-C(23)	120.0(2)
C(19)-C(18)-C(17)	133.1(2)
C(23)-C(18)-C(17)	106.92(18)
C(20)-C(19)-C(18)	118.5(2)

C(20)-C(19)-H(19A)	120.8
C(18)-C(19)-H(19A)	120.8
C(19)-C(20)-C(21)	121.3(2)
C(19)-C(20)-Cl(5)	118.48(17)
C(21)-C(20)-Cl(5)	120.16(18)
C(22)-C(21)-C(20)	121.0(2)
C(22)-C(21)-Cl(6)	118.10(18)
C(20)-C(21)-Cl(6)	120.90(18)
C(21)-C(22)-C(23)	117.9(2)
C(21)-C(22)-H(22A)	121.0
C(23)-C(22)-H(22A)	121.0
C(22)-C(23)-C(18)	121.3(2)
C(22)-C(23)-C(24)	131.4(2)
C(18)-C(23)-C(24)	107.25(19)
N(6)-C(24)-N(5)	122.46(19)
N(6)-C(24)-C(23)	130.4(2)
N(5)-C(24)-C(23)	105.59(18)
C(34)-C(25)-O(1)	121.2(2)
C(34)-C(25)-C(26)	121.1(2)
O(1)-C(25)-C(26)	117.6(2)
C(27)-C(26)-C(25)	119.9(2)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(26)-C(27)-C(28)	120.6(2)
C(26)-C(27)-H(27A)	119.7
C(28)-C(27)-H(27A)	119.7
C(27)-C(28)-C(33)	119.6(2)
C(27)-C(28)-C(29)	122.2(2)
C(33)-C(28)-C(29)	118.2(2)
C(30)-C(29)-C(28)	120.6(3)
C(30)-C(29)-H(29A)	119.7
C(28)-C(29)-H(29A)	119.7
C(29)-C(30)-C(31)	120.6(2)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(32)-C(31)-C(30)	120.5(3)

C(32)-C(31)-H(31A)	119.8
C(30)-C(31)-H(31A)	119.8
C(31)-C(32)-C(33)	120.4(3)
C(31)-C(32)-H(32A)	119.8
C(33)-C(32)-H(32A)	119.8
C(32)-C(33)-C(28)	119.8(2)
C(32)-C(33)-C(34)	121.6(2)
C(28)-C(33)-C(34)	118.7(2)
C(25)-C(34)-C(33)	120.0(2)
C(25)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
O(1)-B(1)-N(5)	116.04(19)
O(1)-B(1)-N(3)	116.55(19)
N(5)-B(1)-N(3)	103.19(17)
O(1)-B(1)-N(1)	111.28(17)
N(5)-B(1)-N(1)	103.87(18)
N(3)-B(1)-N(1)	104.50(18)

Symmetry transformations used to generate equivalent atoms:

Table S 52. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	23(1)	39(1)	40(1)	-4(1)	-2(1)	-9(1)
Cl(2)	22(1)	50(1)	38(1)	6(1)	-9(1)	-2(1)
Cl(3)	30(1)	31(1)	54(1)	3(1)	-2(1)	4(1)
Cl(4)	42(1)	31(1)	32(1)	-6(1)	9(1)	0(1)
Cl(5)	29(1)	47(1)	23(1)	3(1)	2(1)	11(1)
Cl(6)	41(1)	35(1)	40(1)	8(1)	6(1)	4(1)
O(1)	16(1)	45(1)	22(1)	-10(1)	1(1)	-2(1)
N(1)	18(1)	30(1)	19(1)	-4(1)	1(1)	0(1)
N(2)	22(1)	34(1)	20(1)	2(1)	0(1)	-5(1)
N(3)	16(1)	30(1)	19(1)	-2(1)	0(1)	-2(1)
N(4)	17(1)	29(1)	23(1)	-2(1)	0(1)	1(1)
N(5)	19(1)	28(1)	20(1)	-5(1)	-1(1)	2(1)
N(6)	20(1)	27(1)	24(1)	-7(1)	0(1)	2(1)
C(1)	18(1)	27(1)	22(1)	-7(1)	2(1)	1(1)
C(2)	19(1)	31(1)	20(1)	-6(1)	1(1)	0(1)
C(3)	24(1)	27(1)	24(1)	-6(1)	2(1)	-2(1)
C(4)	20(1)	34(1)	23(1)	-7(1)	1(1)	-5(1)
C(5)	18(1)	38(1)	22(1)	-3(1)	-1(1)	-1(1)
C(6)	22(1)	33(1)	21(1)	1(1)	0(1)	-1(1)
C(7)	20(1)	33(1)	17(1)	-4(1)	1(1)	-3(1)
C(8)	20(1)	35(1)	16(1)	-1(1)	1(1)	-2(1)
C(9)	18(1)	32(1)	21(1)	1(1)	2(1)	-5(1)
C(10)	17(1)	30(1)	23(1)	0(1)	3(1)	-6(1)
C(11)	19(1)	32(1)	28(1)	6(1)	-1(1)	-6(1)
C(12)	19(1)	28(1)	35(1)	4(1)	6(1)	-2(1)
C(13)	22(1)	30(1)	26(1)	-4(1)	7(1)	-5(1)
C(14)	21(1)	30(1)	20(1)	0(1)	5(1)	-4(1)
C(15)	17(1)	28(1)	22(1)	0(1)	4(1)	-4(1)
C(16)	14(1)	32(1)	21(1)	-5(1)	0(1)	-3(1)
C(17)	16(1)	32(1)	21(1)	-5(1)	1(1)	2(1)

C(18)	17(1)	30(1)	24(1)	-3(1)	1(1)	5(1)
C(19)	20(1)	32(1)	23(1)	-4(1)	1(1)	5(1)
C(20)	19(1)	39(1)	22(1)	-2(1)	4(1)	10(1)
C(21)	22(1)	31(1)	32(1)	2(1)	7(1)	7(1)
C(22)	18(1)	29(1)	31(1)	-2(1)	1(1)	3(1)
C(23)	17(1)	31(1)	26(1)	-5(1)	1(1)	6(1)
C(24)	17(1)	29(1)	24(1)	-6(1)	2(1)	4(1)
C(25)	17(1)	39(1)	21(1)	-10(1)	2(1)	1(1)
C(26)	29(1)	38(1)	29(1)	1(1)	3(1)	3(1)
C(27)	38(1)	35(1)	36(1)	0(1)	9(1)	-6(1)
C(28)	26(1)	40(1)	26(1)	-9(1)	7(1)	-1(1)
C(29)	29(1)	57(2)	37(1)	-14(1)	11(1)	-10(1)
C(30)	18(1)	76(2)	38(1)	-22(1)	3(1)	-2(1)
C(31)	30(1)	64(2)	39(1)	-10(1)	-5(1)	12(1)
C(32)	34(1)	44(2)	44(2)	2(1)	-2(1)	7(1)
C(33)	25(1)	35(1)	26(1)	-6(1)	3(1)	4(1)
C(34)	27(1)	33(1)	30(1)	-2(1)	4(1)	-2(1)
B(1)	17(1)	32(1)	20(1)	-5(1)	-2(1)	-1(1)

Table S 53. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**.

	x	y	z	U(eq)
H(3A)	11359	4672	5077	30
H(6A)	11661	2776	6526	31
H(11A)	9328	1153	4573	32
H(14A)	6694	1501	1396	28
H(19A)	5813	3681	49	30
H(22A)	8013	5215	1967	32
H(26A)	5019	2467	5183	39
H(27A)	2933	2153	4670	44
H(29A)	746	2304	3612	48
H(30A)	-591	2859	2466	53
H(31A)	122	3747	1864	54
H(32A)	2196	4068	2394	50
H(34A)	4385	3915	3428	36

Table S 54. Torsion angles [°] for **NaphO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087099)**.

C(24)-N(6)-C(1)-N(1)	-11.1(3)
C(24)-N(6)-C(1)-C(2)	153.8(2)
C(8)-N(1)-C(1)-N(6)	157.08(19)
B(1)-N(1)-C(1)-N(6)	-6.7(3)
C(8)-N(1)-C(1)-C(2)	-10.9(2)
B(1)-N(1)-C(1)-C(2)	-174.65(18)
N(6)-C(1)-C(2)-C(3)	9.7(4)
N(1)-C(1)-C(2)-C(3)	176.7(2)
N(6)-C(1)-C(2)-C(7)	-161.7(2)
N(1)-C(1)-C(2)-C(7)	5.4(2)
C(7)-C(2)-C(3)-C(4)	-1.9(3)
C(1)-C(2)-C(3)-C(4)	-172.2(2)
C(2)-C(3)-C(4)-C(5)	0.0(3)
C(2)-C(3)-C(4)-Cl(1)	178.10(16)
C(3)-C(4)-C(5)-C(6)	2.5(3)
Cl(1)-C(4)-C(5)-C(6)	-175.58(17)
C(3)-C(4)-C(5)-Cl(2)	-178.22(17)
Cl(1)-C(4)-C(5)-Cl(2)	3.7(3)
C(4)-C(5)-C(6)-C(7)	-3.0(3)
Cl(2)-C(5)-C(6)-C(7)	177.70(16)
C(5)-C(6)-C(7)-C(2)	1.1(3)
C(5)-C(6)-C(7)-C(8)	171.3(2)
C(3)-C(2)-C(7)-C(6)	1.3(3)
C(1)-C(2)-C(7)-C(6)	173.78(19)
C(3)-C(2)-C(7)-C(8)	-170.99(19)
C(1)-C(2)-C(7)-C(8)	1.5(2)
C(9)-N(2)-C(8)-N(1)	10.0(3)
C(9)-N(2)-C(8)-C(7)	-149.9(2)
C(1)-N(1)-C(8)-N(2)	-152.0(2)
B(1)-N(1)-C(8)-N(2)	11.8(3)
C(1)-N(1)-C(8)-C(7)	11.8(2)
B(1)-N(1)-C(8)-C(7)	175.66(18)
C(6)-C(7)-C(8)-N(2)	-16.2(4)

C(2)-C(7)-C(8)-N(2)	154.9(2)
C(6)-C(7)-C(8)-N(1)	-178.9(2)
C(2)-C(7)-C(8)-N(1)	-7.7(2)
C(8)-N(2)-C(9)-N(3)	-9.9(3)
C(8)-N(2)-C(9)-C(10)	149.9(2)
C(16)-N(3)-C(9)-N(2)	153.1(2)
B(1)-N(3)-C(9)-N(2)	-12.1(3)
C(16)-N(3)-C(9)-C(10)	-10.5(2)
B(1)-N(3)-C(9)-C(10)	-175.69(18)
N(2)-C(9)-C(10)-C(11)	17.1(4)
N(3)-C(9)-C(10)-C(11)	179.6(2)
N(2)-C(9)-C(10)-C(15)	-156.7(2)
N(3)-C(9)-C(10)-C(15)	5.7(2)
C(15)-C(10)-C(11)-C(12)	-2.9(3)
C(9)-C(10)-C(11)-C(12)	-176.1(2)
C(10)-C(11)-C(12)-C(13)	1.3(3)
C(10)-C(11)-C(12)-Cl(3)	-176.47(16)
C(11)-C(12)-C(13)-C(14)	1.4(3)
Cl(3)-C(12)-C(13)-C(14)	179.11(17)
C(11)-C(12)-C(13)-Cl(4)	-175.46(17)
Cl(3)-C(12)-C(13)-Cl(4)	2.2(3)
C(12)-C(13)-C(14)-C(15)	-2.4(3)
Cl(4)-C(13)-C(14)-C(15)	174.54(16)
C(13)-C(14)-C(15)-C(10)	0.7(3)
C(13)-C(14)-C(15)-C(16)	175.6(2)
C(11)-C(10)-C(15)-C(14)	2.0(3)
C(9)-C(10)-C(15)-C(14)	176.56(19)
C(11)-C(10)-C(15)-C(16)	-174.07(19)
C(9)-C(10)-C(15)-C(16)	0.5(2)
C(17)-N(4)-C(16)-N(3)	9.7(3)
C(17)-N(4)-C(16)-C(15)	-153.7(2)
C(9)-N(3)-C(16)-N(4)	-156.10(19)
B(1)-N(3)-C(16)-N(4)	8.9(3)
C(9)-N(3)-C(16)-C(15)	10.8(2)
B(1)-N(3)-C(16)-C(15)	175.72(18)
C(14)-C(15)-C(16)-N(4)	-16.4(4)

C(10)-C(15)-C(16)-N(4)	159.0(2)
C(14)-C(15)-C(16)-N(3)	178.1(2)
C(10)-C(15)-C(16)-N(3)	-6.6(2)
C(16)-N(4)-C(17)-N(5)	-5.3(3)
C(16)-N(4)-C(17)-C(18)	159.1(2)
C(24)-N(5)-C(17)-N(4)	154.21(19)
B(1)-N(5)-C(17)-N(4)	-18.0(3)
C(24)-N(5)-C(17)-C(18)	-13.7(2)
B(1)-N(5)-C(17)-C(18)	174.14(18)
N(4)-C(17)-C(18)-C(19)	20.8(4)
N(5)-C(17)-C(18)-C(19)	-172.9(2)
N(4)-C(17)-C(18)-C(23)	-158.8(2)
N(5)-C(17)-C(18)-C(23)	7.4(2)
C(23)-C(18)-C(19)-C(20)	-1.4(3)
C(17)-C(18)-C(19)-C(20)	179.0(2)
C(18)-C(19)-C(20)-C(21)	1.7(3)
C(18)-C(19)-C(20)-Cl(5)	-176.37(16)
C(19)-C(20)-C(21)-C(22)	-0.6(3)
Cl(5)-C(20)-C(21)-C(22)	177.44(17)
C(19)-C(20)-C(21)-Cl(6)	-178.07(16)
Cl(5)-C(20)-C(21)-Cl(6)	0.0(3)
C(20)-C(21)-C(22)-C(23)	-0.8(3)
Cl(6)-C(21)-C(22)-C(23)	176.70(16)
C(21)-C(22)-C(23)-C(18)	1.1(3)
C(21)-C(22)-C(23)-C(24)	-180.0(2)
C(19)-C(18)-C(23)-C(22)	0.0(3)
C(17)-C(18)-C(23)-C(22)	179.68(19)
C(19)-C(18)-C(23)-C(24)	-179.15(19)
C(17)-C(18)-C(23)-C(24)	0.5(2)
C(1)-N(6)-C(24)-N(5)	4.9(3)
C(1)-N(6)-C(24)-C(23)	-158.6(2)
C(17)-N(5)-C(24)-N(6)	-153.01(19)
B(1)-N(5)-C(24)-N(6)	19.3(3)
C(17)-N(5)-C(24)-C(23)	14.0(2)
B(1)-N(5)-C(24)-C(23)	-173.66(18)
C(22)-C(23)-C(24)-N(6)	-21.8(4)

C(18)-C(23)-C(24)-N(6)	157.2(2)
C(22)-C(23)-C(24)-N(5)	172.6(2)
C(18)-C(23)-C(24)-N(5)	-8.4(2)
B(1)-O(1)-C(25)-C(34)	-85.4(3)
B(1)-O(1)-C(25)-C(26)	98.0(2)
C(34)-C(25)-C(26)-C(27)	0.7(4)
O(1)-C(25)-C(26)-C(27)	177.2(2)
C(25)-C(26)-C(27)-C(28)	0.0(4)
C(26)-C(27)-C(28)-C(33)	-0.5(4)
C(26)-C(27)-C(28)-C(29)	179.4(2)
C(27)-C(28)-C(29)-C(30)	-179.6(2)
C(33)-C(28)-C(29)-C(30)	0.2(3)
C(28)-C(29)-C(30)-C(31)	-0.8(4)
C(29)-C(30)-C(31)-C(32)	0.6(4)
C(30)-C(31)-C(32)-C(33)	0.2(4)
C(31)-C(32)-C(33)-C(28)	-0.8(4)
C(31)-C(32)-C(33)-C(34)	179.3(2)
C(27)-C(28)-C(33)-C(32)	-179.6(2)
C(29)-C(28)-C(33)-C(32)	0.6(3)
C(27)-C(28)-C(33)-C(34)	0.3(3)
C(29)-C(28)-C(33)-C(34)	-179.6(2)
O(1)-C(25)-C(34)-C(33)	-177.25(19)
C(26)-C(25)-C(34)-C(33)	-0.8(3)
C(32)-C(33)-C(34)-C(25)	-179.8(2)
C(28)-C(33)-C(34)-C(25)	0.4(3)
C(25)-O(1)-B(1)-N(5)	69.6(3)
C(25)-O(1)-B(1)-N(3)	-52.3(3)
C(25)-O(1)-B(1)-N(1)	-171.98(19)
C(24)-N(5)-B(1)-O(1)	90.7(2)
C(17)-N(5)-B(1)-O(1)	-97.8(2)
C(24)-N(5)-B(1)-N(3)	-140.56(19)
C(17)-N(5)-B(1)-N(3)	30.9(3)
C(24)-N(5)-B(1)-N(1)	-31.7(3)
C(17)-N(5)-B(1)-N(1)	139.77(19)
C(9)-N(3)-B(1)-O(1)	-94.4(2)
C(16)-N(3)-B(1)-O(1)	102.0(2)

C(9)-N(3)-B(1)-N(5)	137.18(18)
C(16)-N(3)-B(1)-N(5)	-26.4(3)
C(9)-N(3)-B(1)-N(1)	28.8(3)
C(16)-N(3)-B(1)-N(1)	-134.74(19)
C(1)-N(1)-B(1)-O(1)	-99.9(2)
C(8)-N(1)-B(1)-O(1)	97.8(2)
C(1)-N(1)-B(1)-N(5)	25.6(3)
C(8)-N(1)-B(1)-N(5)	-136.65(19)
C(1)-N(1)-B(1)-N(3)	133.47(19)
C(8)-N(1)-B(1)-N(3)	-28.8(3)

Symmetry transformations used to generate equivalent atoms:

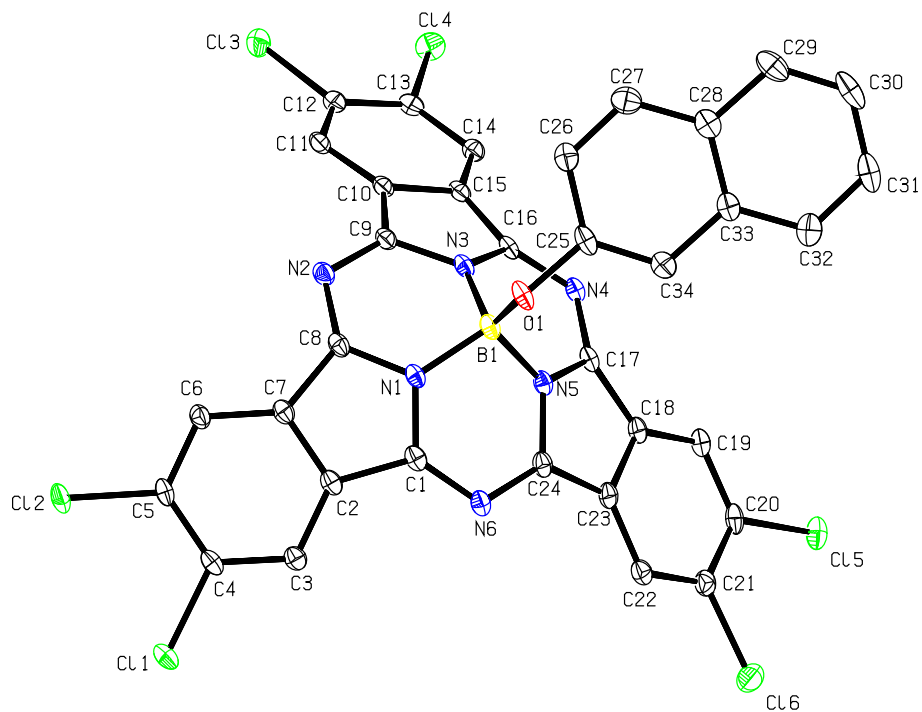


Figure S28: Anisotropic displacement ellipsoid plot of NaphO-Cl₆ BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101).

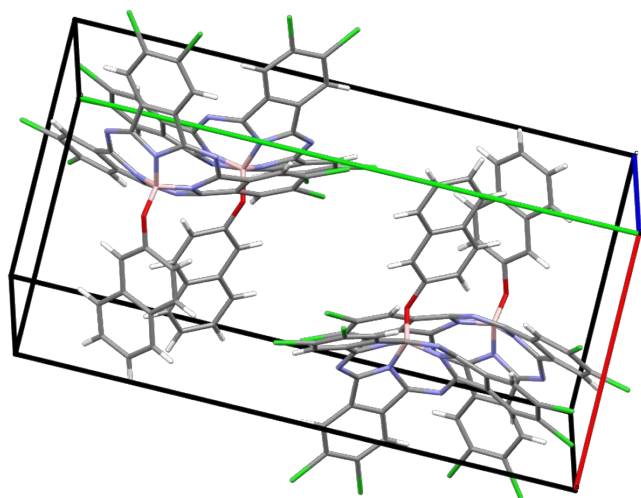


Figure S29: Populated unit cell of NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101).

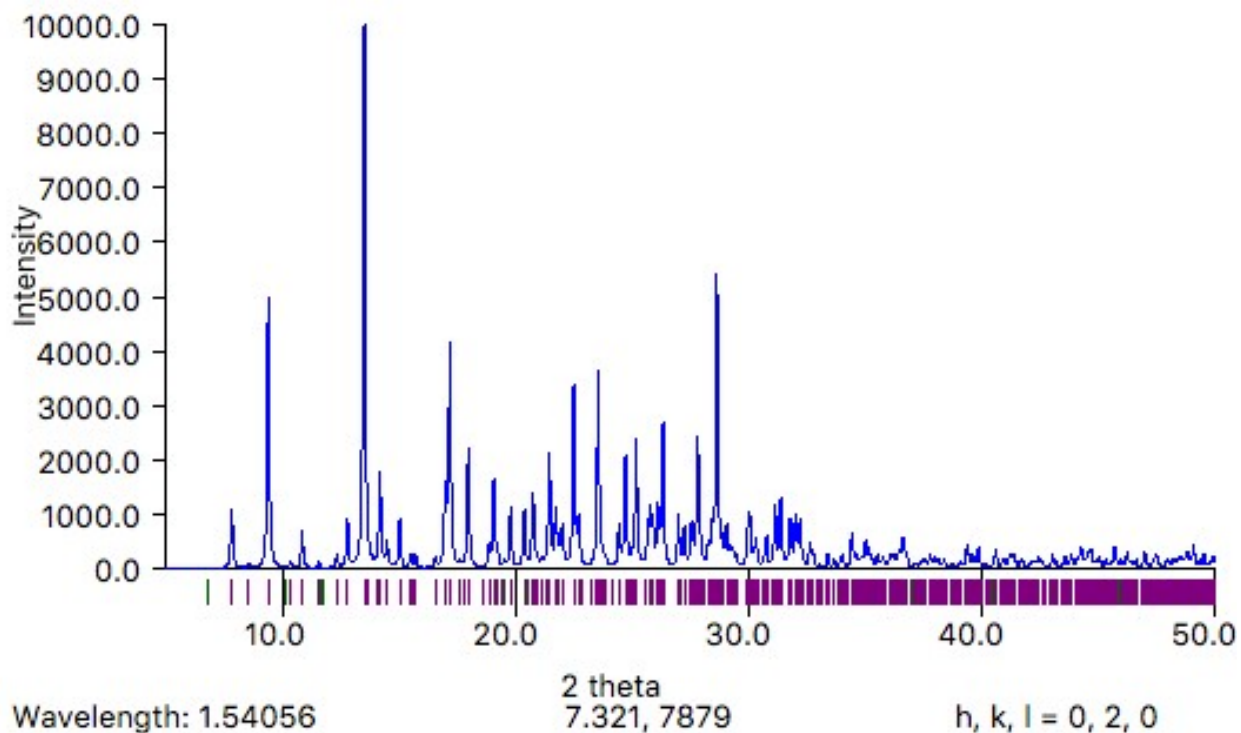


Figure S 30: Powder x-ray diffraction **NaphO-Cl₆BsubPc** (Chlorobenzene:Heptane; CCDC deposit 2087101).

Table S 55. Crystal data and structure refinement for NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101).

Identification code	d19210_a	
Empirical formula	C ₃₄ H ₁₃ B Cl ₆ N ₆ O	
Formula weight	745.01	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.4146(7) Å	α = 90°.
	b = 22.7238(13) Å	β = 98.340(2)°.
	c = 13.0926(9) Å	γ = 90°.
Volume	3065.7(3) Å ³	
Z	4	
Density (calculated)	1.614 Mg/m ³	
Absorption coefficient	0.603 mm ⁻¹	
F(000)	1496	
Crystal size	0.260 x 0.150 x 0.130 mm ³	
Theta range for data collection	1.792 to 27.579°.	
Index ranges	-13 ≤ h ≤ 13, -25 ≤ k ≤ 29, -17 ≤ l ≤ 16	
Reflections collected	51899	
Independent reflections	7075 [R(int) = 0.0875]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6837	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7075 / 0 / 433	
Goodness-of-fit on F ²	1.026	
Final R indices [I > 2σ(I)]	R1 = 0.0431, wR2 = 0.0819	
R indices (all data)	R1 = 0.1010, wR2 = 0.1028	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.434 and -0.442 e.Å ⁻³	

Table S 56. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	13889(1)	4561(1)	6108(1)	34(1)
Cl(2)	14028(1)	3317(1)	7174(1)	38(1)
Cl(3)	9334(1)	117(1)	3450(1)	40(1)
Cl(4)	7506(1)	337(1)	1355(1)	35(1)
Cl(5)	5753(1)	4634(1)	-1286(1)	33(1)
Cl(6)	7251(1)	5665(1)	2(1)	39(1)
O(1)	6140(2)	3408(1)	4705(1)	28(1)
N(1)	8468(2)	3450(1)	4726(2)	22(1)
N(2)	9074(2)	2458(1)	5141(2)	26(1)
N(3)	7337(2)	2671(1)	3790(2)	22(1)
N(4)	6499(2)	2836(1)	2016(2)	22(1)
N(5)	7149(2)	3634(1)	3140(2)	22(1)
N(6)	8689(2)	4348(1)	3836(2)	24(1)
C(1)	9097(3)	3962(1)	4588(2)	23(1)
C(2)	10353(3)	3919(1)	5241(2)	23(1)
C(3)	11411(3)	4297(1)	5378(2)	24(1)
C(4)	12540(3)	4105(1)	5963(2)	25(1)
C(5)	12623(3)	3543(1)	6413(2)	25(1)
C(6)	11591(3)	3157(1)	6251(2)	25(1)
C(7)	10449(3)	3346(1)	5668(2)	23(1)
C(8)	9263(3)	3039(1)	5259(2)	23(1)
C(9)	8171(3)	2287(1)	4355(2)	23(1)
C(10)	8130(2)	1751(1)	3760(2)	23(1)
C(11)	8783(3)	1219(1)	3951(2)	26(1)
C(12)	8605(3)	794(1)	3200(2)	27(1)
C(13)	7804(3)	898(1)	2251(2)	25(1)
C(14)	7198(3)	1431(1)	2036(2)	23(1)
C(15)	7351(2)	1863(1)	2797(2)	23(1)
C(16)	6926(2)	2472(1)	2806(2)	22(1)
C(17)	6662(2)	3415(1)	2188(2)	22(1)

C(18)	6696(2)	3909(1)	1474(2)	24(1)
C(19)	6232(3)	3986(1)	435(2)	25(1)
C(20)	6411(3)	4525(1)	-12(2)	27(1)
C(21)	7072(3)	4983(1)	562(2)	28(1)
C(22)	7563(3)	4912(1)	1590(2)	26(1)
C(23)	7364(2)	4376(1)	2050(2)	24(1)
C(24)	7746(3)	4162(1)	3092(2)	24(1)
C(25)	4889(3)	3228(1)	4334(2)	27(1)
C(26)	4452(3)	2691(1)	4717(2)	32(1)
C(27)	3211(3)	2505(1)	4415(3)	38(1)
C(28)	2359(3)	2839(1)	3713(2)	31(1)
C(29)	1047(3)	2656(2)	3367(3)	42(1)
C(30)	251(3)	2987(2)	2696(3)	44(1)
C(31)	682(3)	3518(2)	2328(3)	45(1)
C(32)	1923(3)	3710(2)	2641(3)	42(1)
C(33)	2772(3)	3378(1)	3329(2)	28(1)
C(34)	4092(3)	3564(1)	3671(2)	31(1)
B(1)	7177(3)	3294(1)	4118(2)	24(1)

Table S 57. Bond lengths [Å] and angles [°] for **NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101)**.

Cl(1)-C(4)	1.733(3)
Cl(2)-C(5)	1.725(3)
Cl(3)-C(12)	1.727(3)
Cl(4)-C(13)	1.730(3)
Cl(5)-C(20)	1.728(3)
Cl(6)-C(21)	1.736(3)
O(1)-C(25)	1.385(3)
O(1)-B(1)	1.437(4)
N(1)-C(1)	1.360(3)
N(1)-C(8)	1.371(3)
N(1)-B(1)	1.502(4)
N(2)-C(8)	1.341(3)
N(2)-C(9)	1.347(3)
N(3)-C(9)	1.370(3)
N(3)-C(16)	1.374(3)
N(3)-B(1)	1.497(4)
N(4)-C(17)	1.341(3)
N(4)-C(16)	1.349(3)
N(5)-C(24)	1.358(3)
N(5)-C(17)	1.370(3)
N(5)-B(1)	1.491(4)
N(6)-C(1)	1.341(3)
N(6)-C(24)	1.346(3)
C(1)-C(2)	1.459(4)
C(2)-C(3)	1.387(4)
C(2)-C(7)	1.414(4)
C(3)-C(4)	1.378(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.404(4)
C(5)-C(6)	1.380(4)
C(6)-C(7)	1.386(4)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.452(4)
C(9)-C(10)	1.443(4)
C(10)-C(11)	1.392(4)
C(10)-C(15)	1.421(4)
C(11)-C(12)	1.370(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.412(4)
C(13)-C(14)	1.376(4)
C(14)-C(15)	1.391(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.453(4)
C(17)-C(18)	1.465(4)
C(18)-C(19)	1.388(4)
C(18)-C(23)	1.423(4)
C(19)-C(20)	1.380(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.404(4)
C(21)-C(22)	1.379(4)
C(22)-C(23)	1.389(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.448(4)
C(25)-C(34)	1.348(4)
C(25)-C(26)	1.418(4)
C(26)-C(27)	1.362(4)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.403(4)
C(27)-H(27A)	0.9500
C(28)-C(33)	1.415(4)
C(28)-C(29)	1.438(4)
C(29)-C(30)	1.346(5)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.399(5)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.369(4)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.391(4)

C(32)-H(32A)	0.9500
C(33)-C(34)	1.445(4)
C(34)-H(34A)	0.9500
C(25)-O(1)-B(1)	120.1(2)
C(1)-N(1)-C(8)	112.6(2)
C(1)-N(1)-B(1)	122.9(2)
C(8)-N(1)-B(1)	122.5(2)
C(8)-N(2)-C(9)	116.5(2)
C(9)-N(3)-C(16)	112.6(2)
C(9)-N(3)-B(1)	122.4(2)
C(16)-N(3)-B(1)	123.3(2)
C(17)-N(4)-C(16)	117.0(2)
C(24)-N(5)-C(17)	112.9(2)
C(24)-N(5)-B(1)	123.0(2)
C(17)-N(5)-B(1)	123.6(2)
C(1)-N(6)-C(24)	116.5(2)
N(6)-C(1)-N(1)	123.4(2)
N(6)-C(1)-C(2)	129.5(3)
N(1)-C(1)-C(2)	105.9(2)
C(3)-C(2)-C(7)	120.6(2)
C(3)-C(2)-C(1)	131.5(3)
C(7)-C(2)-C(1)	107.4(2)
C(4)-C(3)-C(2)	118.3(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(3)
C(3)-C(4)-Cl(1)	119.0(2)
C(5)-C(4)-Cl(1)	119.9(2)
C(6)-C(5)-C(4)	121.0(2)
C(6)-C(5)-Cl(2)	118.4(2)
C(4)-C(5)-Cl(2)	120.5(2)
C(5)-C(6)-C(7)	118.3(3)
C(5)-C(6)-H(6A)	120.9
C(7)-C(6)-H(6A)	120.9
C(6)-C(7)-C(2)	120.7(2)

C(6)-C(7)-C(8)	132.0(3)
C(2)-C(7)-C(8)	106.9(2)
N(2)-C(8)-N(1)	123.0(2)
N(2)-C(8)-C(7)	128.3(2)
N(1)-C(8)-C(7)	106.2(2)
N(2)-C(9)-N(3)	123.1(2)
N(2)-C(9)-C(10)	128.2(2)
N(3)-C(9)-C(10)	106.3(2)
C(11)-C(10)-C(15)	121.1(3)
C(11)-C(10)-C(9)	131.4(3)
C(15)-C(10)-C(9)	107.2(2)
C(12)-C(11)-C(10)	118.1(3)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.1(3)
C(11)-C(12)-Cl(3)	118.7(2)
C(13)-C(12)-Cl(3)	120.2(2)
C(14)-C(13)-C(12)	121.4(3)
C(14)-C(13)-Cl(4)	118.6(2)
C(12)-C(13)-Cl(4)	119.9(2)
C(13)-C(14)-C(15)	118.3(3)
C(13)-C(14)-H(14A)	120.8
C(15)-C(14)-H(14A)	120.8
C(14)-C(15)-C(10)	120.0(3)
C(14)-C(15)-C(16)	132.4(3)
C(10)-C(15)-C(16)	107.4(2)
N(4)-C(16)-N(3)	122.7(2)
N(4)-C(16)-C(15)	130.2(2)
N(3)-C(16)-C(15)	105.5(2)
N(4)-C(17)-N(5)	122.0(2)
N(4)-C(17)-C(18)	131.3(3)
N(5)-C(17)-C(18)	105.2(2)
C(19)-C(18)-C(23)	120.0(3)
C(19)-C(18)-C(17)	133.3(3)
C(23)-C(18)-C(17)	106.8(2)
C(20)-C(19)-C(18)	118.5(3)

C(20)-C(19)-H(19A)	120.7
C(18)-C(19)-H(19A)	120.7
C(19)-C(20)-C(21)	121.1(3)
C(19)-C(20)-Cl(5)	118.5(2)
C(21)-C(20)-Cl(5)	120.3(2)
C(22)-C(21)-C(20)	121.3(3)
C(22)-C(21)-Cl(6)	118.0(2)
C(20)-C(21)-Cl(6)	120.7(2)
C(21)-C(22)-C(23)	117.9(3)
C(21)-C(22)-H(22A)	121.0
C(23)-C(22)-H(22A)	121.0
C(22)-C(23)-C(18)	121.1(3)
C(22)-C(23)-C(24)	131.7(3)
C(18)-C(23)-C(24)	107.2(2)
N(6)-C(24)-N(5)	122.3(2)
N(6)-C(24)-C(23)	130.4(3)
N(5)-C(24)-C(23)	106.0(2)
C(34)-C(25)-O(1)	121.2(3)
C(34)-C(25)-C(26)	121.0(3)
O(1)-C(25)-C(26)	117.7(3)
C(27)-C(26)-C(25)	120.2(3)
C(27)-C(26)-H(26A)	119.9
C(25)-C(26)-H(26A)	119.9
C(26)-C(27)-C(28)	120.4(3)
C(26)-C(27)-H(27A)	119.8
C(28)-C(27)-H(27A)	119.8
C(27)-C(28)-C(33)	120.3(3)
C(27)-C(28)-C(29)	122.2(3)
C(33)-C(28)-C(29)	117.5(3)
C(30)-C(29)-C(28)	120.8(3)
C(30)-C(29)-H(29A)	119.6
C(28)-C(29)-H(29A)	119.6
C(29)-C(30)-C(31)	120.6(3)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(32)-C(31)-C(30)	120.5(3)

C(32)-C(31)-H(31A)	119.7
C(30)-C(31)-H(31A)	119.7
C(31)-C(32)-C(33)	120.3(3)
C(31)-C(32)-H(32A)	119.8
C(33)-C(32)-H(32A)	119.8
C(32)-C(33)-C(28)	120.2(3)
C(32)-C(33)-C(34)	122.0(3)
C(28)-C(33)-C(34)	117.8(3)
C(25)-C(34)-C(33)	120.2(3)
C(25)-C(34)-H(34A)	119.9
C(33)-C(34)-H(34A)	119.9
O(1)-B(1)-N(5)	116.3(2)
O(1)-B(1)-N(3)	116.6(2)
N(5)-B(1)-N(3)	103.4(2)
O(1)-B(1)-N(1)	111.1(2)
N(5)-B(1)-N(1)	103.7(2)
N(3)-B(1)-N(1)	104.3(2)

Symmetry transformations used to generate equivalent atoms:

Table S 58. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	22(1)	39(1)	39(1)	-4(1)	-4(1)	-9(1)
Cl(2)	22(1)	50(1)	38(1)	6(1)	-11(1)	-2(1)
Cl(3)	30(1)	32(1)	55(1)	3(1)	-3(1)	4(1)
Cl(4)	42(1)	32(1)	32(1)	-6(1)	8(1)	1(1)
Cl(5)	29(1)	48(1)	23(1)	3(1)	1(1)	11(1)
Cl(6)	41(1)	36(1)	40(1)	9(1)	6(1)	5(1)
O(1)	15(1)	44(1)	22(1)	-9(1)	-1(1)	-1(1)
N(1)	17(1)	29(1)	18(1)	-3(1)	0(1)	-2(1)
N(2)	22(1)	32(1)	21(1)	2(1)	-1(1)	-5(1)
N(3)	16(1)	31(1)	18(1)	-2(1)	-1(1)	-4(1)
N(4)	16(1)	29(1)	21(1)	-4(1)	-1(1)	1(1)
N(5)	18(1)	26(1)	19(1)	-5(1)	-2(1)	1(1)
N(6)	20(1)	27(1)	24(1)	-5(1)	-1(1)	3(1)
C(1)	21(1)	28(2)	21(2)	-10(1)	2(1)	1(1)
C(2)	21(1)	29(2)	18(2)	-8(1)	1(1)	-1(1)
C(3)	25(2)	26(2)	21(2)	-5(1)	1(1)	-2(1)
C(4)	18(1)	33(2)	24(2)	-8(1)	1(1)	-4(1)
C(5)	18(1)	36(2)	20(2)	-4(1)	-4(1)	2(1)
C(6)	21(1)	33(2)	21(2)	2(1)	-2(1)	-3(1)
C(7)	21(1)	29(2)	18(2)	-4(1)	1(1)	-2(1)
C(8)	19(1)	34(2)	17(2)	-2(1)	1(1)	-3(1)
C(9)	18(1)	30(2)	21(2)	2(1)	2(1)	-4(1)
C(10)	17(1)	28(2)	23(2)	2(1)	1(1)	-5(1)
C(11)	18(1)	33(2)	26(2)	4(1)	-1(1)	-7(1)
C(12)	20(2)	26(2)	34(2)	3(1)	4(1)	-2(1)
C(13)	22(1)	28(2)	26(2)	-3(1)	7(1)	-5(1)
C(14)	22(1)	30(2)	18(2)	1(1)	2(1)	-4(1)
C(15)	16(1)	29(2)	22(2)	0(1)	3(1)	-6(1)
C(16)	13(1)	30(2)	21(2)	-5(1)	-1(1)	-3(1)
C(17)	15(1)	31(2)	21(2)	-6(1)	-1(1)	1(1)

C(18)	17(1)	29(2)	25(2)	-4(1)	1(1)	6(1)
C(19)	20(1)	33(2)	22(2)	-4(1)	-1(1)	6(1)
C(20)	16(1)	41(2)	24(2)	-2(1)	3(1)	11(1)
C(21)	20(1)	31(2)	32(2)	2(1)	4(1)	5(1)
C(22)	19(1)	28(2)	30(2)	-4(1)	1(1)	2(1)
C(23)	17(1)	27(2)	26(2)	-3(1)	2(1)	7(1)
C(24)	19(1)	26(2)	25(2)	-5(1)	1(1)	6(1)
C(25)	18(1)	42(2)	21(2)	-12(1)	2(1)	2(1)
C(26)	28(2)	38(2)	30(2)	0(1)	3(1)	3(1)
C(27)	39(2)	39(2)	37(2)	-2(2)	10(2)	-4(2)
C(28)	29(2)	39(2)	26(2)	-9(1)	6(1)	1(1)
C(29)	30(2)	59(2)	38(2)	-14(2)	12(2)	-11(2)
C(30)	18(2)	74(3)	39(2)	-26(2)	3(1)	-3(2)
C(31)	27(2)	67(3)	36(2)	-11(2)	-7(2)	12(2)
C(32)	37(2)	45(2)	42(2)	2(2)	1(2)	9(2)
C(33)	25(2)	35(2)	25(2)	-6(1)	2(1)	4(1)
C(34)	28(2)	36(2)	30(2)	-2(1)	4(1)	-2(1)
B(1)	19(2)	31(2)	20(2)	-4(1)	-1(1)	0(1)

Table S 59. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **NaphO-Cl₆BsubPc** (Chlorobenzene:Heptane; CCDC deposit 2087101).

	x	y	z	U(eq)
H(3A)	11358	4678	5076	29
H(6A)	11661	2771	6533	31
H(11A)	9336	1152	4584	31
H(14A)	6689	1502	1386	28
H(19A)	5801	3675	39	30
H(22A)	8024	5221	1973	31
H(26A)	5026	2461	5186	39
H(27A)	2921	2148	4680	46
H(29A)	738	2297	3614	50
H(30A)	-611	2858	2470	53
H(31A)	109	3748	1857	54
H(32A)	2205	4072	2386	50
H(34A)	4398	3924	3428	37

Table S 60. Torsion angles [°] for **NaphO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087101)**.

