Molecular engineering of α and β peripherally tri-halogenated substituted boron subphthalocyanines as mixed alloys to control physical and electrochemical properties for organic photovoltaic applications.

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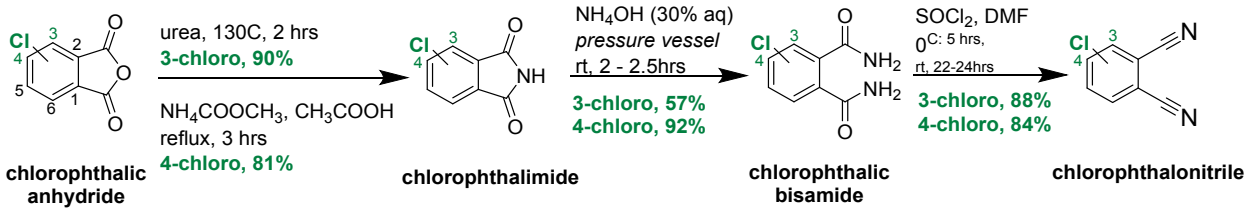
Supporting Information



Scheme S1. The synthesis of mono-chlorinated phthalonitriles from their corresponding anhydrides

Table S1. Process optimization for 3-chlorophthalimide and 3-chlorophthalic bisamide. The highest yielding conditions are shown in green.

Target compound	Reagent (equiv.)	Reaction temperature (°C)	Reaction time (hr)	Yield (%)
3-chlorophthalimide	Ammonium acetate (15)	118	3.5	0
3-chlorophthalimide	Ammonium acetate (15)	118	24	0
3-chlorophthalimide	Urea (2)	120	2	90
3-chlorophthalic bisamide	Ammonium hydroxide (131)	55	1.5	2.5
3-chlorophthalic bisamide	Ammonium hydroxide (131)	23	1	40
3-chlorophthalic bisamide	Ammonium hydroxide (131)	23	2	57
3-chlorophthalic bisamide	Ammonium hydroxide (131)	23	4	36
3-chlorophthalic bisamide	Ammonium hydroxide (131)	23	2.5	92
3-chlorophthalic bisamide	Ammonium hydroxide (131)	23	24	46