C(24)-N(6)-C(1)-N(1)	-11.8(4)
C(24)-N(6)-C(1)-C(2)	153.4(3)
C(8)-N(1)-C(1)-N(6)	157.5(3)
B(1)-N(1)-C(1)-N(6)	-6.5(4)
C(8)-N(1)-C(1)-C(2)	-10.6(3)
B(1)-N(1)-C(1)-C(2)	-174.6(2)
N(6)-C(1)-C(2)-C(3)	9.8(5)
N(1)-C(1)-C(2)-C(3)	176.9(3)
N(6)-C(1)-C(2)-C(7)	-161.6(3)
N(1)-C(1)-C(2)-C(7)	5.5(3)
C(7)-C(2)-C(3)-C(4)	-1.8(4)
C(1)-C(2)-C(3)-C(4)	-172.2(3)
C(2)-C(3)-C(4)-C(5)	-0.2(4)
C(2)-C(3)-C(4)-Cl(1)	177.9(2)
C(3)-C(4)-C(5)-C(6)	2.4(4)
Cl(1)-C(4)-C(5)-C(6)	-175.6(2)
C(3)-C(4)-C(5)-Cl(2)	-178.1(2)
Cl(1)-C(4)-C(5)-Cl(2)	3.8(3)
C(4)-C(5)-C(6)-C(7)	-2.6(4)
Cl(2)-C(5)-C(6)-C(7)	177.9(2)
C(5)-C(6)-C(7)-C(2)	0.6(4)
C(5)-C(6)-C(7)-C(8)	171.7(3)
C(3)-C(2)-C(7)-C(6)	1.6(4)
C(1)-C(2)-C(7)-C(6)	174.1(3)
C(3)-C(2)-C(7)-C(8)	-171.5(2)
C(1)-C(2)-C(7)-C(8)	1.0(3)
C(9)-N(2)-C(8)-N(1)	9.8(4)
C(9)-N(2)-C(8)-C(7)	-149.6(3)
C(1)-N(1)-C(8)-N(2)	-152.0(3)
B(1)-N(1)-C(8)-N(2)	12.1(4)
C(1)-N(1)-C(8)-C(7)	11.2(3)
B(1)-N(1)-C(8)-C(7)	175.4(2)
C(6)-C(7)-C(8)-N(2)	-17.0(5)

C(2)-C(7)-C(8)-N(2)	155.0(3)
C(6)-C(7)-C(8)-N(1)	-179.1(3)
C(2)-C(7)-C(8)-N(1)	-7.1(3)
C(8)-N(2)-C(9)-N(3)	-9.8(4)
C(8)-N(2)-C(9)-C(10)	150.1(3)
C(16)-N(3)-C(9)-N(2)	153.2(3)
B(1)-N(3)-C(9)-N(2)	-12.1(4)
C(16)-N(3)-C(9)-C(10)	-10.5(3)
B(1)-N(3)-C(9)-C(10)	-175.8(2)
N(2)-C(9)-C(10)-C(11)	16.8(5)
N(3)-C(9)-C(10)-C(11)	179.4(3)
N(2)-C(9)-C(10)-C(15)	-156.8(3)
N(3)-C(9)-C(10)-C(15)	5.8(3)
C(15)-C(10)-C(11)-C(12)	-3.0(4)
C(9)-C(10)-C(11)-C(12)	-175.8(3)
C(10)-C(11)-C(12)-C(13)	1.3(4)
C(10)-C(11)-C(12)-Cl(3)	-176.5(2)
C(11)-C(12)-C(13)-C(14)	1.4(4)
Cl(3)-C(12)-C(13)-C(14)	179.2(2)
C(11)-C(12)-C(13)-Cl(4)	-175.4(2)
Cl(3)-C(12)-C(13)-Cl(4)	2.3(3)
C(12)-C(13)-C(14)-C(15)	-2.5(4)
Cl(4)-C(13)-C(14)-C(15)	174.4(2)
C(13)-C(14)-C(15)-C(10)	0.8(4)
C(13)-C(14)-C(15)-C(16)	175.5(3)
C(11)-C(10)-C(15)-C(14)	2.0(4)
C(9)-C(10)-C(15)-C(14)	176.4(2)
C(11)-C(10)-C(15)-C(16)	-174.0(2)
C(9)-C(10)-C(15)-C(16)	0.4(3)
C(17)-N(4)-C(16)-N(3)	9.4(4)
C(17)-N(4)-C(16)-C(15)	-153.8(3)
C(9)-N(3)-C(16)-N(4)	-156.1(2)
B(1)-N(3)-C(16)-N(4)	9.1(4)
C(9)-N(3)-C(16)-C(15)	10.7(3)
B(1)-N(3)-C(16)-C(15)	175.8(2)
C(14)-C(15)-C(16)-N(4)	-16.3(5)

C(10)-C(15)-C(16)-N(4)	158.9(3)
C(14)-C(15)-C(16)-N(3)	178.3(3)
C(10)-C(15)-C(16)-N(3)	-6.4(3)
C(16)-N(4)-C(17)-N(5)	-4.8(4)
C(16)-N(4)-C(17)-C(18)	158.9(3)
C(24)-N(5)-C(17)-N(4)	153.8(2)
B(1)-N(5)-C(17)-N(4)	-18.6(4)
C(24)-N(5)-C(17)-C(18)	-13.6(3)
B(1)-N(5)-C(17)-C(18)	174.0(2)
N(4)-C(17)-C(18)-C(19)	21.3(5)
N(5)-C(17)-C(18)-C(19)	-173.0(3)
N(4)-C(17)-C(18)-C(23)	-158.5(3)
N(5)-C(17)-C(18)-C(23)	7.2(3)
C(23)-C(18)-C(19)-C(20)	-1.3(4)
C(17)-C(18)-C(19)-C(20)	178.9(3)
C(18)-C(19)-C(20)-C(21)	1.4(4)
C(18)-C(19)-C(20)-Cl(5)	-176.4(2)
C(19)-C(20)-C(21)-C(22)	-0.2(4)
Cl(5)-C(20)-C(21)-C(22)	177.6(2)
C(19)-C(20)-C(21)-Cl(6)	-178.2(2)
Cl(5)-C(20)-C(21)-Cl(6)	-0.4(3)
C(20)-C(21)-C(22)-C(23)	-1.1(4)
Cl(6)-C(21)-C(22)-C(23)	176.9(2)
C(21)-C(22)-C(23)-C(18)	1.2(4)
C(21)-C(22)-C(23)-C(24)	179.8(3)
C(19)-C(18)-C(23)-C(22)	0.0(4)
C(17)-C(18)-C(23)-C(22)	179.9(2)
C(19)-C(18)-C(23)-C(24)	-178.9(2)
C(17)-C(18)-C(23)-C(24)	0.9(3)
C(1)-N(6)-C(24)-N(5)	5.9(4)
C(1)-N(6)-C(24)-C(23)	-159.0(3)
C(17)-N(5)-C(24)-N(6)	-153.8(2)
B(1)-N(5)-C(24)-N(6)	18.6(4)
C(17)-N(5)-C(24)-C(23)	14.3(3)
B(1)-N(5)-C(24)-C(23)	-173.3(2)
C(22)-C(23)-C(24)-N(6)	-20.8(5)

C(18)-C(23)-C(24)-N(6)	158.0(3)
C(22)-C(23)-C(24)-N(5)	172.4(3)
C(18)-C(23)-C(24)-N(5)	-8.8(3)
B(1)-O(1)-C(25)-C(34)	-85.2(3)
B(1)-O(1)-C(25)-C(26)	98.0(3)
C(34)-C(25)-C(26)-C(27)	0.3(5)
O(1)-C(25)-C(26)-C(27)	177.1(3)
C(25)-C(26)-C(27)-C(28)	0.7(5)
C(26)-C(27)-C(28)-C(33)	-1.3(5)
C(26)-C(27)-C(28)-C(29)	179.4(3)
C(27)-C(28)-C(29)-C(30)	179.8(3)
C(33)-C(28)-C(29)-C(30)	0.4(5)
C(28)-C(29)-C(30)-C(31)	-0.5(5)
C(29)-C(30)-C(31)-C(32)	0.3(5)
C(30)-C(31)-C(32)-C(33)	0.0(5)
C(31)-C(32)-C(33)-C(28)	-0.1(5)
C(31)-C(32)-C(33)-C(34)	179.5(3)
C(27)-C(28)-C(33)-C(32)	-179.5(3)
C(29)-C(28)-C(33)-C(32)	-0.1(4)
C(27)-C(28)-C(33)-C(34)	0.9(4)
C(29)-C(28)-C(33)-C(34)	-179.7(3)
O(1)-C(25)-C(34)-C(33)	-177.3(2)
C(26)-C(25)-C(34)-C(33)	-0.7(4)
C(32)-C(33)-C(34)-C(25)	-179.5(3)
C(28)-C(33)-C(34)-C(25)	0.1(4)
C(25)-O(1)-B(1)-N(5)	69.6(3)
C(25)-O(1)-B(1)-N(3)	-52.9(4)
C(25)-O(1)-B(1)-N(1)	-172.1(2)
C(24)-N(5)-B(1)-O(1)	90.7(3)
C(17)-N(5)-B(1)-O(1)	-97.7(3)
C(24)-N(5)-B(1)-N(3)	-140.1(2)
C(17)-N(5)-B(1)-N(3)	31.5(3)
C(24)-N(5)-B(1)-N(1)	-31.5(3)
C(17)-N(5)-B(1)-N(1)	140.1(2)
C(9)-N(3)-B(1)-O(1)	-94.0(3)
C(16)-N(3)-B(1)-O(1)	102.2(3)

C(9)-N(3)-B(1)-N(5)	137.0(2)
C(16)-N(3)-B(1)-N(5)	-26.7(3)
C(9)-N(3)-B(1)-N(1)	28.8(3)
C(16)-N(3)-B(1)-N(1)	-134.9(2)
C(1)-N(1)-B(1)-O(1)	-100.0(3)
C(8)-N(1)-B(1)-O(1)	97.5(3)
C(1)-N(1)-B(1)-N(5)	25.6(3)
C(8)-N(1)-B(1)-N(5)	-136.8(2)
C(1)-N(1)-B(1)-N(3)	133.6(3)
C(8)-N(1)-B(1)-N(3)	-28.9(3)

Symmetry transformations used to generate equivalent atoms:

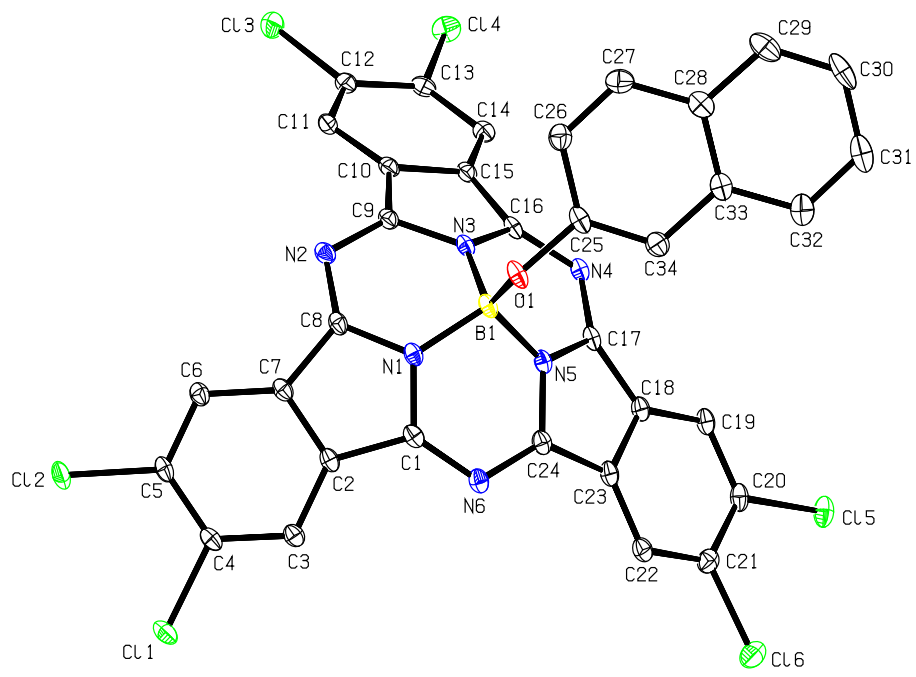


Figure S31: Anisotropic displacement ellipsoid plot of **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**.

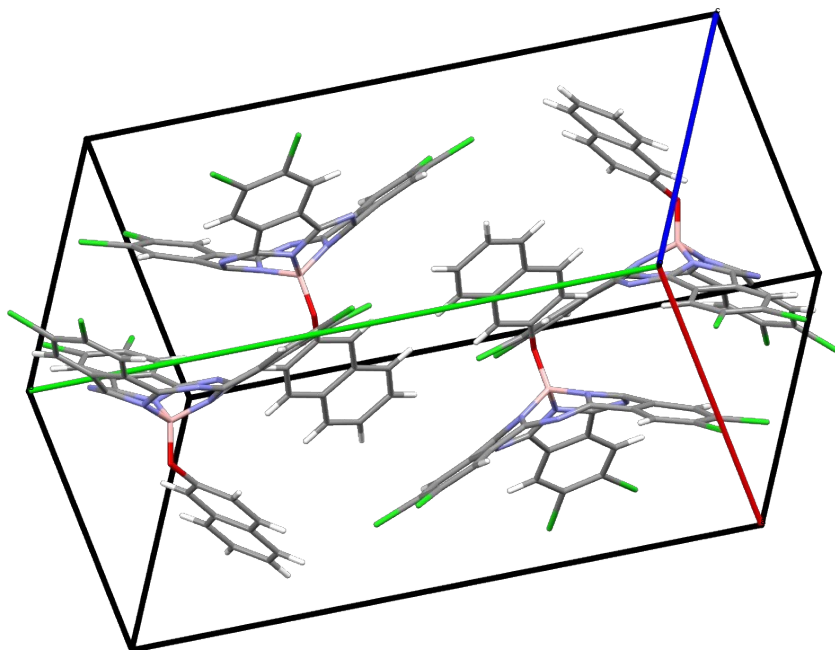


Figure S32: Populated unit cell of **NaphO-Cl₆BsubPc** (Dichlorobenzene:Heptane; CCDC deposit 2087104).

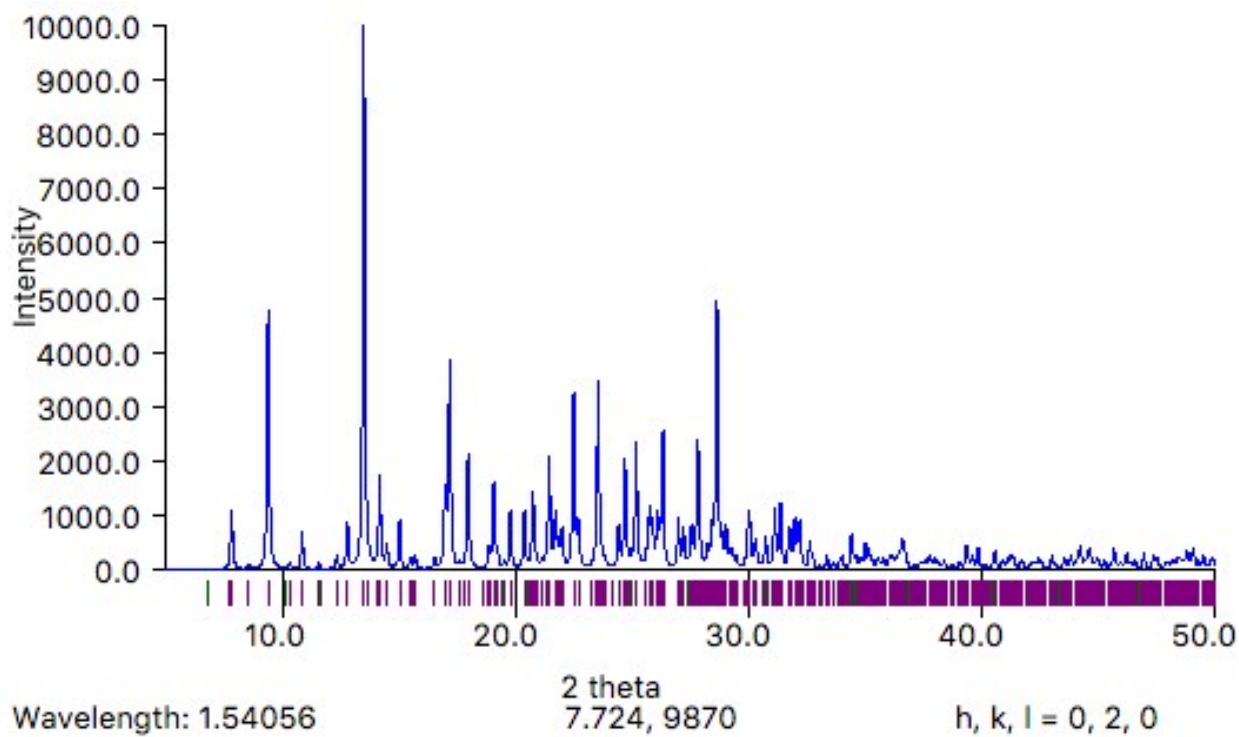


Figure S33: Powder x-ray diffraction **NaphO-Cl₆BsubPc** (Dichlorobenzene:Heptane; CCDC deposit 2087104).

Table S 61. Crystal data and structure refinement for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**.

Identification code	d19218_a	
Empirical formula	C ₃₄ H ₁₃ B Cl ₆ N ₆ O	
Formula weight	745.01	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.4152(3) Å	α = 90°.
	b = 22.7421(7) Å	β = 98.286(1)°.
	c = 13.1005(4) Å	γ = 90°.
Volume	3070.64(16) Å ³	
Z	4	
Density (calculated)	1.612 Mg/m ³	
Absorption coefficient	0.602 mm ⁻¹	
F(000)	1496	
Crystal size	0.220 x 0.160 x 0.120 mm ³	
Theta range for data collection	1.791 to 27.536°.	
Index ranges	-13 ≤ h ≤ 9, -29 ≤ k ≤ 29, -17 ≤ l ≤ 17	
Reflections collected	44864	
Independent reflections	7072 [R(int) = 0.0355]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7094	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7072 / 0 / 433	
Goodness-of-fit on F ²	1.024	
Final R indices [I > 2σ(I)]	R1 = 0.0327, wR2 = 0.0745	
R indices (all data)	R1 = 0.0504, wR2 = 0.0829	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.543 and -0.408 e.Å ⁻³	

Table S 62. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	13885(1)	4560(1)	6105(1)	31(1)
Cl(2)	14020(1)	3318(1)	7176(1)	34(1)
Cl(3)	9330(1)	122(1)	3451(1)	35(1)
Cl(4)	7503(1)	341(1)	1355(1)	31(1)
Cl(5)	5751(1)	4635(1)	-1288(1)	30(1)
Cl(6)	7248(1)	5665(1)	0(1)	35(1)
O(1)	6134(1)	3411(1)	4700(1)	25(1)
N(1)	8461(1)	3452(1)	4725(1)	20(1)
N(2)	9063(2)	2462(1)	5140(1)	22(1)
N(3)	7331(1)	2672(1)	3787(1)	19(1)
N(4)	6496(1)	2839(1)	2014(1)	20(1)
N(5)	7144(1)	3635(1)	3137(1)	19(1)
N(6)	8686(2)	4349(1)	3832(1)	22(1)
C(1)	9091(2)	3964(1)	4586(1)	20(1)
C(2)	10346(2)	3921(1)	5239(1)	20(1)
C(3)	11406(2)	4300(1)	5370(1)	22(1)
C(4)	12535(2)	4105(1)	5960(1)	22(1)
C(5)	12617(2)	3544(1)	6414(1)	23(1)
C(6)	11581(2)	3156(1)	6254(1)	22(1)
C(7)	10438(2)	3349(1)	5666(1)	20(1)
C(8)	9257(2)	3039(1)	5256(1)	20(1)
C(9)	8164(2)	2291(1)	4354(1)	21(1)
C(10)	8124(2)	1754(1)	3759(1)	21(1)
C(11)	8777(2)	1224(1)	3954(1)	23(1)
C(12)	8597(2)	797(1)	3198(2)	24(1)
C(13)	7800(2)	901(1)	2250(1)	22(1)
C(14)	7189(2)	1434(1)	2033(1)	21(1)
C(15)	7344(2)	1866(1)	2795(1)	20(1)
C(16)	6919(2)	2474(1)	2805(1)	20(1)
C(17)	6660(2)	3416(1)	2185(1)	20(1)

C(18)	6693(2)	3911(1)	1476(1)	21(1)
C(19)	6229(2)	3986(1)	432(1)	22(1)
C(20)	6409(2)	4527(1)	-14(1)	24(1)
C(21)	7072(2)	4985(1)	557(2)	25(1)
C(22)	7561(2)	4913(1)	1589(2)	24(1)
C(23)	7361(2)	4378(1)	2047(1)	22(1)
C(24)	7740(2)	4165(1)	3096(1)	21(1)
C(25)	4883(2)	3228(1)	4333(1)	24(1)
C(26)	4449(2)	2693(1)	4718(2)	29(1)
C(27)	3207(2)	2508(1)	4413(2)	33(1)
C(28)	2349(2)	2843(1)	3712(2)	28(1)
C(29)	1039(2)	2659(1)	3366(2)	38(1)
C(30)	242(2)	2989(1)	2690(2)	41(1)
C(31)	676(2)	3524(1)	2319(2)	42(1)
C(32)	1914(2)	3714(1)	2636(2)	39(1)
C(33)	2770(2)	3380(1)	3329(1)	26(1)
C(34)	4082(2)	3565(1)	3669(2)	28(1)
B(1)	7172(2)	3296(1)	4119(2)	21(1)

Table S 63. Bond lengths [\AA] and angles [$^\circ$] for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**.

Cl(1)-C(4)	1.7340(18)
Cl(2)-C(5)	1.7243(18)
Cl(3)-C(12)	1.7255(19)
Cl(4)-C(13)	1.7286(18)
Cl(5)-C(20)	1.7294(19)
Cl(6)-C(21)	1.7294(19)
O(1)-C(25)	1.386(2)
O(1)-B(1)	1.434(2)
N(1)-C(1)	1.363(2)
N(1)-C(8)	1.372(2)
N(1)-B(1)	1.500(2)
N(2)-C(8)	1.335(2)
N(2)-C(9)	1.345(2)
N(3)-C(9)	1.367(2)
N(3)-C(16)	1.373(2)
N(3)-B(1)	1.501(3)
N(4)-C(17)	1.338(2)
N(4)-C(16)	1.351(2)
N(5)-C(24)	1.361(2)
N(5)-C(17)	1.370(2)
N(5)-B(1)	1.496(3)
N(6)-C(1)	1.341(2)
N(6)-C(24)	1.343(2)
C(1)-C(2)	1.459(2)
C(2)-C(3)	1.391(2)
C(2)-C(7)	1.413(3)
C(3)-C(4)	1.384(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.406(3)
C(5)-C(6)	1.384(3)
C(6)-C(7)	1.392(2)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.452(2)
C(9)-C(10)	1.447(3)
C(10)-C(11)	1.389(3)
C(10)-C(15)	1.422(2)
C(11)-C(12)	1.380(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.410(3)
C(13)-C(14)	1.380(3)
C(14)-C(15)	1.393(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.453(3)
C(17)-C(18)	1.463(3)
C(18)-C(19)	1.393(2)
C(18)-C(23)	1.421(3)
C(19)-C(20)	1.385(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.405(3)
C(21)-C(22)	1.384(3)
C(22)-C(23)	1.385(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.457(3)
C(25)-C(34)	1.353(3)
C(25)-C(26)	1.418(3)
C(26)-C(27)	1.365(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.410(3)
C(27)-H(27A)	0.9500
C(28)-C(33)	1.413(3)
C(28)-C(29)	1.436(3)
C(29)-C(30)	1.351(3)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.408(4)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.366(3)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.402(3)

C(32)-H(32A)	0.9500
C(33)-C(34)	1.437(3)
C(34)-H(34A)	0.9500
C(25)-O(1)-B(1)	120.29(14)
C(1)-N(1)-C(8)	112.65(14)
C(1)-N(1)-B(1)	122.79(15)
C(8)-N(1)-B(1)	122.46(15)
C(8)-N(2)-C(9)	116.67(16)
C(9)-N(3)-C(16)	112.94(15)
C(9)-N(3)-B(1)	122.02(15)
C(16)-N(3)-B(1)	123.27(15)
C(17)-N(4)-C(16)	116.98(15)
C(24)-N(5)-C(17)	113.36(15)
C(24)-N(5)-B(1)	122.52(15)
C(17)-N(5)-B(1)	123.69(15)
C(1)-N(6)-C(24)	116.49(16)
N(6)-C(1)-N(1)	123.41(16)
N(6)-C(1)-C(2)	129.53(17)
N(1)-C(1)-C(2)	105.70(15)
C(3)-C(2)-C(7)	120.93(16)
C(3)-C(2)-C(1)	131.10(17)
C(7)-C(2)-C(1)	107.41(15)
C(4)-C(3)-C(2)	117.76(17)
C(4)-C(3)-H(3A)	121.1
C(2)-C(3)-H(3A)	121.1
C(3)-C(4)-C(5)	121.42(17)
C(3)-C(4)-Cl(1)	118.75(15)
C(5)-C(4)-Cl(1)	119.79(14)
C(6)-C(5)-C(4)	121.02(17)
C(6)-C(5)-Cl(2)	118.37(15)
C(4)-C(5)-Cl(2)	120.60(14)
C(5)-C(6)-C(7)	117.97(17)
C(5)-C(6)-H(6A)	121.0
C(7)-C(6)-H(6A)	121.0
C(6)-C(7)-C(2)	120.81(16)

C(6)-C(7)-C(8)	131.59(17)
C(2)-C(7)-C(8)	107.11(15)
N(2)-C(8)-N(1)	122.96(16)
N(2)-C(8)-C(7)	128.76(17)
N(1)-C(8)-C(7)	105.90(15)
N(2)-C(9)-N(3)	123.36(16)
N(2)-C(9)-C(10)	128.26(17)
N(3)-C(9)-C(10)	106.01(15)
C(11)-C(10)-C(15)	121.40(17)
C(11)-C(10)-C(9)	131.15(17)
C(15)-C(10)-C(9)	107.15(16)
C(12)-C(11)-C(10)	117.78(17)
C(12)-C(11)-H(11A)	121.1
C(10)-C(11)-H(11A)	121.1
C(11)-C(12)-C(13)	121.01(17)
C(11)-C(12)-Cl(3)	118.52(15)
C(13)-C(12)-Cl(3)	120.44(15)
C(14)-C(13)-C(12)	121.64(17)
C(14)-C(13)-Cl(4)	118.38(14)
C(12)-C(13)-Cl(4)	119.89(15)
C(13)-C(14)-C(15)	117.98(17)
C(13)-C(14)-H(14A)	121.0
C(15)-C(14)-H(14A)	121.0
C(14)-C(15)-C(10)	120.11(17)
C(14)-C(15)-C(16)	132.32(17)
C(10)-C(15)-C(16)	107.42(15)
N(4)-C(16)-N(3)	122.78(16)
N(4)-C(16)-C(15)	130.12(16)
N(3)-C(16)-C(15)	105.39(15)
N(4)-C(17)-N(5)	122.08(16)
N(4)-C(17)-C(18)	131.41(16)
N(5)-C(17)-C(18)	105.05(15)
C(19)-C(18)-C(23)	119.91(17)
C(19)-C(18)-C(17)	132.98(17)
C(23)-C(18)-C(17)	107.11(15)
C(20)-C(19)-C(18)	118.29(17)

C(20)-C(19)-H(19A)	120.9
C(18)-C(19)-H(19A)	120.9
C(19)-C(20)-C(21)	121.36(17)
C(19)-C(20)-Cl(5)	118.34(15)
C(21)-C(20)-Cl(5)	120.27(15)
C(22)-C(21)-C(20)	120.95(17)
C(22)-C(21)-Cl(6)	118.21(15)
C(20)-C(21)-Cl(6)	120.81(15)
C(21)-C(22)-C(23)	118.07(18)
C(21)-C(22)-H(22A)	121.0
C(23)-C(22)-H(22A)	121.0
C(22)-C(23)-C(18)	121.40(17)
C(22)-C(23)-C(24)	131.45(17)
C(18)-C(23)-C(24)	107.15(16)
N(6)-C(24)-N(5)	122.62(16)
N(6)-C(24)-C(23)	130.23(17)
N(5)-C(24)-C(23)	105.53(15)
C(34)-C(25)-O(1)	121.07(18)
C(34)-C(25)-C(26)	121.10(18)
O(1)-C(25)-C(26)	117.74(17)
C(27)-C(26)-C(25)	119.90(19)
C(27)-C(26)-H(26A)	120.1
C(25)-C(26)-H(26A)	120.1
C(26)-C(27)-C(28)	120.59(19)
C(26)-C(27)-H(27A)	119.7
C(28)-C(27)-H(27A)	119.7
C(27)-C(28)-C(33)	119.91(18)
C(27)-C(28)-C(29)	122.2(2)
C(33)-C(28)-C(29)	117.9(2)
C(30)-C(29)-C(28)	120.8(2)
C(30)-C(29)-H(29A)	119.6
C(28)-C(29)-H(29A)	119.6
C(29)-C(30)-C(31)	120.5(2)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(32)-C(31)-C(30)	120.3(2)

C(32)-C(31)-H(31A)	119.8
C(30)-C(31)-H(31A)	119.8
C(31)-C(32)-C(33)	120.6(2)
C(31)-C(32)-H(32A)	119.7
C(33)-C(32)-H(32A)	119.7
C(32)-C(33)-C(28)	119.82(19)
C(32)-C(33)-C(34)	121.9(2)
C(28)-C(33)-C(34)	118.28(18)
C(25)-C(34)-C(33)	120.22(19)
C(25)-C(34)-H(34A)	119.9
C(33)-C(34)-H(34A)	119.9
O(1)-B(1)-N(5)	116.15(16)
O(1)-B(1)-N(1)	111.22(15)
N(5)-B(1)-N(1)	103.85(15)
O(1)-B(1)-N(3)	116.65(16)
N(5)-B(1)-N(3)	103.15(14)
N(1)-B(1)-N(3)	104.38(15)

Symmetry transformations used to generate equivalent atoms:

Table S 64. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	21(1)	36(1)	36(1)	-4(1)	-2(1)	-9(1)
Cl(2)	19(1)	46(1)	34(1)	6(1)	-9(1)	-2(1)
Cl(3)	27(1)	28(1)	49(1)	2(1)	-2(1)	4(1)
Cl(4)	39(1)	27(1)	28(1)	-6(1)	8(1)	0(1)
Cl(5)	27(1)	44(1)	19(1)	3(1)	2(1)	11(1)
Cl(6)	39(1)	32(1)	36(1)	9(1)	6(1)	5(1)
O(1)	14(1)	40(1)	19(1)	-10(1)	0(1)	-1(1)
N(1)	16(1)	27(1)	16(1)	-3(1)	1(1)	0(1)
N(2)	20(1)	30(1)	16(1)	1(1)	1(1)	-5(1)
N(3)	14(1)	27(1)	15(1)	-2(1)	0(1)	-2(1)
N(4)	15(1)	27(1)	18(1)	-2(1)	0(1)	0(1)
N(5)	16(1)	24(1)	17(1)	-4(1)	-1(1)	2(1)
N(6)	19(1)	24(1)	21(1)	-6(1)	0(1)	3(1)
C(1)	17(1)	24(1)	19(1)	-8(1)	3(1)	0(1)
C(2)	17(1)	26(1)	16(1)	-6(1)	0(1)	0(1)
C(3)	21(1)	24(1)	21(1)	-5(1)	1(1)	-2(1)
C(4)	17(1)	30(1)	20(1)	-6(1)	2(1)	-4(1)
C(5)	16(1)	34(1)	17(1)	-4(1)	-2(1)	-1(1)
C(6)	19(1)	30(1)	18(1)	-1(1)	0(1)	-1(1)
C(7)	18(1)	28(1)	15(1)	-4(1)	1(1)	-3(1)
C(8)	17(1)	30(1)	13(1)	-1(1)	1(1)	-2(1)
C(9)	17(1)	27(1)	17(1)	2(1)	2(1)	-4(1)
C(10)	16(1)	27(1)	20(1)	1(1)	2(1)	-6(1)
C(11)	16(1)	28(1)	24(1)	4(1)	-1(1)	-4(1)
C(12)	18(1)	24(1)	32(1)	4(1)	5(1)	-2(1)
C(13)	21(1)	25(1)	23(1)	-4(1)	7(1)	-5(1)
C(14)	20(1)	27(1)	17(1)	-1(1)	5(1)	-4(1)
C(15)	15(1)	26(1)	20(1)	1(1)	2(1)	-3(1)
C(16)	12(1)	29(1)	18(1)	-4(1)	0(1)	-3(1)
C(17)	14(1)	28(1)	17(1)	-4(1)	-1(1)	2(1)

C(18)	16(1)	26(1)	22(1)	-3(1)	1(1)	5(1)
C(19)	17(1)	29(1)	19(1)	-4(1)	0(1)	6(1)
C(20)	18(1)	36(1)	18(1)	-1(1)	3(1)	9(1)
C(21)	21(1)	26(1)	28(1)	4(1)	8(1)	6(1)
C(22)	17(1)	27(1)	27(1)	-2(1)	2(1)	3(1)
C(23)	16(1)	28(1)	22(1)	-3(1)	1(1)	5(1)
C(24)	17(1)	24(1)	22(1)	-5(1)	2(1)	4(1)
C(25)	16(1)	36(1)	18(1)	-10(1)	2(1)	1(1)
C(26)	28(1)	34(1)	25(1)	1(1)	3(1)	3(1)
C(27)	35(1)	32(1)	33(1)	2(1)	9(1)	-5(1)
C(28)	26(1)	36(1)	23(1)	-8(1)	8(1)	-2(1)
C(29)	28(1)	53(1)	35(1)	-14(1)	12(1)	-10(1)
C(30)	15(1)	71(2)	36(1)	-22(1)	3(1)	-2(1)
C(31)	27(1)	62(2)	36(1)	-10(1)	-4(1)	11(1)
C(32)	32(1)	44(1)	39(1)	1(1)	-1(1)	7(1)
C(33)	23(1)	33(1)	22(1)	-6(1)	4(1)	4(1)
C(34)	26(1)	30(1)	27(1)	-2(1)	4(1)	0(1)
B(1)	16(1)	28(1)	17(1)	-5(1)	-1(1)	-1(1)

Table S 65. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**.

	x	y	z	U(eq)
H(3A)	11355	4679	5064	26
H(6A)	11649	2771	6537	27
H(11A)	9329	1158	4586	28
H(14A)	6679	1505	1383	25
H(19A)	5801	3675	36	27
H(22A)	8020	5221	1973	28
H(26A)	5022	2463	5188	35
H(27A)	2918	2149	4675	40
H(29A)	730	2301	3615	45
H(30A)	-619	2860	2463	49
H(31A)	106	3754	1847	51
H(32A)	2197	4076	2383	46
H(34A)	4386	3926	3426	33

Table S 66. Torsion angles [°] for **NaphO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087104)**.

C(24)-N(6)-C(1)-N(1)	-11.0(2)
C(24)-N(6)-C(1)-C(2)	153.74(18)
C(8)-N(1)-C(1)-N(6)	157.10(16)
B(1)-N(1)-C(1)-N(6)	-6.8(3)
C(8)-N(1)-C(1)-C(2)	-10.72(19)
B(1)-N(1)-C(1)-C(2)	-174.58(15)
N(6)-C(1)-C(2)-C(3)	9.8(3)
N(1)-C(1)-C(2)-C(3)	176.61(18)
N(6)-C(1)-C(2)-C(7)	-161.44(17)
N(1)-C(1)-C(2)-C(7)	5.35(19)
C(7)-C(2)-C(3)-C(4)	-2.2(3)
C(1)-C(2)-C(3)-C(4)	-172.44(18)
C(2)-C(3)-C(4)-C(5)	0.1(3)
C(2)-C(3)-C(4)-Cl(1)	178.17(13)
C(3)-C(4)-C(5)-C(6)	2.4(3)
Cl(1)-C(4)-C(5)-C(6)	-175.66(14)
C(3)-C(4)-C(5)-Cl(2)	-178.21(14)
Cl(1)-C(4)-C(5)-Cl(2)	3.8(2)
C(4)-C(5)-C(6)-C(7)	-2.7(3)
Cl(2)-C(5)-C(6)-C(7)	177.88(14)
C(5)-C(6)-C(7)-C(2)	0.6(3)
C(5)-C(6)-C(7)-C(8)	171.40(18)
C(3)-C(2)-C(7)-C(6)	1.8(3)
C(1)-C(2)-C(7)-C(6)	174.16(16)
C(3)-C(2)-C(7)-C(8)	-170.96(16)
C(1)-C(2)-C(7)-C(8)	1.37(19)
C(9)-N(2)-C(8)-N(1)	10.3(2)
C(9)-N(2)-C(8)-C(7)	-149.67(18)
C(1)-N(1)-C(8)-N(2)	-152.24(16)
B(1)-N(1)-C(8)-N(2)	11.7(3)
C(1)-N(1)-C(8)-C(7)	11.60(19)
B(1)-N(1)-C(8)-C(7)	175.53(15)
C(6)-C(7)-C(8)-N(2)	-16.7(3)

C(2)-C(7)-C(8)-N(2)	155.03(17)
C(6)-C(7)-C(8)-N(1)	-179.26(18)
C(2)-C(7)-C(8)-N(1)	-7.55(19)
C(8)-N(2)-C(9)-N(3)	-10.1(2)
C(8)-N(2)-C(9)-C(10)	149.92(18)
C(16)-N(3)-C(9)-N(2)	153.30(16)
B(1)-N(3)-C(9)-N(2)	-12.0(3)
C(16)-N(3)-C(9)-C(10)	-10.49(19)
B(1)-N(3)-C(9)-C(10)	-175.80(15)
N(2)-C(9)-C(10)-C(11)	16.8(3)
N(3)-C(9)-C(10)-C(11)	179.48(18)
N(2)-C(9)-C(10)-C(15)	-156.91(17)
N(3)-C(9)-C(10)-C(15)	5.82(19)
C(15)-C(10)-C(11)-C(12)	-3.0(3)
C(9)-C(10)-C(11)-C(12)	-175.91(17)
C(10)-C(11)-C(12)-C(13)	1.4(3)
C(10)-C(11)-C(12)-Cl(3)	-176.61(13)
C(11)-C(12)-C(13)-C(14)	1.2(3)
Cl(3)-C(12)-C(13)-C(14)	179.23(14)
C(11)-C(12)-C(13)-Cl(4)	-175.51(14)
Cl(3)-C(12)-C(13)-Cl(4)	2.5(2)
C(12)-C(13)-C(14)-C(15)	-2.3(3)
Cl(4)-C(13)-C(14)-C(15)	174.52(13)
C(13)-C(14)-C(15)-C(10)	0.7(3)
C(13)-C(14)-C(15)-C(16)	175.56(18)
C(11)-C(10)-C(15)-C(14)	2.0(3)
C(9)-C(10)-C(15)-C(14)	176.40(15)
C(11)-C(10)-C(15)-C(16)	-174.04(16)
C(9)-C(10)-C(15)-C(16)	0.37(19)
C(17)-N(4)-C(16)-N(3)	9.2(2)
C(17)-N(4)-C(16)-C(15)	-153.63(18)
C(9)-N(3)-C(16)-N(4)	-155.78(16)
B(1)-N(3)-C(16)-N(4)	9.3(3)
C(9)-N(3)-C(16)-C(15)	10.66(19)
B(1)-N(3)-C(16)-C(15)	175.76(15)
C(14)-C(15)-C(16)-N(4)	-16.7(3)

C(10)-C(15)-C(16)-N(4)	158.69(18)
C(14)-C(15)-C(16)-N(3)	178.27(18)
C(10)-C(15)-C(16)-N(3)	-6.38(18)
C(16)-N(4)-C(17)-N(5)	-4.8(2)
C(16)-N(4)-C(17)-C(18)	159.23(18)
C(24)-N(5)-C(17)-N(4)	154.17(16)
B(1)-N(5)-C(17)-N(4)	-18.5(3)
C(24)-N(5)-C(17)-C(18)	-13.50(19)
B(1)-N(5)-C(17)-C(18)	173.85(15)
N(4)-C(17)-C(18)-C(19)	20.7(3)
N(5)-C(17)-C(18)-C(19)	-173.21(18)
N(4)-C(17)-C(18)-C(23)	-158.60(18)
N(5)-C(17)-C(18)-C(23)	7.45(19)
C(23)-C(18)-C(19)-C(20)	-1.6(3)
C(17)-C(18)-C(19)-C(20)	179.09(18)
C(18)-C(19)-C(20)-C(21)	1.7(3)
C(18)-C(19)-C(20)-Cl(5)	-176.22(13)
C(19)-C(20)-C(21)-C(22)	-0.4(3)
Cl(5)-C(20)-C(21)-C(22)	177.47(14)
C(19)-C(20)-C(21)-Cl(6)	-178.12(14)
Cl(5)-C(20)-C(21)-Cl(6)	-0.2(2)
C(20)-C(21)-C(22)-C(23)	-0.9(3)
Cl(6)-C(21)-C(22)-C(23)	176.80(13)
C(21)-C(22)-C(23)-C(18)	1.0(3)
C(21)-C(22)-C(23)-C(24)	-179.84(18)
C(19)-C(18)-C(23)-C(22)	0.3(3)
C(17)-C(18)-C(23)-C(22)	179.73(16)
C(19)-C(18)-C(23)-C(24)	-179.05(16)
C(17)-C(18)-C(23)-C(24)	0.39(19)
C(1)-N(6)-C(24)-N(5)	4.7(2)
C(1)-N(6)-C(24)-C(23)	-158.67(18)
C(17)-N(5)-C(24)-N(6)	-153.07(16)
B(1)-N(5)-C(24)-N(6)	19.7(3)
C(17)-N(5)-C(24)-C(23)	13.80(19)
B(1)-N(5)-C(24)-C(23)	-173.46(15)
C(22)-C(23)-C(24)-N(6)	-21.9(3)

C(18)-C(23)-C(24)-N(6)	157.33(18)
C(22)-C(23)-C(24)-N(5)	172.60(18)
C(18)-C(23)-C(24)-N(5)	-8.15(19)
B(1)-O(1)-C(25)-C(34)	-85.6(2)
B(1)-O(1)-C(25)-C(26)	97.7(2)
C(34)-C(25)-C(26)-C(27)	0.5(3)
O(1)-C(25)-C(26)-C(27)	177.19(17)
C(25)-C(26)-C(27)-C(28)	0.3(3)
C(26)-C(27)-C(28)-C(33)	-0.7(3)
C(26)-C(27)-C(28)-C(29)	179.35(19)
C(27)-C(28)-C(29)-C(30)	-179.7(2)
C(33)-C(28)-C(29)-C(30)	0.3(3)
C(28)-C(29)-C(30)-C(31)	-0.6(3)
C(29)-C(30)-C(31)-C(32)	0.3(3)
C(30)-C(31)-C(32)-C(33)	0.3(3)
C(31)-C(32)-C(33)-C(28)	-0.6(3)
C(31)-C(32)-C(33)-C(34)	179.4(2)
C(27)-C(28)-C(33)-C(32)	-179.74(19)
C(29)-C(28)-C(33)-C(32)	0.3(3)
C(27)-C(28)-C(33)-C(34)	0.3(3)
C(29)-C(28)-C(33)-C(34)	-179.72(17)
O(1)-C(25)-C(34)-C(33)	-177.44(16)
C(26)-C(25)-C(34)-C(33)	-0.9(3)
C(32)-C(33)-C(34)-C(25)	-179.49(19)
C(28)-C(33)-C(34)-C(25)	0.5(3)
C(25)-O(1)-B(1)-N(5)	69.8(2)
C(25)-O(1)-B(1)-N(1)	-171.75(16)
C(25)-O(1)-B(1)-N(3)	-52.2(2)
C(24)-N(5)-B(1)-O(1)	90.4(2)
C(17)-N(5)-B(1)-O(1)	-97.6(2)
C(24)-N(5)-B(1)-N(1)	-32.0(2)
C(17)-N(5)-B(1)-N(1)	139.99(16)
C(24)-N(5)-B(1)-N(3)	-140.67(16)
C(17)-N(5)-B(1)-N(3)	31.3(2)
C(1)-N(1)-B(1)-O(1)	-99.85(19)
C(8)-N(1)-B(1)-O(1)	97.8(2)

C(1)-N(1)-B(1)-N(5)	25.8(2)
C(8)-N(1)-B(1)-N(5)	-136.52(16)
C(1)-N(1)-B(1)-N(3)	133.55(16)
C(8)-N(1)-B(1)-N(3)	-28.8(2)
C(9)-N(3)-B(1)-O(1)	-94.3(2)
C(16)-N(3)-B(1)-O(1)	101.88(19)
C(9)-N(3)-B(1)-N(5)	137.08(16)
C(16)-N(3)-B(1)-N(5)	-26.7(2)
C(9)-N(3)-B(1)-N(1)	28.8(2)
C(16)-N(3)-B(1)-N(1)	-134.98(16)

Symmetry transformations used to generate equivalent atoms:

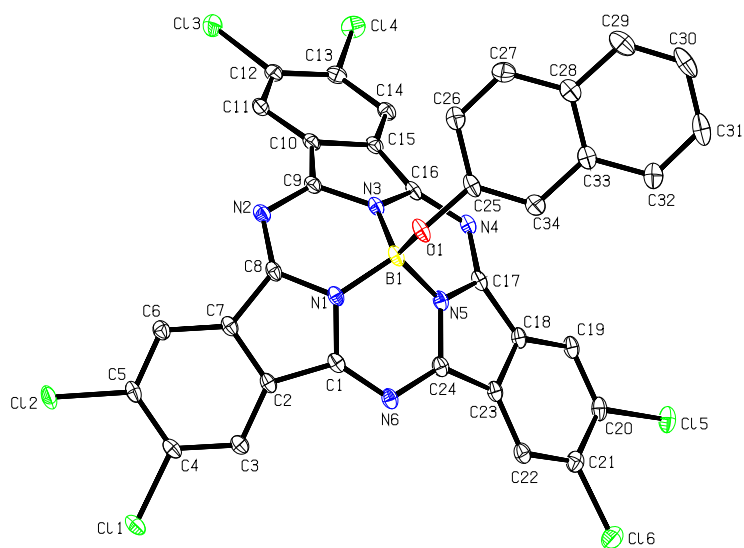


Figure S34: Anisotropic displacement ellipsoid plot of **NaphO-Cl₆ BsubPc** (**Dichlorobenzene:Dimethoxybenzene:Heptane**; CCDC deposit 2087102).

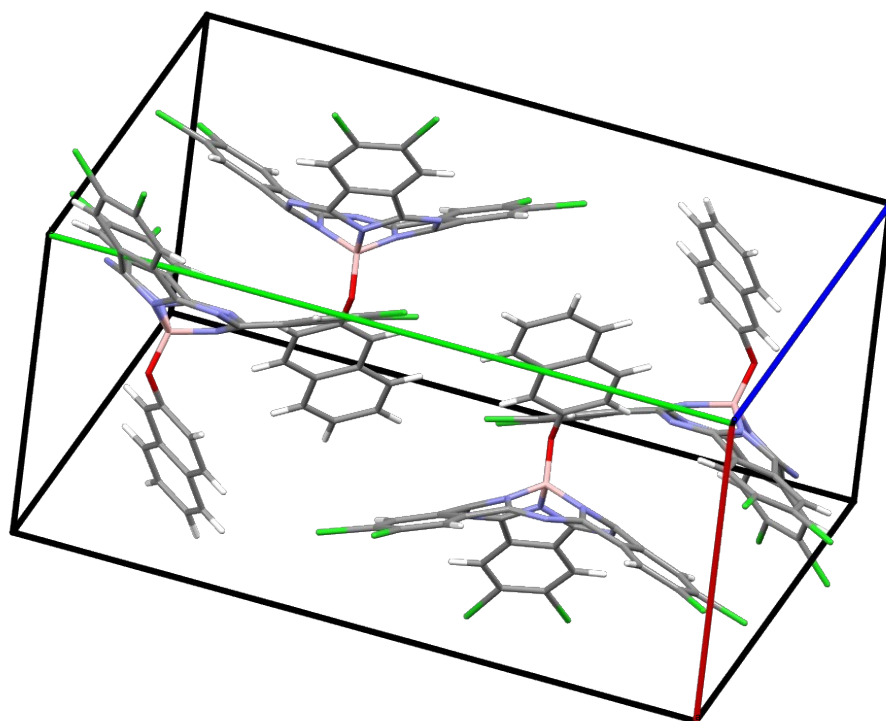


Figure S35: Populated unit cell of NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102).

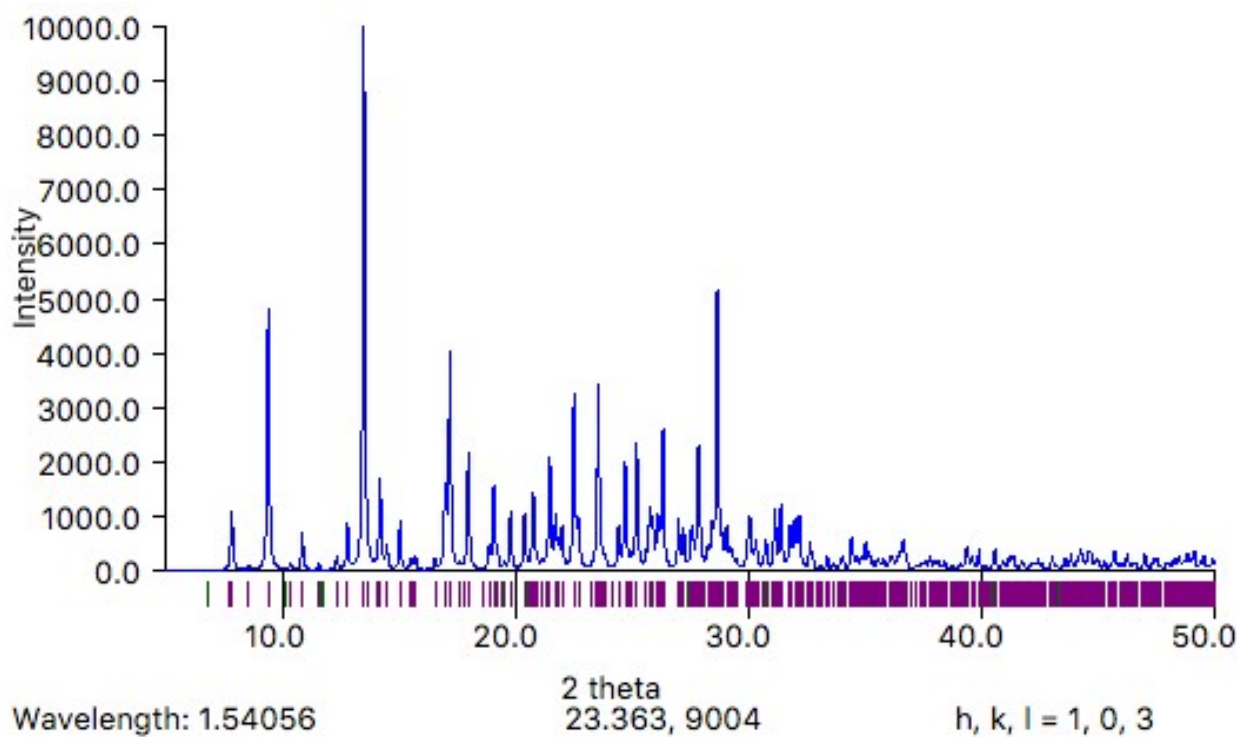


Figure S 36: Powder x-ray diffraction of NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102).

Table S 67. Crystal data and structure refinement for **NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102)**.

Identification code	d19208_a	
Empirical formula	C ₃₄ H ₁₃ B Cl ₆ N ₆ O	
Formula weight	745.01	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.4119(4) Å	α = 90°.
	b = 22.7476(9) Å	β = 98.274(1)°.
	c = 13.0866(5) Å	γ = 90°.
Volume	3067.2(2) Å ³	
Z	4	
Density (calculated)	1.613 Mg/m ³	
Absorption coefficient	0.603 mm ⁻¹	
F(000)	1496	
Crystal size	0.230 x 0.170 x 0.110 mm ³	
Theta range for data collection	1.790 to 27.548°.	
Index ranges	-13<=h<=11, -29<=k<=29, -17<=l<=15	
Reflections collected	46522	
Independent reflections	7066 [R(int) = 0.0483]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7207	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7066 / 0 / 433	
Goodness-of-fit on F ²	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0809	
R indices (all data)	R1 = 0.0666, wR2 = 0.0934	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.504 and -0.374 e.Å ⁻³	

Table S 68. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102)**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	13883(1)	4561(1)	6104(1)	33(1)
Cl(2)	14019(1)	3320(1)	7174(1)	36(1)
Cl(3)	9330(1)	123(1)	3449(1)	37(1)
Cl(4)	7502(1)	342(1)	1354(1)	33(1)
Cl(5)	5750(1)	4636(1)	-1292(1)	32(1)
Cl(6)	7249(1)	5665(1)	-3(1)	37(1)
O(1)	6133(1)	3410(1)	4699(1)	26(1)
N(1)	8460(2)	3452(1)	4724(1)	20(1)
N(2)	9065(2)	2461(1)	5138(1)	23(1)
N(3)	7333(2)	2673(1)	3785(1)	20(1)
N(4)	6496(2)	2840(1)	2012(1)	22(1)
N(5)	7142(2)	3637(1)	3135(1)	21(1)
N(6)	8684(2)	4349(1)	3831(1)	22(1)
C(1)	9094(2)	3964(1)	4586(2)	21(1)
C(2)	10344(2)	3921(1)	5237(2)	21(1)
C(3)	11404(2)	4299(1)	5370(2)	23(1)
C(4)	12534(2)	4106(1)	5958(2)	24(1)
C(5)	12614(2)	3545(1)	6411(2)	24(1)
C(6)	11582(2)	3158(1)	6251(2)	24(1)
C(7)	10437(2)	3351(1)	5663(2)	22(1)
C(8)	9256(2)	3040(1)	5255(2)	22(1)
C(9)	8164(2)	2291(1)	4351(2)	22(1)
C(10)	8127(2)	1756(1)	3758(2)	23(1)
C(11)	8777(2)	1225(1)	3951(2)	25(1)
C(12)	8596(2)	799(1)	3200(2)	25(1)
C(13)	7802(2)	903(1)	2248(2)	24(1)
C(14)	7191(2)	1435(1)	2034(2)	22(1)
C(15)	7345(2)	1866(1)	2792(2)	22(1)
C(16)	6920(2)	2476(1)	2805(2)	21(1)
C(17)	6657(2)	3417(1)	2184(2)	22(1)

C(18)	6694(2)	3912(1)	1473(2)	22(1)
C(19)	6229(2)	3988(1)	430(2)	24(1)
C(20)	6409(2)	4527(1)	-18(2)	26(1)
C(21)	7074(2)	4987(1)	554(2)	26(1)
C(22)	7562(2)	4912(1)	1586(2)	25(1)
C(23)	7361(2)	4378(1)	2045(2)	23(1)
C(24)	7737(2)	4166(1)	3093(2)	22(1)
C(25)	4883(2)	3230(1)	4330(2)	25(1)
C(26)	4447(2)	2694(1)	4714(2)	31(1)
C(27)	3206(2)	2509(1)	4409(2)	34(1)
C(28)	2348(2)	2845(1)	3709(2)	29(1)
C(29)	1040(2)	2660(1)	3363(2)	39(1)
C(30)	241(2)	2992(1)	2690(2)	42(1)
C(31)	676(3)	3525(1)	2320(2)	45(1)
C(32)	1916(3)	3716(1)	2634(2)	40(1)
C(33)	2773(2)	3380(1)	3329(2)	27(1)
C(34)	4082(2)	3567(1)	3668(2)	28(1)
B(1)	7171(2)	3297(1)	4116(2)	22(1)

Table S 69. Bond lengths [\AA] and angles [$^\circ$] for **NaphO-Cl₆BsubPc**
(Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102).

Cl(1)-C(4)	1.732(2)
Cl(2)-C(5)	1.726(2)
Cl(3)-C(12)	1.727(2)
Cl(4)-C(13)	1.728(2)
Cl(5)-C(20)	1.727(2)
Cl(6)-C(21)	1.727(2)
O(1)-C(25)	1.383(3)
O(1)-B(1)	1.434(3)
N(1)-C(1)	1.364(3)
N(1)-C(8)	1.372(3)
N(1)-B(1)	1.500(3)
N(2)-C(8)	1.337(3)
N(2)-C(9)	1.346(3)
N(3)-C(9)	1.367(3)
N(3)-C(16)	1.368(3)
N(3)-B(1)	1.501(3)
N(4)-C(17)	1.338(3)
N(4)-C(16)	1.352(3)
N(5)-C(24)	1.359(3)
N(5)-C(17)	1.368(3)
N(5)-B(1)	1.494(3)
N(6)-C(1)	1.343(3)
N(6)-C(24)	1.344(3)
C(1)-C(2)	1.453(3)
C(2)-C(3)	1.390(3)
C(2)-C(7)	1.409(3)
C(3)-C(4)	1.381(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.404(3)
C(5)-C(6)	1.382(3)
C(6)-C(7)	1.394(3)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.452(3)
C(9)-C(10)	1.442(3)
C(10)-C(11)	1.389(3)
C(10)-C(15)	1.424(3)
C(11)-C(12)	1.373(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.412(3)
C(13)-C(14)	1.378(3)
C(14)-C(15)	1.389(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.455(3)
C(17)-C(18)	1.464(3)
C(18)-C(19)	1.391(3)
C(18)-C(23)	1.421(3)
C(19)-C(20)	1.384(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.409(3)
C(21)-C(22)	1.384(3)
C(22)-C(23)	1.384(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.454(3)
C(25)-C(34)	1.350(3)
C(25)-C(26)	1.418(3)
C(26)-C(27)	1.362(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.409(3)
C(27)-H(27A)	0.9500
C(28)-C(33)	1.411(3)
C(28)-C(29)	1.435(3)
C(29)-C(30)	1.350(4)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.404(4)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.369(4)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.405(3)

C(32)-H(32A)	0.9500
C(33)-C(34)	1.436(3)
C(34)-H(34A)	0.9500
C(25)-O(1)-B(1)	120.26(17)
C(1)-N(1)-C(8)	112.45(17)
C(1)-N(1)-B(1)	122.90(18)
C(8)-N(1)-B(1)	122.52(19)
C(8)-N(2)-C(9)	116.50(19)
C(9)-N(3)-C(16)	112.84(18)
C(9)-N(3)-B(1)	122.26(18)
C(16)-N(3)-B(1)	123.22(18)
C(17)-N(4)-C(16)	116.97(18)
C(24)-N(5)-C(17)	113.42(18)
C(24)-N(5)-B(1)	122.66(18)
C(17)-N(5)-B(1)	123.48(19)
C(1)-N(6)-C(24)	116.65(19)
N(6)-C(1)-N(1)	123.10(18)
N(6)-C(1)-C(2)	129.7(2)
N(1)-C(1)-C(2)	105.93(18)
C(3)-C(2)-C(7)	120.8(2)
C(3)-C(2)-C(1)	131.3(2)
C(7)-C(2)-C(1)	107.38(18)
C(4)-C(3)-C(2)	118.1(2)
C(4)-C(3)-H(3A)	121.0
C(2)-C(3)-H(3A)	121.0
C(3)-C(4)-C(5)	121.2(2)
C(3)-C(4)-Cl(1)	118.94(18)
C(5)-C(4)-Cl(1)	119.88(16)
C(6)-C(5)-C(4)	121.2(2)
C(6)-C(5)-Cl(2)	118.24(18)
C(4)-C(5)-Cl(2)	120.55(17)
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)	131.4(2)
C(2)-C(7)-C(8)	107.25(18)
N(2)-C(8)-N(1)	123.08(19)
N(2)-C(8)-C(7)	128.7(2)
N(1)-C(8)-C(7)	105.75(19)
N(2)-C(9)-N(3)	123.3(2)
N(2)-C(9)-C(10)	128.0(2)
N(3)-C(9)-C(10)	106.23(18)
C(11)-C(10)-C(15)	121.1(2)
C(11)-C(10)-C(9)	131.5(2)
C(15)-C(10)-C(9)	107.19(19)
C(12)-C(11)-C(10)	118.0(2)
C(12)-C(11)-H(11A)	121.0
C(10)-C(11)-H(11A)	121.0
C(11)-C(12)-C(13)	121.1(2)
C(11)-C(12)-Cl(3)	118.74(18)
C(13)-C(12)-Cl(3)	120.11(18)
C(14)-C(13)-C(12)	121.4(2)
C(14)-C(13)-Cl(4)	118.50(17)
C(12)-C(13)-Cl(4)	120.02(18)
C(13)-C(14)-C(15)	118.2(2)
C(13)-C(14)-H(14A)	120.9
C(15)-C(14)-H(14A)	120.9
C(14)-C(15)-C(10)	120.1(2)
C(14)-C(15)-C(16)	132.6(2)
C(10)-C(15)-C(16)	107.12(18)
N(4)-C(16)-N(3)	122.8(2)
N(4)-C(16)-C(15)	129.91(19)
N(3)-C(16)-C(15)	105.58(18)
N(4)-C(17)-N(5)	122.1(2)
N(4)-C(17)-C(18)	131.4(2)
N(5)-C(17)-C(18)	104.92(18)
C(19)-C(18)-C(23)	119.9(2)
C(19)-C(18)-C(17)	132.9(2)
C(23)-C(18)-C(17)	107.16(18)
C(20)-C(19)-C(18)	118.4(2)

C(20)-C(19)-H(19A)	120.8
C(18)-C(19)-H(19A)	120.8
C(19)-C(20)-C(21)	121.3(2)
C(19)-C(20)-Cl(5)	118.53(18)
C(21)-C(20)-Cl(5)	120.13(18)
C(22)-C(21)-C(20)	120.7(2)
C(22)-C(21)-Cl(6)	118.36(18)
C(20)-C(21)-Cl(6)	120.89(18)
C(23)-C(22)-C(21)	118.3(2)
C(23)-C(22)-H(22A)	120.9
C(21)-C(22)-H(22A)	120.9
C(22)-C(23)-C(18)	121.3(2)
C(22)-C(23)-C(24)	131.6(2)
C(18)-C(23)-C(24)	107.04(19)
N(6)-C(24)-N(5)	122.5(2)
N(6)-C(24)-C(23)	130.2(2)
N(5)-C(24)-C(23)	105.68(18)
C(34)-C(25)-O(1)	121.3(2)
C(34)-C(25)-C(26)	121.0(2)
O(1)-C(25)-C(26)	117.6(2)
C(27)-C(26)-C(25)	120.0(2)
C(27)-C(26)-H(26A)	120.0
C(25)-C(26)-H(26A)	120.0
C(26)-C(27)-C(28)	120.6(2)
C(26)-C(27)-H(27A)	119.7
C(28)-C(27)-H(27A)	119.7
C(27)-C(28)-C(33)	119.7(2)
C(27)-C(28)-C(29)	122.1(2)
C(33)-C(28)-C(29)	118.2(2)
C(30)-C(29)-C(28)	120.7(3)
C(30)-C(29)-H(29A)	119.6
C(28)-C(29)-H(29A)	119.6
C(29)-C(30)-C(31)	120.5(2)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(32)-C(31)-C(30)	120.5(3)

C(32)-C(31)-H(31A)	119.7
C(30)-C(31)-H(31A)	119.7
C(31)-C(32)-C(33)	120.3(3)
C(31)-C(32)-H(32A)	119.8
C(33)-C(32)-H(32A)	119.8
C(32)-C(33)-C(28)	119.8(2)
C(32)-C(33)-C(34)	121.7(2)
C(28)-C(33)-C(34)	118.5(2)
C(25)-C(34)-C(33)	120.1(2)
C(25)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
O(1)-B(1)-N(5)	116.21(19)
O(1)-B(1)-N(1)	111.15(18)
N(5)-B(1)-N(1)	103.92(18)
O(1)-B(1)-N(3)	116.6(2)
N(5)-B(1)-N(3)	103.31(18)
N(1)-B(1)-N(3)	104.21(18)

Symmetry transformations used to generate equivalent atoms:

Table S 70. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **NaphO-Cl₆BsubPc** (**Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	21(1)	38(1)	37(1)	-4(1)	-2(1)	-9(1)
Cl(2)	19(1)	49(1)	35(1)	6(1)	-9(1)	-3(1)
Cl(3)	28(1)	31(1)	51(1)	2(1)	-2(1)	4(1)
Cl(4)	40(1)	30(1)	30(1)	-6(1)	9(1)	0(1)
Cl(5)	28(1)	47(1)	21(1)	3(1)	3(1)	12(1)
Cl(6)	40(1)	35(1)	38(1)	9(1)	7(1)	5(1)
O(1)	15(1)	44(1)	20(1)	-10(1)	1(1)	-1(1)
N(1)	16(1)	29(1)	16(1)	-4(1)	2(1)	-1(1)
N(2)	19(1)	31(1)	18(1)	1(1)	0(1)	-5(1)
N(3)	15(1)	29(1)	16(1)	-2(1)	1(1)	-2(1)
N(4)	16(1)	29(1)	20(1)	-3(1)	0(1)	0(1)
N(5)	18(1)	26(1)	18(1)	-5(1)	-1(1)	2(1)
N(6)	19(1)	27(1)	20(1)	-6(1)	0(1)	2(1)
C(1)	17(1)	26(1)	20(1)	-8(1)	3(1)	0(1)
C(2)	17(1)	28(1)	17(1)	-7(1)	1(1)	0(1)
C(3)	23(1)	27(1)	19(1)	-6(1)	1(1)	-2(1)
C(4)	18(1)	32(1)	21(1)	-7(1)	2(1)	-5(1)
C(5)	17(1)	37(1)	19(1)	-2(1)	-1(1)	0(1)
C(6)	21(1)	31(1)	20(1)	0(1)	2(1)	-1(1)
C(7)	18(1)	31(1)	15(1)	-4(1)	2(1)	-2(1)
C(8)	17(1)	34(1)	15(1)	-2(1)	1(1)	-2(1)
C(9)	17(1)	28(1)	19(1)	1(1)	3(1)	-4(1)
C(10)	16(1)	30(1)	21(1)	1(1)	2(1)	-6(1)
C(11)	18(1)	31(1)	25(1)	5(1)	-1(1)	-6(1)
C(12)	17(1)	26(1)	33(1)	4(1)	6(1)	-2(1)
C(13)	22(1)	27(1)	26(1)	-2(1)	9(1)	-3(1)
C(14)	18(1)	30(1)	19(1)	-1(1)	4(1)	-4(1)
C(15)	15(1)	28(1)	22(1)	1(1)	4(1)	-3(1)
C(16)	13(1)	31(1)	18(1)	-5(1)	0(1)	-4(1)
C(17)	14(1)	30(1)	20(1)	-6(1)	0(1)	1(1)

C(18)	16(1)	28(1)	22(1)	-2(1)	1(1)	6(1)
C(19)	18(1)	32(1)	21(1)	-5(1)	1(1)	6(1)
C(20)	18(1)	37(1)	21(1)	-1(1)	3(1)	10(1)
C(21)	21(1)	30(1)	28(1)	2(1)	8(1)	7(1)
C(22)	18(1)	28(1)	28(1)	-3(1)	2(1)	4(1)
C(23)	16(1)	28(1)	24(1)	-3(1)	2(1)	4(1)
C(24)	18(1)	26(1)	23(1)	-5(1)	3(1)	4(1)
C(25)	17(1)	39(1)	19(1)	-10(1)	2(1)	1(1)
C(26)	26(1)	39(1)	27(1)	0(1)	3(1)	3(1)
C(27)	36(1)	34(1)	33(1)	0(1)	9(1)	-5(1)
C(28)	26(1)	38(1)	24(1)	-8(1)	8(1)	-1(1)
C(29)	28(1)	56(2)	36(2)	-14(1)	14(1)	-8(1)
C(30)	18(1)	73(2)	36(2)	-24(1)	4(1)	-3(1)
C(31)	27(1)	68(2)	36(2)	-10(1)	-5(1)	15(1)
C(32)	32(1)	44(2)	40(2)	4(1)	-1(1)	7(1)
C(33)	24(1)	36(1)	22(1)	-6(1)	4(1)	4(1)
C(34)	27(1)	33(1)	26(1)	-2(1)	4(1)	-1(1)
B(1)	16(1)	32(1)	19(1)	-6(1)	-1(1)	-1(1)

Table S 71. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102)**.

	x	y	z	U(eq)
H(3A)	11353	4679	5066	27
H(6A)	11651	2773	6534	29
H(11A)	9331	1158	4583	30
H(14A)	6677	1505	1384	27
H(19A)	5798	3676	35	29
H(22A)	8023	5220	1970	30
H(26A)	5020	2464	5185	37
H(27A)	2918	2150	4671	41
H(29A)	732	2302	3609	47
H(30A)	-621	2863	2465	51
H(31A)	104	3754	1847	54
H(32A)	2199	4078	2381	47
H(34A)	4386	3928	3427	34

Table S 72. Torsion angles [°] for **NaphO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087102)**.

C(24)-N(6)-C(1)-N(1)	-11.3(3)
C(24)-N(6)-C(1)-C(2)	153.7(2)
C(8)-N(1)-C(1)-N(6)	157.3(2)
B(1)-N(1)-C(1)-N(6)	-6.4(3)
C(8)-N(1)-C(1)-C(2)	-10.8(2)
B(1)-N(1)-C(1)-C(2)	-174.54(19)
N(6)-C(1)-C(2)-C(3)	9.7(4)
N(1)-C(1)-C(2)-C(3)	176.7(2)
N(6)-C(1)-C(2)-C(7)	-161.6(2)
N(1)-C(1)-C(2)-C(7)	5.5(2)
C(7)-C(2)-C(3)-C(4)	-2.0(3)
C(1)-C(2)-C(3)-C(4)	-172.3(2)
C(2)-C(3)-C(4)-C(5)	-0.1(3)
C(2)-C(3)-C(4)-Cl(1)	178.14(16)
C(3)-C(4)-C(5)-C(6)	2.6(3)
Cl(1)-C(4)-C(5)-C(6)	-175.68(17)
C(3)-C(4)-C(5)-Cl(2)	-178.06(17)
Cl(1)-C(4)-C(5)-Cl(2)	3.7(3)
C(4)-C(5)-C(6)-C(7)	-2.8(3)
Cl(2)-C(5)-C(6)-C(7)	177.86(17)
C(5)-C(6)-C(7)-C(2)	0.6(3)
C(5)-C(6)-C(7)-C(8)	171.5(2)
C(3)-C(2)-C(7)-C(6)	1.7(3)
C(1)-C(2)-C(7)-C(6)	174.1(2)
C(3)-C(2)-C(7)-C(8)	-171.11(19)
C(1)-C(2)-C(7)-C(8)	1.3(2)
C(9)-N(2)-C(8)-N(1)	10.1(3)
C(9)-N(2)-C(8)-C(7)	-149.6(2)
C(1)-N(1)-C(8)-N(2)	-152.1(2)
B(1)-N(1)-C(8)-N(2)	11.7(3)
C(1)-N(1)-C(8)-C(7)	11.5(2)
B(1)-N(1)-C(8)-C(7)	175.38(19)

C(6)-C(7)-C(8)-N(2)	-16.9(4)
C(2)-C(7)-C(8)-N(2)	154.9(2)
C(6)-C(7)-C(8)-N(1)	-179.3(2)
C(2)-C(7)-C(8)-N(1)	-7.5(2)
C(8)-N(2)-C(9)-N(3)	-9.8(3)
C(8)-N(2)-C(9)-C(10)	150.0(2)
C(16)-N(3)-C(9)-N(2)	153.4(2)
B(1)-N(3)-C(9)-N(2)	-12.3(3)
C(16)-N(3)-C(9)-C(10)	-10.2(2)
B(1)-N(3)-C(9)-C(10)	-175.85(18)
N(2)-C(9)-C(10)-C(11)	17.0(4)
N(3)-C(9)-C(10)-C(11)	179.5(2)
N(2)-C(9)-C(10)-C(15)	-157.0(2)
N(3)-C(9)-C(10)-C(15)	5.5(2)
C(15)-C(10)-C(11)-C(12)	-2.9(3)
C(9)-C(10)-C(11)-C(12)	-176.2(2)
C(10)-C(11)-C(12)-C(13)	1.7(3)
C(10)-C(11)-C(12)-Cl(3)	-176.79(17)
C(11)-C(12)-C(13)-C(14)	0.6(3)
Cl(3)-C(12)-C(13)-C(14)	179.12(17)
C(11)-C(12)-C(13)-Cl(4)	-175.53(17)
Cl(3)-C(12)-C(13)-Cl(4)	3.0(3)
C(12)-C(13)-C(14)-C(15)	-1.8(3)
Cl(4)-C(13)-C(14)-C(15)	174.44(16)
C(13)-C(14)-C(15)-C(10)	0.6(3)
C(13)-C(14)-C(15)-C(16)	175.4(2)
C(11)-C(10)-C(15)-C(14)	1.8(3)
C(9)-C(10)-C(15)-C(14)	176.55(19)
C(11)-C(10)-C(15)-C(16)	-174.2(2)
C(9)-C(10)-C(15)-C(16)	0.6(2)
C(17)-N(4)-C(16)-N(3)	8.9(3)
C(17)-N(4)-C(16)-C(15)	-153.9(2)
C(9)-N(3)-C(16)-N(4)	-155.9(2)
B(1)-N(3)-C(16)-N(4)	9.6(3)
C(9)-N(3)-C(16)-C(15)	10.5(2)
B(1)-N(3)-C(16)-C(15)	175.97(18)

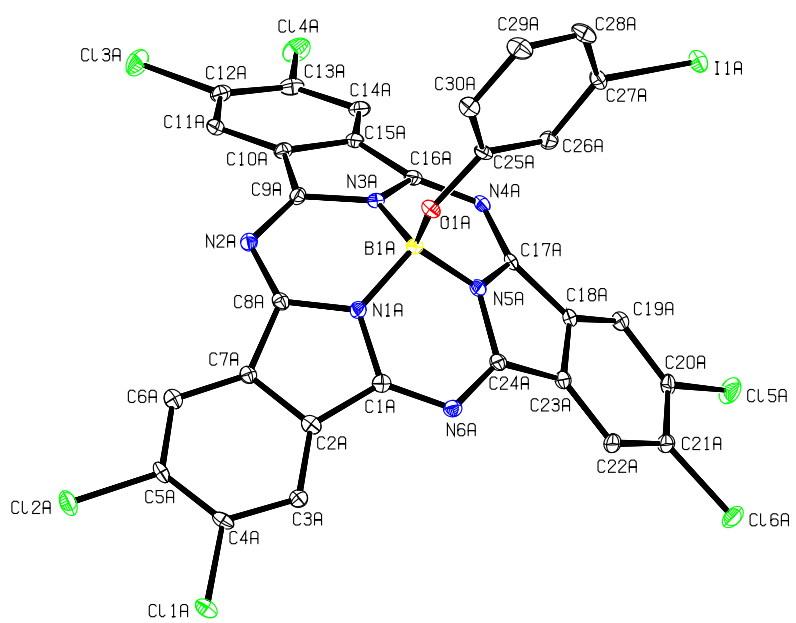
C(14)-C(15)-C(16)-N(4)	-16.6(4)
C(10)-C(15)-C(16)-N(4)	158.7(2)
C(14)-C(15)-C(16)-N(3)	178.3(2)
C(10)-C(15)-C(16)-N(3)	-6.4(2)
C(16)-N(4)-C(17)-N(5)	-4.5(3)
C(16)-N(4)-C(17)-C(18)	158.8(2)
C(24)-N(5)-C(17)-N(4)	153.8(2)
B(1)-N(5)-C(17)-N(4)	-18.7(3)
C(24)-N(5)-C(17)-C(18)	-13.3(2)
B(1)-N(5)-C(17)-C(18)	174.19(18)
N(4)-C(17)-C(18)-C(19)	21.6(4)
N(5)-C(17)-C(18)-C(19)	-172.9(2)
N(4)-C(17)-C(18)-C(23)	-158.3(2)
N(5)-C(17)-C(18)-C(23)	7.2(2)
C(23)-C(18)-C(19)-C(20)	-1.3(3)
C(17)-C(18)-C(19)-C(20)	178.8(2)
C(18)-C(19)-C(20)-C(21)	1.6(3)
C(18)-C(19)-C(20)-Cl(5)	-176.33(16)
C(19)-C(20)-C(21)-C(22)	-0.4(3)
Cl(5)-C(20)-C(21)-C(22)	177.47(17)
C(19)-C(20)-C(21)-Cl(6)	-178.02(16)
Cl(5)-C(20)-C(21)-Cl(6)	-0.1(3)
C(20)-C(21)-C(22)-C(23)	-1.0(3)
Cl(6)-C(21)-C(22)-C(23)	176.65(16)
C(21)-C(22)-C(23)-C(18)	1.2(3)
C(21)-C(22)-C(23)-C(24)	-179.8(2)
C(19)-C(18)-C(23)-C(22)	-0.1(3)
C(17)-C(18)-C(23)-C(22)	179.83(19)
C(19)-C(18)-C(23)-C(24)	-179.25(19)
C(17)-C(18)-C(23)-C(24)	0.7(2)
C(1)-N(6)-C(24)-N(5)	5.0(3)
C(1)-N(6)-C(24)-C(23)	-158.5(2)
C(17)-N(5)-C(24)-N(6)	-153.2(2)
B(1)-N(5)-C(24)-N(6)	19.4(3)
C(17)-N(5)-C(24)-C(23)	13.8(2)
B(1)-N(5)-C(24)-C(23)	-173.62(18)

C(22)-C(23)-C(24)-N(6)	-21.8(4)
C(18)-C(23)-C(24)-N(6)	157.3(2)
C(22)-C(23)-C(24)-N(5)	172.6(2)
C(18)-C(23)-C(24)-N(5)	-8.3(2)
B(1)-O(1)-C(25)-C(34)	-85.5(3)
B(1)-O(1)-C(25)-C(26)	98.0(3)
C(34)-C(25)-C(26)-C(27)	0.7(4)
O(1)-C(25)-C(26)-C(27)	177.2(2)
C(25)-C(26)-C(27)-C(28)	0.2(4)
C(26)-C(27)-C(28)-C(33)	-0.7(4)
C(26)-C(27)-C(28)-C(29)	179.3(2)
C(27)-C(28)-C(29)-C(30)	-179.9(2)
C(33)-C(28)-C(29)-C(30)	0.1(4)
C(28)-C(29)-C(30)-C(31)	-0.3(4)
C(29)-C(30)-C(31)-C(32)	0.1(4)
C(30)-C(31)-C(32)-C(33)	0.2(4)
C(31)-C(32)-C(33)-C(28)	-0.4(4)
C(31)-C(32)-C(33)-C(34)	179.5(2)
C(27)-C(28)-C(33)-C(32)	-179.8(2)
C(29)-C(28)-C(33)-C(32)	0.2(3)
C(27)-C(28)-C(33)-C(34)	0.3(3)
C(29)-C(28)-C(33)-C(34)	-179.7(2)
O(1)-C(25)-C(34)-C(33)	-177.46(19)
C(26)-C(25)-C(34)-C(33)	-1.0(3)
C(32)-C(33)-C(34)-C(25)	-179.4(2)
C(28)-C(33)-C(34)-C(25)	0.5(3)
C(25)-O(1)-B(1)-N(5)	69.5(3)
C(25)-O(1)-B(1)-N(1)	-171.98(19)
C(25)-O(1)-B(1)-N(3)	-52.8(3)
C(24)-N(5)-B(1)-O(1)	90.6(2)
C(17)-N(5)-B(1)-O(1)	-97.6(2)
C(24)-N(5)-B(1)-N(1)	-31.8(3)
C(17)-N(5)-B(1)-N(1)	140.02(19)
C(24)-N(5)-B(1)-N(3)	-140.36(19)
C(17)-N(5)-B(1)-N(3)	31.4(3)
C(1)-N(1)-B(1)-O(1)	-100.2(2)

C(8)-N(1)-B(1)-O(1)	97.7(2)
C(1)-N(1)-B(1)-N(5)	25.6(3)
C(8)-N(1)-B(1)-N(5)	-136.60(19)
C(1)-N(1)-B(1)-N(3)	133.5(2)
C(8)-N(1)-B(1)-N(3)	-28.7(3)
C(9)-N(3)-B(1)-O(1)	-94.0(2)
C(16)-N(3)-B(1)-O(1)	101.8(2)
C(9)-N(3)-B(1)-N(5)	137.24(19)
C(16)-N(3)-B(1)-N(5)	-26.9(3)
C(9)-N(3)-B(1)-N(1)	28.9(3)
C(16)-N(3)-B(1)-N(1)	-135.26(19)

Symmetry transformations used to generate equivalent atoms:

a)



b)

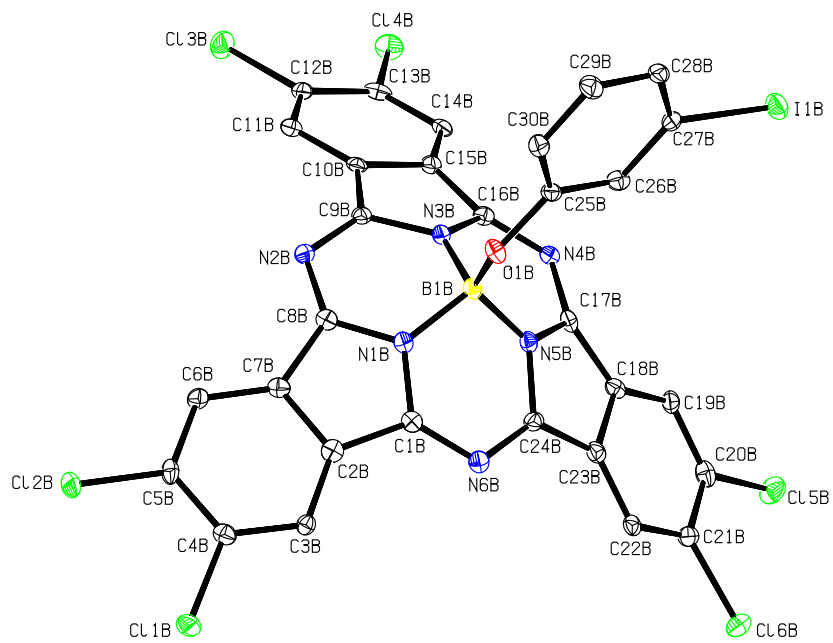


Figure S37: Anisotropic displacement ellipsoid plots of individual co-crystals of *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

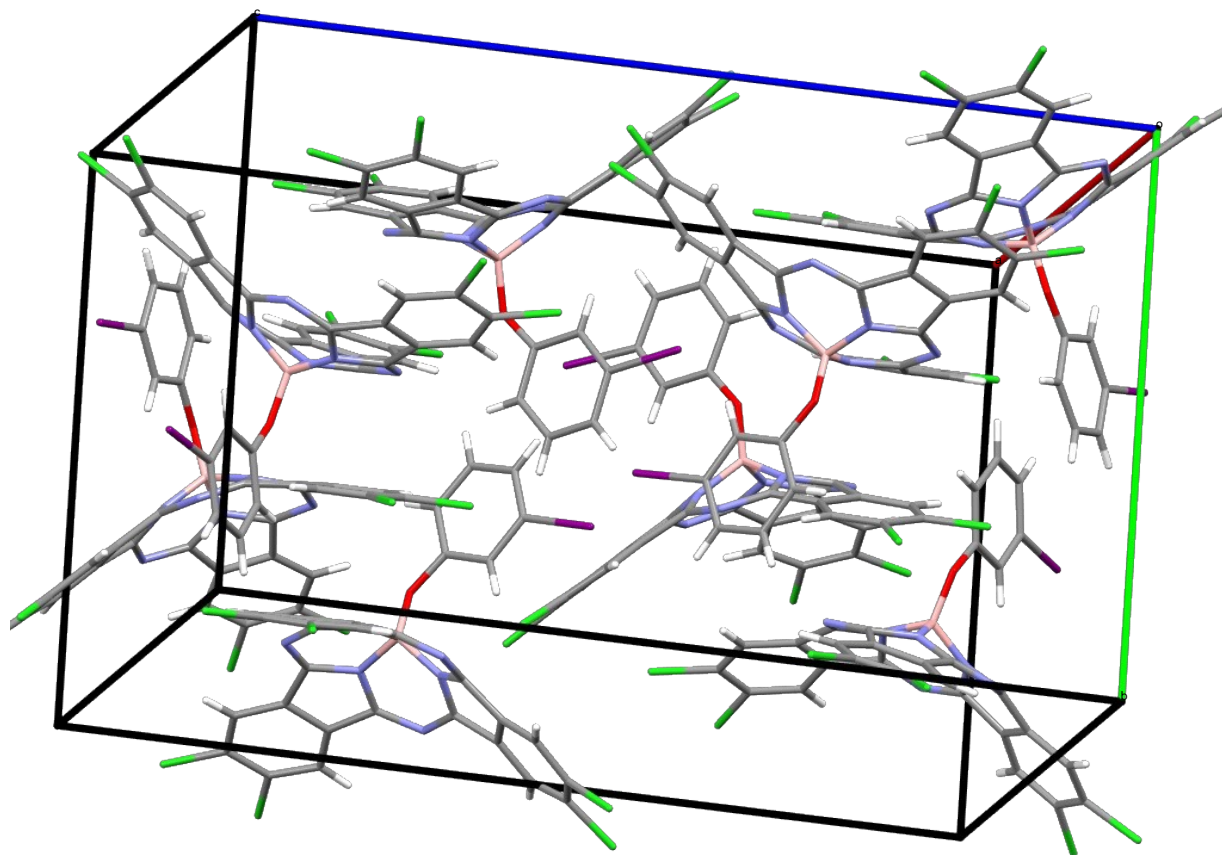


Figure S38: Populated unit cell of *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

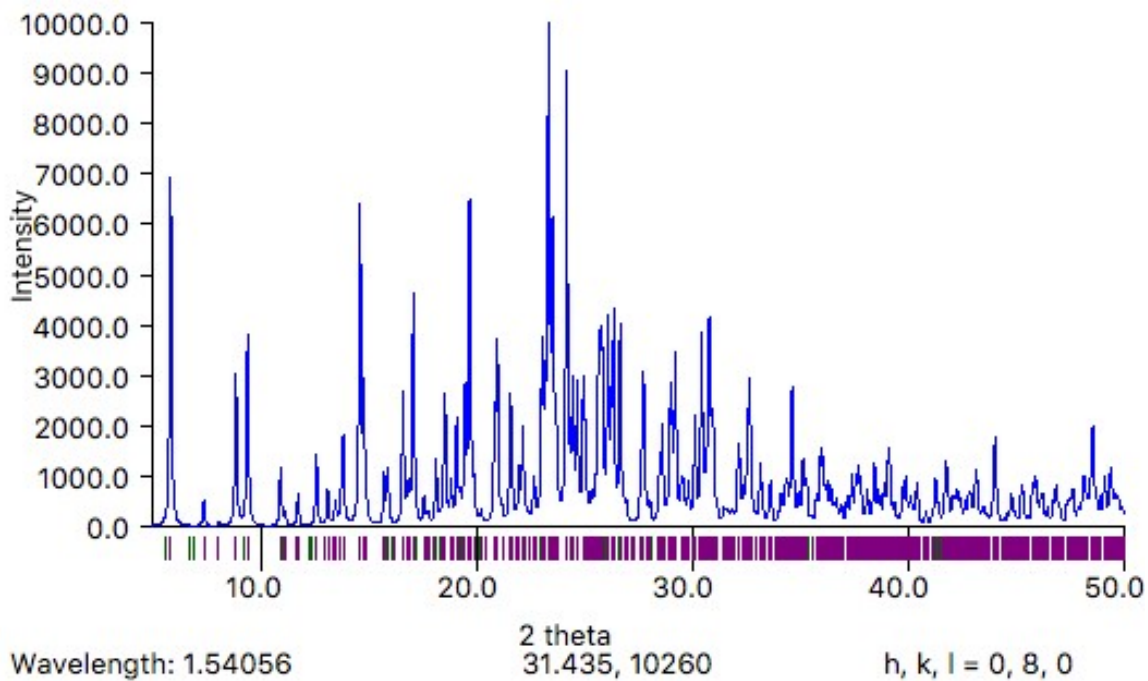


Figure S39: Powder x-ray diffraction of *m*IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

Table S 73. Crystal data and structure refinement for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

Identification code	d19227a_a	
Empirical formula	C ₃₀ H ₁₀ B Cl ₆ I N ₆ O	
Formula weight	820.85	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2 ₁	
Unit cell dimensions	a = 15.8587(3) Å	α = 90°.
	b = 15.1167(3) Å	β = 90°.
	c = 23.9409(5) Å	γ = 90°.
Volume	5739.4(2) Å ³	
Z	8	
Density (calculated)	1.900 Mg/m ³	
Absorption coefficient	1.715 mm ⁻¹	
F(000)	3200	
Crystal size	0.230 x 0.170 x 0.130 mm ³	
Theta range for data collection	1.701 to 27.501°.	
Index ranges	-20 ≤ h ≤ 20, -19 ≤ k ≤ 19, -31 ≤ l ≤ 31	
Reflections collected	63792	
Independent reflections	13120 [R(int) = 0.0440]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6956	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13120 / 1 / 811	
Goodness-of-fit on F ²	1.032	
Final R indices [I > 2σ(I)]	R1 = 0.0302, wR2 = 0.0751	
R indices (all data)	R1 = 0.0366, wR2 = 0.0772	
Absolute structure parameter	-0.008(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.808 and -1.007 e.Å ⁻³	

Table S 74. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1A)	2972(1)	4048(1)	4617(1)	23(1)
Cl(1A)	9256(1)	20(1)	7023(1)	22(1)
Cl(2A)	8593(1)	523(1)	8208(1)	28(1)
Cl(3A)	2331(1)	1580(1)	8900(1)	32(1)
Cl(4A)	1065(1)	1135(1)	7920(1)	32(1)
Cl(5A)	2909(1)	-818(1)	4231(1)	33(1)
Cl(6A)	4797(1)	-961(1)	3850(1)	28(1)
O(1A)	5368(2)	3156(2)	6158(2)	17(1)
N(1A)	5819(3)	1822(3)	6581(2)	15(1)
N(2A)	5314(3)	2009(3)	7507(2)	16(1)
N(3A)	4390(3)	2203(3)	6727(2)	15(1)
N(4A)	3397(3)	1593(3)	6093(2)	16(1)
N(5A)	4842(3)	1653(3)	5853(2)	15(1)
N(6A)	6209(3)	1022(3)	5766(2)	17(1)
C(1A)	6370(3)	1310(3)	6283(2)	16(1)
C(2A)	7009(3)	1045(3)	6686(2)	16(1)
C(3A)	7765(3)	595(3)	6625(2)	16(1)
C(4A)	8257(3)	469(3)	7098(2)	18(1)
C(5A)	7971(3)	720(4)	7627(2)	18(1)
C(6A)	7197(3)	1142(3)	7697(2)	18(1)
C(7A)	6736(3)	1331(3)	7223(2)	14(1)
C(8A)	5926(3)	1793(3)	7145(2)	15(1)
C(9A)	4547(3)	2155(3)	7287(2)	16(1)
C(10A)	3713(3)	2020(3)	7550(2)	16(1)
C(11A)	3475(3)	1929(3)	8104(2)	19(1)
C(12A)	2640(4)	1681(3)	8213(2)	21(1)
C(13A)	2085(3)	1509(3)	7777(3)	22(1)
C(14A)	2312(3)	1608(3)	7224(2)	20(1)
C(15A)	3137(3)	1881(3)	7113(2)	16(1)
C(16A)	3591(3)	1934(3)	6588(2)	16(1)

C(17A)	4035(3)	1414(3)	5746(2)	15(1)
C(18A)	4070(3)	801(3)	5276(2)	17(1)
C(19A)	3446(3)	347(3)	4998(2)	21(1)
C(20A)	3678(3)	-225(3)	4574(2)	20(1)
C(21A)	4538(3)	-323(3)	4425(2)	20(1)
C(22A)	5174(3)	86(3)	4723(2)	20(1)
C(23A)	4941(3)	653(3)	5159(2)	16(1)
C(24A)	5429(3)	1150(3)	5573(2)	17(1)
C(25A)	4946(3)	3789(3)	5861(2)	15(1)
C(26A)	4309(3)	3602(3)	5482(2)	18(1)
C(27A)	3920(3)	4313(3)	5203(2)	19(1)
C(28A)	4159(3)	5171(3)	5295(2)	25(1)
C(29A)	4818(4)	5340(4)	5660(3)	26(1)
C(30A)	5210(3)	4657(3)	5946(2)	19(1)
B(1A)	5087(4)	2288(4)	6305(2)	16(1)
I(1B)	2030(1)	6531(1)	5151(1)	31(1)
Cl(1B)	-4232(1)	2503(1)	2428(1)	30(1)
Cl(2B)	-3400(1)	3176(1)	1325(1)	38(1)
Cl(3B)	2920(1)	3903(1)	1108(1)	35(1)
Cl(4B)	4051(1)	3489(1)	2156(1)	32(1)
Cl(5B)	1425(1)	1415(1)	5722(1)	34(1)
Cl(6B)	-529(1)	1268(1)	5877(1)	29(1)
O(1B)	-403(2)	5560(2)	3646(2)	24(1)
N(1B)	-897(3)	4279(3)	3183(2)	19(1)
N(2B)	-224(3)	4433(3)	2300(2)	20(1)
N(3B)	571(3)	4544(3)	3144(2)	19(1)
N(4B)	1424(3)	3865(3)	3840(2)	20(1)
N(5B)	-63(3)	4014(3)	3969(2)	18(1)
N(6B)	-1462(3)	3443(3)	3935(2)	20(1)
C(1B)	-1529(3)	3793(3)	3419(2)	19(1)
C(2B)	-2117(3)	3591(4)	2967(2)	21(1)
C(3B)	-2893(3)	3170(3)	2967(2)	18(1)
C(4B)	-3283(3)	3046(4)	2454(2)	23(1)
C(5B)	-2893(4)	3318(4)	1946(2)	22(1)
C(6B)	-2107(3)	3722(4)	1955(2)	21(1)
C(7B)	-1723(3)	3872(3)	2464(2)	20(1)

C(8B)	-912(3)	4270(3)	2618(2)	20(1)
C(9B)	510(3)	4515(3)	2568(2)	18(1)
C(10B)	1368(3)	4360(3)	2375(2)	19(1)
C(11B)	1688(4)	4272(3)	1833(2)	22(1)
C(12B)	2509(4)	4019(3)	1772(2)	21(1)
C(13B)	3022(3)	3836(4)	2247(3)	24(1)
C(14B)	2709(3)	3925(3)	2779(2)	19(1)
C(15B)	1879(3)	4184(3)	2839(3)	20(1)
C(16B)	1330(3)	4238(3)	3334(2)	19(1)
C(17B)	718(3)	3709(4)	4140(2)	20(1)
C(18B)	564(3)	3083(3)	4574(2)	19(1)
C(19B)	1105(4)	2581(3)	4923(2)	22(1)
C(20B)	761(4)	2032(4)	5301(2)	25(1)
C(21B)	-132(3)	1943(3)	5361(2)	22(1)
C(22B)	-656(3)	2386(3)	5009(2)	19(1)
C(23B)	-327(3)	2963(3)	4621(2)	21(1)
C(24B)	-699(3)	3512(3)	4182(2)	20(1)
C(25B)	85(3)	6200(4)	3902(2)	21(1)
C(26B)	723(4)	6030(3)	4285(2)	22(1)
C(27B)	1128(3)	6747(4)	4532(2)	20(1)
C(28B)	928(4)	7603(4)	4396(2)	24(1)
C(29B)	279(4)	7753(4)	4012(3)	28(1)
C(30B)	-133(4)	7060(4)	3773(3)	28(1)
B(1B)	-187(4)	4672(4)	3516(3)	19(1)

Table S 75. Bond lengths [Å] and angles [°] for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

I(1A)-C(27A)	2.094(5)
Cl(1A)-C(4A)	1.733(5)
Cl(2A)-C(5A)	1.731(5)
Cl(3A)-C(12A)	1.723(6)
Cl(4A)-C(13A)	1.747(5)
Cl(5A)-C(20A)	1.722(5)
Cl(6A)-C(21A)	1.731(5)
O(1A)-C(25A)	1.366(6)
O(1A)-B(1A)	1.430(7)
N(1A)-C(8A)	1.360(7)
N(1A)-C(1A)	1.370(6)
N(1A)-B(1A)	1.510(7)
N(2A)-C(8A)	1.342(7)
N(2A)-C(9A)	1.344(7)
N(3A)-C(9A)	1.366(6)
N(3A)-C(16A)	1.371(6)
N(3A)-B(1A)	1.504(7)
N(4A)-C(16A)	1.330(7)
N(4A)-C(17A)	1.336(7)
N(5A)-C(17A)	1.355(6)
N(5A)-C(24A)	1.377(6)
N(5A)-B(1A)	1.499(7)
N(6A)-C(24A)	1.335(7)
N(6A)-C(1A)	1.335(7)
C(1A)-C(2A)	1.456(7)
C(2A)-C(3A)	1.386(7)
C(2A)-C(7A)	1.424(8)
C(3A)-C(4A)	1.389(8)
C(3A)-H(3AA)	0.9300
C(4A)-C(5A)	1.398(8)
C(5A)-C(6A)	1.394(8)
C(6A)-C(7A)	1.380(7)

C(6A)-H(6AA)	0.9300
C(7A)-C(8A)	1.473(7)
C(9A)-C(10A)	1.480(7)
C(10A)-C(11A)	1.384(7)
C(10A)-C(15A)	1.406(7)
C(11A)-C(12A)	1.401(8)
C(11A)-H(11A)	0.9300
C(12A)-C(13A)	1.388(9)
C(13A)-C(14A)	1.382(8)
C(14A)-C(15A)	1.396(7)
C(14A)-H(14A)	0.9300
C(15A)-C(16A)	1.451(7)
C(17A)-C(18A)	1.459(7)
C(18A)-C(19A)	1.377(7)
C(18A)-C(23A)	1.427(7)
C(19A)-C(20A)	1.383(7)
C(19A)-H(19A)	0.9300
C(20A)-C(21A)	1.417(7)
C(21A)-C(22A)	1.382(8)
C(22A)-C(23A)	1.400(7)
C(22A)-H(22A)	0.9300
C(23A)-C(24A)	1.465(7)
C(25A)-C(26A)	1.388(7)
C(25A)-C(30A)	1.392(7)
C(26A)-C(27A)	1.408(7)
C(26A)-H(26A)	0.9300
C(27A)-C(28A)	1.369(8)
C(28A)-C(29A)	1.387(8)
C(28A)-H(28A)	0.9300
C(29A)-C(30A)	1.386(7)
C(29A)-H(29A)	0.9300
C(30A)-H(30A)	0.9300
I(1B)-C(27B)	2.084(5)
Cl(1B)-C(4B)	1.715(6)
Cl(2B)-C(5B)	1.704(6)
Cl(3B)-C(12B)	1.726(6)

Cl(4B)-C(13B)	1.727(5)
Cl(5B)-C(20B)	1.729(6)
Cl(6B)-C(21B)	1.722(6)
O(1B)-C(25B)	1.382(6)
O(1B)-B(1B)	1.421(7)
N(1B)-C(8B)	1.354(7)
N(1B)-C(1B)	1.365(7)
N(1B)-B(1B)	1.502(7)
N(2B)-C(9B)	1.335(7)
N(2B)-C(8B)	1.353(7)
N(3B)-C(16B)	1.368(7)
N(3B)-C(9B)	1.382(7)
N(3B)-B(1B)	1.509(7)
N(4B)-C(16B)	1.343(7)
N(4B)-C(17B)	1.352(7)
N(5B)-C(24B)	1.361(7)
N(5B)-C(17B)	1.384(7)
N(5B)-B(1B)	1.484(8)
N(6B)-C(1B)	1.349(7)
N(6B)-C(24B)	1.351(7)
C(1B)-C(2B)	1.461(8)
C(2B)-C(3B)	1.385(7)
C(2B)-C(7B)	1.422(8)
C(3B)-C(4B)	1.389(8)
C(3B)-H(3BA)	0.9300
C(4B)-C(5B)	1.424(8)
C(5B)-C(6B)	1.388(8)
C(6B)-C(7B)	1.381(8)
C(6B)-H(6BA)	0.9300
C(7B)-C(8B)	1.467(8)
C(9B)-C(10B)	1.455(7)
C(10B)-C(11B)	1.400(8)
C(10B)-C(15B)	1.400(8)
C(11B)-C(12B)	1.365(8)
C(11B)-H(11B)	0.9300
C(12B)-C(13B)	1.424(9)