Mass Spectroscopy

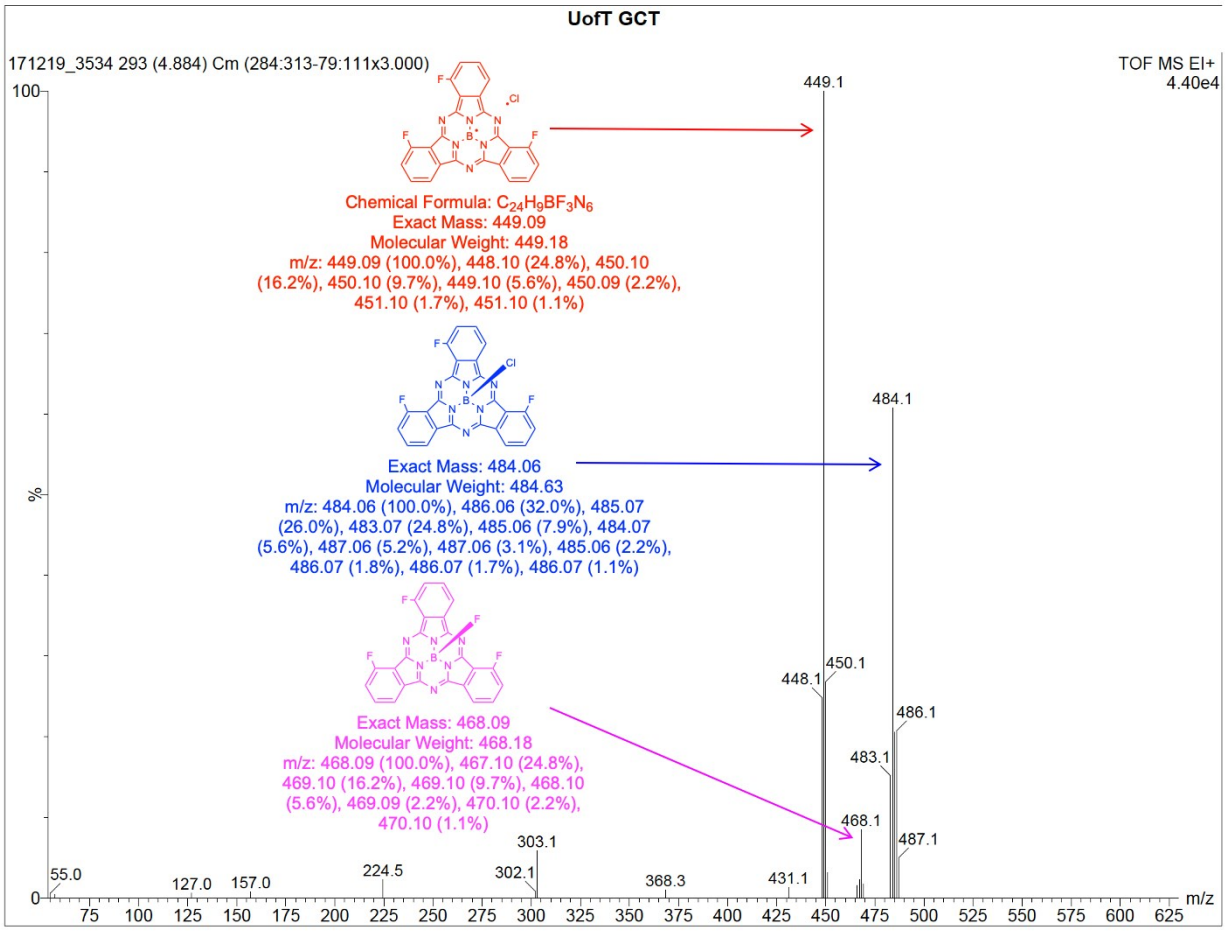


Figure S1. Mass spectrum of Cl-αF_3BsubPc (sublimed product, depicting the presence of it and F-αF_3BsubPc impurity)