C(13B)-C(14B)	1.374(9)
C(14B)-C(15B)	1.381(7)
C(14B)-H(14B)	0.9300
C(15B)-C(16B)	1.473(8)
C(17B)-C(18B)	1.426(8)
C(18B)-C(19B)	1.418(8)
C(18B)-C(23B)	1.429(7)
C(19B)-C(20B)	1.345(8)
C(19B)-H(19B)	0.9300
C(20B)-C(21B)	1.430(8)
C(21B)-C(22B)	1.360(8)
C(22B)-C(23B)	1.376(8)
C(22B)-H(22B)	0.9300
C(23B)-C(24B)	1.464(8)
C(25B)-C(30B)	1.380(8)
C(25B)-C(26B)	1.390(8)
C(26B)-C(27B)	1.392(7)
C(26B)-H(26B)	0.9300
C(27B)-C(28B)	1.372(8)
C(28B)-C(29B)	1.399(8)
C(28B)-H(28B)	0.9300
C(29B)-C(30B)	1.361(8)
C(29B)-H(29B)	0.9300
C(30B)-H(30B)	0.9300
C(25A)-O(1A)-B(1A)	128.2(4)
C(8A)-N(1A)-C(1A)	114.8(4)
C(8A)-N(1A)-B(1A)	123.1(4)
C(1A)-N(1A)-B(1A)	121.7(4)
C(8A)-N(2A)-C(9A)	116.2(4)
C(9A)-N(3A)-C(16A)	113.0(4)
C(9A)-N(3A)-B(1A)	122.0(4)
C(16A)-N(3A)-B(1A)	122.8(4)
C(16A)-N(4A)-C(17A)	117.2(4)
C(17A)-N(5A)-C(24A)	113.6(4)
C(17A)-N(5A)-B(1A)	123.5(4)

C(24A)-N(5A)-B(1A)	122.0(4)
C(24A)-N(6A)-C(1A)	116.8(4)
N(6A)-C(1A)-N(1A)	123.1(4)
N(6A)-C(1A)-C(2A)	131.1(5)
N(1A)-C(1A)-C(2A)	104.7(4)
C(3A)-C(2A)-C(7A)	120.5(5)
C(3A)-C(2A)-C(1A)	131.8(5)
C(7A)-C(2A)-C(1A)	107.7(4)
C(2A)-C(3A)-C(4A)	117.8(5)
C(2A)-C(3A)-H(3AA)	121.1
C(4A)-C(3A)-H(3AA)	121.1
C(3A)-C(4A)-C(5A)	121.3(5)
C(3A)-C(4A)-Cl(1A)	118.9(4)
C(5A)-C(4A)-Cl(1A)	119.8(4)
C(6A)-C(5A)-C(4A)	121.3(5)
C(6A)-C(5A)-Cl(2A)	118.9(5)
C(4A)-C(5A)-Cl(2A)	119.8(4)
C(7A)-C(6A)-C(5A)	117.6(5)
C(7A)-C(6A)-H(6AA)	121.2
C(5A)-C(6A)-H(6AA)	121.2
C(6A)-C(7A)-C(2A)	121.2(5)
C(6A)-C(7A)-C(8A)	131.7(5)
C(2A)-C(7A)-C(8A)	107.1(4)
N(2A)-C(8A)-N(1A)	122.9(4)
N(2A)-C(8A)-C(7A)	131.5(5)
N(1A)-C(8A)-C(7A)	104.5(4)
N(2A)-C(9A)-N(3A)	124.0(4)
N(2A)-C(9A)-C(10A)	128.3(4)
N(3A)-C(9A)-C(10A)	105.2(4)
C(11A)-C(10A)-C(15A)	121.4(5)
C(11A)-C(10A)-C(9A)	131.7(5)
C(15A)-C(10A)-C(9A)	106.6(4)
C(10A)-C(11A)-C(12A)	117.5(5)
C(10A)-C(11A)-H(11A)	121.2
C(12A)-C(11A)-H(11A)	121.2
C(13A)-C(12A)-C(11A)	120.6(5)

C(13A)-C(12A)-Cl(3A)	121.4(4)
C(11A)-C(12A)-Cl(3A)	118.0(4)
C(14A)-C(13A)-C(12A)	122.3(5)
C(14A)-C(13A)-Cl(4A)	117.6(4)
C(12A)-C(13A)-Cl(4A)	120.0(4)
C(13A)-C(14A)-C(15A)	117.3(5)
C(13A)-C(14A)-H(14A)	121.4
C(15A)-C(14A)-H(14A)	121.4
C(14A)-C(15A)-C(10A)	120.8(5)
C(14A)-C(15A)-C(16A)	130.3(5)
C(10A)-C(15A)-C(16A)	108.3(4)
N(4A)-C(16A)-N(3A)	123.1(5)
N(4A)-C(16A)-C(15A)	129.4(5)
N(3A)-C(16A)-C(15A)	105.4(4)
N(4A)-C(17A)-N(5A)	123.0(5)
N(4A)-C(17A)-C(18A)	129.6(5)
N(5A)-C(17A)-C(18A)	106.1(4)
C(19A)-C(18A)-C(23A)	121.5(5)
C(19A)-C(18A)-C(17A)	131.4(5)
C(23A)-C(18A)-C(17A)	106.8(4)
C(18A)-C(19A)-C(20A)	118.4(5)
C(18A)-C(19A)-H(19A)	120.8
C(20A)-C(19A)-H(19A)	120.8
C(19A)-C(20A)-C(21A)	120.5(5)
C(19A)-C(20A)-Cl(5A)	119.1(4)
C(21A)-C(20A)-Cl(5A)	120.5(4)
C(22A)-C(21A)-C(20A)	121.7(5)
C(22A)-C(21A)-Cl(6A)	119.1(4)
C(20A)-C(21A)-Cl(6A)	119.2(4)
C(21A)-C(22A)-C(23A)	117.7(5)
C(21A)-C(22A)-H(22A)	121.1
C(23A)-C(22A)-H(22A)	121.1
C(22A)-C(23A)-C(18A)	119.9(5)
C(22A)-C(23A)-C(24A)	132.7(5)
C(18A)-C(23A)-C(24A)	107.3(4)
N(6A)-C(24A)-N(5A)	122.5(5)

N(6A)-C(24A)-C(23A)	130.6(5)
N(5A)-C(24A)-C(23A)	104.8(4)
O(1A)-C(25A)-C(26A)	123.7(4)
O(1A)-C(25A)-C(30A)	115.9(4)
C(26A)-C(25A)-C(30A)	120.4(5)
C(25A)-C(26A)-C(27A)	118.3(5)
C(25A)-C(26A)-H(26A)	120.8
C(27A)-C(26A)-H(26A)	120.8
C(28A)-C(27A)-C(26A)	121.7(5)
C(28A)-C(27A)-I(1A)	119.2(4)
C(26A)-C(27A)-I(1A)	119.1(4)
C(27A)-C(28A)-C(29A)	119.0(5)
C(27A)-C(28A)-H(28A)	120.5
C(29A)-C(28A)-H(28A)	120.5
C(30A)-C(29A)-C(28A)	120.8(5)
C(30A)-C(29A)-H(29A)	119.6
C(28A)-C(29A)-H(29A)	119.6
C(29A)-C(30A)-C(25A)	119.7(5)
C(29A)-C(30A)-H(30A)	120.1
C(25A)-C(30A)-H(30A)	120.1
O(1A)-B(1A)-N(5A)	119.4(5)
O(1A)-B(1A)-N(3A)	118.2(4)
N(5A)-B(1A)-N(3A)	103.9(4)
O(1A)-B(1A)-N(1A)	107.3(4)
N(5A)-B(1A)-N(1A)	102.5(4)
N(3A)-B(1A)-N(1A)	103.4(4)
C(25B)-O(1B)-B(1B)	128.6(4)
C(8B)-N(1B)-C(1B)	113.3(5)
C(8B)-N(1B)-B(1B)	123.1(5)
C(1B)-N(1B)-B(1B)	123.0(5)
C(9B)-N(2B)-C(8B)	116.7(5)
C(16B)-N(3B)-C(9B)	112.5(4)
C(16B)-N(3B)-B(1B)	123.3(5)
C(9B)-N(3B)-B(1B)	122.4(4)
C(16B)-N(4B)-C(17B)	117.4(5)
C(24B)-N(5B)-C(17B)	111.5(4)

C(24B)-N(5B)-B(1B)	123.3(5)
C(17B)-N(5B)-B(1B)	123.9(5)
C(1B)-N(6B)-C(24B)	116.2(5)
N(6B)-C(1B)-N(1B)	122.2(5)
N(6B)-C(1B)-C(2B)	130.4(5)
N(1B)-C(1B)-C(2B)	105.9(5)
C(3B)-C(2B)-C(7B)	121.9(5)
C(3B)-C(2B)-C(1B)	131.5(5)
C(7B)-C(2B)-C(1B)	106.5(5)
C(2B)-C(3B)-C(4B)	117.2(5)
C(2B)-C(3B)-H(3BA)	121.4
C(4B)-C(3B)-H(3BA)	121.4
C(3B)-C(4B)-C(5B)	121.5(5)
C(3B)-C(4B)-Cl(1B)	119.2(4)
C(5B)-C(4B)-Cl(1B)	119.2(4)
C(6B)-C(5B)-C(4B)	120.2(5)
C(6B)-C(5B)-Cl(2B)	119.5(5)
C(4B)-C(5B)-Cl(2B)	120.3(4)
C(7B)-C(6B)-C(5B)	118.9(5)
C(7B)-C(6B)-H(6BA)	120.6
C(5B)-C(6B)-H(6BA)	120.6
C(6B)-C(7B)-C(2B)	120.2(5)
C(6B)-C(7B)-C(8B)	132.6(5)
C(2B)-C(7B)-C(8B)	107.2(5)
N(2B)-C(8B)-N(1B)	123.2(5)
N(2B)-C(8B)-C(7B)	129.8(5)
N(1B)-C(8B)-C(7B)	105.7(5)
N(2B)-C(9B)-N(3B)	122.9(5)
N(2B)-C(9B)-C(10B)	130.3(5)
N(3B)-C(9B)-C(10B)	104.8(4)
C(11B)-C(10B)-C(15B)	120.4(5)
C(11B)-C(10B)-C(9B)	130.4(5)
C(15B)-C(10B)-C(9B)	108.7(5)
C(12B)-C(11B)-C(10B)	118.2(5)
C(12B)-C(11B)-H(11B)	120.9
C(10B)-C(11B)-H(11B)	120.9

C(11B)-C(12B)-C(13B)	120.9(5)
C(11B)-C(12B)-Cl(3B)	119.1(5)
C(13B)-C(12B)-Cl(3B)	119.9(4)
C(14B)-C(13B)-C(12B)	120.9(5)
C(14B)-C(13B)-Cl(4B)	119.1(5)
C(12B)-C(13B)-Cl(4B)	119.9(5)
C(13B)-C(14B)-C(15B)	117.9(5)
C(13B)-C(14B)-H(14B)	121.0
C(15B)-C(14B)-H(14B)	121.0
C(14B)-C(15B)-C(10B)	121.6(5)
C(14B)-C(15B)-C(16B)	131.5(5)
C(10B)-C(15B)-C(16B)	106.6(5)
N(4B)-C(16B)-N(3B)	122.6(5)
N(4B)-C(16B)-C(15B)	129.6(5)
N(3B)-C(16B)-C(15B)	105.7(5)
N(4B)-C(17B)-N(5B)	121.7(5)
N(4B)-C(17B)-C(18B)	130.1(5)
N(5B)-C(17B)-C(18B)	106.5(4)
C(19B)-C(18B)-C(17B)	132.9(5)
C(19B)-C(18B)-C(23B)	118.9(5)
C(17B)-C(18B)-C(23B)	108.1(5)
C(20B)-C(19B)-C(18B)	118.8(5)
C(20B)-C(19B)-H(19B)	120.6
C(18B)-C(19B)-H(19B)	120.6
C(19B)-C(20B)-C(21B)	121.9(5)
C(19B)-C(20B)-Cl(5B)	118.5(4)
C(21B)-C(20B)-Cl(5B)	119.6(4)
C(22B)-C(21B)-C(20B)	119.7(5)
C(22B)-C(21B)-Cl(6B)	121.0(4)
C(20B)-C(21B)-Cl(6B)	119.3(4)
C(21B)-C(22B)-C(23B)	119.9(5)
C(21B)-C(22B)-H(22B)	120.0
C(23B)-C(22B)-H(22B)	120.0
C(22B)-C(23B)-C(18B)	120.6(5)
C(22B)-C(23B)-C(24B)	133.7(5)
C(18B)-C(23B)-C(24B)	105.6(5)

N(6B)-C(24B)-N(5B)	122.9(5)
N(6B)-C(24B)-C(23B)	129.2(5)
N(5B)-C(24B)-C(23B)	106.7(5)
C(30B)-C(25B)-O(1B)	114.8(5)
C(30B)-C(25B)-C(26B)	120.3(5)
O(1B)-C(25B)-C(26B)	124.8(5)
C(25B)-C(26B)-C(27B)	118.2(5)
C(25B)-C(26B)-H(26B)	120.9
C(27B)-C(26B)-H(26B)	120.9
C(28B)-C(27B)-C(26B)	121.8(5)
C(28B)-C(27B)-I(1B)	118.4(4)
C(26B)-C(27B)-I(1B)	119.8(4)
C(27B)-C(28B)-C(29B)	118.6(5)
C(27B)-C(28B)-H(28B)	120.7
C(29B)-C(28B)-H(28B)	120.7
C(30B)-C(29B)-C(28B)	120.3(6)
C(30B)-C(29B)-H(29B)	119.8
C(28B)-C(29B)-H(29B)	119.8
C(29B)-C(30B)-C(25B)	120.8(6)
C(29B)-C(30B)-H(30B)	119.6
C(25B)-C(30B)-H(30B)	119.6
O(1B)-B(1B)-N(5B)	120.3(5)
O(1B)-B(1B)-N(1B)	108.0(4)
N(5B)-B(1B)-N(1B)	102.8(4)
O(1B)-B(1B)-N(3B)	116.3(5)
N(5B)-B(1B)-N(3B)	103.9(4)
N(1B)-B(1B)-N(3B)	103.5(4)

Symmetry transformations used to generate equivalent atoms:

Table S 76. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1A)	23(1)	24(1)	21(1)	3(1)	-6(1)	1(1)
Cl(1A)	16(1)	21(1)	28(1)	5(1)	-3(1)	3(1)
Cl(2A)	24(1)	40(1)	21(1)	8(1)	-6(1)	4(1)
Cl(3A)	38(1)	39(1)	20(1)	0(1)	10(1)	-2(1)
Cl(4A)	23(1)	38(1)	34(1)	-5(1)	11(1)	-5(1)
Cl(5A)	31(1)	42(1)	27(1)	-16(1)	-7(1)	-2(1)
Cl(6A)	38(1)	26(1)	19(1)	-7(1)	5(1)	3(1)
O(1A)	17(2)	16(2)	20(2)	3(1)	-2(2)	2(1)
N(1A)	17(2)	14(2)	14(2)	-1(2)	-1(2)	0(2)
N(2A)	19(2)	13(2)	15(2)	0(2)	-2(2)	-1(2)
N(3A)	16(2)	14(2)	15(2)	-2(2)	0(2)	4(2)
N(4A)	15(2)	18(2)	16(2)	3(2)	-3(2)	4(2)
N(5A)	19(2)	12(2)	14(2)	3(2)	-1(2)	1(2)
N(6A)	17(2)	16(2)	17(2)	1(2)	2(2)	2(2)
C(1A)	14(2)	15(2)	17(3)	2(2)	3(2)	-3(2)
C(2A)	13(2)	12(2)	22(3)	3(2)	-1(2)	-5(2)
C(3A)	17(2)	13(2)	18(3)	-1(2)	-1(2)	-2(2)
C(4A)	14(2)	12(2)	27(3)	5(2)	-3(2)	1(2)
C(5A)	18(3)	19(3)	18(3)	7(2)	-6(2)	0(2)
C(6A)	17(2)	16(2)	19(3)	3(2)	-1(2)	-3(2)
C(7A)	16(2)	12(2)	15(2)	3(2)	0(2)	-2(2)
C(8A)	17(2)	11(2)	17(3)	2(2)	-3(2)	-1(2)
C(9A)	20(2)	15(2)	12(2)	0(2)	2(2)	1(2)
C(10A)	18(2)	13(2)	17(3)	-1(2)	2(2)	1(2)
C(11A)	22(3)	16(2)	18(3)	-1(2)	-4(2)	6(2)
C(12A)	29(3)	16(2)	19(3)	1(2)	7(2)	5(2)
C(13A)	19(3)	19(3)	29(3)	-2(2)	7(2)	2(2)
C(14A)	18(3)	17(2)	24(3)	-4(2)	1(2)	4(2)
C(15A)	16(2)	15(2)	17(3)	0(2)	1(2)	4(2)
C(16A)	14(2)	16(2)	18(3)	-2(2)	-1(2)	4(2)

C(17A)	16(2)	16(2)	12(2)	3(2)	-4(2)	4(2)
C(18A)	21(2)	19(2)	12(2)	2(2)	-4(2)	5(2)
C(19A)	19(3)	25(3)	17(3)	-1(2)	-4(2)	5(2)
C(20A)	23(2)	23(2)	14(2)	-2(2)	-7(2)	1(2)
C(21A)	26(3)	19(2)	14(2)	2(2)	3(2)	4(2)
C(22A)	25(3)	20(2)	13(3)	3(2)	4(2)	3(2)
C(23A)	19(2)	16(2)	13(2)	3(2)	1(2)	1(2)
C(24A)	22(3)	14(2)	14(2)	4(2)	2(2)	4(2)
C(25A)	14(2)	14(2)	18(3)	4(2)	1(2)	4(2)
C(26A)	23(3)	14(2)	18(3)	0(2)	0(2)	0(2)
C(27A)	17(2)	22(2)	18(3)	3(2)	-4(2)	2(2)
C(28A)	24(3)	17(3)	33(3)	9(2)	-1(2)	3(2)
C(29A)	27(3)	14(2)	38(4)	2(2)	-4(3)	-3(2)
C(30A)	15(2)	19(2)	23(3)	2(2)	0(2)	-3(2)
B(1A)	18(3)	16(3)	15(3)	-2(2)	-2(2)	5(2)
I(1B)	24(1)	40(1)	29(1)	-5(1)	-4(1)	-3(1)
Cl(1B)	19(1)	38(1)	33(1)	4(1)	-4(1)	-7(1)
Cl(2B)	30(1)	60(1)	23(1)	1(1)	-9(1)	-16(1)
Cl(3B)	27(1)	53(1)	25(1)	-4(1)	7(1)	-2(1)
Cl(4B)	19(1)	37(1)	38(1)	0(1)	3(1)	3(1)
Cl(5B)	32(1)	38(1)	31(1)	12(1)	-4(1)	6(1)
Cl(6B)	34(1)	29(1)	25(1)	6(1)	5(1)	-1(1)
O(1B)	23(2)	24(2)	25(2)	-7(2)	-4(2)	0(2)
N(1B)	17(2)	20(2)	19(2)	-2(2)	-1(2)	2(2)
N(2B)	19(2)	21(2)	19(2)	1(2)	0(2)	-1(2)
N(3B)	20(2)	20(2)	17(2)	0(2)	-3(2)	-2(2)
N(4B)	21(2)	19(2)	20(2)	0(2)	-2(2)	-4(2)
N(5B)	18(2)	22(2)	16(2)	-4(2)	-1(2)	0(2)
N(6B)	16(2)	25(2)	20(2)	-3(2)	1(2)	3(2)
C(1B)	18(2)	16(2)	23(3)	-1(2)	-1(2)	4(2)
C(2B)	21(3)	19(2)	24(3)	-2(2)	2(2)	6(2)
C(3B)	18(2)	20(2)	17(3)	1(2)	0(2)	2(2)
C(4B)	20(3)	20(3)	29(3)	2(2)	-4(2)	0(2)
C(5B)	27(3)	23(3)	17(3)	0(2)	-7(2)	5(2)
C(6B)	16(2)	25(3)	20(3)	-1(2)	4(2)	2(2)
C(7B)	15(2)	19(3)	26(3)	2(2)	0(2)	2(2)

C(8B)	17(3)	18(2)	24(3)	0(2)	-1(2)	3(2)
C(9B)	20(3)	15(2)	20(3)	3(2)	-2(2)	-3(2)
C(10B)	19(3)	13(2)	24(3)	2(2)	-2(2)	-6(2)
C(11B)	21(3)	20(3)	24(3)	1(2)	-1(2)	-6(2)
C(12B)	24(3)	19(2)	21(3)	-1(2)	3(2)	-7(2)
C(13B)	15(3)	17(3)	40(4)	0(2)	2(2)	-3(2)
C(14B)	16(2)	15(2)	24(3)	2(2)	-6(2)	-3(2)
C(15B)	22(3)	17(2)	21(3)	2(2)	-2(2)	-4(2)
C(16B)	19(2)	17(2)	22(3)	-1(2)	1(2)	-1(2)
C(17B)	17(2)	25(3)	18(3)	-7(2)	-3(2)	0(2)
C(18B)	17(2)	18(2)	22(3)	-8(2)	3(2)	-1(2)
C(19B)	25(3)	24(3)	16(3)	-3(2)	-3(2)	-1(2)
C(20B)	29(3)	20(3)	25(3)	-5(2)	-8(2)	6(2)
C(21B)	26(3)	20(3)	20(3)	-4(2)	5(2)	-3(2)
C(22B)	22(2)	18(2)	17(3)	-6(2)	0(2)	-1(2)
C(23B)	23(2)	21(2)	20(2)	-5(2)	-1(2)	-2(2)
C(24B)	23(3)	18(2)	18(3)	-1(2)	3(2)	-2(2)
C(25B)	22(3)	21(3)	20(3)	-4(2)	5(2)	-6(2)
C(26B)	25(3)	17(2)	25(3)	-3(2)	6(2)	-1(2)
C(27B)	18(2)	26(3)	16(3)	-2(2)	5(2)	-2(2)
C(28B)	29(3)	22(3)	21(3)	-5(2)	4(2)	-8(2)
C(29B)	36(3)	20(3)	30(3)	-3(2)	-3(3)	-3(2)
C(30B)	35(3)	26(3)	22(3)	-1(2)	-3(2)	-6(2)
B(1B)	15(3)	24(3)	18(3)	-3(2)	0(2)	0(2)

Table S 77. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

	x	y	z	U(eq)
H(3AA)	7937	384	6278	19
H(6AA)	6999	1292	8050	21
H(11A)	3856	2028	8392	23
H(14A)	1932	1498	6936	24
H(19A)	2882	422	5093	25
H(22A)	5739	-13	4637	24
H(26A)	4144	3022	5413	22
H(28A)	3882	5633	5116	30
H(29A)	5000	5919	5713	31
H(30A)	5646	4778	6194	23
H(3BA)	-3142	2978	3297	22
H(6BA)	-1844	3888	1624	25
H(11B)	1351	4383	1523	26
H(14B)	3046	3814	3089	22
H(19B)	1688	2630	4891	26
H(22B)	-1235	2298	5029	23
H(26B)	876	5453	4374	27
H(28B)	1217	8074	4556	29
H(29B)	129	8329	3918	34
H(30B)	-567	7166	3521	33

Table S 78. Torsion angles [°] for *m*-IPhO-Cl₆BsubPc (Toluene:Heptane; CCDC deposit 2087103).

C(24A)-N(6A)-C(1A)-N(1A)	-9.0(7)
C(24A)-N(6A)-C(1A)-C(2A)	156.9(5)
C(8A)-N(1A)-C(1A)-N(6A)	157.4(5)
B(1A)-N(1A)-C(1A)-N(6A)	-15.4(7)
C(8A)-N(1A)-C(1A)-C(2A)	-11.6(5)
B(1A)-N(1A)-C(1A)-C(2A)	175.5(4)
N(6A)-C(1A)-C(2A)-C(3A)	19.0(9)
N(1A)-C(1A)-C(2A)-C(3A)	-173.2(5)
N(6A)-C(1A)-C(2A)-C(7A)	-160.5(5)
N(1A)-C(1A)-C(2A)-C(7A)	7.3(5)
C(7A)-C(2A)-C(3A)-C(4A)	-2.7(7)
C(1A)-C(2A)-C(3A)-C(4A)	177.8(5)
C(2A)-C(3A)-C(4A)-C(5A)	5.3(7)
C(2A)-C(3A)-C(4A)-Cl(1A)	-172.9(4)
C(3A)-C(4A)-C(5A)-C(6A)	-3.0(8)
Cl(1A)-C(4A)-C(5A)-C(6A)	175.2(4)
C(3A)-C(4A)-C(5A)-Cl(2A)	178.2(4)
Cl(1A)-C(4A)-C(5A)-Cl(2A)	-3.6(6)
C(4A)-C(5A)-C(6A)-C(7A)	-2.1(8)
Cl(2A)-C(5A)-C(6A)-C(7A)	176.7(4)
C(5A)-C(6A)-C(7A)-C(2A)	4.6(7)
C(5A)-C(6A)-C(7A)-C(8A)	-177.3(5)
C(3A)-C(2A)-C(7A)-C(6A)	-2.3(7)
C(1A)-C(2A)-C(7A)-C(6A)	177.3(5)
C(3A)-C(2A)-C(7A)-C(8A)	179.2(4)
C(1A)-C(2A)-C(7A)-C(8A)	-1.2(5)
C(9A)-N(2A)-C(8A)-N(1A)	7.9(7)
C(9A)-N(2A)-C(8A)-C(7A)	-158.3(5)
C(1A)-N(1A)-C(8A)-N(2A)	-158.5(4)
B(1A)-N(1A)-C(8A)-N(2A)	14.2(7)
C(1A)-N(1A)-C(8A)-C(7A)	10.9(5)
B(1A)-N(1A)-C(8A)-C(7A)	-176.4(4)
C(6A)-C(7A)-C(8A)-N(2A)	-15.7(9)

C(2A)-C(7A)-C(8A)-N(2A)	162.6(5)
C(6A)-C(7A)-C(8A)-N(1A)	176.3(5)
C(2A)-C(7A)-C(8A)-N(1A)	-5.4(5)
C(8A)-N(2A)-C(9A)-N(3A)	-8.4(7)
C(8A)-N(2A)-C(9A)-C(10A)	150.8(5)
C(16A)-N(3A)-C(9A)-N(2A)	150.4(5)
B(1A)-N(3A)-C(9A)-N(2A)	-13.3(7)
C(16A)-N(3A)-C(9A)-C(10A)	-12.8(5)
B(1A)-N(3A)-C(9A)-C(10A)	-176.5(4)
N(2A)-C(9A)-C(10A)-C(11A)	18.2(9)
N(3A)-C(9A)-C(10A)-C(11A)	-179.6(5)
N(2A)-C(9A)-C(10A)-C(15A)	-154.5(5)
N(3A)-C(9A)-C(10A)-C(15A)	7.7(5)
C(15A)-C(10A)-C(11A)-C(12A)	0.8(7)
C(9A)-C(10A)-C(11A)-C(12A)	-171.0(5)
C(10A)-C(11A)-C(12A)-C(13A)	1.9(7)
C(10A)-C(11A)-C(12A)-Cl(3A)	-179.1(4)
C(11A)-C(12A)-C(13A)-C(14A)	-2.7(8)
Cl(3A)-C(12A)-C(13A)-C(14A)	178.2(4)
C(11A)-C(12A)-C(13A)-Cl(4A)	176.0(4)
Cl(3A)-C(12A)-C(13A)-Cl(4A)	-3.0(6)
C(12A)-C(13A)-C(14A)-C(15A)	0.8(7)
Cl(4A)-C(13A)-C(14A)-C(15A)	-178.0(4)
C(13A)-C(14A)-C(15A)-C(10A)	1.9(7)
C(13A)-C(14A)-C(15A)-C(16A)	171.2(5)
C(11A)-C(10A)-C(15A)-C(14A)	-2.8(7)
C(9A)-C(10A)-C(15A)-C(14A)	170.9(4)
C(11A)-C(10A)-C(15A)-C(16A)	-174.1(4)
C(9A)-C(10A)-C(15A)-C(16A)	-0.5(5)
C(17A)-N(4A)-C(16A)-N(3A)	8.0(7)
C(17A)-N(4A)-C(16A)-C(15A)	-153.1(5)
C(9A)-N(3A)-C(16A)-N(4A)	-152.5(5)
B(1A)-N(3A)-C(16A)-N(4A)	11.1(7)
C(9A)-N(3A)-C(16A)-C(15A)	12.5(5)
B(1A)-N(3A)-C(16A)-C(15A)	176.0(4)
C(14A)-C(15A)-C(16A)-N(4A)	-13.5(9)

C(10A)-C(15A)-C(16A)-N(4A)	156.8(5)
C(14A)-C(15A)-C(16A)-N(3A)	-177.1(5)
C(10A)-C(15A)-C(16A)-N(3A)	-6.9(5)
C(16A)-N(4A)-C(17A)-N(5A)	-7.4(7)
C(16A)-N(4A)-C(17A)-C(18A)	157.7(5)
C(24A)-N(5A)-C(17A)-N(4A)	157.2(5)
B(1A)-N(5A)-C(17A)-N(4A)	-12.4(7)
C(24A)-N(5A)-C(17A)-C(18A)	-11.0(5)
B(1A)-N(5A)-C(17A)-C(18A)	179.4(4)
N(4A)-C(17A)-C(18A)-C(19A)	12.1(9)
N(5A)-C(17A)-C(18A)-C(19A)	179.2(5)
N(4A)-C(17A)-C(18A)-C(23A)	-162.2(5)
N(5A)-C(17A)-C(18A)-C(23A)	4.9(5)
C(23A)-C(18A)-C(19A)-C(20A)	-3.8(8)
C(17A)-C(18A)-C(19A)-C(20A)	-177.4(5)
C(18A)-C(19A)-C(20A)-C(21A)	-1.3(8)
C(18A)-C(19A)-C(20A)-Cl(5A)	178.6(4)
C(19A)-C(20A)-C(21A)-C(22A)	5.5(8)
Cl(5A)-C(20A)-C(21A)-C(22A)	-174.4(4)
C(19A)-C(20A)-C(21A)-Cl(6A)	-173.8(4)
Cl(5A)-C(20A)-C(21A)-Cl(6A)	6.3(6)
C(20A)-C(21A)-C(22A)-C(23A)	-4.3(7)
Cl(6A)-C(21A)-C(22A)-C(23A)	175.0(4)
C(21A)-C(22A)-C(23A)-C(18A)	-0.8(7)
C(21A)-C(22A)-C(23A)-C(24A)	176.3(5)
C(19A)-C(18A)-C(23A)-C(22A)	5.0(8)
C(17A)-C(18A)-C(23A)-C(22A)	180.0(4)
C(19A)-C(18A)-C(23A)-C(24A)	-172.8(5)
C(17A)-C(18A)-C(23A)-C(24A)	2.2(5)
C(1A)-N(6A)-C(24A)-N(5A)	8.3(7)
C(1A)-N(6A)-C(24A)-C(23A)	-152.5(5)
C(17A)-N(5A)-C(24A)-N(6A)	-152.7(5)
B(1A)-N(5A)-C(24A)-N(6A)	17.0(7)
C(17A)-N(5A)-C(24A)-C(23A)	12.2(5)
B(1A)-N(5A)-C(24A)-C(23A)	-178.0(4)
C(22A)-C(23A)-C(24A)-N(6A)	-22.4(9)

C(18A)-C(23A)-C(24A)-N(6A)	154.9(5)
C(22A)-C(23A)-C(24A)-N(5A)	174.3(5)
C(18A)-C(23A)-C(24A)-N(5A)	-8.3(5)
B(1A)-O(1A)-C(25A)-C(26A)	-24.5(8)
B(1A)-O(1A)-C(25A)-C(30A)	157.4(5)
O(1A)-C(25A)-C(26A)-C(27A)	179.7(5)
C(30A)-C(25A)-C(26A)-C(27A)	-2.2(8)
C(25A)-C(26A)-C(27A)-C(28A)	0.4(8)
C(25A)-C(26A)-C(27A)-I(1A)	178.9(4)
C(26A)-C(27A)-C(28A)-C(29A)	2.1(9)
I(1A)-C(27A)-C(28A)-C(29A)	-176.4(4)
C(27A)-C(28A)-C(29A)-C(30A)	-2.7(9)
C(28A)-C(29A)-C(30A)-C(25A)	0.9(9)
O(1A)-C(25A)-C(30A)-C(29A)	179.8(5)
C(26A)-C(25A)-C(30A)-C(29A)	1.6(8)
C(25A)-O(1A)-B(1A)-N(5A)	58.4(7)
C(25A)-O(1A)-B(1A)-N(3A)	-69.5(7)
C(25A)-O(1A)-B(1A)-N(1A)	174.3(4)
C(17A)-N(5A)-B(1A)-O(1A)	-107.8(6)
C(24A)-N(5A)-B(1A)-O(1A)	83.5(6)
C(17A)-N(5A)-B(1A)-N(3A)	26.5(6)
C(24A)-N(5A)-B(1A)-N(3A)	-142.2(4)
C(17A)-N(5A)-B(1A)-N(1A)	133.9(4)
C(24A)-N(5A)-B(1A)-N(1A)	-34.8(6)
C(9A)-N(3A)-B(1A)-O(1A)	-88.7(6)
C(16A)-N(3A)-B(1A)-O(1A)	109.2(5)
C(9A)-N(3A)-B(1A)-N(5A)	136.4(4)
C(16A)-N(3A)-B(1A)-N(5A)	-25.7(6)
C(9A)-N(3A)-B(1A)-N(1A)	29.6(6)
C(16A)-N(3A)-B(1A)-N(1A)	-132.5(4)
C(8A)-N(1A)-B(1A)-O(1A)	95.2(5)
C(1A)-N(1A)-B(1A)-O(1A)	-92.6(5)
C(8A)-N(1A)-B(1A)-N(5A)	-138.2(4)
C(1A)-N(1A)-B(1A)-N(5A)	34.0(6)
C(8A)-N(1A)-B(1A)-N(3A)	-30.4(6)
C(1A)-N(1A)-B(1A)-N(3A)	141.8(4)

C(24B)-N(6B)-C(1B)-N(1B)	-7.4(7)
C(24B)-N(6B)-C(1B)-C(2B)	156.3(5)
C(8B)-N(1B)-C(1B)-N(6B)	154.7(5)
B(1B)-N(1B)-C(1B)-N(6B)	-16.9(8)
C(8B)-N(1B)-C(1B)-C(2B)	-12.4(6)
B(1B)-N(1B)-C(1B)-C(2B)	176.0(5)
N(6B)-C(1B)-C(2B)-C(3B)	19.1(9)
N(1B)-C(1B)-C(2B)-C(3B)	-175.3(5)
N(6B)-C(1B)-C(2B)-C(7B)	-157.4(5)
N(1B)-C(1B)-C(2B)-C(7B)	8.3(5)
C(7B)-C(2B)-C(3B)-C(4B)	-1.2(8)
C(1B)-C(2B)-C(3B)-C(4B)	-177.2(5)
C(2B)-C(3B)-C(4B)-C(5B)	1.7(8)
C(2B)-C(3B)-C(4B)-Cl(1B)	178.3(4)
C(3B)-C(4B)-C(5B)-C(6B)	-0.4(8)
Cl(1B)-C(4B)-C(5B)-C(6B)	-177.0(4)
C(3B)-C(4B)-C(5B)-Cl(2B)	-178.7(4)
Cl(1B)-C(4B)-C(5B)-Cl(2B)	4.7(7)
C(4B)-C(5B)-C(6B)-C(7B)	-1.5(8)
Cl(2B)-C(5B)-C(6B)-C(7B)	176.8(4)
C(5B)-C(6B)-C(7B)-C(2B)	1.9(8)
C(5B)-C(6B)-C(7B)-C(8B)	179.6(5)
C(3B)-C(2B)-C(7B)-C(6B)	-0.6(8)
C(1B)-C(2B)-C(7B)-C(6B)	176.3(5)
C(3B)-C(2B)-C(7B)-C(8B)	-178.8(5)
C(1B)-C(2B)-C(7B)-C(8B)	-1.9(6)
C(9B)-N(2B)-C(8B)-N(1B)	6.8(7)
C(9B)-N(2B)-C(8B)-C(7B)	-157.8(5)
C(1B)-N(1B)-C(8B)-N(2B)	-156.7(5)
B(1B)-N(1B)-C(8B)-N(2B)	14.9(8)
C(1B)-N(1B)-C(8B)-C(7B)	11.1(6)
B(1B)-N(1B)-C(8B)-C(7B)	-177.3(5)
C(6B)-C(7B)-C(8B)-N(2B)	-16.3(10)
C(2B)-C(7B)-C(8B)-N(2B)	161.6(5)
C(6B)-C(7B)-C(8B)-N(1B)	176.9(6)
C(2B)-C(7B)-C(8B)-N(1B)	-5.1(6)

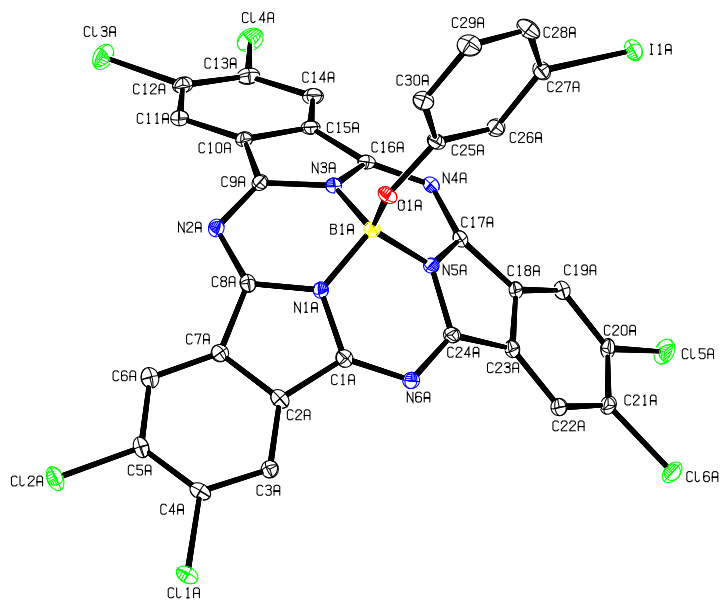
C(8B)-N(2B)-C(9B)-N(3B)	-7.7(7)
C(8B)-N(2B)-C(9B)-C(10B)	154.1(5)
C(16B)-N(3B)-C(9B)-N(2B)	152.5(5)
B(1B)-N(3B)-C(9B)-N(2B)	-12.8(8)
C(16B)-N(3B)-C(9B)-C(10B)	-13.2(6)
B(1B)-N(3B)-C(9B)-C(10B)	-178.5(4)
N(2B)-C(9B)-C(10B)-C(11B)	15.9(9)
N(3B)-C(9B)-C(10B)-C(11B)	-179.9(5)
N(2B)-C(9B)-C(10B)-C(15B)	-156.3(5)
N(3B)-C(9B)-C(10B)-C(15B)	8.0(5)
C(15B)-C(10B)-C(11B)-C(12B)	-0.6(8)
C(9B)-C(10B)-C(11B)-C(12B)	-171.9(5)
C(10B)-C(11B)-C(12B)-C(13B)	1.0(8)
C(10B)-C(11B)-C(12B)-Cl(3B)	179.9(4)
C(11B)-C(12B)-C(13B)-C(14B)	-1.2(8)
Cl(3B)-C(12B)-C(13B)-C(14B)	179.9(4)
C(11B)-C(12B)-C(13B)-Cl(4B)	178.3(4)
Cl(3B)-C(12B)-C(13B)-Cl(4B)	-0.6(6)
C(12B)-C(13B)-C(14B)-C(15B)	0.9(8)
Cl(4B)-C(13B)-C(14B)-C(15B)	-178.6(4)
C(13B)-C(14B)-C(15B)-C(10B)	-0.5(8)
C(13B)-C(14B)-C(15B)-C(16B)	171.7(5)
C(11B)-C(10B)-C(15B)-C(14B)	0.3(8)
C(9B)-C(10B)-C(15B)-C(14B)	173.4(5)
C(11B)-C(10B)-C(15B)-C(16B)	-173.6(5)
C(9B)-C(10B)-C(15B)-C(16B)	-0.5(6)
C(17B)-N(4B)-C(16B)-N(3B)	7.2(8)
C(17B)-N(4B)-C(16B)-C(15B)	-154.0(5)
C(9B)-N(3B)-C(16B)-N(4B)	-152.0(5)
B(1B)-N(3B)-C(16B)-N(4B)	13.2(8)
C(9B)-N(3B)-C(16B)-C(15B)	13.0(6)
B(1B)-N(3B)-C(16B)-C(15B)	178.2(4)
C(14B)-C(15B)-C(16B)-N(4B)	-16.8(10)
C(10B)-C(15B)-C(16B)-N(4B)	156.3(5)
C(14B)-C(15B)-C(16B)-N(3B)	179.7(5)
C(10B)-C(15B)-C(16B)-N(3B)	-7.3(5)

C(16B)-N(4B)-C(17B)-N(5B)	-7.7(7)
C(16B)-N(4B)-C(17B)-C(18B)	155.7(5)
C(24B)-N(5B)-C(17B)-N(4B)	155.1(5)
B(1B)-N(5B)-C(17B)-N(4B)	-12.3(8)
C(24B)-N(5B)-C(17B)-C(18B)	-11.8(6)
B(1B)-N(5B)-C(17B)-C(18B)	-179.2(4)
N(4B)-C(17B)-C(18B)-C(19B)	17.6(10)
N(5B)-C(17B)-C(18B)-C(19B)	-177.1(5)
N(4B)-C(17B)-C(18B)-C(23B)	-160.1(5)
N(5B)-C(17B)-C(18B)-C(23B)	5.2(6)
C(17B)-C(18B)-C(19B)-C(20B)	-179.9(5)
C(23B)-C(18B)-C(19B)-C(20B)	-2.4(7)
C(18B)-C(19B)-C(20B)-C(21B)	-0.1(8)
C(18B)-C(19B)-C(20B)-Cl(5B)	179.5(4)
C(19B)-C(20B)-C(21B)-C(22B)	3.6(8)
Cl(5B)-C(20B)-C(21B)-C(22B)	-175.9(4)
C(19B)-C(20B)-C(21B)-Cl(6B)	-176.9(4)
Cl(5B)-C(20B)-C(21B)-Cl(6B)	3.5(6)
C(20B)-C(21B)-C(22B)-C(23B)	-4.5(8)
Cl(6B)-C(21B)-C(22B)-C(23B)	176.1(4)
C(21B)-C(22B)-C(23B)-C(18B)	1.9(8)
C(21B)-C(22B)-C(23B)-C(24B)	178.1(5)
C(19B)-C(18B)-C(23B)-C(22B)	1.5(7)
C(17B)-C(18B)-C(23B)-C(22B)	179.6(5)
C(19B)-C(18B)-C(23B)-C(24B)	-175.6(5)
C(17B)-C(18B)-C(23B)-C(24B)	2.5(6)
C(1B)-N(6B)-C(24B)-N(5B)	9.6(7)
C(1B)-N(6B)-C(24B)-C(23B)	-155.7(5)
C(17B)-N(5B)-C(24B)-N(6B)	-154.8(5)
B(1B)-N(5B)-C(24B)-N(6B)	12.7(8)
C(17B)-N(5B)-C(24B)-C(23B)	13.3(6)
B(1B)-N(5B)-C(24B)-C(23B)	-179.2(5)
C(22B)-C(23B)-C(24B)-N(6B)	-18.9(10)
C(18B)-C(23B)-C(24B)-N(6B)	157.7(5)
C(22B)-C(23B)-C(24B)-N(5B)	174.0(5)
C(18B)-C(23B)-C(24B)-N(5B)	-9.4(6)

B(1B)-O(1B)-C(25B)-C(30B)	154.5(5)
B(1B)-O(1B)-C(25B)-C(26B)	-28.9(9)
C(30B)-C(25B)-C(26B)-C(27B)	0.2(8)
O(1B)-C(25B)-C(26B)-C(27B)	-176.3(5)
C(25B)-C(26B)-C(27B)-C(28B)	-1.8(8)
C(25B)-C(26B)-C(27B)-I(1B)	175.7(4)
C(26B)-C(27B)-C(28B)-C(29B)	2.1(8)
I(1B)-C(27B)-C(28B)-C(29B)	-175.3(4)
C(27B)-C(28B)-C(29B)-C(30B)	-0.9(9)
C(28B)-C(29B)-C(30B)-C(25B)	-0.6(9)
O(1B)-C(25B)-C(30B)-C(29B)	177.8(5)
C(26B)-C(25B)-C(30B)-C(29B)	1.0(9)
C(25B)-O(1B)-B(1B)-N(5B)	68.8(7)
C(25B)-O(1B)-B(1B)-N(1B)	-173.8(5)
C(25B)-O(1B)-B(1B)-N(3B)	-58.0(8)
C(24B)-N(5B)-B(1B)-O(1B)	89.1(6)
C(17B)-N(5B)-B(1B)-O(1B)	-104.9(6)
C(24B)-N(5B)-B(1B)-N(1B)	-30.9(6)
C(17B)-N(5B)-B(1B)-N(1B)	135.1(5)
C(24B)-N(5B)-B(1B)-N(3B)	-138.5(5)
C(17B)-N(5B)-B(1B)-N(3B)	27.4(6)
C(8B)-N(1B)-B(1B)-O(1B)	94.0(6)
C(1B)-N(1B)-B(1B)-O(1B)	-95.2(6)
C(8B)-N(1B)-B(1B)-N(5B)	-137.8(5)
C(1B)-N(1B)-B(1B)-N(5B)	33.0(6)
C(8B)-N(1B)-B(1B)-N(3B)	-29.9(7)
C(1B)-N(1B)-B(1B)-N(3B)	140.9(5)
C(16B)-N(3B)-B(1B)-O(1B)	106.7(6)
C(9B)-N(3B)-B(1B)-O(1B)	-89.5(6)
C(16B)-N(3B)-B(1B)-N(5B)	-27.8(6)
C(9B)-N(3B)-B(1B)-N(5B)	135.9(5)
C(16B)-N(3B)-B(1B)-N(1B)	-135.0(5)
C(9B)-N(3B)-B(1B)-N(1B)	28.8(6)

Symmetry transformations used to generate equivalent atoms:

a)



b)

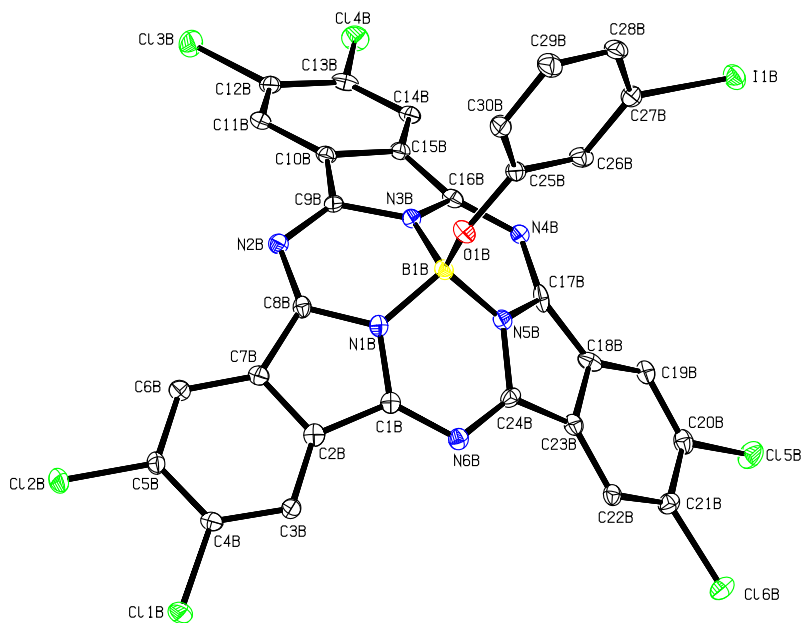


Figure S40: Anisotropic displacement ellipsoid plots of individual co-crystals of *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

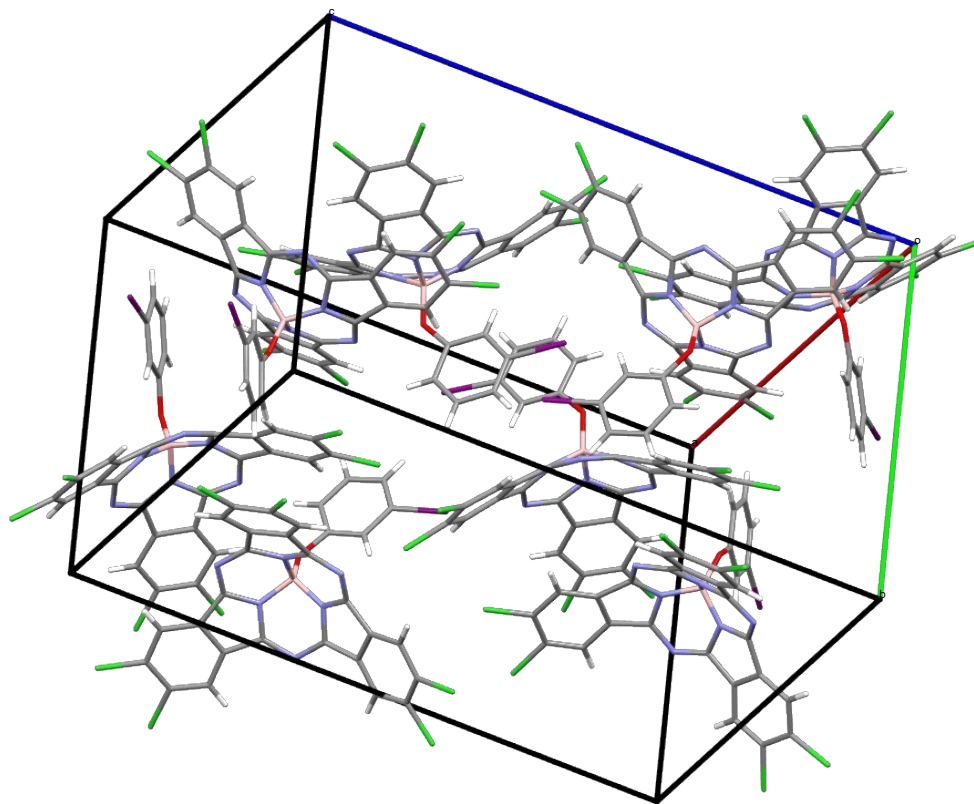


Figure S41: Populated unit cell of *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

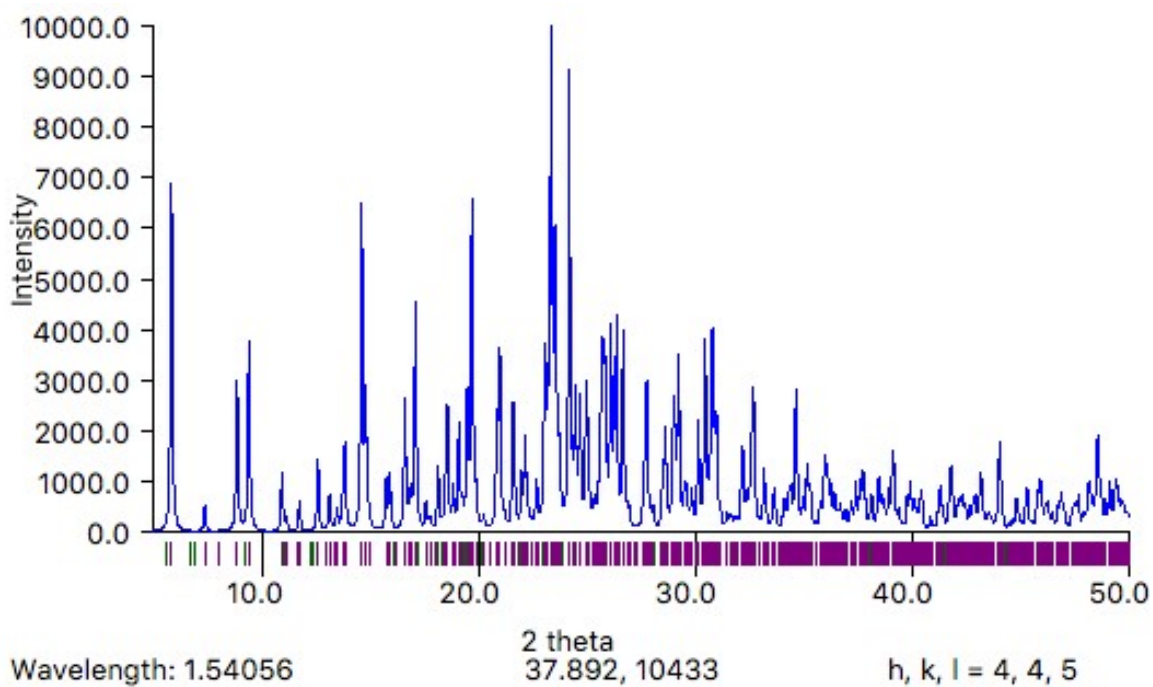


Figure S 42: Powder x-ray diffraction of *m*IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

Table S 79. Crystal data and structure refinement for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

Identification code	d19232a_a	
Empirical formula	C ₃₀ H ₁₀ B Cl ₆ I N ₆ O	
Formula weight	820.85	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2 ₁	
Unit cell dimensions	a = 15.8551(3) Å	α = 90°.
	b = 15.1122(3) Å	β = 90°.
	c = 23.9203(5) Å	γ = 90°.
Volume	5731.4(2) Å ³	
Z	8	
Density (calculated)	1.903 Mg/m ³	
Absorption coefficient	1.718 mm ⁻¹	
F(000)	3200	
Crystal size	0.350 x 0.320 x 0.300 mm ³	
Theta range for data collection	1.862 to 27.490°.	
Index ranges	-20 ≤ h ≤ 20, -19 ≤ k ≤ 19, -31 ≤ l ≤ 31	
Reflections collected	130895	
Independent reflections	13117 [R(int) = 0.0361]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6732	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13117 / 1 / 811	
Goodness-of-fit on F ²	1.025	
Final R indices [I > 2σ(I)]	R1 = 0.0255, wR2 = 0.0652	
R indices (all data)	R1 = 0.0289, wR2 = 0.0665	
Absolute structure parameter	-0.015(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.252 and -0.757 e.Å ⁻³	

Table S 80. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1A)	2973(1)	4044(1)	4614(1)	25(1)
Cl(1A)	9253(1)	20(1)	7024(1)	24(1)
Cl(2A)	8589(1)	522(1)	8209(1)	30(1)
Cl(3A)	2329(1)	1579(1)	8902(1)	34(1)
Cl(4A)	1065(1)	1134(1)	7921(1)	33(1)
Cl(5A)	2912(1)	-819(1)	4232(1)	34(1)
Cl(6A)	4799(1)	-960(1)	3851(1)	28(1)
O(1A)	5364(2)	3158(2)	6160(1)	19(1)
N(1A)	5817(2)	1823(2)	6580(2)	16(1)
N(2A)	5314(2)	2010(2)	7508(2)	18(1)
N(3A)	4388(2)	2205(2)	6728(2)	17(1)
N(4A)	3393(2)	1587(2)	6093(2)	18(1)
N(5A)	4841(2)	1655(2)	5852(2)	16(1)
N(6A)	6208(2)	1021(2)	5766(2)	17(1)
C(1A)	6370(3)	1314(3)	6283(2)	18(1)
C(2A)	7010(3)	1053(3)	6686(2)	18(1)
C(3A)	7765(3)	595(3)	6627(2)	17(1)
C(4A)	8255(3)	471(3)	7099(2)	18(1)
C(5A)	7967(3)	720(3)	7629(2)	20(1)
C(6A)	7193(3)	1143(3)	7700(2)	20(1)
C(7A)	6730(3)	1334(3)	7223(2)	18(1)
C(8A)	5925(3)	1794(3)	7146(2)	17(1)
C(9A)	4542(3)	2157(3)	7290(2)	18(1)
C(10A)	3713(3)	2022(3)	7552(2)	18(1)
C(11A)	3477(3)	1929(3)	8106(2)	21(1)
C(12A)	2642(3)	1682(3)	8213(2)	23(1)
C(13A)	2081(3)	1506(3)	7778(2)	23(1)
C(14A)	2306(3)	1603(3)	7224(2)	22(1)
C(15A)	3135(3)	1879(3)	7113(2)	19(1)
C(16A)	3591(3)	1935(3)	6588(2)	17(1)

C(17A)	4031(3)	1413(3)	5747(2)	17(1)
C(18A)	4074(3)	803(3)	5276(2)	18(1)
C(19A)	3442(3)	348(3)	4999(2)	22(1)
C(20A)	3682(3)	-221(3)	4575(2)	21(1)
C(21A)	4540(3)	-324(3)	4425(2)	21(1)
C(22A)	5174(3)	88(3)	4725(2)	20(1)
C(23A)	4939(3)	658(3)	5157(2)	17(1)
C(24A)	5428(3)	1151(3)	5573(2)	18(1)
C(25A)	4943(3)	3787(3)	5857(2)	18(1)
C(26A)	4307(3)	3603(3)	5481(2)	20(1)
C(27A)	3916(3)	4310(3)	5200(2)	22(1)
C(28A)	4159(3)	5172(3)	5292(2)	27(1)
C(29A)	4819(3)	5342(3)	5660(2)	28(1)
C(30A)	5206(3)	4659(3)	5943(2)	22(1)
B(1A)	5091(3)	2289(3)	6306(2)	17(1)
I(1B)	2031(1)	6529(1)	5154(1)	31(1)
Cl(1B)	-4231(1)	2503(1)	2430(1)	29(1)
Cl(2B)	-3405(1)	3182(1)	1327(1)	38(1)
Cl(3B)	2921(1)	3905(1)	1107(1)	35(1)
Cl(4B)	4050(1)	3488(1)	2155(1)	32(1)
Cl(5B)	1425(1)	1414(1)	5722(1)	34(1)
Cl(6B)	-529(1)	1268(1)	5877(1)	29(1)
O(1B)	-399(2)	5560(2)	3646(1)	24(1)
N(1B)	-897(2)	4277(2)	3184(2)	19(1)
N(2B)	-222(2)	4433(2)	2301(2)	20(1)
N(3B)	577(2)	4541(2)	3142(2)	19(1)
N(4B)	1426(2)	3863(2)	3839(2)	20(1)
N(5B)	-59(2)	4010(2)	3972(2)	19(1)
N(6B)	-1459(2)	3446(2)	3936(2)	21(1)
C(1B)	-1527(3)	3795(3)	3420(2)	20(1)
C(2B)	-2112(3)	3592(3)	2970(2)	21(1)
C(3B)	-2889(3)	3172(3)	2968(2)	20(1)
C(4B)	-3276(3)	3048(3)	2455(2)	22(1)
C(5B)	-2894(3)	3323(3)	1950(2)	22(1)
C(6B)	-2109(3)	3725(3)	1957(2)	21(1)
C(7B)	-1719(3)	3874(3)	2465(2)	20(1)

C(8B)	-911(3)	4269(3)	2615(2)	19(1)
C(9B)	514(3)	4514(3)	2574(2)	19(1)
C(10B)	1364(3)	4357(3)	2373(2)	20(1)
C(11B)	1689(3)	4278(3)	1829(2)	22(1)
C(12B)	2512(3)	4018(3)	1768(2)	22(1)
C(13B)	3023(3)	3837(3)	2243(2)	24(1)
C(14B)	2711(3)	3922(3)	2779(2)	20(1)
C(15B)	1878(3)	4186(3)	2841(2)	21(1)
C(16B)	1331(3)	4237(3)	3332(2)	21(1)
C(17B)	721(3)	3696(3)	4139(2)	23(1)
C(18B)	563(3)	3082(3)	4572(2)	21(1)
C(19B)	1106(3)	2586(3)	4920(2)	23(1)
C(20B)	758(3)	2032(3)	5304(2)	24(1)
C(21B)	-131(3)	1945(3)	5362(2)	23(1)
C(22B)	-660(3)	2389(3)	5008(2)	20(1)
C(23B)	-323(3)	2962(3)	4619(2)	21(1)
C(24B)	-701(3)	3512(3)	4182(2)	20(1)
C(25B)	83(3)	6201(3)	3901(2)	22(1)
C(26B)	717(3)	6029(3)	4285(2)	24(1)
C(27B)	1130(3)	6744(3)	4537(2)	23(1)
C(28B)	934(3)	7601(3)	4401(2)	26(1)
C(29B)	289(4)	7756(3)	4015(2)	32(1)
C(30B)	-139(3)	7061(3)	3772(2)	28(1)
B(1B)	-182(3)	4670(3)	3514(2)	20(1)

Table S 81. Bond lengths [Å] and angles [°] for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

I(1A)-C(27A)	2.088(5)
Cl(1A)-C(4A)	1.732(4)
Cl(2A)-C(5A)	1.727(5)
Cl(3A)-C(12A)	1.726(5)
Cl(4A)-C(13A)	1.740(5)
Cl(5A)-C(20A)	1.726(4)
Cl(6A)-C(21A)	1.727(4)
O(1A)-C(25A)	1.369(5)
O(1A)-B(1A)	1.425(6)
N(1A)-C(1A)	1.366(6)
N(1A)-C(8A)	1.366(5)
N(1A)-B(1A)	1.500(6)
N(2A)-C(8A)	1.340(6)
N(2A)-C(9A)	1.348(6)
N(3A)-C(9A)	1.369(5)
N(3A)-C(16A)	1.370(6)
N(3A)-B(1A)	1.509(6)
N(4A)-C(17A)	1.332(6)
N(4A)-C(16A)	1.334(6)
N(5A)-C(17A)	1.359(6)
N(5A)-C(24A)	1.376(5)
N(5A)-B(1A)	1.501(6)
N(6A)-C(24A)	1.336(6)
N(6A)-C(1A)	1.338(6)
C(1A)-C(2A)	1.453(6)
C(2A)-C(3A)	1.390(6)
C(2A)-C(7A)	1.423(7)
C(3A)-C(4A)	1.383(6)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.400(7)
C(5A)-C(6A)	1.395(7)
C(6A)-C(7A)	1.387(6)

C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.465(6)
C(9A)-C(10A)	1.469(6)
C(10A)-C(11A)	1.385(6)
C(10A)-C(15A)	1.411(6)
C(11A)-C(12A)	1.400(7)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.395(7)
C(13A)-C(14A)	1.381(7)
C(14A)-C(15A)	1.405(6)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.451(6)
C(17A)-C(18A)	1.459(6)
C(18A)-C(19A)	1.384(6)
C(18A)-C(23A)	1.418(6)
C(19A)-C(20A)	1.383(6)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.415(6)
C(21A)-C(22A)	1.383(7)
C(22A)-C(23A)	1.397(6)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.465(6)
C(25A)-C(26A)	1.380(7)
C(25A)-C(30A)	1.397(6)
C(26A)-C(27A)	1.406(6)
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.377(7)
C(28A)-C(29A)	1.392(7)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.378(7)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
I(1B)-C(27B)	2.079(5)
Cl(1B)-C(4B)	1.725(5)
Cl(2B)-C(5B)	1.711(5)
Cl(3B)-C(12B)	1.718(5)

Cl(4B)-C(13B)	1.725(5)
Cl(5B)-C(20B)	1.729(5)
Cl(6B)-C(21B)	1.721(5)
O(1B)-C(25B)	1.375(6)
O(1B)-B(1B)	1.425(6)
N(1B)-C(1B)	1.358(6)
N(1B)-C(8B)	1.360(6)
N(1B)-B(1B)	1.504(6)
N(2B)-C(9B)	1.343(6)
N(2B)-C(8B)	1.349(6)
N(3B)-C(16B)	1.358(6)
N(3B)-C(9B)	1.363(5)
N(3B)-B(1B)	1.510(6)
N(4B)-C(16B)	1.348(6)
N(4B)-C(17B)	1.352(6)
N(5B)-C(24B)	1.363(6)
N(5B)-C(17B)	1.382(6)
N(5B)-B(1B)	1.493(6)
N(6B)-C(24B)	1.343(6)
N(6B)-C(1B)	1.348(6)
C(1B)-C(2B)	1.453(6)
C(2B)-C(3B)	1.385(6)
C(2B)-C(7B)	1.425(7)
C(3B)-C(4B)	1.383(6)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.414(7)
C(5B)-C(6B)	1.385(6)
C(6B)-C(7B)	1.381(7)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.458(6)
C(9B)-C(10B)	1.451(6)
C(10B)-C(11B)	1.405(7)
C(10B)-C(15B)	1.407(6)
C(11B)-C(12B)	1.370(7)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.422(7)

C(13B)-C(14B)	1.378(7)
C(14B)-C(15B)	1.387(6)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.462(7)
C(17B)-C(18B)	1.413(7)
C(18B)-C(19B)	1.414(6)
C(18B)-C(23B)	1.422(6)
C(19B)-C(20B)	1.360(7)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.422(7)
C(21B)-C(22B)	1.367(7)
C(22B)-C(23B)	1.380(6)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.463(6)
C(25B)-C(30B)	1.382(7)
C(25B)-C(26B)	1.387(7)
C(26B)-C(27B)	1.400(6)
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.372(7)
C(28B)-C(29B)	1.398(7)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.378(7)
C(29B)-H(29B)	0.9500
C(30B)-H(30B)	0.9500
C(25A)-O(1A)-B(1A)	128.4(4)
C(1A)-N(1A)-C(8A)	114.6(4)
C(1A)-N(1A)-B(1A)	122.0(4)
C(8A)-N(1A)-B(1A)	123.0(4)
C(8A)-N(2A)-C(9A)	116.5(4)
C(9A)-N(3A)-C(16A)	112.8(4)
C(9A)-N(3A)-B(1A)	122.1(4)
C(16A)-N(3A)-B(1A)	122.9(4)
C(17A)-N(4A)-C(16A)	116.8(4)
C(17A)-N(5A)-C(24A)	113.7(4)
C(17A)-N(5A)-B(1A)	123.7(4)

C(24A)-N(5A)-B(1A)	121.7(4)
C(24A)-N(6A)-C(1A)	116.8(4)
N(6A)-C(1A)-N(1A)	122.9(4)
N(6A)-C(1A)-C(2A)	131.1(4)
N(1A)-C(1A)-C(2A)	104.8(4)
C(3A)-C(2A)-C(7A)	120.6(4)
C(3A)-C(2A)-C(1A)	131.9(4)
C(7A)-C(2A)-C(1A)	107.5(4)
C(4A)-C(3A)-C(2A)	117.9(4)
C(4A)-C(3A)-H(3AA)	121.0
C(2A)-C(3A)-H(3AA)	121.0
C(3A)-C(4A)-C(5A)	121.3(4)
C(3A)-C(4A)-Cl(1A)	118.8(4)
C(5A)-C(4A)-Cl(1A)	119.8(3)
C(6A)-C(5A)-C(4A)	121.3(4)
C(6A)-C(5A)-Cl(2A)	119.0(4)
C(4A)-C(5A)-Cl(2A)	119.6(3)
C(7A)-C(6A)-C(5A)	117.5(4)
C(7A)-C(6A)-H(6AA)	121.3
C(5A)-C(6A)-H(6AA)	121.3
C(6A)-C(7A)-C(2A)	121.0(4)
C(6A)-C(7A)-C(8A)	131.5(4)
C(2A)-C(7A)-C(8A)	107.5(4)
N(2A)-C(8A)-N(1A)	122.8(4)
N(2A)-C(8A)-C(7A)	131.7(4)
N(1A)-C(8A)-C(7A)	104.4(4)
N(2A)-C(9A)-N(3A)	123.4(4)
N(2A)-C(9A)-C(10A)	128.6(4)
N(3A)-C(9A)-C(10A)	105.5(4)
C(11A)-C(10A)-C(15A)	121.4(4)
C(11A)-C(10A)-C(9A)	131.6(4)
C(15A)-C(10A)-C(9A)	106.6(4)
C(10A)-C(11A)-C(12A)	117.3(4)
C(10A)-C(11A)-H(11A)	121.4
C(12A)-C(11A)-H(11A)	121.4
C(13A)-C(12A)-C(11A)	121.1(4)

C(13A)-C(12A)-Cl(3A)	120.8(4)
C(11A)-C(12A)-Cl(3A)	118.1(4)
C(14A)-C(13A)-C(12A)	122.1(4)
C(14A)-C(13A)-Cl(4A)	117.5(4)
C(12A)-C(13A)-Cl(4A)	120.3(4)
C(13A)-C(14A)-C(15A)	117.1(4)
C(13A)-C(14A)-H(14A)	121.5
C(15A)-C(14A)-H(14A)	121.5
C(14A)-C(15A)-C(10A)	120.9(4)
C(14A)-C(15A)-C(16A)	130.3(4)
C(10A)-C(15A)-C(16A)	108.1(4)
N(4A)-C(16A)-N(3A)	123.4(4)
N(4A)-C(16A)-C(15A)	128.9(4)
N(3A)-C(16A)-C(15A)	105.5(4)
N(4A)-C(17A)-N(5A)	123.4(4)
N(4A)-C(17A)-C(18A)	129.8(4)
N(5A)-C(17A)-C(18A)	105.6(4)
C(19A)-C(18A)-C(23A)	121.8(4)
C(19A)-C(18A)-C(17A)	130.6(4)
C(23A)-C(18A)-C(17A)	107.3(4)
C(20A)-C(19A)-C(18A)	117.4(4)
C(20A)-C(19A)-H(19A)	121.3
C(18A)-C(19A)-H(19A)	121.3
C(19A)-C(20A)-C(21A)	121.3(4)
C(19A)-C(20A)-Cl(5A)	118.6(4)
C(21A)-C(20A)-Cl(5A)	120.1(3)
C(22A)-C(21A)-C(20A)	121.2(4)
C(22A)-C(21A)-Cl(6A)	119.3(4)
C(20A)-C(21A)-Cl(6A)	119.5(4)
C(21A)-C(22A)-C(23A)	117.8(4)
C(21A)-C(22A)-H(22A)	121.1
C(23A)-C(22A)-H(22A)	121.1
C(22A)-C(23A)-C(18A)	120.2(4)
C(22A)-C(23A)-C(24A)	132.4(4)
C(18A)-C(23A)-C(24A)	107.3(4)
N(6A)-C(24A)-N(5A)	122.6(4)

N(6A)-C(24A)-C(23A)	130.6(4)
N(5A)-C(24A)-C(23A)	104.7(4)
O(1A)-C(25A)-C(26A)	124.2(4)
O(1A)-C(25A)-C(30A)	115.6(4)
C(26A)-C(25A)-C(30A)	120.2(4)
C(25A)-C(26A)-C(27A)	118.7(4)
C(25A)-C(26A)-H(26A)	120.6
C(27A)-C(26A)-H(26A)	120.6
C(28A)-C(27A)-C(26A)	121.3(4)
C(28A)-C(27A)-I(1A)	119.3(3)
C(26A)-C(27A)-I(1A)	119.4(3)
C(27A)-C(28A)-C(29A)	119.1(4)
C(27A)-C(28A)-H(28A)	120.5
C(29A)-C(28A)-H(28A)	120.5
C(30A)-C(29A)-C(28A)	120.5(4)
C(30A)-C(29A)-H(29A)	119.8
C(28A)-C(29A)-H(29A)	119.8
C(29A)-C(30A)-C(25A)	120.1(4)
C(29A)-C(30A)-H(30A)	119.9
C(25A)-C(30A)-H(30A)	119.9
O(1A)-B(1A)-N(1A)	107.8(4)
O(1A)-B(1A)-N(5A)	119.5(4)
N(1A)-B(1A)-N(5A)	102.7(3)
O(1A)-B(1A)-N(3A)	117.7(4)
N(1A)-B(1A)-N(3A)	103.6(3)
N(5A)-B(1A)-N(3A)	103.6(4)
C(25B)-O(1B)-B(1B)	129.0(4)
C(1B)-N(1B)-C(8B)	113.5(4)
C(1B)-N(1B)-B(1B)	123.2(4)
C(8B)-N(1B)-B(1B)	122.7(4)
C(9B)-N(2B)-C(8B)	116.7(4)
C(16B)-N(3B)-C(9B)	112.8(4)
C(16B)-N(3B)-B(1B)	123.2(4)
C(9B)-N(3B)-B(1B)	122.2(4)
C(16B)-N(4B)-C(17B)	117.6(4)
C(24B)-N(5B)-C(17B)	111.8(4)

C(24B)-N(5B)-B(1B)	122.8(4)
C(17B)-N(5B)-B(1B)	124.0(4)
C(24B)-N(6B)-C(1B)	116.4(4)
N(6B)-C(1B)-N(1B)	122.1(4)
N(6B)-C(1B)-C(2B)	130.3(4)
N(1B)-C(1B)-C(2B)	106.0(4)
C(3B)-C(2B)-C(7B)	121.5(4)
C(3B)-C(2B)-C(1B)	131.9(4)
C(7B)-C(2B)-C(1B)	106.5(4)
C(4B)-C(3B)-C(2B)	117.4(4)
C(4B)-C(3B)-H(3BA)	121.3
C(2B)-C(3B)-H(3BA)	121.3
C(3B)-C(4B)-C(5B)	121.8(4)
C(3B)-C(4B)-Cl(1B)	119.1(4)
C(5B)-C(4B)-Cl(1B)	119.1(4)
C(6B)-C(5B)-C(4B)	120.3(4)
C(6B)-C(5B)-Cl(2B)	119.4(4)
C(4B)-C(5B)-Cl(2B)	120.3(4)
C(7B)-C(6B)-C(5B)	119.0(4)
C(7B)-C(6B)-H(6BA)	120.5
C(5B)-C(6B)-H(6BA)	120.5
C(6B)-C(7B)-C(2B)	120.0(4)
C(6B)-C(7B)-C(8B)	132.7(4)
C(2B)-C(7B)-C(8B)	107.3(4)
N(2B)-C(8B)-N(1B)	122.8(4)
N(2B)-C(8B)-C(7B)	130.5(4)
N(1B)-C(8B)-C(7B)	105.4(4)
N(2B)-C(9B)-N(3B)	123.4(4)
N(2B)-C(9B)-C(10B)	129.2(4)
N(3B)-C(9B)-C(10B)	105.5(4)
C(11B)-C(10B)-C(15B)	120.5(4)
C(11B)-C(10B)-C(9B)	131.4(4)
C(15B)-C(10B)-C(9B)	107.8(4)
C(12B)-C(11B)-C(10B)	118.2(4)
C(12B)-C(11B)-H(11B)	120.9
C(10B)-C(11B)-H(11B)	120.9

C(11B)-C(12B)-C(13B)	120.8(4)
C(11B)-C(12B)-Cl(3B)	119.1(4)
C(13B)-C(12B)-Cl(3B)	120.1(4)
C(14B)-C(13B)-C(12B)	121.3(4)
C(14B)-C(13B)-Cl(4B)	118.8(4)
C(12B)-C(13B)-Cl(4B)	119.9(4)
C(13B)-C(14B)-C(15B)	117.9(4)
C(13B)-C(14B)-H(14B)	121.0
C(15B)-C(14B)-H(14B)	121.0
C(14B)-C(15B)-C(10B)	121.2(5)
C(14B)-C(15B)-C(16B)	131.8(4)
C(10B)-C(15B)-C(16B)	106.5(4)
N(4B)-C(16B)-N(3B)	122.8(4)
N(4B)-C(16B)-C(15B)	129.4(4)
N(3B)-C(16B)-C(15B)	105.8(4)
N(4B)-C(17B)-N(5B)	121.5(4)
N(4B)-C(17B)-C(18B)	131.1(4)
N(5B)-C(17B)-C(18B)	106.2(4)
C(17B)-C(18B)-C(19B)	132.3(4)
C(17B)-C(18B)-C(23B)	108.5(4)
C(19B)-C(18B)-C(23B)	119.2(4)
C(20B)-C(19B)-C(18B)	118.5(4)
C(20B)-C(19B)-H(19B)	120.7
C(18B)-C(19B)-H(19B)	120.7
C(19B)-C(20B)-C(21B)	121.7(4)
C(19B)-C(20B)-Cl(5B)	118.4(4)
C(21B)-C(20B)-Cl(5B)	120.0(4)
C(22B)-C(21B)-C(20B)	120.1(4)
C(22B)-C(21B)-Cl(6B)	120.6(4)
C(20B)-C(21B)-Cl(6B)	119.3(4)
C(21B)-C(22B)-C(23B)	119.2(4)
C(21B)-C(22B)-H(22B)	120.4
C(23B)-C(22B)-H(22B)	120.4
C(22B)-C(23B)-C(18B)	121.1(4)
C(22B)-C(23B)-C(24B)	132.9(4)
C(18B)-C(23B)-C(24B)	106.0(4)

N(6B)-C(24B)-N(5B)	123.2(4)
N(6B)-C(24B)-C(23B)	129.6(4)
N(5B)-C(24B)-C(23B)	105.8(4)
O(1B)-C(25B)-C(30B)	115.0(4)
O(1B)-C(25B)-C(26B)	124.4(4)
C(30B)-C(25B)-C(26B)	120.6(4)
C(25B)-C(26B)-C(27B)	118.7(4)
C(25B)-C(26B)-H(26B)	120.7
C(27B)-C(26B)-H(26B)	120.7
C(28B)-C(27B)-C(26B)	121.4(5)
C(28B)-C(27B)-I(1B)	118.2(3)
C(26B)-C(27B)-I(1B)	120.4(4)
C(27B)-C(28B)-C(29B)	118.7(4)
C(27B)-C(28B)-H(28B)	120.6
C(29B)-C(28B)-H(28B)	120.6
C(30B)-C(29B)-C(28B)	120.8(5)
C(30B)-C(29B)-H(29B)	119.6
C(28B)-C(29B)-H(29B)	119.6
C(29B)-C(30B)-C(25B)	119.8(5)
C(29B)-C(30B)-H(30B)	120.1
C(25B)-C(30B)-H(30B)	120.1
O(1B)-B(1B)-N(5B)	119.9(4)
O(1B)-B(1B)-N(1B)	107.9(4)
N(5B)-B(1B)-N(1B)	102.8(4)
O(1B)-B(1B)-N(3B)	116.4(4)
N(5B)-B(1B)-N(3B)	104.0(4)
N(1B)-B(1B)-N(3B)	103.9(4)

Symmetry transformations used to generate equivalent atoms:

Table S 82. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1A)	26(1)	25(1)	23(1)	3(1)	-6(1)	1(1)
Cl(1A)	18(1)	22(1)	31(1)	4(1)	-2(1)	4(1)
Cl(2A)	25(1)	41(1)	23(1)	8(1)	-7(1)	3(1)
Cl(3A)	40(1)	41(1)	21(1)	1(1)	10(1)	-1(1)
Cl(4A)	26(1)	39(1)	35(1)	-5(1)	11(1)	-4(1)
Cl(5A)	31(1)	44(1)	28(1)	-16(1)	-7(1)	-2(1)
Cl(6A)	39(1)	27(1)	19(1)	-6(1)	5(1)	3(1)
O(1A)	20(2)	16(2)	22(2)	5(1)	-1(1)	2(1)
N(1A)	19(2)	15(2)	14(2)	1(1)	0(1)	1(1)
N(2A)	20(2)	17(2)	15(2)	-2(1)	-2(1)	0(1)
N(3A)	18(2)	16(2)	16(2)	-2(1)	-1(1)	3(1)
N(4A)	18(2)	19(2)	17(2)	2(1)	-2(1)	4(1)
N(5A)	19(2)	13(2)	14(2)	1(1)	1(1)	2(1)
N(6A)	18(2)	17(2)	16(2)	2(1)	2(1)	2(1)
C(1A)	16(2)	18(2)	18(2)	3(2)	1(2)	-1(2)
C(2A)	15(2)	16(2)	22(2)	5(2)	-3(2)	-4(2)
C(3A)	18(2)	17(2)	18(2)	0(2)	-1(2)	-1(2)
C(4A)	14(2)	14(2)	28(2)	4(2)	-3(2)	-2(2)
C(5A)	21(2)	21(2)	17(2)	4(2)	-4(2)	-3(2)
C(6A)	21(2)	20(2)	20(2)	3(2)	-1(2)	-4(2)
C(7A)	19(2)	16(2)	18(2)	2(2)	1(2)	-1(2)
C(8A)	21(2)	13(2)	16(2)	1(2)	-3(2)	-2(2)
C(9A)	24(2)	16(2)	14(2)	0(2)	2(2)	3(2)
C(10A)	21(2)	14(2)	17(2)	-1(2)	1(2)	3(2)
C(11A)	25(2)	18(2)	19(2)	-1(2)	0(2)	6(2)
C(12A)	30(3)	16(2)	22(2)	2(2)	7(2)	5(2)
C(13A)	20(2)	20(2)	29(3)	-1(2)	7(2)	2(2)
C(14A)	18(2)	21(2)	27(2)	-4(2)	-1(2)	4(2)
C(15A)	19(2)	17(2)	20(2)	0(2)	4(2)	6(2)
C(16A)	17(2)	16(2)	19(2)	-1(2)	-1(2)	5(2)

C(17A)	18(2)	18(2)	15(2)	1(2)	-4(2)	3(2)
C(18A)	25(2)	18(2)	12(2)	1(2)	-2(2)	5(2)
C(19A)	23(2)	25(2)	17(2)	0(2)	-4(2)	5(2)
C(20A)	26(2)	24(2)	14(2)	-2(2)	-6(2)	0(2)
C(21A)	31(2)	19(2)	14(2)	2(2)	3(2)	4(2)
C(22A)	26(2)	20(2)	15(2)	3(2)	2(2)	5(2)
C(23A)	21(2)	18(2)	13(2)	3(2)	0(2)	1(2)
C(24A)	21(2)	16(2)	17(2)	3(2)	2(2)	4(2)
C(25A)	17(2)	17(2)	20(2)	4(2)	1(2)	4(2)
C(26A)	25(2)	17(2)	19(2)	1(2)	2(2)	2(2)
C(27A)	22(2)	23(2)	20(2)	3(2)	-1(2)	3(2)
C(28A)	27(2)	20(2)	35(3)	9(2)	-4(2)	2(2)
C(29A)	31(3)	15(2)	37(3)	0(2)	-2(2)	-5(2)
C(30A)	22(2)	19(2)	26(2)	2(2)	0(2)	-1(2)
B(1A)	21(2)	15(2)	16(2)	1(2)	1(2)	4(2)
I(1B)	24(1)	40(1)	28(1)	-5(1)	-4(1)	-3(1)
Cl(1B)	19(1)	36(1)	33(1)	3(1)	-3(1)	-6(1)
Cl(2B)	30(1)	60(1)	24(1)	2(1)	-8(1)	-16(1)
Cl(3B)	27(1)	53(1)	26(1)	-4(1)	6(1)	-3(1)
Cl(4B)	19(1)	38(1)	38(1)	-1(1)	3(1)	3(1)
Cl(5B)	32(1)	39(1)	31(1)	12(1)	-3(1)	6(1)
Cl(6B)	35(1)	29(1)	24(1)	6(1)	6(1)	-1(1)
O(1B)	23(2)	23(2)	27(2)	-5(1)	-4(1)	-1(1)
N(1B)	20(2)	20(2)	18(2)	-1(1)	-2(1)	2(1)
N(2B)	20(2)	20(2)	21(2)	1(1)	-1(1)	-1(1)
N(3B)	21(2)	18(2)	18(2)	0(1)	-2(2)	-2(1)
N(4B)	21(2)	20(2)	18(2)	1(1)	-3(2)	-4(2)
N(5B)	19(2)	20(2)	19(2)	-3(1)	-1(1)	-1(1)
N(6B)	21(2)	23(2)	19(2)	-3(2)	2(2)	2(2)
C(1B)	21(2)	18(2)	20(2)	-1(2)	-1(2)	3(2)
C(2B)	20(2)	19(2)	23(2)	0(2)	-1(2)	6(2)
C(3B)	18(2)	23(2)	19(2)	2(2)	0(2)	1(2)
C(4B)	19(2)	19(2)	27(2)	2(2)	-2(2)	-2(2)
C(5B)	24(2)	24(2)	18(2)	0(2)	-5(2)	0(2)
C(6B)	16(2)	23(2)	23(2)	-3(2)	3(2)	1(2)
C(7B)	18(2)	18(2)	23(2)	1(2)	-2(2)	1(2)

C(8B)	21(2)	19(2)	18(2)	1(2)	-4(2)	4(2)
C(9B)	25(2)	14(2)	18(2)	2(2)	-1(2)	-4(2)
C(10B)	20(2)	16(2)	23(2)	1(2)	-3(2)	-4(2)
C(11B)	25(2)	19(2)	23(2)	-1(2)	-1(2)	-8(2)
C(12B)	23(2)	20(2)	23(2)	-1(2)	4(2)	-6(2)
C(13B)	16(2)	20(2)	38(3)	-1(2)	3(2)	-4(2)
C(14B)	17(2)	16(2)	26(2)	2(2)	-3(2)	-2(2)
C(15B)	22(2)	18(2)	22(2)	3(2)	-4(2)	-5(2)
C(16B)	20(2)	17(2)	24(2)	-2(2)	-2(2)	-3(2)
C(17B)	19(2)	34(2)	16(2)	-11(2)	-5(2)	8(2)
C(18B)	16(2)	16(2)	32(2)	-7(2)	3(2)	0(2)
C(19B)	25(2)	24(2)	20(2)	-4(2)	-4(2)	0(2)
C(20B)	29(2)	20(2)	23(2)	-3(2)	-6(2)	4(2)
C(21B)	28(2)	20(2)	21(2)	-1(2)	5(2)	1(2)
C(22B)	23(2)	21(2)	17(2)	-5(2)	1(2)	0(2)
C(23B)	23(2)	20(2)	20(2)	-3(2)	-2(2)	0(2)
C(24B)	26(2)	17(2)	17(2)	-1(2)	5(2)	0(2)
C(25B)	26(2)	21(2)	19(2)	-5(2)	5(2)	-5(2)
C(26B)	26(2)	17(2)	28(2)	-4(2)	5(2)	-2(2)
C(27B)	22(2)	26(2)	21(2)	-2(2)	4(2)	-1(2)
C(28B)	30(2)	21(2)	28(2)	-6(2)	4(2)	-8(2)
C(29B)	40(3)	21(2)	34(3)	-2(2)	-4(2)	-3(2)
C(30B)	36(3)	23(2)	23(2)	-1(2)	-2(2)	-5(2)
B(1B)	16(2)	24(2)	19(2)	-1(2)	-1(2)	-1(2)

Table S 83. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

	x	y	z	U(eq)
H(3AA)	7939	375	6273	21
H(6AA)	6989	1294	8061	24
H(11A)	3866	2029	8402	25
H(14A)	1917	1488	6931	26
H(19A)	2865	423	5097	26
H(22A)	5752	-15	4640	24
H(26A)	4136	3010	5413	24
H(28A)	3879	5645	5107	33
H(29A)	5005	5933	5716	33
H(30A)	5653	4781	6196	27
H(3BA)	-3146	2977	3305	24
H(6BA)	-1843	3895	1618	25
H(11B)	1348	4402	1512	27
H(14B)	3055	3803	3095	23
H(19B)	1701	2638	4887	27
H(22B)	-1252	2303	5031	24
H(26B)	869	5438	4375	29
H(28B)	1230	8081	4566	32
H(29B)	144	8346	3918	38
H(30B)	-585	7174	3516	33

Table S 84. Torsion angles [°] for *m*-IPhO-Cl₆BsubPc (Chlorobenzene:Heptane; CCDC deposit 2087106).

C(24A)-N(6A)-C(1A)-N(1A)	-8.5(6)
C(24A)-N(6A)-C(1A)-C(2A)	157.1(4)
C(8A)-N(1A)-C(1A)-N(6A)	157.2(4)
B(1A)-N(1A)-C(1A)-N(6A)	-16.0(6)
C(8A)-N(1A)-C(1A)-C(2A)	-11.7(5)
B(1A)-N(1A)-C(1A)-C(2A)	175.1(4)
N(6A)-C(1A)-C(2A)-C(3A)	18.4(8)
N(1A)-C(1A)-C(2A)-C(3A)	-174.1(4)
N(6A)-C(1A)-C(2A)-C(7A)	-160.0(4)
N(1A)-C(1A)-C(2A)-C(7A)	7.6(5)
C(7A)-C(2A)-C(3A)-C(4A)	-3.7(6)
C(1A)-C(2A)-C(3A)-C(4A)	178.1(4)
C(2A)-C(3A)-C(4A)-C(5A)	6.0(6)
C(2A)-C(3A)-C(4A)-Cl(1A)	-172.5(3)
C(3A)-C(4A)-C(5A)-C(6A)	-3.2(7)
Cl(1A)-C(4A)-C(5A)-C(6A)	175.3(4)
C(3A)-C(4A)-C(5A)-Cl(2A)	178.1(3)
Cl(1A)-C(4A)-C(5A)-Cl(2A)	-3.4(5)
C(4A)-C(5A)-C(6A)-C(7A)	-2.1(7)
Cl(2A)-C(5A)-C(6A)-C(7A)	176.6(3)
C(5A)-C(6A)-C(7A)-C(2A)	4.4(6)
C(5A)-C(6A)-C(7A)-C(8A)	-177.4(4)
C(3A)-C(2A)-C(7A)-C(6A)	-1.5(6)
C(1A)-C(2A)-C(7A)-C(6A)	177.0(4)
C(3A)-C(2A)-C(7A)-C(8A)	179.8(4)
C(1A)-C(2A)-C(7A)-C(8A)	-1.6(5)
C(9A)-N(2A)-C(8A)-N(1A)	8.0(6)
C(9A)-N(2A)-C(8A)-C(7A)	-158.2(4)
C(1A)-N(1A)-C(8A)-N(2A)	-158.7(4)
B(1A)-N(1A)-C(8A)-N(2A)	14.4(6)
C(1A)-N(1A)-C(8A)-C(7A)	10.7(5)
B(1A)-N(1A)-C(8A)-C(7A)	-176.2(4)
C(6A)-C(7A)-C(8A)-N(2A)	-15.5(8)

C(2A)-C(7A)-C(8A)-N(2A)	163.0(4)
C(6A)-C(7A)-C(8A)-N(1A)	176.5(5)
C(2A)-C(7A)-C(8A)-N(1A)	-5.0(5)
C(8A)-N(2A)-C(9A)-N(3A)	-8.5(6)
C(8A)-N(2A)-C(9A)-C(10A)	150.6(4)
C(16A)-N(3A)-C(9A)-N(2A)	150.4(4)
B(1A)-N(3A)-C(9A)-N(2A)	-13.1(6)
C(16A)-N(3A)-C(9A)-C(10A)	-12.8(5)
B(1A)-N(3A)-C(9A)-C(10A)	-176.3(4)
N(2A)-C(9A)-C(10A)-C(11A)	18.3(8)
N(3A)-C(9A)-C(10A)-C(11A)	-179.7(4)
N(2A)-C(9A)-C(10A)-C(15A)	-154.2(4)
N(3A)-C(9A)-C(10A)-C(15A)	7.8(5)
C(15A)-C(10A)-C(11A)-C(12A)	0.4(6)
C(9A)-C(10A)-C(11A)-C(12A)	-171.1(4)
C(10A)-C(11A)-C(12A)-C(13A)	2.2(6)
C(10A)-C(11A)-C(12A)-Cl(3A)	-179.0(3)
C(11A)-C(12A)-C(13A)-C(14A)	-2.9(7)
Cl(3A)-C(12A)-C(13A)-C(14A)	178.4(4)
C(11A)-C(12A)-C(13A)-Cl(4A)	176.0(3)
Cl(3A)-C(12A)-C(13A)-Cl(4A)	-2.7(5)
C(12A)-C(13A)-C(14A)-C(15A)	0.7(7)
Cl(4A)-C(13A)-C(14A)-C(15A)	-178.2(3)
C(13A)-C(14A)-C(15A)-C(10A)	1.9(6)
C(13A)-C(14A)-C(15A)-C(16A)	171.3(4)
C(11A)-C(10A)-C(15A)-C(14A)	-2.5(6)
C(9A)-C(10A)-C(15A)-C(14A)	170.8(4)
C(11A)-C(10A)-C(15A)-C(16A)	-174.0(4)
C(9A)-C(10A)-C(15A)-C(16A)	-0.7(5)
C(17A)-N(4A)-C(16A)-N(3A)	7.5(6)
C(17A)-N(4A)-C(16A)-C(15A)	-153.4(4)
C(9A)-N(3A)-C(16A)-N(4A)	-152.2(4)
B(1A)-N(3A)-C(16A)-N(4A)	11.1(6)
C(9A)-N(3A)-C(16A)-C(15A)	12.4(5)
B(1A)-N(3A)-C(16A)-C(15A)	175.8(4)
C(14A)-C(15A)-C(16A)-N(4A)	-13.7(8)

C(10A)-C(15A)-C(16A)-N(4A)	156.7(4)
C(14A)-C(15A)-C(16A)-N(3A)	-177.2(4)
C(10A)-C(15A)-C(16A)-N(3A)	-6.7(5)
C(16A)-N(4A)-C(17A)-N(5A)	-7.0(6)
C(16A)-N(4A)-C(17A)-C(18A)	158.1(4)
C(24A)-N(5A)-C(17A)-N(4A)	156.9(4)
B(1A)-N(5A)-C(17A)-N(4A)	-12.3(6)
C(24A)-N(5A)-C(17A)-C(18A)	-11.3(5)
B(1A)-N(5A)-C(17A)-C(18A)	179.5(4)
N(4A)-C(17A)-C(18A)-C(19A)	12.1(8)
N(5A)-C(17A)-C(18A)-C(19A)	179.3(4)
N(4A)-C(17A)-C(18A)-C(23A)	-162.2(4)
N(5A)-C(17A)-C(18A)-C(23A)	5.0(5)
C(23A)-C(18A)-C(19A)-C(20A)	-3.8(6)
C(17A)-C(18A)-C(19A)-C(20A)	-177.4(4)
C(18A)-C(19A)-C(20A)-C(21A)	-0.8(7)
C(18A)-C(19A)-C(20A)-Cl(5A)	178.5(3)
C(19A)-C(20A)-C(21A)-C(22A)	5.1(7)
Cl(5A)-C(20A)-C(21A)-C(22A)	-174.2(3)
C(19A)-C(20A)-C(21A)-Cl(6A)	-173.9(3)
Cl(5A)-C(20A)-C(21A)-Cl(6A)	6.8(5)
C(20A)-C(21A)-C(22A)-C(23A)	-4.4(6)
Cl(6A)-C(21A)-C(22A)-C(23A)	174.6(3)
C(21A)-C(22A)-C(23A)-C(18A)	-0.2(6)
C(21A)-C(22A)-C(23A)-C(24A)	175.8(4)
C(19A)-C(18A)-C(23A)-C(22A)	4.4(6)
C(17A)-C(18A)-C(23A)-C(22A)	179.3(4)
C(19A)-C(18A)-C(23A)-C(24A)	-172.5(4)
C(17A)-C(18A)-C(23A)-C(24A)	2.4(5)
C(1A)-N(6A)-C(24A)-N(5A)	8.0(6)
C(1A)-N(6A)-C(24A)-C(23A)	-153.0(4)
C(17A)-N(5A)-C(24A)-N(6A)	-152.5(4)
B(1A)-N(5A)-C(24A)-N(6A)	16.9(6)
C(17A)-N(5A)-C(24A)-C(23A)	12.7(5)
B(1A)-N(5A)-C(24A)-C(23A)	-177.9(4)
C(22A)-C(23A)-C(24A)-N(6A)	-21.6(8)