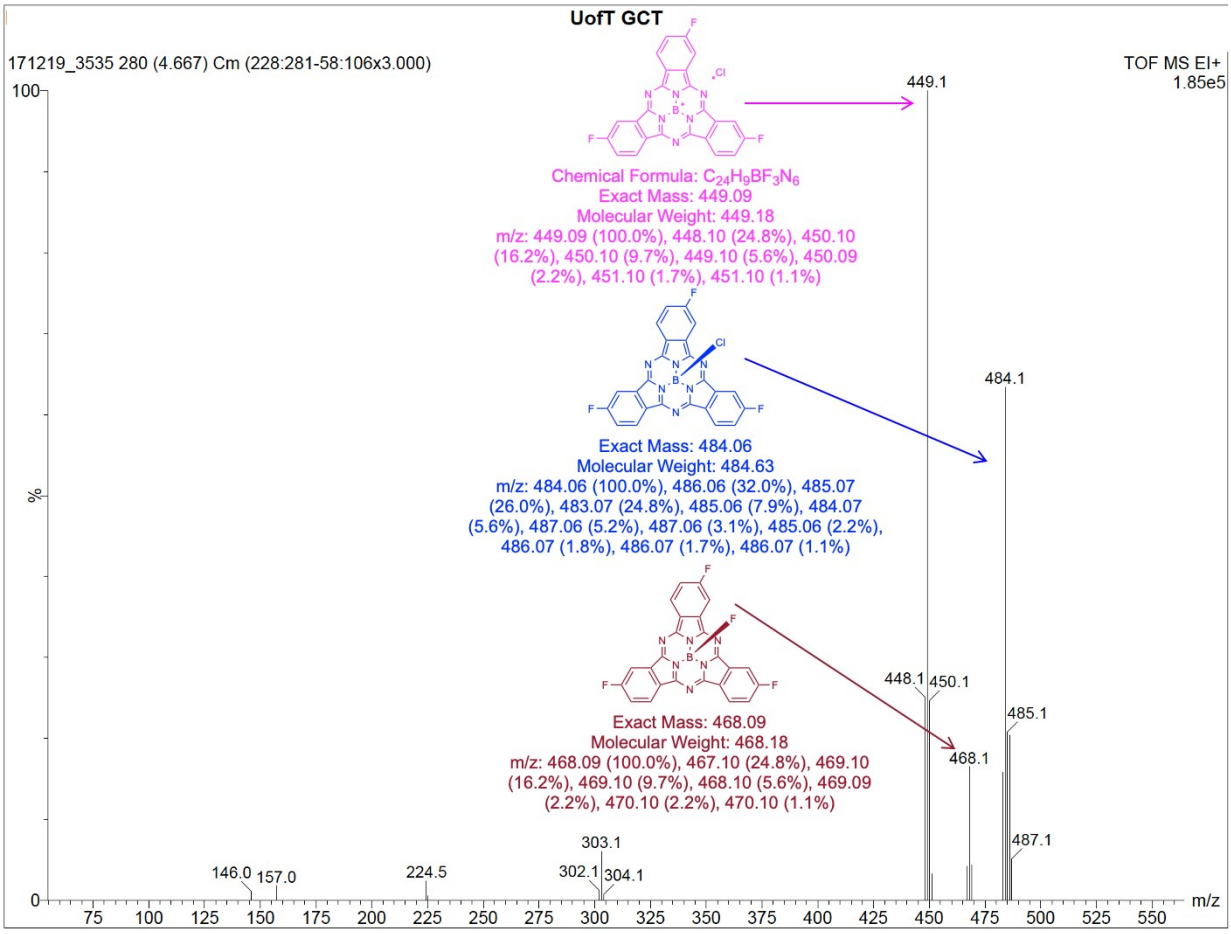


Figure S2. Mass spectrum of Cl-βF_3BsubPc (sublimed product, depicting the presence of it and F-αF_3BsubPc impurity)