C(18A)-C(23A)-C(24A)-N(6A)	154.8(4)
C(22A)-C(23A)-C(24A)-N(5A)	174.9(4)
C(18A)-C(23A)-C(24A)-N(5A)	-8.7(5)
B(1A)-O(1A)-C(25A)-C(26A)	-23.2(7)
B(1A)-O(1A)-C(25A)-C(30A)	158.0(4)
O(1A)-C(25A)-C(26A)-C(27A)	179.3(4)
C(30A)-C(25A)-C(26A)-C(27A)	-1.9(7)
C(25A)-C(26A)-C(27A)-C(28A)	0.3(7)
C(25A)-C(26A)-C(27A)-I(1A)	178.5(3)
C(26A)-C(27A)-C(28A)-C(29A)	1.7(8)
I(1A)-C(27A)-C(28A)-C(29A)	-176.4(4)
C(27A)-C(28A)-C(29A)-C(30A)	-2.2(8)
C(28A)-C(29A)-C(30A)-C(25A)	0.7(8)
O(1A)-C(25A)-C(30A)-C(29A)	-179.7(4)
C(26A)-C(25A)-C(30A)-C(29A)	1.4(7)
C(25A)-O(1A)-B(1A)-N(1A)	173.4(4)
C(25A)-O(1A)-B(1A)-N(5A)	56.9(6)
C(25A)-O(1A)-B(1A)-N(3A)	-70.0(6)
C(1A)-N(1A)-B(1A)-O(1A)	-92.5(5)
C(8A)-N(1A)-B(1A)-O(1A)	94.9(5)
C(1A)-N(1A)-B(1A)-N(5A)	34.5(5)
C(8A)-N(1A)-B(1A)-N(5A)	-138.1(4)
C(1A)-N(1A)-B(1A)-N(3A)	142.0(4)
C(8A)-N(1A)-B(1A)-N(3A)	-30.6(5)
C(17A)-N(5A)-B(1A)-O(1A)	-107.4(5)
C(24A)-N(5A)-B(1A)-O(1A)	84.3(5)
C(17A)-N(5A)-B(1A)-N(1A)	133.5(4)
C(24A)-N(5A)-B(1A)-N(1A)	-34.8(5)
C(17A)-N(5A)-B(1A)-N(3A)	25.9(5)
C(24A)-N(5A)-B(1A)-N(3A)	-142.4(4)
C(9A)-N(3A)-B(1A)-O(1A)	-89.1(5)
C(16A)-N(3A)-B(1A)-O(1A)	109.1(5)
C(9A)-N(3A)-B(1A)-N(1A)	29.7(5)
C(16A)-N(3A)-B(1A)-N(1A)	-132.1(4)
C(9A)-N(3A)-B(1A)-N(5A)	136.6(4)
C(16A)-N(3A)-B(1A)-N(5A)	-25.2(5)

C(24B)-N(6B)-C(1B)-N(1B)	-7.3(6)
C(24B)-N(6B)-C(1B)-C(2B)	156.1(5)
C(8B)-N(1B)-C(1B)-N(6B)	154.7(4)
B(1B)-N(1B)-C(1B)-N(6B)	-16.9(7)
C(8B)-N(1B)-C(1B)-C(2B)	-12.1(5)
B(1B)-N(1B)-C(1B)-C(2B)	176.2(4)
N(6B)-C(1B)-C(2B)-C(3B)	19.3(8)
N(1B)-C(1B)-C(2B)-C(3B)	-175.3(5)
N(6B)-C(1B)-C(2B)-C(7B)	-157.5(5)
N(1B)-C(1B)-C(2B)-C(7B)	8.0(5)
C(7B)-C(2B)-C(3B)-C(4B)	-0.9(7)
C(1B)-C(2B)-C(3B)-C(4B)	-177.3(5)
C(2B)-C(3B)-C(4B)-C(5B)	1.0(7)
C(2B)-C(3B)-C(4B)-Cl(1B)	178.4(3)
C(3B)-C(4B)-C(5B)-C(6B)	0.3(7)
Cl(1B)-C(4B)-C(5B)-C(6B)	-177.0(4)
C(3B)-C(4B)-C(5B)-Cl(2B)	-178.3(4)
Cl(1B)-C(4B)-C(5B)-Cl(2B)	4.3(6)
C(4B)-C(5B)-C(6B)-C(7B)	-1.8(7)
Cl(2B)-C(5B)-C(6B)-C(7B)	176.9(4)
C(5B)-C(6B)-C(7B)-C(2B)	1.9(7)
C(5B)-C(6B)-C(7B)-C(8B)	179.6(5)
C(3B)-C(2B)-C(7B)-C(6B)	-0.6(7)
C(1B)-C(2B)-C(7B)-C(6B)	176.6(4)
C(3B)-C(2B)-C(7B)-C(8B)	-178.8(4)
C(1B)-C(2B)-C(7B)-C(8B)	-1.6(5)
C(9B)-N(2B)-C(8B)-N(1B)	7.0(6)
C(9B)-N(2B)-C(8B)-C(7B)	-157.7(4)
C(1B)-N(1B)-C(8B)-N(2B)	-157.0(4)
B(1B)-N(1B)-C(8B)-N(2B)	14.7(7)
C(1B)-N(1B)-C(8B)-C(7B)	11.0(5)
B(1B)-N(1B)-C(8B)-C(7B)	-177.3(4)
C(6B)-C(7B)-C(8B)-N(2B)	-16.4(8)
C(2B)-C(7B)-C(8B)-N(2B)	161.5(4)
C(6B)-C(7B)-C(8B)-N(1B)	176.8(5)
C(2B)-C(7B)-C(8B)-N(1B)	-5.3(5)

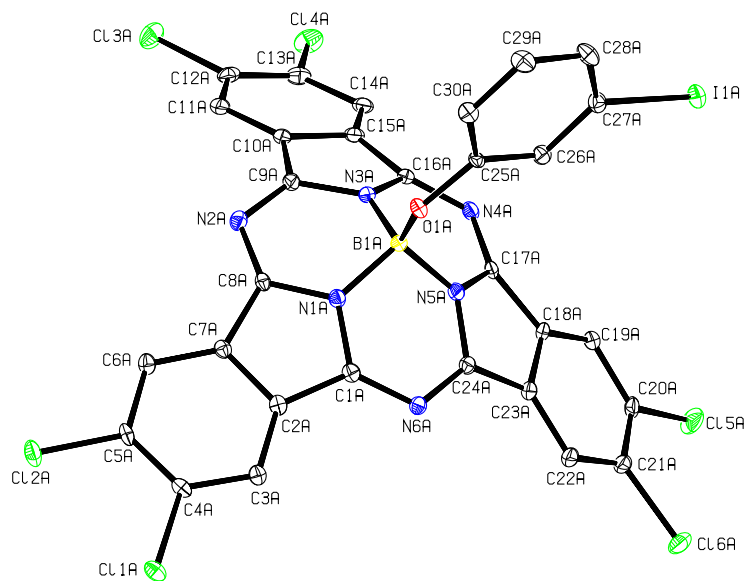
C(8B)-N(2B)-C(9B)-N(3B)	-7.9(6)
C(8B)-N(2B)-C(9B)-C(10B)	154.1(4)
C(16B)-N(3B)-C(9B)-N(2B)	152.6(4)
B(1B)-N(3B)-C(9B)-N(2B)	-12.7(6)
C(16B)-N(3B)-C(9B)-C(10B)	-13.0(5)
B(1B)-N(3B)-C(9B)-C(10B)	-178.4(4)
N(2B)-C(9B)-C(10B)-C(11B)	16.5(8)
N(3B)-C(9B)-C(10B)-C(11B)	-179.0(5)
N(2B)-C(9B)-C(10B)-C(15B)	-157.1(4)
N(3B)-C(9B)-C(10B)-C(15B)	7.4(5)
C(15B)-C(10B)-C(11B)-C(12B)	1.0(6)
C(9B)-C(10B)-C(11B)-C(12B)	-172.0(4)
C(10B)-C(11B)-C(12B)-C(13B)	-0.4(7)
C(10B)-C(11B)-C(12B)-Cl(3B)	179.3(3)
C(11B)-C(12B)-C(13B)-C(14B)	-0.3(7)
Cl(3B)-C(12B)-C(13B)-C(14B)	-179.9(4)
C(11B)-C(12B)-C(13B)-Cl(4B)	178.6(3)
Cl(3B)-C(12B)-C(13B)-Cl(4B)	-1.0(5)
C(12B)-C(13B)-C(14B)-C(15B)	0.3(7)
Cl(4B)-C(13B)-C(14B)-C(15B)	-178.7(3)
C(13B)-C(14B)-C(15B)-C(10B)	0.4(7)
C(13B)-C(14B)-C(15B)-C(16B)	171.7(5)
C(11B)-C(10B)-C(15B)-C(14B)	-1.1(7)
C(9B)-C(10B)-C(15B)-C(14B)	173.4(4)
C(11B)-C(10B)-C(15B)-C(16B)	-174.3(4)
C(9B)-C(10B)-C(15B)-C(16B)	0.2(5)
C(17B)-N(4B)-C(16B)-N(3B)	7.8(6)
C(17B)-N(4B)-C(16B)-C(15B)	-153.4(5)
C(9B)-N(3B)-C(16B)-N(4B)	-151.9(4)
B(1B)-N(3B)-C(16B)-N(4B)	13.3(7)
C(9B)-N(3B)-C(16B)-C(15B)	13.2(5)
B(1B)-N(3B)-C(16B)-C(15B)	178.3(4)
C(14B)-C(15B)-C(16B)-N(4B)	-16.2(8)
C(10B)-C(15B)-C(16B)-N(4B)	156.0(5)
C(14B)-C(15B)-C(16B)-N(3B)	-179.9(5)
C(10B)-C(15B)-C(16B)-N(3B)	-7.7(5)

C(16B)-N(4B)-C(17B)-N(5B)	-9.3(6)
C(16B)-N(4B)-C(17B)-C(18B)	156.3(5)
C(24B)-N(5B)-C(17B)-N(4B)	156.0(4)
B(1B)-N(5B)-C(17B)-N(4B)	-10.4(7)
C(24B)-N(5B)-C(17B)-C(18B)	-12.8(5)
B(1B)-N(5B)-C(17B)-C(18B)	-179.1(4)
N(4B)-C(17B)-C(18B)-C(19B)	16.4(8)
N(5B)-C(17B)-C(18B)-C(19B)	-176.4(5)
N(4B)-C(17B)-C(18B)-C(23B)	-160.9(5)
N(5B)-C(17B)-C(18B)-C(23B)	6.3(5)
C(17B)-C(18B)-C(19B)-C(20B)	-179.5(5)
C(23B)-C(18B)-C(19B)-C(20B)	-2.4(6)
C(18B)-C(19B)-C(20B)-C(21B)	-0.2(7)
C(18B)-C(19B)-C(20B)-Cl(5B)	179.1(3)
C(19B)-C(20B)-C(21B)-C(22B)	3.5(7)
Cl(5B)-C(20B)-C(21B)-C(22B)	-175.8(3)
C(19B)-C(20B)-C(21B)-Cl(6B)	-177.2(4)
Cl(5B)-C(20B)-C(21B)-Cl(6B)	3.5(5)
C(20B)-C(21B)-C(22B)-C(23B)	-4.0(7)
Cl(6B)-C(21B)-C(22B)-C(23B)	176.7(3)
C(21B)-C(22B)-C(23B)-C(18B)	1.4(7)
C(21B)-C(22B)-C(23B)-C(24B)	178.6(5)
C(17B)-C(18B)-C(23B)-C(22B)	179.6(4)
C(19B)-C(18B)-C(23B)-C(22B)	1.8(7)
C(17B)-C(18B)-C(23B)-C(24B)	1.7(5)
C(19B)-C(18B)-C(23B)-C(24B)	-176.1(4)
C(1B)-N(6B)-C(24B)-N(5B)	9.5(6)
C(1B)-N(6B)-C(24B)-C(23B)	-155.1(5)
C(17B)-N(5B)-C(24B)-N(6B)	-154.0(4)
B(1B)-N(5B)-C(24B)-N(6B)	12.5(6)
C(17B)-N(5B)-C(24B)-C(23B)	13.7(5)
B(1B)-N(5B)-C(24B)-C(23B)	-179.7(4)
C(22B)-C(23B)-C(24B)-N(6B)	-20.0(8)
C(18B)-C(23B)-C(24B)-N(6B)	157.6(4)
C(22B)-C(23B)-C(24B)-N(5B)	173.4(5)
C(18B)-C(23B)-C(24B)-N(5B)	-9.1(5)

B(1B)-O(1B)-C(25B)-C(30B)	154.3(5)
B(1B)-O(1B)-C(25B)-C(26B)	-29.2(7)
O(1B)-C(25B)-C(26B)-C(27B)	-176.5(4)
C(30B)-C(25B)-C(26B)-C(27B)	-0.2(7)
C(25B)-C(26B)-C(27B)-C(28B)	-1.7(7)
C(25B)-C(26B)-C(27B)-I(1B)	176.0(3)
C(26B)-C(27B)-C(28B)-C(29B)	2.0(7)
I(1B)-C(27B)-C(28B)-C(29B)	-175.7(4)
C(27B)-C(28B)-C(29B)-C(30B)	-0.3(8)
C(28B)-C(29B)-C(30B)-C(25B)	-1.5(8)
O(1B)-C(25B)-C(30B)-C(29B)	178.4(5)
C(26B)-C(25B)-C(30B)-C(29B)	1.8(8)
C(25B)-O(1B)-B(1B)-N(5B)	68.9(6)
C(25B)-O(1B)-B(1B)-N(1B)	-174.0(4)
C(25B)-O(1B)-B(1B)-N(3B)	-57.7(6)
C(24B)-N(5B)-B(1B)-O(1B)	89.2(5)
C(17B)-N(5B)-B(1B)-O(1B)	-105.9(5)
C(24B)-N(5B)-B(1B)-N(1B)	-30.5(5)
C(17B)-N(5B)-B(1B)-N(1B)	134.4(4)
C(24B)-N(5B)-B(1B)-N(3B)	-138.6(4)
C(17B)-N(5B)-B(1B)-N(3B)	26.4(5)
C(1B)-N(1B)-B(1B)-O(1B)	-94.9(5)
C(8B)-N(1B)-B(1B)-O(1B)	94.3(5)
C(1B)-N(1B)-B(1B)-N(5B)	32.8(5)
C(8B)-N(1B)-B(1B)-N(5B)	-138.0(4)
C(1B)-N(1B)-B(1B)-N(3B)	140.9(4)
C(8B)-N(1B)-B(1B)-N(3B)	-29.9(6)
C(16B)-N(3B)-B(1B)-O(1B)	106.6(5)
C(9B)-N(3B)-B(1B)-O(1B)	-89.6(5)
C(16B)-N(3B)-B(1B)-N(5B)	-27.7(5)
C(9B)-N(3B)-B(1B)-N(5B)	136.1(4)
C(16B)-N(3B)-B(1B)-N(1B)	-134.9(4)
C(9B)-N(3B)-B(1B)-N(1B)	28.9(5)

Symmetry transformations used to generate equivalent atoms:

a)



b)

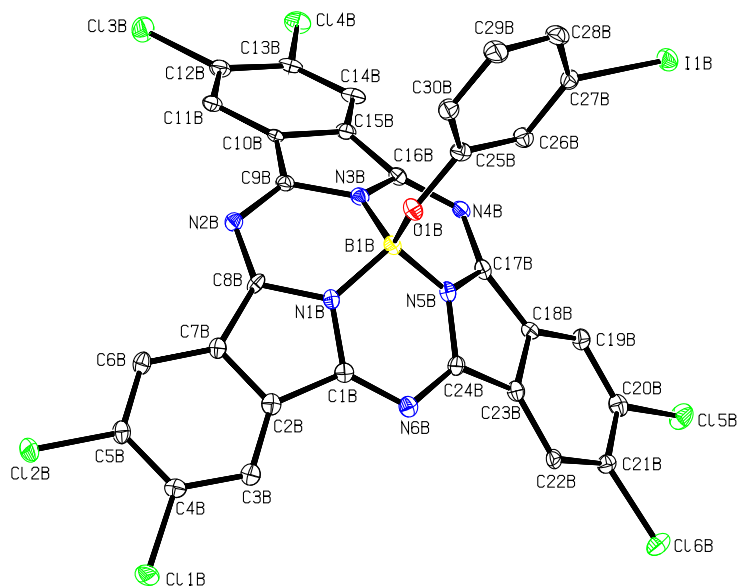


Figure S43: Anisotropic displacement ellipsoid plots of individual co-crystals of *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

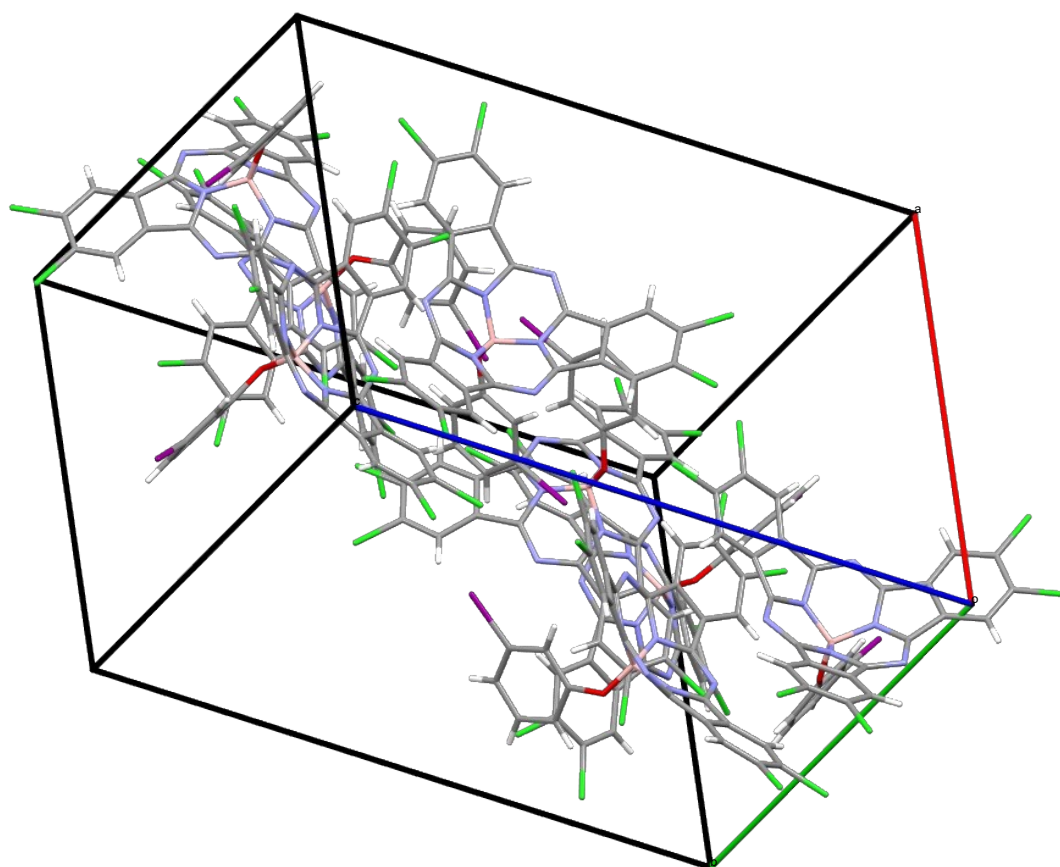


Figure S44: Populated unit cell of *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

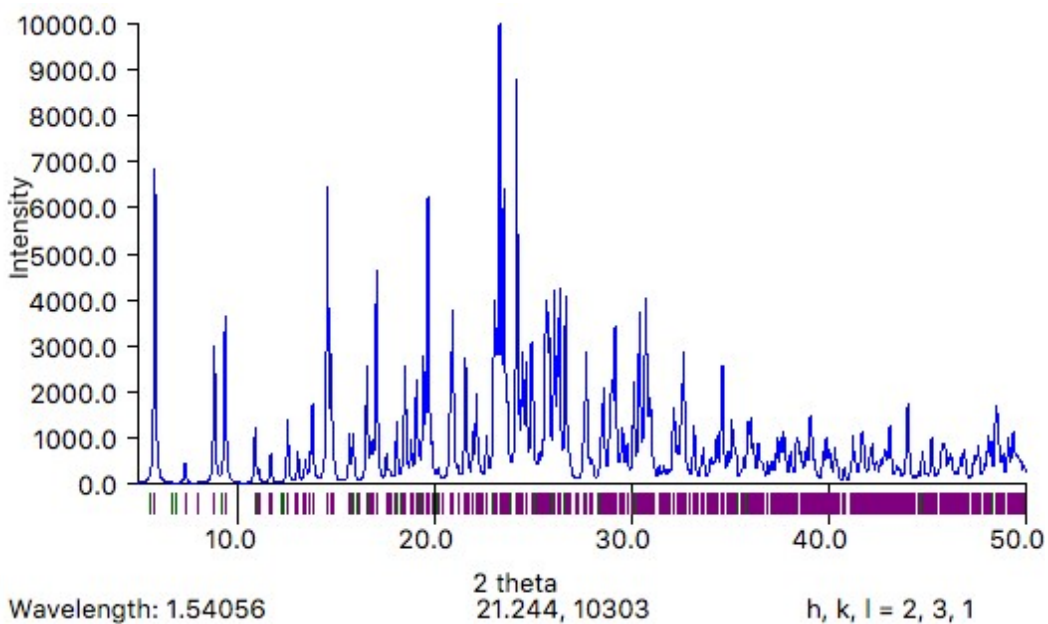


Figure S 45: Powder x-ray diffraction of *m*IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

Table S 85. Crystal data and structure refinement for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

Identification code	d2016a_a	
Empirical formula	C ₃₀ H ₁₀ B Cl ₆ I N ₆ O	
Formula weight	820.85	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2 ₁	
Unit cell dimensions	a = 15.8910(5) Å	α = 90°.
	b = 15.1094(5) Å	β = 90°.
	c = 23.9482(7) Å	γ = 90°.
Volume	5750.0(3) Å ³	
Z	8	
Density (calculated)	1.896 Mg/m ³	
Absorption coefficient	1.712 mm ⁻¹	
F(000)	3200	
Crystal size	0.230 x 0.170 x 0.140 mm ³	
Theta range for data collection	1.701 to 27.503°.	
Index ranges	-20 ≤ h ≤ 20, -19 ≤ k ≤ 19, -31 ≤ l ≤ 31	
Reflections collected	145967	
Independent reflections	13192 [R(int) = 0.0485]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7006	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13192 / 1 / 811	
Goodness-of-fit on F ²	1.044	
Final R indices [I > 2σ(I)]	R1 = 0.0301, wR2 = 0.0787	
R indices (all data)	R1 = 0.0329, wR2 = 0.0801	
Absolute structure parameter	0.097(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.035 and -0.864 e.Å ⁻³	

Table S 86. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1A)	2981(1)	4029(1)	4614(1)	24(1)
Cl(1A)	9251(1)	30(1)	7029(1)	23(1)
Cl(2A)	8584(1)	536(1)	8213(1)	30(1)
Cl(3A)	2330(1)	1576(1)	8899(1)	34(1)
Cl(4A)	1070(1)	1140(1)	7918(1)	34(1)
Cl(5A)	2926(1)	-812(1)	4231(1)	35(1)
Cl(6A)	4809(1)	-953(1)	3853(1)	30(1)
O(1A)	5365(2)	3154(2)	6163(2)	18(1)
N(1A)	5813(3)	1824(3)	6585(2)	17(1)
N(2A)	5308(3)	2009(3)	7512(2)	19(1)
N(3A)	4391(3)	2204(3)	6731(2)	17(1)
N(4A)	3401(3)	1586(3)	6094(2)	18(1)
N(5A)	4850(3)	1648(3)	5857(2)	16(1)
N(6A)	6209(3)	1020(3)	5771(2)	17(1)
C(1A)	6374(3)	1314(3)	6290(2)	17(1)
C(2A)	7009(3)	1049(3)	6692(2)	16(1)
C(3A)	7763(3)	603(3)	6631(2)	17(1)
C(4A)	8252(3)	478(3)	7104(2)	18(1)
C(5A)	7964(3)	722(4)	7634(2)	19(1)
C(6A)	7185(3)	1150(4)	7703(2)	19(1)
C(7A)	6731(3)	1338(3)	7227(2)	17(1)
C(8A)	5923(3)	1794(3)	7147(2)	15(1)
C(9A)	4545(3)	2153(3)	7292(2)	17(1)
C(10A)	3719(3)	2019(3)	7555(2)	17(1)
C(11A)	3475(3)	1927(3)	8103(2)	20(1)
C(12A)	2647(4)	1677(3)	8215(2)	23(1)
C(13A)	2085(3)	1505(4)	7781(3)	24(1)
C(14A)	2312(3)	1600(3)	7222(2)	21(1)
C(15A)	3137(3)	1877(3)	7112(2)	19(1)
C(16A)	3588(3)	1937(3)	6595(2)	17(1)

C(17A)	4036(3)	1408(3)	5754(2)	17(1)
C(18A)	4083(3)	799(3)	5280(2)	17(1)
C(19A)	3452(3)	344(3)	5003(2)	20(1)
C(20A)	3690(3)	-221(3)	4575(2)	23(1)
C(21A)	4549(3)	-317(3)	4429(2)	21(1)
C(22A)	5179(4)	90(3)	4730(2)	21(1)
C(23A)	4944(3)	648(3)	5164(2)	18(1)
C(24A)	5428(3)	1151(3)	5581(2)	17(1)
C(25A)	4945(3)	3775(3)	5860(2)	16(1)
C(26A)	4306(3)	3596(3)	5482(2)	19(1)
C(27A)	3922(3)	4295(3)	5198(2)	21(1)
C(28A)	4159(3)	5165(4)	5291(2)	25(1)
C(29A)	4809(4)	5329(4)	5661(3)	27(1)
C(30A)	5199(3)	4655(3)	5943(2)	20(1)
B(1A)	5091(4)	2291(4)	6311(2)	17(1)
I(1B)	2030(1)	6516(1)	5153(1)	29(1)
Cl(1B)	-4221(1)	2515(1)	2430(1)	29(1)
Cl(2B)	-3394(1)	3192(1)	1327(1)	38(1)
Cl(3B)	2920(1)	3910(1)	1110(1)	34(1)
Cl(4B)	4046(1)	3487(1)	2156(1)	30(1)
Cl(5B)	1422(1)	1420(1)	5724(1)	33(1)
Cl(6B)	-526(1)	1282(1)	5880(1)	30(1)
O(1B)	-392(2)	5559(2)	3646(2)	23(1)
N(1B)	-888(3)	4278(3)	3183(2)	18(1)
N(2B)	-219(3)	4433(3)	2302(2)	19(1)
N(3B)	579(3)	4537(3)	3142(2)	18(1)
N(4B)	1425(3)	3860(3)	3838(2)	20(1)
N(5B)	-50(3)	4009(3)	3969(2)	19(1)
N(6B)	-1453(3)	3446(3)	3936(2)	20(1)
C(1B)	-1516(3)	3797(3)	3422(2)	19(1)
C(2B)	-2104(3)	3595(3)	2967(2)	21(1)
C(3B)	-2874(3)	3173(4)	2964(2)	21(1)
C(4B)	-3270(3)	3050(3)	2454(2)	22(1)
C(5B)	-2879(4)	3328(4)	1949(2)	23(1)
C(6B)	-2104(3)	3725(4)	1952(2)	22(1)
C(7B)	-1716(3)	3878(3)	2465(2)	18(1)

C(8B)	-915(3)	4248(3)	2604(2)	16(1)
C(9B)	518(3)	4511(3)	2573(2)	18(1)
C(10B)	1351(3)	4369(3)	2370(2)	16(1)
C(11B)	1688(3)	4278(3)	1829(2)	21(1)
C(12B)	2511(4)	4021(3)	1771(2)	22(1)
C(13B)	3015(3)	3838(3)	2249(3)	22(1)
C(14B)	2712(3)	3919(3)	2781(2)	22(1)
C(15B)	1878(3)	4182(3)	2842(2)	20(1)
C(16B)	1336(3)	4232(3)	3333(2)	18(1)
C(17B)	725(3)	3711(3)	4135(2)	19(1)
C(18B)	572(3)	3074(3)	4574(2)	19(1)
C(19B)	1105(4)	2588(3)	4915(2)	22(1)
C(20B)	754(3)	2038(3)	5302(2)	22(1)
C(21B)	-122(3)	1953(3)	5363(2)	19(1)
C(22B)	-677(3)	2391(3)	5014(2)	20(1)
C(23B)	-322(3)	2966(3)	4618(2)	20(1)
C(24B)	-691(3)	3515(3)	4178(2)	20(1)
C(25B)	79(3)	6200(3)	3893(2)	21(1)
C(26B)	716(4)	6025(3)	4285(2)	22(1)
C(27B)	1121(3)	6736(4)	4528(2)	22(1)
C(28B)	928(4)	7605(4)	4403(2)	28(1)
C(29B)	267(4)	7771(4)	4023(3)	34(1)
C(30B)	-141(4)	7065(4)	3774(2)	26(1)
B(1B)	-175(4)	4667(4)	3513(2)	18(1)

Table S 87. Bond lengths [\AA] and angles [$^\circ$] for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

I(1A)-C(27A)	2.087(5)
Cl(1A)-C(4A)	1.735(5)
Cl(2A)-C(5A)	1.724(5)
Cl(3A)-C(12A)	1.721(6)
Cl(4A)-C(13A)	1.737(5)
Cl(5A)-C(20A)	1.717(5)
Cl(6A)-C(21A)	1.733(5)
O(1A)-C(25A)	1.361(6)
O(1A)-B(1A)	1.419(7)
N(1A)-C(8A)	1.359(6)
N(1A)-C(1A)	1.373(6)
N(1A)-B(1A)	1.498(7)
N(2A)-C(9A)	1.340(7)
N(2A)-C(8A)	1.349(7)
N(3A)-C(9A)	1.369(6)
N(3A)-C(16A)	1.377(6)
N(3A)-B(1A)	1.505(7)
N(4A)-C(17A)	1.325(7)
N(4A)-C(16A)	1.346(7)
N(5A)-C(24A)	1.359(6)
N(5A)-C(17A)	1.366(6)
N(5A)-B(1A)	1.507(7)
N(6A)-C(24A)	1.338(6)
N(6A)-C(1A)	1.345(7)
C(1A)-C(2A)	1.451(7)
C(2A)-C(3A)	1.382(7)
C(2A)-C(7A)	1.425(7)
C(3A)-C(4A)	1.388(7)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.398(8)
C(5A)-C(6A)	1.406(7)
C(6A)-C(7A)	1.378(7)

C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.471(7)
C(9A)-C(10A)	1.469(7)
C(10A)-C(11A)	1.375(7)
C(10A)-C(15A)	1.425(7)
C(11A)-C(12A)	1.394(8)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.393(9)
C(13A)-C(14A)	1.393(8)
C(14A)-C(15A)	1.401(7)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.433(7)
C(17A)-C(18A)	1.463(7)
C(18A)-C(19A)	1.386(7)
C(18A)-C(23A)	1.414(7)
C(19A)-C(20A)	1.387(7)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.416(7)
C(21A)-C(22A)	1.378(8)
C(22A)-C(23A)	1.391(7)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.470(7)
C(25A)-C(26A)	1.387(7)
C(25A)-C(30A)	1.403(7)
C(26A)-C(27A)	1.397(7)
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.385(8)
C(28A)-C(29A)	1.383(8)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.370(7)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
I(1B)-C(27B)	2.107(5)
Cl(1B)-C(4B)	1.716(5)
Cl(2B)-C(5B)	1.712(6)
Cl(3B)-C(12B)	1.720(6)

Cl(4B)-C(13B)	1.736(5)
Cl(5B)-C(20B)	1.739(5)
Cl(6B)-C(21B)	1.725(5)
O(1B)-C(25B)	1.360(6)
O(1B)-B(1B)	1.427(7)
N(1B)-C(1B)	1.360(7)
N(1B)-C(8B)	1.390(6)
N(1B)-B(1B)	1.501(7)
N(2B)-C(9B)	1.344(7)
N(2B)-C(8B)	1.350(7)
N(3B)-C(16B)	1.367(7)
N(3B)-C(9B)	1.368(6)
N(3B)-B(1B)	1.505(7)
N(4B)-C(17B)	1.340(7)
N(4B)-C(16B)	1.341(7)
N(5B)-C(24B)	1.358(7)
N(5B)-C(17B)	1.371(6)
N(5B)-B(1B)	1.490(7)
N(6B)-C(1B)	1.343(7)
N(6B)-C(24B)	1.348(7)
C(1B)-C(2B)	1.468(7)
C(2B)-C(3B)	1.379(7)
C(2B)-C(7B)	1.416(7)
C(3B)-C(4B)	1.387(8)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.424(8)
C(5B)-C(6B)	1.370(8)
C(6B)-C(7B)	1.394(7)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.430(7)
C(9B)-C(10B)	1.426(7)
C(10B)-C(11B)	1.409(7)
C(10B)-C(15B)	1.436(7)
C(11B)-C(12B)	1.371(8)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.423(8)

C(13B)-C(14B)	1.368(8)
C(14B)-C(15B)	1.391(7)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.459(7)
C(17B)-C(18B)	1.446(7)
C(18B)-C(19B)	1.387(7)
C(18B)-C(23B)	1.433(7)
C(19B)-C(20B)	1.363(8)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.406(7)
C(21B)-C(22B)	1.383(7)
C(22B)-C(23B)	1.405(7)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.462(7)
C(25B)-C(30B)	1.382(8)
C(25B)-C(26B)	1.406(8)
C(26B)-C(27B)	1.380(7)
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.381(8)
C(28B)-C(29B)	1.413(9)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.382(8)
C(29B)-H(29B)	0.9500
C(30B)-H(30B)	0.9500
C(25A)-O(1A)-B(1A)	128.0(4)
C(8A)-N(1A)-C(1A)	114.1(4)
C(8A)-N(1A)-B(1A)	123.2(4)
C(1A)-N(1A)-B(1A)	122.4(4)
C(9A)-N(2A)-C(8A)	116.1(4)
C(9A)-N(3A)-C(16A)	112.3(4)
C(9A)-N(3A)-B(1A)	122.0(4)
C(16A)-N(3A)-B(1A)	123.6(4)
C(17A)-N(4A)-C(16A)	117.4(4)
C(24A)-N(5A)-C(17A)	113.9(4)
C(24A)-N(5A)-B(1A)	122.4(4)

C(17A)-N(5A)-B(1A)	122.9(4)
C(24A)-N(6A)-C(1A)	116.5(4)
N(6A)-C(1A)-N(1A)	122.3(4)
N(6A)-C(1A)-C(2A)	131.0(5)
N(1A)-C(1A)-C(2A)	105.4(4)
C(3A)-C(2A)-C(7A)	120.9(5)
C(3A)-C(2A)-C(1A)	131.8(5)
C(7A)-C(2A)-C(1A)	107.3(4)
C(2A)-C(3A)-C(4A)	117.7(5)
C(2A)-C(3A)-H(3AA)	121.1
C(4A)-C(3A)-H(3AA)	121.1
C(3A)-C(4A)-C(5A)	121.5(5)
C(3A)-C(4A)-Cl(1A)	118.8(4)
C(5A)-C(4A)-Cl(1A)	119.7(4)
C(4A)-C(5A)-C(6A)	121.1(5)
C(4A)-C(5A)-Cl(2A)	120.0(4)
C(6A)-C(5A)-Cl(2A)	118.8(4)
C(7A)-C(6A)-C(5A)	117.2(5)
C(7A)-C(6A)-H(6AA)	121.4
C(5A)-C(6A)-H(6AA)	121.4
C(6A)-C(7A)-C(2A)	121.3(5)
C(6A)-C(7A)-C(8A)	131.4(5)
C(2A)-C(7A)-C(8A)	107.3(4)
N(2A)-C(8A)-N(1A)	122.7(4)
N(2A)-C(8A)-C(7A)	131.4(4)
N(1A)-C(8A)-C(7A)	104.9(4)
N(2A)-C(9A)-N(3A)	123.8(5)
N(2A)-C(9A)-C(10A)	128.2(4)
N(3A)-C(9A)-C(10A)	105.7(4)
C(11A)-C(10A)-C(15A)	120.8(5)
C(11A)-C(10A)-C(9A)	132.5(5)
C(15A)-C(10A)-C(9A)	106.3(4)
C(10A)-C(11A)-C(12A)	118.5(5)
C(10A)-C(11A)-H(11A)	120.8
C(12A)-C(11A)-H(11A)	120.8
C(13A)-C(12A)-C(11A)	120.8(5)

C(13A)-C(12A)-Cl(3A)	120.3(4)
C(11A)-C(12A)-Cl(3A)	118.8(4)
C(14A)-C(13A)-C(12A)	122.0(5)
C(14A)-C(13A)-Cl(4A)	117.1(4)
C(12A)-C(13A)-Cl(4A)	120.9(4)
C(13A)-C(14A)-C(15A)	117.0(5)
C(13A)-C(14A)-H(14A)	121.5
C(15A)-C(14A)-H(14A)	121.5
C(14A)-C(15A)-C(10A)	120.8(5)
C(14A)-C(15A)-C(16A)	130.5(5)
C(10A)-C(15A)-C(16A)	108.0(4)
N(4A)-C(16A)-N(3A)	122.0(4)
N(4A)-C(16A)-C(15A)	129.4(5)
N(3A)-C(16A)-C(15A)	106.2(4)
N(4A)-C(17A)-N(5A)	123.8(4)
N(4A)-C(17A)-C(18A)	130.0(5)
N(5A)-C(17A)-C(18A)	105.0(4)
C(19A)-C(18A)-C(23A)	121.8(4)
C(19A)-C(18A)-C(17A)	130.3(5)
C(23A)-C(18A)-C(17A)	107.6(4)
C(20A)-C(19A)-C(18A)	117.5(5)
C(20A)-C(19A)-H(19A)	121.2
C(18A)-C(19A)-H(19A)	121.2
C(19A)-C(20A)-C(21A)	120.5(5)
C(19A)-C(20A)-Cl(5A)	118.8(4)
C(21A)-C(20A)-Cl(5A)	120.7(4)
C(22A)-C(21A)-C(20A)	121.8(5)
C(22A)-C(21A)-Cl(6A)	119.3(4)
C(20A)-C(21A)-Cl(6A)	118.9(4)
C(21A)-C(22A)-C(23A)	117.8(5)
C(21A)-C(22A)-H(22A)	121.1
C(23A)-C(22A)-H(22A)	121.1
C(22A)-C(23A)-C(18A)	120.3(5)
C(22A)-C(23A)-C(24A)	132.9(5)
C(18A)-C(23A)-C(24A)	106.8(4)
N(6A)-C(24A)-N(5A)	122.8(4)

N(6A)-C(24A)-C(23A)	129.8(5)
N(5A)-C(24A)-C(23A)	105.2(4)
O(1A)-C(25A)-C(26A)	124.9(4)
O(1A)-C(25A)-C(30A)	115.9(4)
C(26A)-C(25A)-C(30A)	119.2(4)
C(25A)-C(26A)-C(27A)	119.3(5)
C(25A)-C(26A)-H(26A)	120.3
C(27A)-C(26A)-H(26A)	120.3
C(28A)-C(27A)-C(26A)	121.3(5)
C(28A)-C(27A)-I(1A)	119.0(4)
C(26A)-C(27A)-I(1A)	119.6(4)
C(29A)-C(28A)-C(27A)	118.4(5)
C(29A)-C(28A)-H(28A)	120.8
C(27A)-C(28A)-H(28A)	120.8
C(30A)-C(29A)-C(28A)	121.4(5)
C(30A)-C(29A)-H(29A)	119.3
C(28A)-C(29A)-H(29A)	119.3
C(29A)-C(30A)-C(25A)	120.2(5)
C(29A)-C(30A)-H(30A)	119.9
C(25A)-C(30A)-H(30A)	119.9
O(1A)-B(1A)-N(1A)	107.9(4)
O(1A)-B(1A)-N(3A)	118.2(4)
N(1A)-B(1A)-N(3A)	103.4(4)
O(1A)-B(1A)-N(5A)	119.4(4)
N(1A)-B(1A)-N(5A)	102.0(4)
N(3A)-B(1A)-N(5A)	103.7(4)
C(25B)-O(1B)-B(1B)	129.5(4)
C(1B)-N(1B)-C(8B)	112.3(4)
C(1B)-N(1B)-B(1B)	122.8(4)
C(8B)-N(1B)-B(1B)	124.2(4)
C(9B)-N(2B)-C(8B)	118.3(4)
C(16B)-N(3B)-C(9B)	112.7(4)
C(16B)-N(3B)-B(1B)	123.2(4)
C(9B)-N(3B)-B(1B)	122.4(4)
C(17B)-N(4B)-C(16B)	117.5(4)
C(24B)-N(5B)-C(17B)	112.7(4)

C(24B)-N(5B)-B(1B)	122.5(4)
C(17B)-N(5B)-B(1B)	123.5(4)
C(1B)-N(6B)-C(24B)	115.5(5)
N(6B)-C(1B)-N(1B)	122.7(5)
N(6B)-C(1B)-C(2B)	130.2(5)
N(1B)-C(1B)-C(2B)	105.5(4)
C(3B)-C(2B)-C(7B)	121.5(5)
C(3B)-C(2B)-C(1B)	131.6(5)
C(7B)-C(2B)-C(1B)	106.8(4)
C(2B)-C(3B)-C(4B)	117.9(5)
C(2B)-C(3B)-H(3BA)	121.1
C(4B)-C(3B)-H(3BA)	121.1
C(3B)-C(4B)-C(5B)	120.7(5)
C(3B)-C(4B)-Cl(1B)	119.6(4)
C(5B)-C(4B)-Cl(1B)	119.6(4)
C(6B)-C(5B)-C(4B)	121.1(5)
C(6B)-C(5B)-Cl(2B)	119.1(4)
C(4B)-C(5B)-Cl(2B)	119.7(4)
C(5B)-C(6B)-C(7B)	118.3(5)
C(5B)-C(6B)-H(6BA)	120.8
C(7B)-C(6B)-H(6BA)	120.8
C(6B)-C(7B)-C(2B)	120.3(5)
C(6B)-C(7B)-C(8B)	131.5(5)
C(2B)-C(7B)-C(8B)	108.0(4)
N(2B)-C(8B)-N(1B)	120.2(5)
N(2B)-C(8B)-C(7B)	133.3(5)
N(1B)-C(8B)-C(7B)	105.8(4)
N(2B)-C(9B)-N(3B)	123.1(5)
N(2B)-C(9B)-C(10B)	129.1(5)
N(3B)-C(9B)-C(10B)	106.2(4)
C(11B)-C(10B)-C(9B)	133.0(5)
C(11B)-C(10B)-C(15B)	118.9(5)
C(9B)-C(10B)-C(15B)	107.6(4)
C(12B)-C(11B)-C(10B)	118.8(5)
C(12B)-C(11B)-H(11B)	120.6
C(10B)-C(11B)-H(11B)	120.6

C(11B)-C(12B)-C(13B)	120.7(5)
C(11B)-C(12B)-Cl(3B)	118.6(4)
C(13B)-C(12B)-Cl(3B)	120.6(4)
C(14B)-C(13B)-C(12B)	122.2(5)
C(14B)-C(13B)-Cl(4B)	118.7(4)
C(12B)-C(13B)-Cl(4B)	119.1(4)
C(13B)-C(14B)-C(15B)	117.3(5)
C(13B)-C(14B)-H(14B)	121.3
C(15B)-C(14B)-H(14B)	121.3
C(14B)-C(15B)-C(10B)	121.9(5)
C(14B)-C(15B)-C(16B)	131.4(5)
C(10B)-C(15B)-C(16B)	106.3(4)
N(4B)-C(16B)-N(3B)	122.4(5)
N(4B)-C(16B)-C(15B)	130.0(5)
N(3B)-C(16B)-C(15B)	105.5(4)
N(4B)-C(17B)-N(5B)	122.4(5)
N(4B)-C(17B)-C(18B)	129.7(5)
N(5B)-C(17B)-C(18B)	106.1(4)
C(19B)-C(18B)-C(23B)	120.2(5)
C(19B)-C(18B)-C(17B)	132.6(5)
C(23B)-C(18B)-C(17B)	107.2(4)
C(20B)-C(19B)-C(18B)	118.2(5)
C(20B)-C(19B)-H(19B)	120.9
C(18B)-C(19B)-H(19B)	120.9
C(19B)-C(20B)-C(21B)	122.1(5)
C(19B)-C(20B)-Cl(5B)	118.2(4)
C(21B)-C(20B)-Cl(5B)	119.7(4)
C(22B)-C(21B)-C(20B)	121.6(5)
C(22B)-C(21B)-Cl(6B)	118.5(4)
C(20B)-C(21B)-Cl(6B)	119.8(4)
C(21B)-C(22B)-C(23B)	116.6(5)
C(21B)-C(22B)-H(22B)	121.7
C(23B)-C(22B)-H(22B)	121.7
C(22B)-C(23B)-C(18B)	121.1(5)
C(22B)-C(23B)-C(24B)	132.5(5)
C(18B)-C(23B)-C(24B)	106.3(4)

N(6B)-C(24B)-N(5B)	123.9(5)
N(6B)-C(24B)-C(23B)	128.8(5)
N(5B)-C(24B)-C(23B)	106.1(4)
O(1B)-C(25B)-C(30B)	116.4(5)
O(1B)-C(25B)-C(26B)	123.6(5)
C(30B)-C(25B)-C(26B)	119.8(5)
C(27B)-C(26B)-C(25B)	118.1(5)
C(27B)-C(26B)-H(26B)	121.0
C(25B)-C(26B)-H(26B)	121.0
C(26B)-C(27B)-C(28B)	123.1(5)
C(26B)-C(27B)-I(1B)	119.8(4)
C(28B)-C(27B)-I(1B)	117.1(4)
C(27B)-C(28B)-C(29B)	118.2(5)
C(27B)-C(28B)-H(28B)	120.9
C(29B)-C(28B)-H(28B)	120.9
C(30B)-C(29B)-C(28B)	119.3(6)
C(30B)-C(29B)-H(29B)	120.3
C(28B)-C(29B)-H(29B)	120.3
C(29B)-C(30B)-C(25B)	121.4(5)
C(29B)-C(30B)-H(30B)	119.3
C(25B)-C(30B)-H(30B)	119.3
O(1B)-B(1B)-N(5B)	120.0(4)
O(1B)-B(1B)-N(1B)	107.8(4)
N(5B)-B(1B)-N(1B)	103.0(4)
O(1B)-B(1B)-N(3B)	116.5(4)
N(5B)-B(1B)-N(3B)	103.8(4)
N(1B)-B(1B)-N(3B)	103.9(4)

Symmetry transformations used to generate equivalent atoms:

Table S 88. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1A)	21(1)	29(1)	22(1)	3(1)	-6(1)	-1(1)
Cl(1A)	16(1)	23(1)	30(1)	5(1)	-2(1)	2(1)
Cl(2A)	24(1)	44(1)	22(1)	9(1)	-7(1)	3(1)
Cl(3A)	40(1)	41(1)	22(1)	1(1)	11(1)	-2(1)
Cl(4A)	24(1)	40(1)	38(1)	-5(1)	11(1)	-5(1)
Cl(5A)	33(1)	45(1)	28(1)	-17(1)	-7(1)	-3(1)
Cl(6A)	40(1)	28(1)	21(1)	-8(1)	6(1)	1(1)
O(1A)	16(2)	19(2)	19(2)	4(1)	-3(1)	1(1)
N(1A)	16(2)	19(2)	16(2)	1(2)	-1(2)	0(2)
N(2A)	22(2)	19(2)	16(2)	-1(2)	-2(2)	-2(2)
N(3A)	17(2)	18(2)	16(2)	-2(2)	-2(2)	4(2)
N(4A)	16(2)	21(2)	18(2)	2(2)	-3(2)	2(2)
N(5A)	19(2)	15(2)	15(2)	3(2)	-1(2)	1(2)
N(6A)	18(2)	18(2)	15(2)	2(2)	2(2)	0(2)
C(1A)	14(2)	19(2)	19(2)	1(2)	0(2)	-2(2)
C(2A)	15(2)	16(2)	18(2)	3(2)	-1(2)	-5(2)
C(3A)	16(2)	19(2)	17(2)	4(2)	0(2)	-2(2)
C(4A)	13(2)	15(2)	25(2)	5(2)	-2(2)	-1(2)
C(5A)	19(2)	19(2)	18(2)	7(2)	-7(2)	-2(2)
C(6A)	17(2)	23(2)	17(2)	3(2)	-1(2)	-2(2)
C(7A)	18(2)	14(2)	18(2)	2(2)	-2(2)	-1(2)
C(8A)	17(2)	14(2)	15(2)	3(2)	-2(2)	-1(2)
C(9A)	21(2)	15(2)	16(2)	1(2)	-1(2)	1(2)
C(10A)	22(2)	12(2)	18(2)	0(2)	0(2)	4(2)
C(11A)	24(3)	16(2)	21(2)	0(2)	1(2)	5(2)
C(12A)	33(3)	14(2)	23(3)	-1(2)	8(2)	5(2)
C(13A)	20(3)	21(2)	30(3)	-1(2)	7(2)	2(2)
C(14A)	18(3)	18(2)	25(3)	-3(2)	0(2)	6(2)
C(15A)	19(2)	16(2)	22(2)	-2(2)	2(2)	5(2)
C(16A)	20(2)	15(2)	17(2)	-1(2)	-2(2)	6(2)

C(17A)	18(2)	18(2)	14(2)	1(2)	-6(2)	3(2)
C(18A)	22(2)	20(2)	10(2)	-1(2)	-2(2)	2(2)
C(19A)	20(2)	22(2)	17(2)	-1(2)	-4(2)	4(2)
C(20A)	27(2)	25(2)	15(2)	-2(2)	-9(2)	1(2)
C(21A)	28(3)	19(2)	15(2)	0(2)	2(2)	3(2)
C(22A)	29(3)	22(2)	14(2)	1(2)	1(2)	4(2)
C(23A)	22(2)	20(2)	13(2)	1(2)	0(2)	2(2)
C(24A)	18(2)	20(2)	14(2)	2(2)	2(2)	2(2)
C(25A)	17(2)	15(2)	14(2)	4(2)	2(2)	4(2)
C(26A)	22(2)	17(2)	18(2)	2(2)	1(2)	-1(2)
C(27A)	20(2)	24(2)	18(2)	3(2)	0(2)	0(2)
C(28A)	24(3)	19(2)	32(3)	11(2)	-2(2)	0(2)
C(29A)	27(3)	16(2)	37(3)	0(2)	-4(2)	-4(2)
C(30A)	17(2)	21(2)	22(2)	4(2)	2(2)	-3(2)
B(1A)	20(3)	17(3)	15(2)	-2(2)	-2(2)	4(2)
I(1B)	21(1)	41(1)	26(1)	-3(1)	-1(1)	-5(1)
Cl(1B)	17(1)	36(1)	35(1)	3(1)	-4(1)	-4(1)
Cl(2B)	30(1)	60(1)	24(1)	2(1)	-9(1)	-16(1)
Cl(3B)	24(1)	52(1)	26(1)	-5(1)	6(1)	-2(1)
Cl(4B)	17(1)	32(1)	39(1)	-1(1)	2(1)	1(1)
Cl(5B)	30(1)	38(1)	30(1)	12(1)	-4(1)	7(1)
Cl(6B)	37(1)	27(1)	25(1)	6(1)	8(1)	1(1)
O(1B)	24(2)	22(2)	24(2)	-5(2)	-3(2)	1(2)
N(1B)	20(2)	18(2)	16(2)	-1(2)	-3(2)	2(2)
N(2B)	21(2)	18(2)	18(2)	2(2)	-2(2)	0(2)
N(3B)	20(2)	15(2)	20(2)	0(2)	-2(2)	-1(2)
N(4B)	19(2)	19(2)	20(2)	-1(2)	-4(2)	-4(2)
N(5B)	20(2)	20(2)	16(2)	-3(2)	-2(2)	2(2)
N(6B)	20(2)	21(2)	20(2)	-4(2)	1(2)	3(2)
C(1B)	18(2)	20(2)	20(2)	-1(2)	1(2)	2(2)
C(2B)	23(3)	19(2)	21(3)	-2(2)	0(2)	4(2)
C(3B)	20(2)	22(2)	22(3)	1(2)	-1(2)	5(2)
C(4B)	19(2)	18(2)	27(3)	2(2)	-1(2)	1(2)
C(5B)	24(3)	24(3)	20(3)	1(2)	-5(2)	5(2)
C(6B)	21(3)	26(3)	18(2)	2(2)	-2(2)	6(2)
C(7B)	19(2)	19(2)	17(2)	0(2)	-1(2)	4(2)

C(8B)	15(2)	18(2)	15(2)	8(2)	1(2)	9(2)
C(9B)	19(2)	14(2)	20(2)	1(2)	-2(2)	-2(2)
C(10B)	21(2)	12(2)	16(2)	-1(2)	-1(2)	-8(2)
C(11B)	20(2)	20(2)	23(2)	2(2)	-3(2)	-7(2)
C(12B)	19(3)	22(2)	25(3)	-4(2)	4(2)	-5(2)
C(13B)	15(2)	16(2)	34(3)	-1(2)	0(2)	-6(2)
C(14B)	15(2)	15(2)	35(3)	2(2)	-2(2)	-3(2)
C(15B)	19(2)	18(2)	24(3)	1(2)	-1(2)	-5(2)
C(16B)	19(2)	16(2)	19(2)	-3(2)	-1(2)	-1(2)
C(17B)	17(2)	22(2)	17(2)	-4(2)	-3(2)	1(2)
C(18B)	17(2)	21(2)	19(2)	-1(2)	-2(2)	-4(2)
C(19B)	26(3)	24(3)	18(2)	-2(2)	-1(2)	-1(2)
C(20B)	26(3)	16(2)	23(2)	-5(2)	-3(2)	4(2)
C(21B)	22(2)	18(2)	18(2)	-2(2)	4(2)	1(2)
C(22B)	28(3)	17(2)	14(2)	-3(2)	-2(2)	-2(2)
C(23B)	21(2)	20(2)	18(2)	-3(2)	-1(2)	2(2)
C(24B)	23(2)	21(2)	15(2)	-4(2)	4(2)	-1(2)
C(25B)	18(2)	20(2)	24(3)	-3(2)	5(2)	0(2)
C(26B)	24(3)	19(2)	23(3)	-2(2)	1(2)	0(2)
C(27B)	21(2)	27(3)	17(2)	-1(2)	2(2)	-2(2)
C(28B)	30(3)	23(3)	31(3)	-6(2)	3(2)	-7(2)
C(29B)	46(4)	19(3)	37(3)	7(2)	-11(3)	-6(2)
C(30B)	31(3)	22(3)	24(3)	2(2)	-3(2)	-1(2)
B(1B)	16(2)	20(3)	18(3)	-3(2)	-1(2)	0(2)

Table S 89. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

	x	y	z	U(eq)
H(3AA)	7940	390	6276	21
H(6AA)	6980	1303	8063	23
H(11A)	3861	2032	8399	24
H(14A)	1926	1481	6929	25
H(19A)	2877	417	5102	24
H(22A)	5755	-9	4643	26
H(26A)	4130	3004	5418	23
H(28A)	3880	5637	5106	30
H(29A)	4989	5921	5720	32
H(30A)	5643	4784	6196	24
H(3BA)	-3124	2972	3302	26
H(6BA)	-1837	3891	1613	26
H(11B)	1352	4394	1509	25
H(14B)	3057	3801	3096	26
H(19B)	1699	2638	4881	27
H(22B)	-1268	2308	5041	23
H(26B)	864	5435	4380	26
H(28B)	1232	8078	4568	34
H(29B)	104	8361	3939	41
H(30B)	-581	7177	3515	31

Table S 90. Torsion angles [°] for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Heptane; CCDC deposit 2087107).

C(24A)-N(6A)-C(1A)-N(1A)	-8.3(7)
C(24A)-N(6A)-C(1A)-C(2A)	156.6(5)
C(8A)-N(1A)-C(1A)-N(6A)	157.1(5)
B(1A)-N(1A)-C(1A)-N(6A)	-16.6(7)
C(8A)-N(1A)-C(1A)-C(2A)	-11.1(5)
B(1A)-N(1A)-C(1A)-C(2A)	175.1(4)
N(6A)-C(1A)-C(2A)-C(3A)	19.9(9)
N(1A)-C(1A)-C(2A)-C(3A)	-173.3(5)
N(6A)-C(1A)-C(2A)-C(7A)	-160.1(5)
N(1A)-C(1A)-C(2A)-C(7A)	6.7(5)
C(7A)-C(2A)-C(3A)-C(4A)	-2.4(7)
C(1A)-C(2A)-C(3A)-C(4A)	177.6(5)
C(2A)-C(3A)-C(4A)-C(5A)	5.6(7)
C(2A)-C(3A)-C(4A)-Cl(1A)	-173.0(4)
C(3A)-C(4A)-C(5A)-C(6A)	-3.6(8)
Cl(1A)-C(4A)-C(5A)-C(6A)	175.0(4)
C(3A)-C(4A)-C(5A)-Cl(2A)	178.8(4)
Cl(1A)-C(4A)-C(5A)-Cl(2A)	-2.7(6)
C(4A)-C(5A)-C(6A)-C(7A)	-1.7(8)
Cl(2A)-C(5A)-C(6A)-C(7A)	176.0(4)
C(5A)-C(6A)-C(7A)-C(2A)	4.8(7)
C(5A)-C(6A)-C(7A)-C(8A)	-177.9(5)
C(3A)-C(2A)-C(7A)-C(6A)	-2.8(7)
C(1A)-C(2A)-C(7A)-C(6A)	177.2(5)
C(3A)-C(2A)-C(7A)-C(8A)	179.3(4)
C(1A)-C(2A)-C(7A)-C(8A)	-0.7(5)
C(9A)-N(2A)-C(8A)-N(1A)	8.0(7)
C(9A)-N(2A)-C(8A)-C(7A)	-158.5(5)
C(1A)-N(1A)-C(8A)-N(2A)	-158.9(5)
B(1A)-N(1A)-C(8A)-N(2A)	14.8(7)
C(1A)-N(1A)-C(8A)-C(7A)	10.6(5)
B(1A)-N(1A)-C(8A)-C(7A)	-175.7(4)
C(6A)-C(7A)-C(8A)-N(2A)	-15.0(9)

C(2A)-C(7A)-C(8A)-N(2A)	162.6(5)
C(6A)-C(7A)-C(8A)-N(1A)	176.8(5)
C(2A)-C(7A)-C(8A)-N(1A)	-5.6(5)
C(8A)-N(2A)-C(9A)-N(3A)	-8.7(7)
C(8A)-N(2A)-C(9A)-C(10A)	151.1(5)
C(16A)-N(3A)-C(9A)-N(2A)	151.1(5)
B(1A)-N(3A)-C(9A)-N(2A)	-13.0(7)
C(16A)-N(3A)-C(9A)-C(10A)	-12.5(5)
B(1A)-N(3A)-C(9A)-C(10A)	-176.6(4)
N(2A)-C(9A)-C(10A)-C(11A)	17.8(9)
N(3A)-C(9A)-C(10A)-C(11A)	-179.5(5)
N(2A)-C(9A)-C(10A)-C(15A)	-154.8(5)
N(3A)-C(9A)-C(10A)-C(15A)	7.9(5)
C(15A)-C(10A)-C(11A)-C(12A)	1.1(7)
C(9A)-C(10A)-C(11A)-C(12A)	-170.6(5)
C(10A)-C(11A)-C(12A)-C(13A)	1.3(7)
C(10A)-C(11A)-C(12A)-Cl(3A)	-179.0(4)
C(11A)-C(12A)-C(13A)-C(14A)	-1.9(8)
Cl(3A)-C(12A)-C(13A)-C(14A)	178.4(4)
C(11A)-C(12A)-C(13A)-Cl(4A)	176.7(4)
Cl(3A)-C(12A)-C(13A)-Cl(4A)	-2.9(6)
C(12A)-C(13A)-C(14A)-C(15A)	0.0(7)
Cl(4A)-C(13A)-C(14A)-C(15A)	-178.7(4)
C(13A)-C(14A)-C(15A)-C(10A)	2.5(7)
C(13A)-C(14A)-C(15A)-C(16A)	171.8(5)
C(11A)-C(10A)-C(15A)-C(14A)	-3.1(7)
C(9A)-C(10A)-C(15A)-C(14A)	170.6(4)
C(11A)-C(10A)-C(15A)-C(16A)	-174.6(5)
C(9A)-C(10A)-C(15A)-C(16A)	-0.9(5)
C(17A)-N(4A)-C(16A)-N(3A)	7.6(7)
C(17A)-N(4A)-C(16A)-C(15A)	-152.3(5)
C(9A)-N(3A)-C(16A)-N(4A)	-151.9(5)
B(1A)-N(3A)-C(16A)-N(4A)	11.9(7)
C(9A)-N(3A)-C(16A)-C(15A)	12.0(5)
B(1A)-N(3A)-C(16A)-C(15A)	175.8(4)
C(14A)-C(15A)-C(16A)-N(4A)	-14.4(9)

C(10A)-C(15A)-C(16A)-N(4A)	156.0(5)
C(14A)-C(15A)-C(16A)-N(3A)	-176.7(5)
C(10A)-C(15A)-C(16A)-N(3A)	-6.3(5)
C(16A)-N(4A)-C(17A)-N(5A)	-7.5(7)
C(16A)-N(4A)-C(17A)-C(18A)	158.6(5)
C(24A)-N(5A)-C(17A)-N(4A)	157.5(5)
B(1A)-N(5A)-C(17A)-N(4A)	-12.2(7)
C(24A)-N(5A)-C(17A)-C(18A)	-11.5(5)
B(1A)-N(5A)-C(17A)-C(18A)	178.8(4)
N(4A)-C(17A)-C(18A)-C(19A)	11.3(9)
N(5A)-C(17A)-C(18A)-C(19A)	179.3(5)
N(4A)-C(17A)-C(18A)-C(23A)	-162.5(5)
N(5A)-C(17A)-C(18A)-C(23A)	5.5(5)
C(23A)-C(18A)-C(19A)-C(20A)	-4.6(7)
C(17A)-C(18A)-C(19A)-C(20A)	-177.6(5)
C(18A)-C(19A)-C(20A)-C(21A)	-0.6(8)
C(18A)-C(19A)-C(20A)-Cl(5A)	178.7(4)
C(19A)-C(20A)-C(21A)-C(22A)	5.1(8)
Cl(5A)-C(20A)-C(21A)-C(22A)	-174.2(4)
C(19A)-C(20A)-C(21A)-Cl(6A)	-174.3(4)
Cl(5A)-C(20A)-C(21A)-Cl(6A)	6.4(6)
C(20A)-C(21A)-C(22A)-C(23A)	-4.1(8)
Cl(6A)-C(21A)-C(22A)-C(23A)	175.3(4)
C(21A)-C(22A)-C(23A)-C(18A)	-1.1(7)
C(21A)-C(22A)-C(23A)-C(24A)	176.9(5)
C(19A)-C(18A)-C(23A)-C(22A)	5.6(8)
C(17A)-C(18A)-C(23A)-C(22A)	-180.0(4)
C(19A)-C(18A)-C(23A)-C(24A)	-172.9(5)
C(17A)-C(18A)-C(23A)-C(24A)	1.6(5)
C(1A)-N(6A)-C(24A)-N(5A)	8.0(7)
C(1A)-N(6A)-C(24A)-C(23A)	-153.1(5)
C(17A)-N(5A)-C(24A)-N(6A)	-152.6(5)
B(1A)-N(5A)-C(24A)-N(6A)	17.1(7)
C(17A)-N(5A)-C(24A)-C(23A)	12.5(5)
B(1A)-N(5A)-C(24A)-C(23A)	-177.8(4)
C(22A)-C(23A)-C(24A)-N(6A)	-22.7(9)

C(18A)-C(23A)-C(24A)-N(6A)	155.5(5)
C(22A)-C(23A)-C(24A)-N(5A)	173.7(5)
C(18A)-C(23A)-C(24A)-N(5A)	-8.1(5)
B(1A)-O(1A)-C(25A)-C(26A)	-23.0(8)
B(1A)-O(1A)-C(25A)-C(30A)	157.4(5)
O(1A)-C(25A)-C(26A)-C(27A)	179.8(5)
C(30A)-C(25A)-C(26A)-C(27A)	-0.7(7)
C(25A)-C(26A)-C(27A)-C(28A)	-1.1(8)
C(25A)-C(26A)-C(27A)-I(1A)	178.4(4)
C(26A)-C(27A)-C(28A)-C(29A)	2.4(8)
I(1A)-C(27A)-C(28A)-C(29A)	-177.1(4)
C(27A)-C(28A)-C(29A)-C(30A)	-2.0(9)
C(28A)-C(29A)-C(30A)-C(25A)	0.3(9)
O(1A)-C(25A)-C(30A)-C(29A)	-179.4(5)
C(26A)-C(25A)-C(30A)-C(29A)	1.0(8)
C(25A)-O(1A)-B(1A)-N(1A)	173.2(4)
C(25A)-O(1A)-B(1A)-N(3A)	-70.1(7)
C(25A)-O(1A)-B(1A)-N(5A)	57.6(7)
C(8A)-N(1A)-B(1A)-O(1A)	95.1(5)
C(1A)-N(1A)-B(1A)-O(1A)	-91.8(5)
C(8A)-N(1A)-B(1A)-N(3A)	-31.0(6)
C(1A)-N(1A)-B(1A)-N(3A)	142.2(4)
C(8A)-N(1A)-B(1A)-N(5A)	-138.4(4)
C(1A)-N(1A)-B(1A)-N(5A)	34.8(6)
C(9A)-N(3A)-B(1A)-O(1A)	-89.3(6)
C(16A)-N(3A)-B(1A)-O(1A)	108.4(5)
C(9A)-N(3A)-B(1A)-N(1A)	29.8(6)
C(16A)-N(3A)-B(1A)-N(1A)	-132.5(5)
C(9A)-N(3A)-B(1A)-N(5A)	135.9(4)
C(16A)-N(3A)-B(1A)-N(5A)	-26.4(6)
C(24A)-N(5A)-B(1A)-O(1A)	83.5(6)
C(17A)-N(5A)-B(1A)-O(1A)	-107.7(6)
C(24A)-N(5A)-B(1A)-N(1A)	-35.2(6)
C(17A)-N(5A)-B(1A)-N(1A)	133.6(4)
C(24A)-N(5A)-B(1A)-N(3A)	-142.4(4)
C(17A)-N(5A)-B(1A)-N(3A)	26.4(6)

C(24B)-N(6B)-C(1B)-N(1B)	-7.2(7)
C(24B)-N(6B)-C(1B)-C(2B)	156.2(5)
C(8B)-N(1B)-C(1B)-N(6B)	154.0(5)
B(1B)-N(1B)-C(1B)-N(6B)	-16.8(8)
C(8B)-N(1B)-C(1B)-C(2B)	-12.9(6)
B(1B)-N(1B)-C(1B)-C(2B)	176.3(4)
N(6B)-C(1B)-C(2B)-C(3B)	18.6(9)
N(1B)-C(1B)-C(2B)-C(3B)	-175.8(5)
N(6B)-C(1B)-C(2B)-C(7B)	-157.7(5)
N(1B)-C(1B)-C(2B)-C(7B)	7.8(5)
C(7B)-C(2B)-C(3B)-C(4B)	-1.5(8)
C(1B)-C(2B)-C(3B)-C(4B)	-177.4(5)
C(2B)-C(3B)-C(4B)-C(5B)	1.9(8)
C(2B)-C(3B)-C(4B)-Cl(1B)	179.1(4)
C(3B)-C(4B)-C(5B)-C(6B)	-0.1(8)
Cl(1B)-C(4B)-C(5B)-C(6B)	-177.3(4)
C(3B)-C(4B)-C(5B)-Cl(2B)	-178.5(4)
Cl(1B)-C(4B)-C(5B)-Cl(2B)	4.3(6)
C(4B)-C(5B)-C(6B)-C(7B)	-2.1(8)
Cl(2B)-C(5B)-C(6B)-C(7B)	176.3(4)
C(5B)-C(6B)-C(7B)-C(2B)	2.5(8)
C(5B)-C(6B)-C(7B)-C(8B)	178.0(5)
C(3B)-C(2B)-C(7B)-C(6B)	-0.7(8)
C(1B)-C(2B)-C(7B)-C(6B)	176.1(5)
C(3B)-C(2B)-C(7B)-C(8B)	-177.2(5)
C(1B)-C(2B)-C(7B)-C(8B)	-0.4(6)
C(9B)-N(2B)-C(8B)-N(1B)	9.9(7)
C(9B)-N(2B)-C(8B)-C(7B)	-158.8(5)
C(1B)-N(1B)-C(8B)-N(2B)	-158.7(4)
B(1B)-N(1B)-C(8B)-N(2B)	12.0(7)
C(1B)-N(1B)-C(8B)-C(7B)	12.8(6)
B(1B)-N(1B)-C(8B)-C(7B)	-176.5(4)
C(6B)-C(7B)-C(8B)-N(2B)	-13.1(10)
C(2B)-C(7B)-C(8B)-N(2B)	162.8(5)
C(6B)-C(7B)-C(8B)-N(1B)	177.0(5)
C(2B)-C(7B)-C(8B)-N(1B)	-7.1(5)

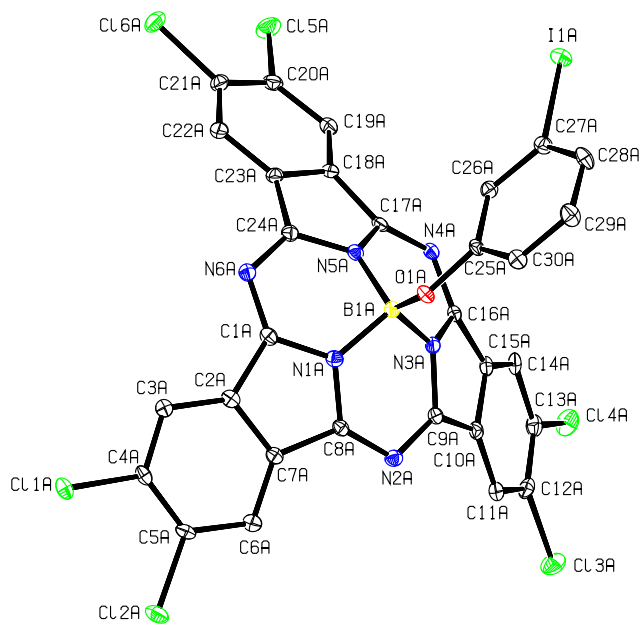
C(8B)-N(2B)-C(9B)-N(3B)	-9.6(7)
C(8B)-N(2B)-C(9B)-C(10B)	153.7(5)
C(16B)-N(3B)-C(9B)-N(2B)	152.9(5)
B(1B)-N(3B)-C(9B)-N(2B)	-12.7(7)
C(16B)-N(3B)-C(9B)-C(10B)	-13.6(6)
B(1B)-N(3B)-C(9B)-C(10B)	-179.2(4)
N(2B)-C(9B)-C(10B)-C(11B)	14.3(9)
N(3B)-C(9B)-C(10B)-C(11B)	179.7(5)
N(2B)-C(9B)-C(10B)-C(15B)	-157.0(5)
N(3B)-C(9B)-C(10B)-C(15B)	8.4(5)
C(9B)-C(10B)-C(11B)-C(12B)	-170.9(5)
C(15B)-C(10B)-C(11B)-C(12B)	-0.4(7)
C(10B)-C(11B)-C(12B)-C(13B)	0.7(8)
C(10B)-C(11B)-C(12B)-Cl(3B)	179.9(4)
C(11B)-C(12B)-C(13B)-C(14B)	-0.8(8)
Cl(3B)-C(12B)-C(13B)-C(14B)	179.9(4)
C(11B)-C(12B)-C(13B)-Cl(4B)	178.4(4)
Cl(3B)-C(12B)-C(13B)-Cl(4B)	-0.8(6)
C(12B)-C(13B)-C(14B)-C(15B)	0.7(8)
Cl(4B)-C(13B)-C(14B)-C(15B)	-178.5(4)
C(13B)-C(14B)-C(15B)-C(10B)	-0.5(7)
C(13B)-C(14B)-C(15B)-C(16B)	171.9(5)
C(11B)-C(10B)-C(15B)-C(14B)	0.4(7)
C(9B)-C(10B)-C(15B)-C(14B)	173.1(5)
C(11B)-C(10B)-C(15B)-C(16B)	-173.7(4)
C(9B)-C(10B)-C(15B)-C(16B)	-1.0(5)
C(17B)-N(4B)-C(16B)-N(3B)	6.6(7)
C(17B)-N(4B)-C(16B)-C(15B)	-154.2(5)
C(9B)-N(3B)-C(16B)-N(4B)	-151.9(5)
B(1B)-N(3B)-C(16B)-N(4B)	13.5(7)
C(9B)-N(3B)-C(16B)-C(15B)	12.9(6)
B(1B)-N(3B)-C(16B)-C(15B)	178.4(4)
C(14B)-C(15B)-C(16B)-N(4B)	-16.8(9)
C(10B)-C(15B)-C(16B)-N(4B)	156.4(5)
C(14B)-C(15B)-C(16B)-N(3B)	179.9(5)
C(10B)-C(15B)-C(16B)-N(3B)	-6.9(5)

C(16B)-N(4B)-C(17B)-N(5B)	-7.3(7)
C(16B)-N(4B)-C(17B)-C(18B)	155.6(5)
C(24B)-N(5B)-C(17B)-N(4B)	154.8(5)
B(1B)-N(5B)-C(17B)-N(4B)	-12.5(7)
C(24B)-N(5B)-C(17B)-C(18B)	-11.6(6)
B(1B)-N(5B)-C(17B)-C(18B)	-178.9(4)
N(4B)-C(17B)-C(18B)-C(19B)	18.3(9)
N(5B)-C(17B)-C(18B)-C(19B)	-176.7(5)
N(4B)-C(17B)-C(18B)-C(23B)	-160.2(5)
N(5B)-C(17B)-C(18B)-C(23B)	4.8(5)
C(23B)-C(18B)-C(19B)-C(20B)	-2.4(7)
C(17B)-C(18B)-C(19B)-C(20B)	179.3(5)
C(18B)-C(19B)-C(20B)-C(21B)	-0.2(8)
C(18B)-C(19B)-C(20B)-Cl(5B)	179.3(4)
C(19B)-C(20B)-C(21B)-C(22B)	3.4(8)
Cl(5B)-C(20B)-C(21B)-C(22B)	-176.1(4)
C(19B)-C(20B)-C(21B)-Cl(6B)	-177.2(4)
Cl(5B)-C(20B)-C(21B)-Cl(6B)	3.4(6)
C(20B)-C(21B)-C(22B)-C(23B)	-3.7(7)
Cl(6B)-C(21B)-C(22B)-C(23B)	176.8(4)
C(21B)-C(22B)-C(23B)-C(18B)	1.2(7)
C(21B)-C(22B)-C(23B)-C(24B)	178.3(5)
C(19B)-C(18B)-C(23B)-C(22B)	1.9(8)
C(17B)-C(18B)-C(23B)-C(22B)	-179.4(4)
C(19B)-C(18B)-C(23B)-C(24B)	-175.9(5)
C(17B)-C(18B)-C(23B)-C(24B)	2.8(5)
C(1B)-N(6B)-C(24B)-N(5B)	9.2(7)
C(1B)-N(6B)-C(24B)-C(23B)	-155.9(5)
C(17B)-N(5B)-C(24B)-N(6B)	-154.7(5)
B(1B)-N(5B)-C(24B)-N(6B)	12.8(7)
C(17B)-N(5B)-C(24B)-C(23B)	13.3(6)
B(1B)-N(5B)-C(24B)-C(23B)	-179.2(4)
C(22B)-C(23B)-C(24B)-N(6B)	-19.7(9)
C(18B)-C(23B)-C(24B)-N(6B)	157.7(5)
C(22B)-C(23B)-C(24B)-N(5B)	173.0(5)
C(18B)-C(23B)-C(24B)-N(5B)	-9.5(5)

B(1B)-O(1B)-C(25B)-C(30B)	154.8(5)
B(1B)-O(1B)-C(25B)-C(26B)	-30.1(8)
O(1B)-C(25B)-C(26B)-C(27B)	-176.8(5)
C(30B)-C(25B)-C(26B)-C(27B)	-1.8(8)
C(25B)-C(26B)-C(27B)-C(28B)	-0.1(8)
C(25B)-C(26B)-C(27B)-I(1B)	176.3(4)
C(26B)-C(27B)-C(28B)-C(29B)	2.2(9)
I(1B)-C(27B)-C(28B)-C(29B)	-174.3(5)
C(27B)-C(28B)-C(29B)-C(30B)	-2.4(9)
C(28B)-C(29B)-C(30B)-C(25B)	0.7(10)
O(1B)-C(25B)-C(30B)-C(29B)	176.8(5)
C(26B)-C(25B)-C(30B)-C(29B)	1.5(9)
C(25B)-O(1B)-B(1B)-N(5B)	69.3(7)
C(25B)-O(1B)-B(1B)-N(1B)	-173.5(5)
C(25B)-O(1B)-B(1B)-N(3B)	-57.3(7)
C(24B)-N(5B)-B(1B)-O(1B)	88.9(6)
C(17B)-N(5B)-B(1B)-O(1B)	-105.0(6)
C(24B)-N(5B)-B(1B)-N(1B)	-30.7(6)
C(17B)-N(5B)-B(1B)-N(1B)	135.4(5)
C(24B)-N(5B)-B(1B)-N(3B)	-138.7(5)
C(17B)-N(5B)-B(1B)-N(3B)	27.3(6)
C(1B)-N(1B)-B(1B)-O(1B)	-94.9(6)
C(8B)-N(1B)-B(1B)-O(1B)	95.3(5)
C(1B)-N(1B)-B(1B)-N(5B)	32.9(6)
C(8B)-N(1B)-B(1B)-N(5B)	-136.9(5)
C(1B)-N(1B)-B(1B)-N(3B)	140.9(5)
C(8B)-N(1B)-B(1B)-N(3B)	-28.9(6)
C(16B)-N(3B)-B(1B)-O(1B)	106.5(5)
C(9B)-N(3B)-B(1B)-O(1B)	-89.5(6)
C(16B)-N(3B)-B(1B)-N(5B)	-27.8(6)
C(9B)-N(3B)-B(1B)-N(5B)	136.3(4)
C(16B)-N(3B)-B(1B)-N(1B)	-135.2(5)
C(9B)-N(3B)-B(1B)-N(1B)	28.9(6)

Symmetry transformations used to generate equivalent atoms:

a)



b)

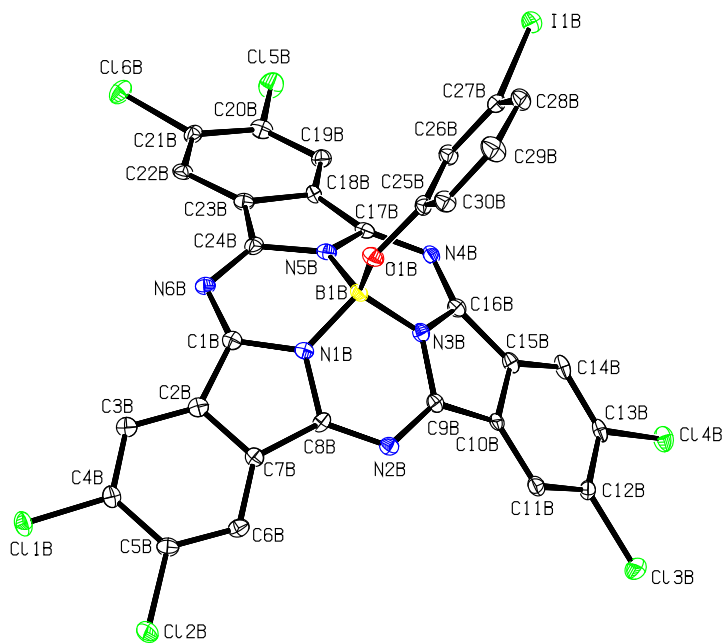


Figure S46: Anisotropic displacement ellipsoid plots of individual co-crystals of *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

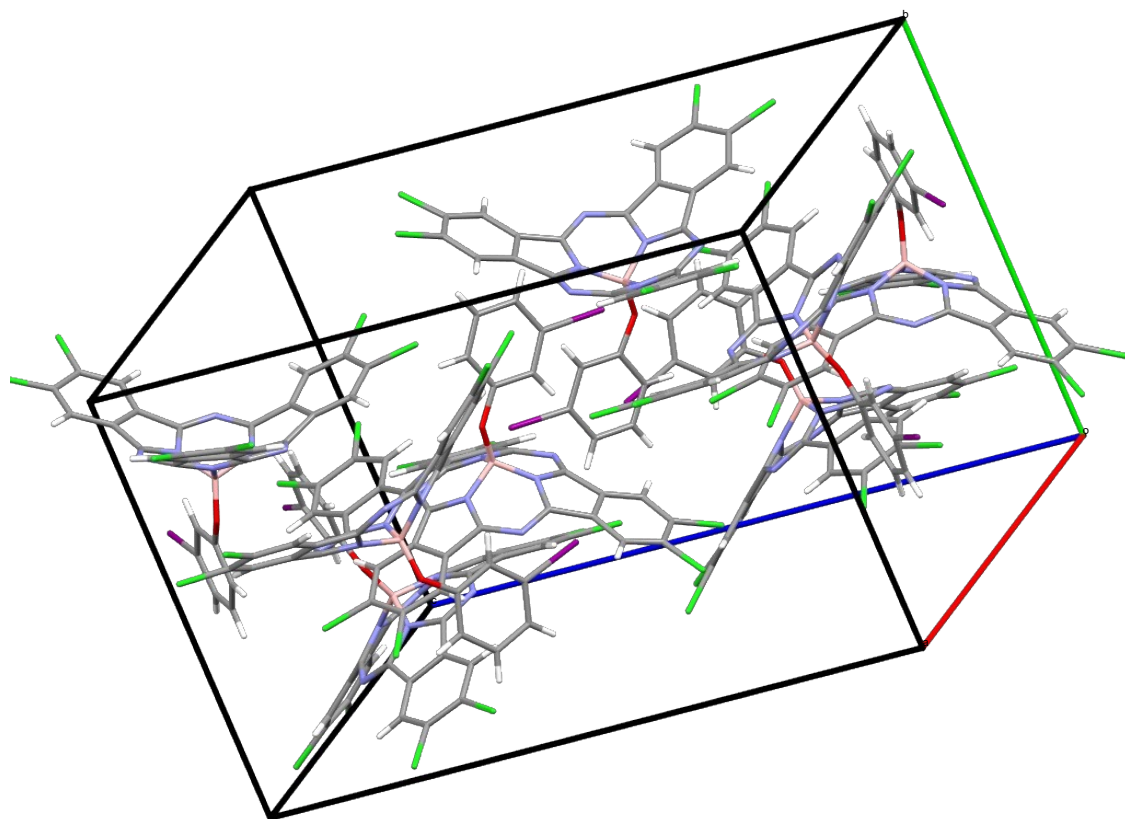


Figure S47: Populated unit cell of *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

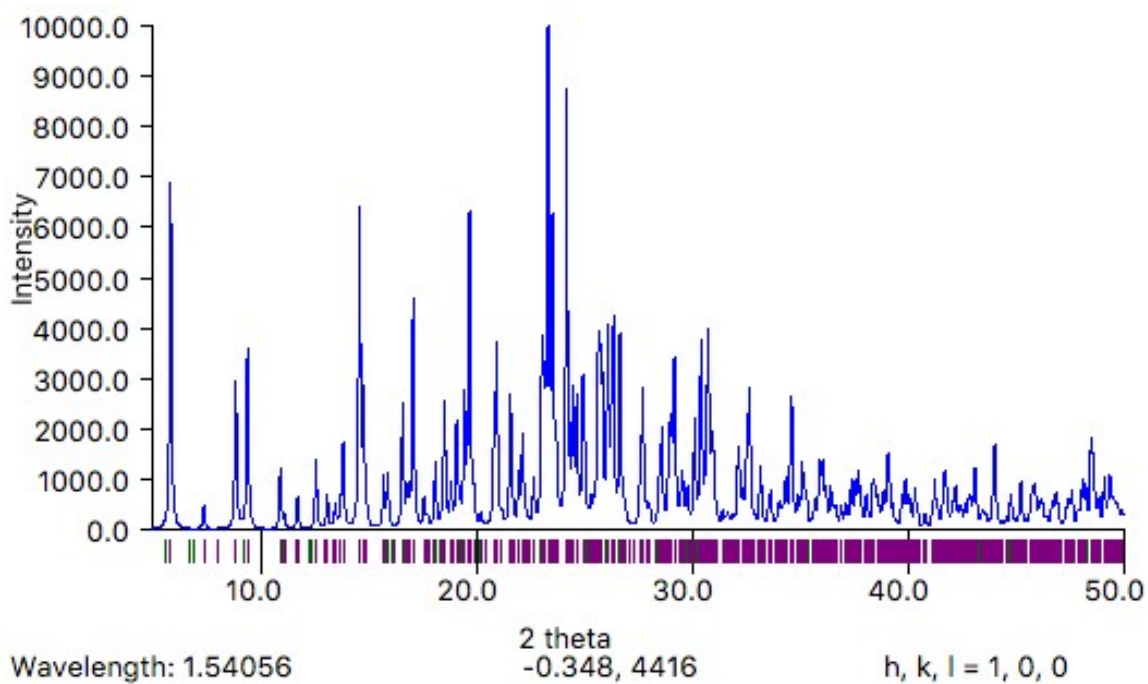


Figure S 48: Powder x-ray diffraction of *m*IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

Table S 91. Crystal data and structure refinement for *m*-IPhO-Cl₆BsubPc
(Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

Identification code	d2017a_a	
Empirical formula	C ₃₀ H ₁₀ B Cl ₆ I N ₆ O	
Formula weight	820.85	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2 ₁	
Unit cell dimensions	a = 15.8915(6) Å	α = 90°.
	b = 15.1172(6) Å	β = 90°.
	c = 23.9514(9) Å	γ = 90°.
Volume	5754.0(4) Å ³	
Z	8	
Density (calculated)	1.895 Mg/m ³	
Absorption coefficient	1.711 mm ⁻¹	
F(000)	3200	
Crystal size	0.330 x 0.260 x 0.250 mm ³	
Theta range for data collection	1.859 to 27.493°.	
Index ranges	-20 ≤ h ≤ 20, -19 ≤ k ≤ 19, -31 ≤ l ≤ 31	
Reflections collected	143954	
Independent reflections	13197 [R(int) = 0.0491]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6639	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13197 / 1 / 811	
Goodness-of-fit on F ²	1.040	
Final R indices [I > 2σ(I)]	R1 = 0.0284, wR2 = 0.0735	
R indices (all data)	R1 = 0.0320, wR2 = 0.0750	
Absolute structure parameter	0.014(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.326 and -0.683 e.Å ⁻³	

Table S 92. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1A)	7021(1)	5969(1)	5386(1)	25(1)
Cl(1A)	749(1)	9973(1)	2971(1)	24(1)
Cl(2A)	1418(1)	9470(1)	1787(1)	30(1)
Cl(3A)	7670(1)	8421(1)	1102(1)	35(1)
Cl(4A)	8929(1)	8860(1)	2082(1)	34(1)
Cl(5A)	7074(1)	10810(1)	5769(1)	36(1)
Cl(6A)	5190(1)	10953(1)	6147(1)	30(1)
O(1A)	4633(2)	6844(2)	3838(1)	19(1)
N(1A)	4185(2)	8175(3)	3414(2)	18(1)
N(2A)	4689(3)	7987(3)	2488(2)	19(1)
N(3A)	5607(2)	7794(3)	3271(2)	18(1)
N(4A)	6597(2)	8411(3)	3907(2)	18(1)
N(5A)	5151(2)	8351(2)	4144(2)	16(1)
N(6A)	3791(2)	8977(3)	4229(2)	18(1)
C(1A)	3627(3)	8686(3)	3712(2)	19(1)
C(2A)	2992(3)	8950(3)	3306(2)	18(1)
C(3A)	2235(3)	9399(3)	3371(2)	18(1)
C(4A)	1750(3)	9522(3)	2896(2)	19(1)
C(5A)	2038(3)	9278(4)	2367(2)	20(1)
C(6A)	2812(3)	8848(3)	2294(2)	20(1)
C(7A)	3267(3)	8663(3)	2774(2)	17(1)
C(8A)	4076(3)	8206(3)	2855(2)	17(1)
C(9A)	5453(3)	7844(3)	2708(2)	18(1)
C(10A)	6282(3)	7978(3)	2445(2)	18(1)
C(11A)	6524(3)	8070(3)	1897(2)	21(1)
C(12A)	7356(4)	8319(3)	1787(2)	24(1)
C(13A)	7913(3)	8489(3)	2222(2)	24(1)
C(14A)	7688(3)	8398(3)	2777(2)	22(1)
C(15A)	6861(3)	8120(3)	2889(2)	20(1)
C(16A)	6409(3)	8061(3)	3406(2)	18(1)

C(17A)	5962(3)	8589(3)	4247(2)	18(1)
C(18A)	5918(3)	9200(3)	4721(2)	19(1)
C(19A)	6548(3)	9653(3)	4999(2)	22(1)
C(20A)	6311(3)	10221(3)	5424(2)	24(1)
C(21A)	5448(3)	10317(3)	5572(2)	22(1)
C(22A)	4818(3)	9907(3)	5272(2)	23(1)
C(23A)	5054(3)	9347(3)	4836(2)	19(1)
C(24A)	4572(3)	8848(3)	4421(2)	18(1)
C(25A)	5055(3)	6221(3)	4139(2)	17(1)
C(26A)	5696(3)	6403(3)	4518(2)	19(1)
C(27A)	6078(3)	5701(3)	4804(2)	21(1)
C(28A)	5841(3)	4836(3)	4709(2)	25(1)
C(29A)	5189(4)	4670(3)	4340(2)	28(1)
C(30A)	4798(3)	5343(3)	4057(2)	21(1)
B(1A)	4906(3)	7706(4)	3691(2)	19(1)
I(1B)	7971(1)	3483(1)	4848(1)	30(1)
Cl(1B)	14223(1)	7489(1)	7570(1)	29(1)
Cl(2B)	13395(1)	6810(1)	8674(1)	38(1)
Cl(3B)	7082(1)	6090(1)	8889(1)	34(1)
Cl(4B)	5956(1)	6513(1)	7844(1)	30(1)
Cl(5B)	8577(1)	8582(1)	4277(1)	34(1)
Cl(6B)	10526(1)	8723(1)	4120(1)	30(1)
O(1B)	10395(2)	4444(2)	6353(2)	24(1)
N(1B)	10891(3)	5725(3)	6818(2)	18(1)
N(2B)	10221(3)	5566(3)	7697(2)	20(1)
N(3B)	9423(2)	5464(3)	6859(2)	18(1)
N(4B)	8577(3)	6141(3)	6162(2)	20(1)
N(5B)	10053(3)	5992(3)	6031(2)	19(1)
N(6B)	11455(3)	6558(3)	6065(2)	20(1)
C(1B)	11519(3)	6207(3)	6578(2)	20(1)
C(2B)	12104(3)	6407(3)	7031(2)	21(1)
C(3B)	12877(3)	6829(3)	7036(2)	22(1)
C(4B)	13270(3)	6952(3)	7546(2)	21(1)
C(5B)	12882(3)	6674(4)	8052(2)	23(1)
C(6B)	12105(3)	6279(4)	8048(2)	22(1)
C(7B)	11717(3)	6124(3)	7534(2)	19(1)

C(8B)	10918(3)	5752(3)	7398(2)	16(1)
C(9B)	9484(3)	5491(3)	7426(2)	18(1)
C(10B)	8649(3)	5635(3)	7630(2)	17(1)
C(11B)	8313(3)	5722(3)	8170(2)	21(1)
C(12B)	7489(3)	5979(3)	8228(2)	21(1)
C(13B)	6985(3)	6162(3)	7749(2)	22(1)
C(14B)	7291(3)	6083(3)	7216(2)	22(1)
C(15B)	8123(3)	5819(3)	7156(2)	20(1)
C(16B)	8667(3)	5768(3)	6665(2)	19(1)
C(17B)	9276(3)	6292(3)	5866(2)	19(1)
C(18B)	9430(3)	6929(3)	5425(2)	19(1)
C(19B)	8897(3)	7416(3)	5084(2)	22(1)
C(20B)	9246(3)	7966(3)	4698(2)	23(1)
C(21B)	10123(3)	8053(3)	4640(2)	20(1)
C(22B)	10678(3)	7609(3)	4986(2)	20(1)
C(23B)	10323(3)	7038(3)	5382(2)	20(1)
C(24B)	10692(3)	6491(3)	5820(2)	20(1)
C(25B)	9921(3)	3800(3)	6105(2)	21(1)
C(26B)	9289(3)	3973(3)	5715(2)	23(1)
C(27B)	8882(3)	3265(3)	5474(2)	23(1)
C(28B)	9073(4)	2399(4)	5600(2)	29(1)
C(29B)	9730(4)	2233(4)	5979(3)	35(1)
C(30B)	10142(3)	2939(3)	6227(2)	26(1)
B(1B)	10177(3)	5334(4)	6488(2)	19(1)

Table S 93. Bond lengths [\AA] and angles [$^\circ$] for *m*-IPhO-Cl₆BsubPc
(Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

I(1A)-C(27A)	2.086(5)
Cl(1A)-C(4A)	1.739(5)
Cl(2A)-C(5A)	1.727(5)
Cl(3A)-C(12A)	1.720(5)
Cl(4A)-C(13A)	1.742(5)
Cl(5A)-C(20A)	1.717(5)
Cl(6A)-C(21A)	1.729(5)
O(1A)-C(25A)	1.362(5)
O(1A)-B(1A)	1.418(7)
N(1A)-C(8A)	1.352(6)
N(1A)-C(1A)	1.375(6)
N(1A)-B(1A)	1.502(6)
N(2A)-C(9A)	1.340(6)
N(2A)-C(8A)	1.353(6)
N(3A)-C(9A)	1.372(6)
N(3A)-C(16A)	1.376(6)
N(3A)-B(1A)	1.507(7)
N(4A)-C(17A)	1.325(6)
N(4A)-C(16A)	1.344(6)
N(5A)-C(17A)	1.360(6)
N(5A)-C(24A)	1.362(6)
N(5A)-B(1A)	1.509(6)
N(6A)-C(24A)	1.338(6)
N(6A)-C(1A)	1.340(6)
C(1A)-C(2A)	1.457(7)
C(2A)-C(3A)	1.390(7)
C(2A)-C(7A)	1.417(7)
C(3A)-C(4A)	1.387(7)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.399(7)
C(5A)-C(6A)	1.403(7)
C(6A)-C(7A)	1.385(7)