NMR Spectroscopy

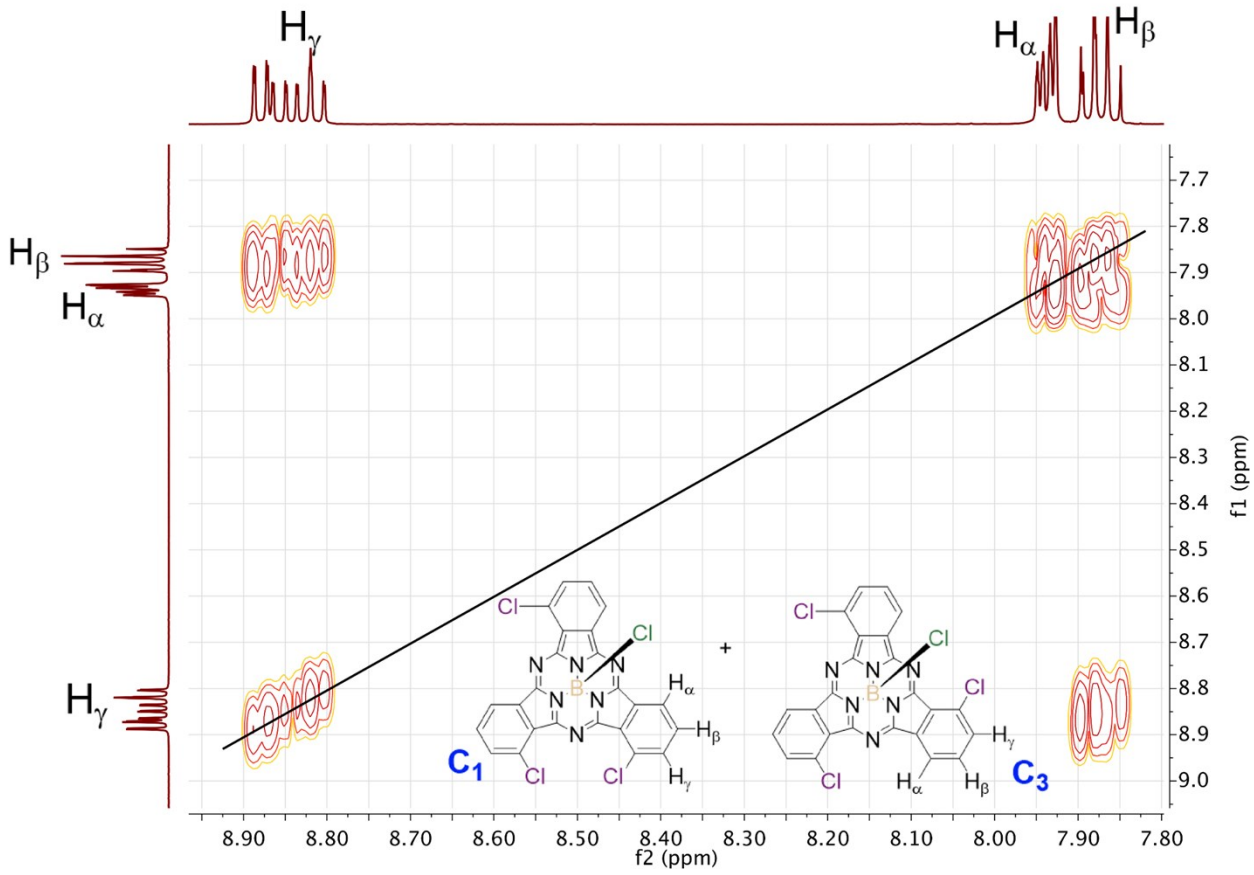


Figure S3. COSY spectrum for Cl-αCl_3BsubPc.

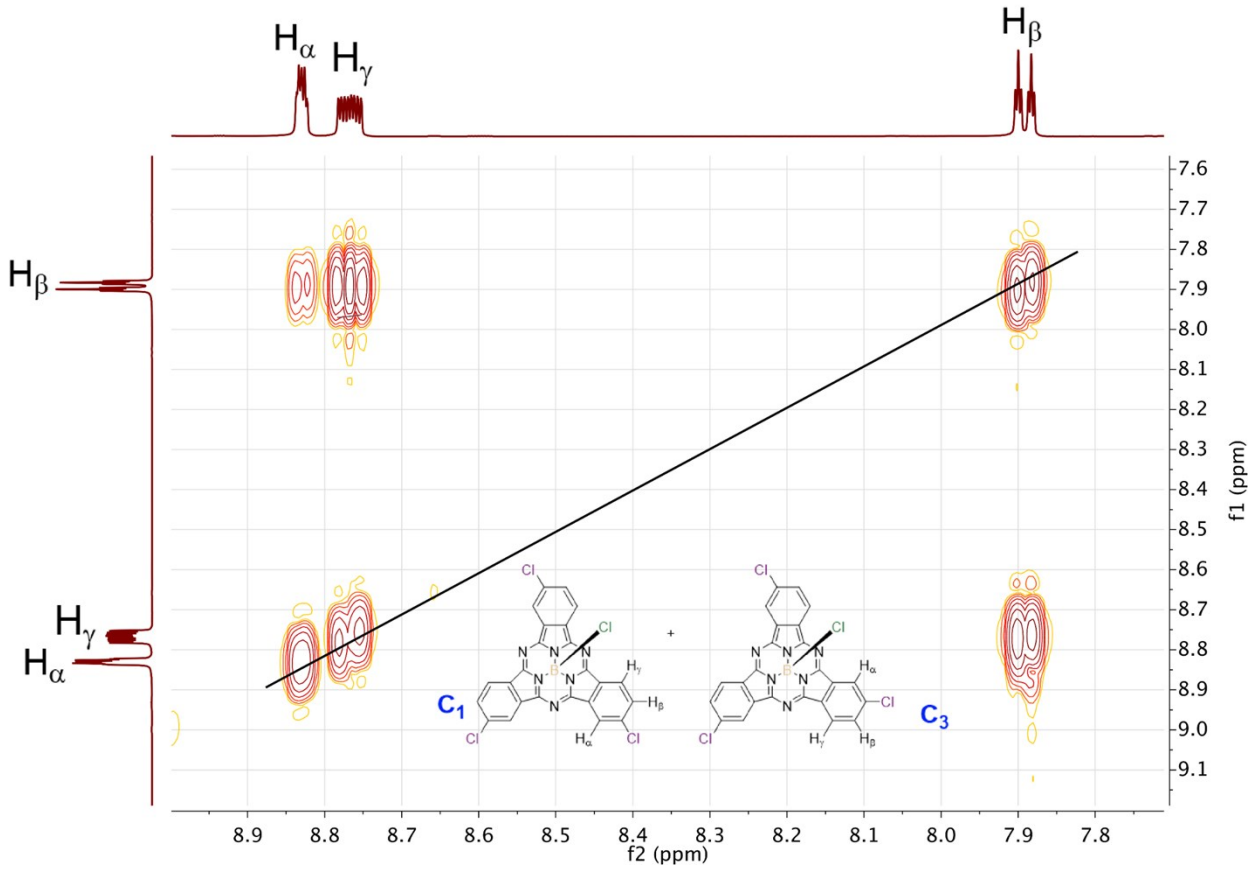


Figure S4. COSY spectrum for Cl-βCl_3BsubPc.

Other characterization (TGA & DSC)

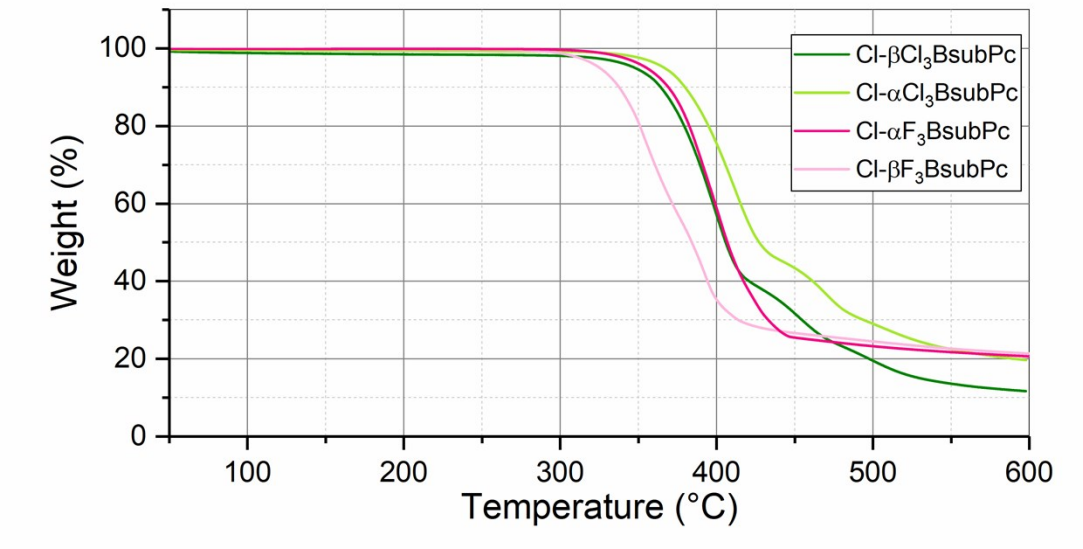


Figure S5. Thermal gravimetric analysis of trichlorinated and trifluorinated BsubPcs

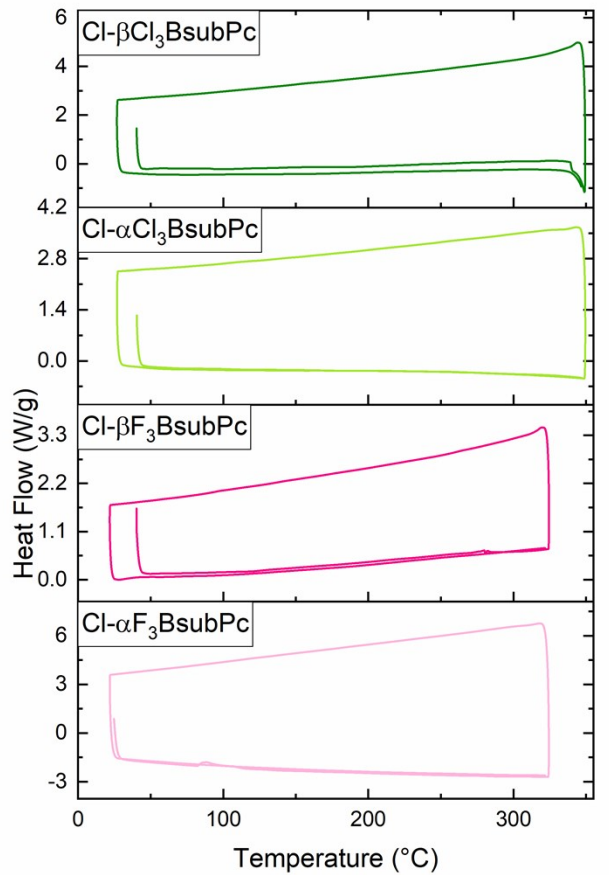


Figure S6. Differential scanning calorimetry of trichlorinated and trifluorinated BsubPcs

Hirshfeld Surface (HS) Analysis

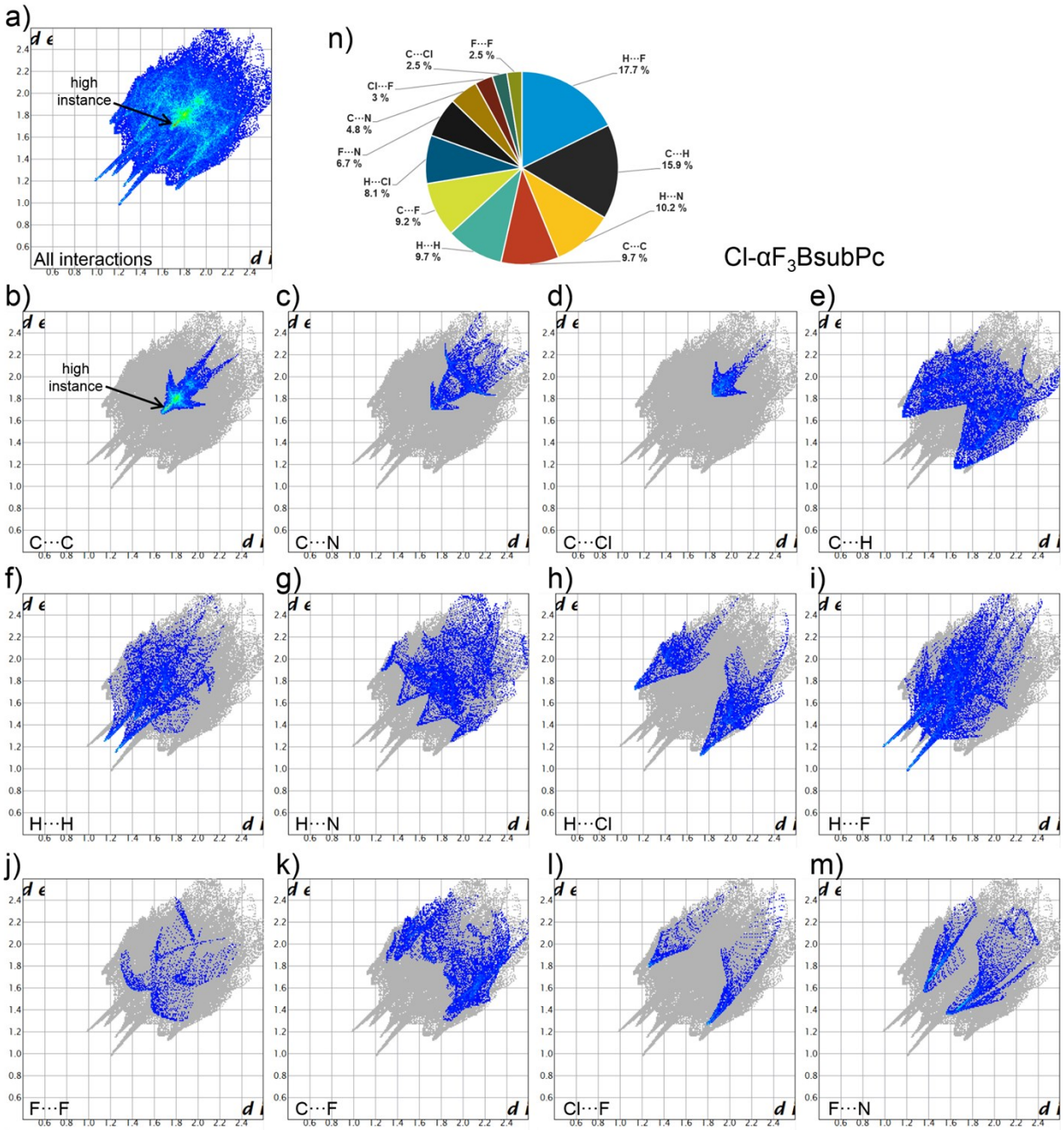


Figure S7. Summary of close contacts in the Cl-αF$_3$BsubPc crystal. (a)-(m) Fingerprint plots of $d_{external}$ (d_e) vs. $d_{internal}$ (d_i) showing instances of each interaction type from low occurrence (blue) to high occurrence (red). For (a) and (b), small red and orange regions of high bond occurrence are indicated using arrows. (n) Pie chart summarizing percentage contributions from each interaction type.