C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.472(6)
C(9A)-C(10A)	1.474(7)
C(10A)-C(11A)	1.375(7)
C(10A)-C(15A)	1.420(7)
C(11A)-C(12A)	1.400(7)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.392(8)
C(13A)-C(14A)	1.385(8)
C(14A)-C(15A)	1.406(7)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.435(7)
C(17A)-C(18A)	1.466(6)
C(18A)-C(19A)	1.384(7)
C(18A)-C(23A)	1.418(7)
C(19A)-C(20A)	1.384(7)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.423(7)
C(21A)-C(22A)	1.380(7)
C(22A)-C(23A)	1.397(7)
C(22A)-H(22A)	0.9500
C(23A)-C(24A)	1.464(7)
C(25A)-C(26A)	1.392(7)
C(25A)-C(30A)	1.402(7)
C(26A)-C(27A)	1.402(7)
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.379(7)
C(28A)-C(29A)	1.384(8)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.372(7)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
I(1B)-C(27B)	2.111(5)
Cl(1B)-C(4B)	1.720(5)
Cl(2B)-C(5B)	1.711(5)
Cl(3B)-C(12B)	1.720(5)

Cl(4B)-C(13B)	1.734(5)
Cl(5B)-C(20B)	1.737(5)
Cl(6B)-C(21B)	1.729(5)
O(1B)-C(25B)	1.365(6)
O(1B)-B(1B)	1.427(6)
N(1B)-C(1B)	1.363(6)
N(1B)-C(8B)	1.391(6)
N(1B)-B(1B)	1.503(6)
N(2B)-C(9B)	1.343(6)
N(2B)-C(8B)	1.349(6)
N(3B)-C(9B)	1.362(6)
N(3B)-C(16B)	1.368(6)
N(3B)-B(1B)	1.506(7)
N(4B)-C(16B)	1.337(6)
N(4B)-C(17B)	1.339(6)
N(5B)-C(24B)	1.363(6)
N(5B)-C(17B)	1.373(6)
N(5B)-B(1B)	1.492(7)
N(6B)-C(1B)	1.343(7)
N(6B)-C(24B)	1.350(7)
C(1B)-C(2B)	1.460(7)
C(2B)-C(3B)	1.384(7)
C(2B)-C(7B)	1.419(7)
C(3B)-C(4B)	1.384(7)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.423(7)
C(5B)-C(6B)	1.373(7)
C(6B)-C(7B)	1.397(7)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.426(7)
C(9B)-C(10B)	1.430(7)
C(10B)-C(11B)	1.406(7)
C(10B)-C(15B)	1.437(7)
C(11B)-C(12B)	1.373(7)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.425(8)

C(13B)-C(14B)	1.372(8)
C(14B)-C(15B)	1.388(7)
C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.461(7)
C(17B)-C(18B)	1.450(7)
C(18B)-C(19B)	1.386(7)
C(18B)-C(23B)	1.433(6)
C(19B)-C(20B)	1.363(7)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.405(7)
C(21B)-C(22B)	1.384(7)
C(22B)-C(23B)	1.401(7)
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.459(7)
C(25B)-C(30B)	1.380(7)
C(25B)-C(26B)	1.398(7)
C(26B)-C(27B)	1.377(7)
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.378(8)
C(28B)-C(29B)	1.405(8)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.386(8)
C(29B)-H(29B)	0.9500
C(30B)-H(30B)	0.9500
C(25A)-O(1A)-B(1A)	128.1(4)
C(8A)-N(1A)-C(1A)	114.3(4)
C(8A)-N(1A)-B(1A)	123.5(4)
C(1A)-N(1A)-B(1A)	121.9(4)
C(9A)-N(2A)-C(8A)	115.9(4)
C(9A)-N(3A)-C(16A)	112.3(4)
C(9A)-N(3A)-B(1A)	122.0(4)
C(16A)-N(3A)-B(1A)	123.6(4)
C(17A)-N(4A)-C(16A)	117.3(4)
C(17A)-N(5A)-C(24A)	114.0(4)
C(17A)-N(5A)-B(1A)	123.0(4)

C(24A)-N(5A)-B(1A)	122.2(4)
C(24A)-N(6A)-C(1A)	116.7(4)
N(6A)-C(1A)-N(1A)	122.6(4)
N(6A)-C(1A)-C(2A)	131.4(4)
N(1A)-C(1A)-C(2A)	104.8(4)
C(3A)-C(2A)-C(7A)	121.2(5)
C(3A)-C(2A)-C(1A)	131.2(5)
C(7A)-C(2A)-C(1A)	107.6(4)
C(4A)-C(3A)-C(2A)	117.1(5)
C(4A)-C(3A)-H(3AA)	121.5
C(2A)-C(3A)-H(3AA)	121.5
C(3A)-C(4A)-C(5A)	121.8(4)
C(3A)-C(4A)-Cl(1A)	118.5(4)
C(5A)-C(4A)-Cl(1A)	119.7(4)
C(4A)-C(5A)-C(6A)	121.5(5)
C(4A)-C(5A)-Cl(2A)	119.9(4)
C(6A)-C(5A)-Cl(2A)	118.6(4)
C(7A)-C(6A)-C(5A)	116.7(5)
C(7A)-C(6A)-H(6AA)	121.7
C(5A)-C(6A)-H(6AA)	121.7
C(6A)-C(7A)-C(2A)	121.6(4)
C(6A)-C(7A)-C(8A)	131.3(5)
C(2A)-C(7A)-C(8A)	107.1(4)
N(1A)-C(8A)-N(2A)	122.9(4)
N(1A)-C(8A)-C(7A)	105.0(4)
N(2A)-C(8A)-C(7A)	131.1(4)
N(2A)-C(9A)-N(3A)	123.8(4)
N(2A)-C(9A)-C(10A)	128.3(4)
N(3A)-C(9A)-C(10A)	105.5(4)
C(11A)-C(10A)-C(15A)	121.2(4)
C(11A)-C(10A)-C(9A)	132.1(4)
C(15A)-C(10A)-C(9A)	106.3(4)
C(10A)-C(11A)-C(12A)	118.1(5)
C(10A)-C(11A)-H(11A)	120.9
C(12A)-C(11A)-H(11A)	120.9
C(13A)-C(12A)-C(11A)	120.6(5)

C(13A)-C(12A)-Cl(3A)	120.8(4)
C(11A)-C(12A)-Cl(3A)	118.6(4)
C(14A)-C(13A)-C(12A)	122.5(5)
C(14A)-C(13A)-Cl(4A)	117.1(4)
C(12A)-C(13A)-Cl(4A)	120.4(4)
C(13A)-C(14A)-C(15A)	117.0(5)
C(13A)-C(14A)-H(14A)	121.5
C(15A)-C(14A)-H(14A)	121.5
C(14A)-C(15A)-C(10A)	120.6(5)
C(14A)-C(15A)-C(16A)	130.5(5)
C(10A)-C(15A)-C(16A)	108.2(4)
N(4A)-C(16A)-N(3A)	122.1(4)
N(4A)-C(16A)-C(15A)	129.4(5)
N(3A)-C(16A)-C(15A)	106.2(4)
N(4A)-C(17A)-N(5A)	123.8(4)
N(4A)-C(17A)-C(18A)	129.8(4)
N(5A)-C(17A)-C(18A)	105.2(4)
C(19A)-C(18A)-C(23A)	122.0(4)
C(19A)-C(18A)-C(17A)	130.6(5)
C(23A)-C(18A)-C(17A)	107.2(4)
C(20A)-C(19A)-C(18A)	117.6(5)
C(20A)-C(19A)-H(19A)	121.2
C(18A)-C(19A)-H(19A)	121.2
C(19A)-C(20A)-C(21A)	120.7(4)
C(19A)-C(20A)-Cl(5A)	118.9(4)
C(21A)-C(20A)-Cl(5A)	120.5(4)
C(22A)-C(21A)-C(20A)	121.5(5)
C(22A)-C(21A)-Cl(6A)	119.5(4)
C(20A)-C(21A)-Cl(6A)	119.0(4)
C(21A)-C(22A)-C(23A)	117.8(5)
C(21A)-C(22A)-H(22A)	121.1
C(23A)-C(22A)-H(22A)	121.1
C(22A)-C(23A)-C(18A)	120.0(4)
C(22A)-C(23A)-C(24A)	132.8(4)
C(18A)-C(23A)-C(24A)	107.2(4)
N(6A)-C(24A)-N(5A)	122.7(4)

N(6A)-C(24A)-C(23A)	130.1(4)
N(5A)-C(24A)-C(23A)	105.1(4)
O(1A)-C(25A)-C(26A)	124.6(4)
O(1A)-C(25A)-C(30A)	115.9(4)
C(26A)-C(25A)-C(30A)	119.4(4)
C(25A)-C(26A)-C(27A)	119.1(4)
C(25A)-C(26A)-H(26A)	120.5
C(27A)-C(26A)-H(26A)	120.5
C(28A)-C(27A)-C(26A)	121.2(5)
C(28A)-C(27A)-I(1A)	119.4(4)
C(26A)-C(27A)-I(1A)	119.4(4)
C(27A)-C(28A)-C(29A)	118.8(5)
C(27A)-C(28A)-H(28A)	120.6
C(29A)-C(28A)-H(28A)	120.6
C(30A)-C(29A)-C(28A)	121.3(5)
C(30A)-C(29A)-H(29A)	119.3
C(28A)-C(29A)-H(29A)	119.3
C(29A)-C(30A)-C(25A)	120.1(5)
C(29A)-C(30A)-H(30A)	120.0
C(25A)-C(30A)-H(30A)	120.0
O(1A)-B(1A)-N(1A)	108.1(4)
O(1A)-B(1A)-N(3A)	118.2(4)
N(1A)-B(1A)-N(3A)	103.2(4)
O(1A)-B(1A)-N(5A)	119.6(4)
N(1A)-B(1A)-N(5A)	102.1(4)
N(3A)-B(1A)-N(5A)	103.5(4)
C(25B)-O(1B)-B(1B)	129.6(4)
C(1B)-N(1B)-C(8B)	112.4(4)
C(1B)-N(1B)-B(1B)	122.8(4)
C(8B)-N(1B)-B(1B)	124.1(4)
C(9B)-N(2B)-C(8B)	118.5(4)
C(9B)-N(3B)-C(16B)	113.1(4)
C(9B)-N(3B)-B(1B)	122.4(4)
C(16B)-N(3B)-B(1B)	122.8(4)
C(16B)-N(4B)-C(17B)	117.5(4)
C(24B)-N(5B)-C(17B)	112.4(4)

C(24B)-N(5B)-B(1B)	122.8(4)
C(17B)-N(5B)-B(1B)	123.4(4)
C(1B)-N(6B)-C(24B)	115.9(4)
N(6B)-C(1B)-N(1B)	122.7(4)
N(6B)-C(1B)-C(2B)	130.3(5)
N(1B)-C(1B)-C(2B)	105.3(4)
C(3B)-C(2B)-C(7B)	121.1(5)
C(3B)-C(2B)-C(1B)	131.8(5)
C(7B)-C(2B)-C(1B)	107.0(4)
C(2B)-C(3B)-C(4B)	118.0(5)
C(2B)-C(3B)-H(3BA)	121.0
C(4B)-C(3B)-H(3BA)	121.0
C(3B)-C(4B)-C(5B)	121.1(5)
C(3B)-C(4B)-Cl(1B)	119.4(4)
C(5B)-C(4B)-Cl(1B)	119.4(4)
C(6B)-C(5B)-C(4B)	120.9(5)
C(6B)-C(5B)-Cl(2B)	119.1(4)
C(4B)-C(5B)-Cl(2B)	120.0(4)
C(5B)-C(6B)-C(7B)	118.4(5)
C(5B)-C(6B)-H(6BA)	120.8
C(7B)-C(6B)-H(6BA)	120.8
C(6B)-C(7B)-C(2B)	120.5(5)
C(6B)-C(7B)-C(8B)	131.4(5)
C(2B)-C(7B)-C(8B)	108.0(4)
N(2B)-C(8B)-N(1B)	119.9(4)
N(2B)-C(8B)-C(7B)	133.7(5)
N(1B)-C(8B)-C(7B)	105.6(4)
N(2B)-C(9B)-N(3B)	123.1(4)
N(2B)-C(9B)-C(10B)	129.2(4)
N(3B)-C(9B)-C(10B)	106.1(4)
C(11B)-C(10B)-C(9B)	132.8(5)
C(11B)-C(10B)-C(15B)	119.2(4)
C(9B)-C(10B)-C(15B)	107.5(4)
C(12B)-C(11B)-C(10B)	118.8(5)
C(12B)-C(11B)-H(11B)	120.6
C(10B)-C(11B)-H(11B)	120.6

C(11B)-C(12B)-C(13B)	120.7(5)
C(11B)-C(12B)-Cl(3B)	118.6(4)
C(13B)-C(12B)-Cl(3B)	120.7(4)
C(14B)-C(13B)-C(12B)	122.1(5)
C(14B)-C(13B)-Cl(4B)	118.9(4)
C(12B)-C(13B)-Cl(4B)	119.0(4)
C(13B)-C(14B)-C(15B)	117.4(5)
C(13B)-C(14B)-H(14B)	121.3
C(15B)-C(14B)-H(14B)	121.3
C(14B)-C(15B)-C(10B)	121.9(5)
C(14B)-C(15B)-C(16B)	131.5(5)
C(10B)-C(15B)-C(16B)	106.3(4)
N(4B)-C(16B)-N(3B)	122.8(4)
N(4B)-C(16B)-C(15B)	129.7(4)
N(3B)-C(16B)-C(15B)	105.3(4)
N(4B)-C(17B)-N(5B)	122.5(4)
N(4B)-C(17B)-C(18B)	129.8(4)
N(5B)-C(17B)-C(18B)	106.1(4)
C(19B)-C(18B)-C(23B)	120.2(4)
C(19B)-C(18B)-C(17B)	132.6(4)
C(23B)-C(18B)-C(17B)	107.1(4)
C(20B)-C(19B)-C(18B)	118.3(5)
C(20B)-C(19B)-H(19B)	120.9
C(18B)-C(19B)-H(19B)	120.9
C(19B)-C(20B)-C(21B)	121.8(5)
C(19B)-C(20B)-Cl(5B)	118.2(4)
C(21B)-C(20B)-Cl(5B)	120.0(4)
C(22B)-C(21B)-C(20B)	121.9(5)
C(22B)-C(21B)-Cl(6B)	118.6(4)
C(20B)-C(21B)-Cl(6B)	119.5(4)
C(21B)-C(22B)-C(23B)	116.5(5)
C(21B)-C(22B)-H(22B)	121.7
C(23B)-C(22B)-H(22B)	121.7
C(22B)-C(23B)-C(18B)	121.2(4)
C(22B)-C(23B)-C(24B)	132.4(4)
C(18B)-C(23B)-C(24B)	106.4(4)

N(6B)-C(24B)-N(5B)	123.4(4)
N(6B)-C(24B)-C(23B)	129.1(4)
N(5B)-C(24B)-C(23B)	106.2(4)
O(1B)-C(25B)-C(30B)	116.1(5)
O(1B)-C(25B)-C(26B)	123.6(5)
C(30B)-C(25B)-C(26B)	120.1(5)
C(27B)-C(26B)-C(25B)	118.2(5)
C(27B)-C(26B)-H(26B)	120.9
C(25B)-C(26B)-H(26B)	120.9
C(26B)-C(27B)-C(28B)	122.9(5)
C(26B)-C(27B)-I(1B)	119.9(4)
C(28B)-C(27B)-I(1B)	117.1(4)
C(27B)-C(28B)-C(29B)	118.3(5)
C(27B)-C(28B)-H(28B)	120.8
C(29B)-C(28B)-H(28B)	120.8
C(30B)-C(29B)-C(28B)	119.4(5)
C(30B)-C(29B)-H(29B)	120.3
C(28B)-C(29B)-H(29B)	120.3
C(25B)-C(30B)-C(29B)	121.0(5)
C(25B)-C(30B)-H(30B)	119.5
C(29B)-C(30B)-H(30B)	119.5
O(1B)-B(1B)-N(5B)	119.7(4)
O(1B)-B(1B)-N(1B)	107.9(4)
N(5B)-B(1B)-N(1B)	102.9(4)
O(1B)-B(1B)-N(3B)	116.7(4)
N(5B)-B(1B)-N(3B)	104.0(4)
N(1B)-B(1B)-N(3B)	103.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S 94. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *m*-IPhO-Cl₆BsubPc (**Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1A)	22(1)	29(1)	24(1)	4(1)	-6(1)	-1(1)
Cl(1A)	17(1)	22(1)	33(1)	5(1)	-2(1)	2(1)
Cl(2A)	24(1)	42(1)	25(1)	9(1)	-7(1)	3(1)
Cl(3A)	41(1)	40(1)	24(1)	1(1)	11(1)	-3(1)
Cl(4A)	24(1)	39(1)	41(1)	-4(1)	11(1)	-5(1)
Cl(5A)	33(1)	44(1)	29(1)	-16(1)	-7(1)	-3(1)
Cl(6A)	40(1)	28(1)	23(1)	-7(1)	5(1)	2(1)
O(1A)	17(2)	18(2)	21(2)	4(1)	-3(1)	1(1)
N(1A)	15(2)	20(2)	18(2)	0(2)	-1(2)	-1(2)
N(2A)	22(2)	18(2)	18(2)	0(2)	-1(2)	-1(2)
N(3A)	17(2)	17(2)	19(2)	-3(2)	-2(2)	3(2)
N(4A)	16(2)	19(2)	19(2)	1(2)	-3(2)	3(2)
N(5A)	19(2)	14(2)	17(2)	3(2)	-1(2)	1(1)
N(6A)	18(2)	18(2)	19(2)	2(2)	2(2)	0(2)
C(1A)	13(2)	21(2)	22(2)	2(2)	-1(2)	-1(2)
C(2A)	16(2)	17(2)	21(2)	4(2)	-1(2)	-4(2)
C(3A)	17(2)	17(2)	20(2)	2(2)	1(2)	-2(2)
C(4A)	16(2)	15(2)	27(2)	5(2)	-2(2)	0(2)
C(5A)	21(2)	21(2)	18(2)	5(2)	-7(2)	-3(2)
C(6A)	18(2)	22(2)	20(2)	2(2)	-1(2)	-2(2)
C(7A)	19(2)	14(2)	19(2)	3(2)	-1(2)	-2(2)
C(8A)	18(2)	13(2)	19(2)	3(2)	-2(2)	-1(2)
C(9A)	21(2)	14(2)	18(2)	1(2)	-1(2)	3(2)
C(10A)	21(2)	11(2)	22(2)	0(2)	-1(2)	3(2)
C(11A)	22(2)	18(2)	23(2)	0(2)	0(2)	6(2)
C(12A)	33(3)	16(2)	23(2)	-1(2)	9(2)	4(2)
C(13A)	20(2)	22(2)	30(3)	1(2)	6(2)	3(2)
C(14A)	17(2)	17(2)	31(3)	-3(2)	2(2)	6(2)
C(15A)	19(2)	16(2)	25(2)	0(2)	3(2)	6(2)
C(16A)	20(2)	15(2)	19(2)	-1(2)	-3(2)	6(2)

C(17A)	19(2)	18(2)	17(2)	2(2)	-7(2)	3(2)
C(18A)	23(2)	20(2)	13(2)	1(2)	-3(2)	3(2)
C(19A)	20(2)	23(2)	22(2)	1(2)	-4(2)	3(2)
C(20A)	29(2)	23(2)	19(2)	-1(2)	-9(2)	1(2)
C(21A)	29(3)	20(2)	17(2)	0(2)	2(2)	2(2)
C(22A)	29(2)	22(2)	17(2)	2(2)	0(2)	4(2)
C(23A)	24(2)	18(2)	14(2)	1(2)	-1(2)	0(2)
C(24A)	20(2)	18(2)	17(2)	3(2)	2(2)	1(2)
C(25A)	18(2)	16(2)	17(2)	6(2)	2(2)	4(2)
C(26A)	21(2)	17(2)	19(2)	0(2)	1(2)	-1(2)
C(27A)	18(2)	23(2)	21(2)	2(2)	0(2)	0(2)
C(28A)	24(2)	17(2)	34(3)	11(2)	-2(2)	1(2)
C(29A)	29(3)	16(2)	38(3)	1(2)	-6(2)	-3(2)
C(30A)	18(2)	21(2)	24(2)	4(2)	1(2)	-2(2)
B(1A)	22(3)	17(2)	18(2)	-2(2)	-3(2)	4(2)
I(1B)	22(1)	40(1)	28(1)	-3(1)	-2(1)	-5(1)
Cl(1B)	17(1)	34(1)	36(1)	4(1)	-4(1)	-5(1)
Cl(2B)	30(1)	59(1)	26(1)	2(1)	-9(1)	-15(1)
Cl(3B)	25(1)	51(1)	27(1)	-5(1)	6(1)	-3(1)
Cl(4B)	18(1)	32(1)	40(1)	-1(1)	2(1)	2(1)
Cl(5B)	30(1)	38(1)	32(1)	12(1)	-4(1)	7(1)
Cl(6B)	37(1)	26(1)	27(1)	7(1)	7(1)	1(1)
O(1B)	25(2)	22(2)	26(2)	-5(2)	-3(2)	0(1)
N(1B)	20(2)	19(2)	17(2)	-1(2)	-2(2)	0(2)
N(2B)	21(2)	19(2)	19(2)	1(2)	-3(2)	1(2)
N(3B)	18(2)	16(2)	21(2)	1(2)	-1(2)	-1(2)
N(4B)	20(2)	19(2)	21(2)	0(2)	-2(2)	-5(2)
N(5B)	20(2)	21(2)	17(2)	-4(2)	-2(2)	2(2)
N(6B)	22(2)	20(2)	19(2)	-3(2)	1(2)	2(2)
C(1B)	20(2)	18(2)	22(2)	-2(2)	0(2)	4(2)
C(2B)	22(2)	18(2)	22(3)	0(2)	0(2)	4(2)
C(3B)	21(2)	22(2)	23(3)	0(2)	-2(2)	5(2)
C(4B)	20(2)	17(2)	28(3)	3(2)	-1(2)	1(2)
C(5B)	25(3)	25(3)	20(2)	1(2)	-5(2)	3(2)
C(6B)	21(2)	27(3)	18(2)	1(2)	0(2)	6(2)
C(7B)	17(2)	19(2)	21(2)	1(2)	-2(2)	3(2)

C(8B)	14(2)	18(2)	17(2)	7(2)	1(2)	9(2)
C(9B)	20(2)	12(2)	22(2)	1(2)	-1(2)	-1(2)
C(10B)	21(2)	13(2)	18(2)	0(2)	-1(2)	-8(2)
C(11B)	21(2)	20(2)	24(2)	1(2)	-2(2)	-6(2)
C(12B)	18(2)	23(2)	23(2)	-2(2)	4(2)	-5(2)
C(13B)	15(2)	15(2)	35(3)	-2(2)	-1(2)	-5(2)
C(14B)	16(2)	16(2)	36(3)	2(2)	-3(2)	-3(2)
C(15B)	19(2)	14(2)	27(3)	1(2)	-3(2)	-3(2)
C(16B)	21(2)	16(2)	22(2)	-1(2)	-1(2)	0(2)
C(17B)	19(2)	21(2)	18(2)	-5(2)	-4(2)	1(2)
C(18B)	17(2)	20(2)	20(2)	-2(2)	0(2)	-6(2)
C(19B)	27(2)	22(2)	19(2)	-2(2)	1(2)	-2(2)
C(20B)	26(2)	16(2)	25(2)	-3(2)	-4(2)	5(2)
C(21B)	25(2)	17(2)	19(2)	-2(2)	5(2)	-1(2)
C(22B)	27(2)	16(2)	17(2)	-4(2)	-1(2)	-2(2)
C(23B)	22(2)	19(2)	19(2)	-3(2)	-1(2)	3(2)
C(24B)	24(2)	18(2)	19(2)	-3(2)	4(2)	0(2)
C(25B)	18(2)	21(2)	25(2)	-3(2)	5(2)	-2(2)
C(26B)	24(2)	19(2)	26(3)	-2(2)	2(2)	-2(2)
C(27B)	22(2)	28(2)	18(2)	0(2)	2(2)	-3(2)
C(28B)	31(3)	23(3)	32(3)	-6(2)	3(2)	-8(2)
C(29B)	45(3)	21(3)	39(3)	6(2)	-10(3)	-6(2)
C(30B)	29(3)	22(2)	28(3)	0(2)	-2(2)	0(2)
B(1B)	15(2)	21(3)	20(3)	-4(2)	-2(2)	-1(2)

Table S 95. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

	x	y	z	U(eq)
H(3AA)	2058	9612	3726	22
H(6AA)	3015	8690	1934	24
H(11A)	6137	7967	1602	25
H(14A)	8075	8519	3070	26
H(19A)	7123	9577	4902	26
H(22A)	4242	10003	5360	27
H(26A)	5872	6995	4582	23
H(28A)	6120	4363	4893	30
H(29A)	5009	4078	4282	33
H(30A)	4352	5214	3805	25
H(3BA)	13130	7029	6699	26
H(6BA)	11837	6114	8387	27
H(11B)	8650	5605	8489	26
H(14B)	6947	6204	6901	27
H(19B)	8303	7367	5120	27
H(22B)	11270	7687	4956	24
H(26B)	9143	4563	5618	27
H(28B)	8768	1926	5436	35
H(29B)	9891	1643	6063	42
H(30B)	10583	2828	6486	31

Table S 96. Torsion angles [°] for *m*-IPhO-Cl₆BsubPc (Dichlorobenzene:Dimethoxybenzene:Heptane; CCDC deposit 2087105).

C(24A)-N(6A)-C(1A)-N(1A)	8.4(7)
C(24A)-N(6A)-C(1A)-C(2A)	-156.5(5)
C(8A)-N(1A)-C(1A)-N(6A)	-157.2(4)
B(1A)-N(1A)-C(1A)-N(6A)	16.7(7)
C(8A)-N(1A)-C(1A)-C(2A)	11.1(5)
B(1A)-N(1A)-C(1A)-C(2A)	-175.0(4)
N(6A)-C(1A)-C(2A)-C(3A)	-19.9(9)
N(1A)-C(1A)-C(2A)-C(3A)	173.2(5)
N(6A)-C(1A)-C(2A)-C(7A)	160.2(5)
N(1A)-C(1A)-C(2A)-C(7A)	-6.7(5)
C(7A)-C(2A)-C(3A)-C(4A)	2.3(7)
C(1A)-C(2A)-C(3A)-C(4A)	-177.6(5)
C(2A)-C(3A)-C(4A)-C(5A)	-5.6(7)
C(2A)-C(3A)-C(4A)-Cl(1A)	173.2(3)
C(3A)-C(4A)-C(5A)-C(6A)	4.0(7)
Cl(1A)-C(4A)-C(5A)-C(6A)	-174.8(4)
C(3A)-C(4A)-C(5A)-Cl(2A)	-178.5(4)
Cl(1A)-C(4A)-C(5A)-Cl(2A)	2.7(6)
C(4A)-C(5A)-C(6A)-C(7A)	1.1(7)
Cl(2A)-C(5A)-C(6A)-C(7A)	-176.4(4)
C(5A)-C(6A)-C(7A)-C(2A)	-4.3(7)
C(5A)-C(6A)-C(7A)-C(8A)	178.1(5)
C(3A)-C(2A)-C(7A)-C(6A)	2.7(7)
C(1A)-C(2A)-C(7A)-C(6A)	-177.4(4)
C(3A)-C(2A)-C(7A)-C(8A)	-179.2(4)
C(1A)-C(2A)-C(7A)-C(8A)	0.7(5)
C(1A)-N(1A)-C(8A)-N(2A)	159.1(4)
B(1A)-N(1A)-C(8A)-N(2A)	-14.7(7)
C(1A)-N(1A)-C(8A)-C(7A)	-10.7(5)
B(1A)-N(1A)-C(8A)-C(7A)	175.5(4)
C(9A)-N(2A)-C(8A)-N(1A)	-8.2(7)
C(9A)-N(2A)-C(8A)-C(7A)	158.6(5)

C(6A)-C(7A)-C(8A)-N(1A)	-176.5(5)
C(2A)-C(7A)-C(8A)-N(1A)	5.6(5)
C(6A)-C(7A)-C(8A)-N(2A)	14.9(9)
C(2A)-C(7A)-C(8A)-N(2A)	-162.9(5)
C(8A)-N(2A)-C(9A)-N(3A)	9.0(7)
C(8A)-N(2A)-C(9A)-C(10A)	-150.9(5)
C(16A)-N(3A)-C(9A)-N(2A)	-151.1(4)
B(1A)-N(3A)-C(9A)-N(2A)	12.9(7)
C(16A)-N(3A)-C(9A)-C(10A)	12.6(5)
B(1A)-N(3A)-C(9A)-C(10A)	176.6(4)
N(2A)-C(9A)-C(10A)-C(11A)	-17.8(8)
N(3A)-C(9A)-C(10A)-C(11A)	179.5(5)
N(2A)-C(9A)-C(10A)-C(15A)	154.8(5)
N(3A)-C(9A)-C(10A)-C(15A)	-7.9(5)
C(15A)-C(10A)-C(11A)-C(12A)	-0.9(7)
C(9A)-C(10A)-C(11A)-C(12A)	170.8(5)
C(10A)-C(11A)-C(12A)-C(13A)	-1.6(7)
C(10A)-C(11A)-C(12A)-Cl(3A)	179.1(4)
C(11A)-C(12A)-C(13A)-C(14A)	1.9(7)
Cl(3A)-C(12A)-C(13A)-C(14A)	-178.8(4)
C(11A)-C(12A)-C(13A)-Cl(4A)	-176.3(4)
Cl(3A)-C(12A)-C(13A)-Cl(4A)	3.0(6)
C(12A)-C(13A)-C(14A)-C(15A)	0.2(7)
Cl(4A)-C(13A)-C(14A)-C(15A)	178.5(3)
C(13A)-C(14A)-C(15A)-C(10A)	-2.6(7)
C(13A)-C(14A)-C(15A)-C(16A)	-171.9(5)
C(11A)-C(10A)-C(15A)-C(14A)	3.0(7)
C(9A)-C(10A)-C(15A)-C(14A)	-170.6(4)
C(11A)-C(10A)-C(15A)-C(16A)	174.5(4)
C(9A)-C(10A)-C(15A)-C(16A)	0.9(5)
C(17A)-N(4A)-C(16A)-N(3A)	-7.8(7)
C(17A)-N(4A)-C(16A)-C(15A)	152.4(5)
C(9A)-N(3A)-C(16A)-N(4A)	152.0(4)
B(1A)-N(3A)-C(16A)-N(4A)	-11.7(7)
C(9A)-N(3A)-C(16A)-C(15A)	-12.2(5)
B(1A)-N(3A)-C(16A)-C(15A)	-175.9(4)

C(14A)-C(15A)-C(16A)-N(4A)	14.2(8)
C(10A)-C(15A)-C(16A)-N(4A)	-156.1(5)
C(14A)-C(15A)-C(16A)-N(3A)	176.8(5)
C(10A)-C(15A)-C(16A)-N(3A)	6.5(5)
C(16A)-N(4A)-C(17A)-N(5A)	7.4(7)
C(16A)-N(4A)-C(17A)-C(18A)	-158.5(5)
C(24A)-N(5A)-C(17A)-N(4A)	-157.5(4)
B(1A)-N(5A)-C(17A)-N(4A)	12.4(7)
C(24A)-N(5A)-C(17A)-C(18A)	11.4(5)
B(1A)-N(5A)-C(17A)-C(18A)	-178.8(4)
N(4A)-C(17A)-C(18A)-C(19A)	-11.4(9)
N(5A)-C(17A)-C(18A)-C(19A)	-179.4(5)
N(4A)-C(17A)-C(18A)-C(23A)	162.5(5)
N(5A)-C(17A)-C(18A)-C(23A)	-5.4(5)
C(23A)-C(18A)-C(19A)-C(20A)	4.1(7)
C(17A)-C(18A)-C(19A)-C(20A)	177.3(5)
C(18A)-C(19A)-C(20A)-C(21A)	1.2(7)
C(18A)-C(19A)-C(20A)-Cl(5A)	-178.8(4)
C(19A)-C(20A)-C(21A)-C(22A)	-5.4(8)
Cl(5A)-C(20A)-C(21A)-C(22A)	174.7(4)
C(19A)-C(20A)-C(21A)-Cl(6A)	174.0(4)
Cl(5A)-C(20A)-C(21A)-Cl(6A)	-6.0(6)
C(20A)-C(21A)-C(22A)-C(23A)	3.9(7)
Cl(6A)-C(21A)-C(22A)-C(23A)	-175.4(4)
C(21A)-C(22A)-C(23A)-C(18A)	1.4(7)
C(21A)-C(22A)-C(23A)-C(24A)	-176.7(5)
C(19A)-C(18A)-C(23A)-C(22A)	-5.6(7)
C(17A)-C(18A)-C(23A)-C(22A)	179.9(4)
C(19A)-C(18A)-C(23A)-C(24A)	172.9(4)
C(17A)-C(18A)-C(23A)-C(24A)	-1.7(5)
C(1A)-N(6A)-C(24A)-N(5A)	-8.1(7)
C(1A)-N(6A)-C(24A)-C(23A)	152.8(5)
C(17A)-N(5A)-C(24A)-N(6A)	152.6(4)
B(1A)-N(5A)-C(24A)-N(6A)	-17.4(7)
C(17A)-N(5A)-C(24A)-C(23A)	-12.4(5)
B(1A)-N(5A)-C(24A)-C(23A)	177.6(4)

C(22A)-C(23A)-C(24A)-N(6A)	22.9(9)
C(18A)-C(23A)-C(24A)-N(6A)	-155.3(5)
C(22A)-C(23A)-C(24A)-N(5A)	-173.7(5)
C(18A)-C(23A)-C(24A)-N(5A)	8.1(5)
B(1A)-O(1A)-C(25A)-C(26A)	23.5(7)
B(1A)-O(1A)-C(25A)-C(30A)	-157.6(4)
O(1A)-C(25A)-C(26A)-C(27A)	179.6(4)
C(30A)-C(25A)-C(26A)-C(27A)	0.9(7)
C(25A)-C(26A)-C(27A)-C(28A)	1.2(8)
C(25A)-C(26A)-C(27A)-I(1A)	-178.7(4)
C(26A)-C(27A)-C(28A)-C(29A)	-2.7(8)
I(1A)-C(27A)-C(28A)-C(29A)	177.2(4)
C(27A)-C(28A)-C(29A)-C(30A)	2.1(9)
C(28A)-C(29A)-C(30A)-C(25A)	-0.1(8)
O(1A)-C(25A)-C(30A)-C(29A)	179.7(5)
C(26A)-C(25A)-C(30A)-C(29A)	-1.4(7)
C(25A)-O(1A)-B(1A)-N(1A)	-173.8(4)
C(25A)-O(1A)-B(1A)-N(3A)	69.7(6)
C(25A)-O(1A)-B(1A)-N(5A)	-57.8(7)
C(8A)-N(1A)-B(1A)-O(1A)	-94.8(5)
C(1A)-N(1A)-B(1A)-O(1A)	91.8(5)
C(8A)-N(1A)-B(1A)-N(3A)	31.1(6)
C(1A)-N(1A)-B(1A)-N(3A)	-142.2(4)
C(8A)-N(1A)-B(1A)-N(5A)	138.2(4)
C(1A)-N(1A)-B(1A)-N(5A)	-35.1(6)
C(9A)-N(3A)-B(1A)-O(1A)	89.3(6)
C(16A)-N(3A)-B(1A)-O(1A)	-108.5(5)
C(9A)-N(3A)-B(1A)-N(1A)	-29.9(6)
C(16A)-N(3A)-B(1A)-N(1A)	132.3(4)
C(9A)-N(3A)-B(1A)-N(5A)	-135.9(4)
C(16A)-N(3A)-B(1A)-N(5A)	26.3(6)
C(17A)-N(5A)-B(1A)-O(1A)	107.5(5)
C(24A)-N(5A)-B(1A)-O(1A)	-83.5(6)
C(17A)-N(5A)-B(1A)-N(1A)	-133.4(4)
C(24A)-N(5A)-B(1A)-N(1A)	35.6(6)
C(17A)-N(5A)-B(1A)-N(3A)	-26.5(6)

C(24A)-N(5A)-B(1A)-N(3A)	142.5(4)
C(24B)-N(6B)-C(1B)-N(1B)	7.3(7)
C(24B)-N(6B)-C(1B)-C(2B)	-156.1(5)
C(8B)-N(1B)-C(1B)-N(6B)	-154.1(4)
B(1B)-N(1B)-C(1B)-N(6B)	16.9(7)
C(8B)-N(1B)-C(1B)-C(2B)	12.8(5)
B(1B)-N(1B)-C(1B)-C(2B)	-176.2(4)
N(6B)-C(1B)-C(2B)-C(3B)	-18.7(9)
N(1B)-C(1B)-C(2B)-C(3B)	175.8(5)
N(6B)-C(1B)-C(2B)-C(7B)	157.7(5)
N(1B)-C(1B)-C(2B)-C(7B)	-7.9(5)
C(7B)-C(2B)-C(3B)-C(4B)	1.3(7)
C(1B)-C(2B)-C(3B)-C(4B)	177.3(5)
C(2B)-C(3B)-C(4B)-C(5B)	-1.7(7)
C(2B)-C(3B)-C(4B)-Cl(1B)	-179.0(4)
C(3B)-C(4B)-C(5B)-C(6B)	-0.2(8)
Cl(1B)-C(4B)-C(5B)-C(6B)	177.1(4)
C(3B)-C(4B)-C(5B)-Cl(2B)	178.4(4)
Cl(1B)-C(4B)-C(5B)-Cl(2B)	-4.3(6)
C(4B)-C(5B)-C(6B)-C(7B)	2.5(8)
Cl(2B)-C(5B)-C(6B)-C(7B)	-176.1(4)
C(5B)-C(6B)-C(7B)-C(2B)	-2.8(7)
C(5B)-C(6B)-C(7B)-C(8B)	-178.3(5)
C(3B)-C(2B)-C(7B)-C(6B)	0.9(7)
C(1B)-C(2B)-C(7B)-C(6B)	-175.9(5)
C(3B)-C(2B)-C(7B)-C(8B)	177.3(4)
C(1B)-C(2B)-C(7B)-C(8B)	0.5(5)
C(9B)-N(2B)-C(8B)-N(1B)	-10.0(7)
C(9B)-N(2B)-C(8B)-C(7B)	158.4(5)
C(1B)-N(1B)-C(8B)-N(2B)	158.7(4)
B(1B)-N(1B)-C(8B)-N(2B)	-12.1(7)
C(1B)-N(1B)-C(8B)-C(7B)	-12.6(5)
B(1B)-N(1B)-C(8B)-C(7B)	176.5(4)
C(6B)-C(7B)-C(8B)-N(2B)	13.2(9)
C(2B)-C(7B)-C(8B)-N(2B)	-162.7(5)
C(6B)-C(7B)-C(8B)-N(1B)	-177.2(5)

C(2B)-C(7B)-C(8B)-N(1B)	6.9(5)
C(8B)-N(2B)-C(9B)-N(3B)	9.9(7)
C(8B)-N(2B)-C(9B)-C(10B)	-153.5(5)
C(16B)-N(3B)-C(9B)-N(2B)	-153.0(4)
B(1B)-N(3B)-C(9B)-N(2B)	12.5(7)
C(16B)-N(3B)-C(9B)-C(10B)	13.6(5)
B(1B)-N(3B)-C(9B)-C(10B)	179.2(4)
N(2B)-C(9B)-C(10B)-C(11B)	-14.5(9)
N(3B)-C(9B)-C(10B)-C(11B)	180.0(5)
N(2B)-C(9B)-C(10B)-C(15B)	157.2(5)
N(3B)-C(9B)-C(10B)-C(15B)	-8.3(5)
C(9B)-C(10B)-C(11B)-C(12B)	171.1(5)
C(15B)-C(10B)-C(11B)-C(12B)	0.2(7)
C(10B)-C(11B)-C(12B)-C(13B)	-0.5(7)
C(10B)-C(11B)-C(12B)-Cl(3B)	-179.7(4)
C(11B)-C(12B)-C(13B)-C(14B)	0.6(8)
Cl(3B)-C(12B)-C(13B)-C(14B)	179.8(4)
C(11B)-C(12B)-C(13B)-Cl(4B)	-178.3(4)
Cl(3B)-C(12B)-C(13B)-Cl(4B)	0.8(6)
C(12B)-C(13B)-C(14B)-C(15B)	-0.3(7)
Cl(4B)-C(13B)-C(14B)-C(15B)	178.6(4)
C(13B)-C(14B)-C(15B)-C(10B)	0.0(7)
C(13B)-C(14B)-C(15B)-C(16B)	-172.0(5)
C(11B)-C(10B)-C(15B)-C(14B)	0.1(7)
C(9B)-C(10B)-C(15B)-C(14B)	-173.0(4)
C(11B)-C(10B)-C(15B)-C(16B)	173.8(4)
C(9B)-C(10B)-C(15B)-C(16B)	0.8(5)
C(17B)-N(4B)-C(16B)-N(3B)	-6.5(7)
C(17B)-N(4B)-C(16B)-C(15B)	154.2(5)
C(9B)-N(3B)-C(16B)-N(4B)	151.7(4)
B(1B)-N(3B)-C(16B)-N(4B)	-13.8(7)
C(9B)-N(3B)-C(16B)-C(15B)	-13.0(5)
B(1B)-N(3B)-C(16B)-C(15B)	-178.5(4)
C(14B)-C(15B)-C(16B)-N(4B)	16.6(9)
C(10B)-C(15B)-C(16B)-N(4B)	-156.3(5)
C(14B)-C(15B)-C(16B)-N(3B)	179.9(5)

C(10B)-C(15B)-C(16B)-N(3B)	7.0(5)
C(16B)-N(4B)-C(17B)-N(5B)	7.4(7)
C(16B)-N(4B)-C(17B)-C(18B)	-155.9(5)
C(24B)-N(5B)-C(17B)-N(4B)	-154.8(5)
B(1B)-N(5B)-C(17B)-N(4B)	12.1(7)
C(24B)-N(5B)-C(17B)-C(18B)	12.0(5)
B(1B)-N(5B)-C(17B)-C(18B)	178.8(4)
N(4B)-C(17B)-C(18B)-C(19B)	-17.9(9)
N(5B)-C(17B)-C(18B)-C(19B)	176.7(5)
N(4B)-C(17B)-C(18B)-C(23B)	160.2(5)
N(5B)-C(17B)-C(18B)-C(23B)	-5.2(5)
C(23B)-C(18B)-C(19B)-C(20B)	2.7(7)
C(17B)-C(18B)-C(19B)-C(20B)	-179.4(5)
C(18B)-C(19B)-C(20B)-C(21B)	-0.5(7)
C(18B)-C(19B)-C(20B)-Cl(5B)	-179.4(4)
C(19B)-C(20B)-C(21B)-C(22B)	-2.3(8)
Cl(5B)-C(20B)-C(21B)-C(22B)	176.7(4)
C(19B)-C(20B)-C(21B)-Cl(6B)	177.1(4)
Cl(5B)-C(20B)-C(21B)-Cl(6B)	-4.0(6)
C(20B)-C(21B)-C(22B)-C(23B)	2.6(7)
Cl(6B)-C(21B)-C(22B)-C(23B)	-176.8(3)
C(21B)-C(22B)-C(23B)-C(18B)	-0.3(7)
C(21B)-C(22B)-C(23B)-C(24B)	-177.8(5)
C(19B)-C(18B)-C(23B)-C(22B)	-2.3(7)
C(17B)-C(18B)-C(23B)-C(22B)	179.3(4)
C(19B)-C(18B)-C(23B)-C(24B)	175.7(4)
C(17B)-C(18B)-C(23B)-C(24B)	-2.7(5)
C(1B)-N(6B)-C(24B)-N(5B)	-9.6(7)
C(1B)-N(6B)-C(24B)-C(23B)	155.9(5)
C(17B)-N(5B)-C(24B)-N(6B)	154.7(4)
B(1B)-N(5B)-C(24B)-N(6B)	-12.2(7)
C(17B)-N(5B)-C(24B)-C(23B)	-13.7(5)
B(1B)-N(5B)-C(24B)-C(23B)	179.4(4)
C(22B)-C(23B)-C(24B)-N(6B)	19.9(9)
C(18B)-C(23B)-C(24B)-N(6B)	-157.8(5)
C(22B)-C(23B)-C(24B)-N(5B)	-172.6(5)

C(18B)-C(23B)-C(24B)-N(5B)	9.6(5)
B(1B)-O(1B)-C(25B)-C(30B)	-154.2(5)
B(1B)-O(1B)-C(25B)-C(26B)	30.7(8)
O(1B)-C(25B)-C(26B)-C(27B)	176.9(4)
C(30B)-C(25B)-C(26B)-C(27B)	2.0(8)
C(25B)-C(26B)-C(27B)-C(28B)	-0.2(8)
C(25B)-C(26B)-C(27B)-I(1B)	-176.4(4)
C(26B)-C(27B)-C(28B)-C(29B)	-2.0(8)
I(1B)-C(27B)-C(28B)-C(29B)	174.3(4)
C(27B)-C(28B)-C(29B)-C(30B)	2.4(9)
O(1B)-C(25B)-C(30B)-C(29B)	-176.9(5)
C(26B)-C(25B)-C(30B)-C(29B)	-1.6(8)
C(28B)-C(29B)-C(30B)-C(25B)	-0.6(9)
C(25B)-O(1B)-B(1B)-N(5B)	-69.7(7)
C(25B)-O(1B)-B(1B)-N(1B)	173.3(4)
C(25B)-O(1B)-B(1B)-N(3B)	57.0(7)
C(24B)-N(5B)-B(1B)-O(1B)	-89.2(6)
C(17B)-N(5B)-B(1B)-O(1B)	105.3(5)
C(24B)-N(5B)-B(1B)-N(1B)	30.4(6)
C(17B)-N(5B)-B(1B)-N(1B)	-135.1(4)
C(24B)-N(5B)-B(1B)-N(3B)	138.4(4)
C(17B)-N(5B)-B(1B)-N(3B)	-27.1(6)
C(1B)-N(1B)-B(1B)-O(1B)	94.7(5)
C(8B)-N(1B)-B(1B)-O(1B)	-95.4(5)
C(1B)-N(1B)-B(1B)-N(5B)	-32.8(6)
C(8B)-N(1B)-B(1B)-N(5B)	137.2(4)
C(1B)-N(1B)-B(1B)-N(3B)	-140.9(4)
C(8B)-N(1B)-B(1B)-N(3B)	29.1(6)
C(9B)-N(3B)-B(1B)-O(1B)	89.7(5)
C(16B)-N(3B)-B(1B)-O(1B)	-106.2(5)
C(9B)-N(3B)-B(1B)-N(5B)	-136.2(4)
C(16B)-N(3B)-B(1B)-N(5B)	27.9(6)
C(9B)-N(3B)-B(1B)-N(1B)	-28.9(6)
C(16B)-N(3B)-B(1B)-N(1B)	135.2(4)

Symmetry transformations used to generate equivalent atoms: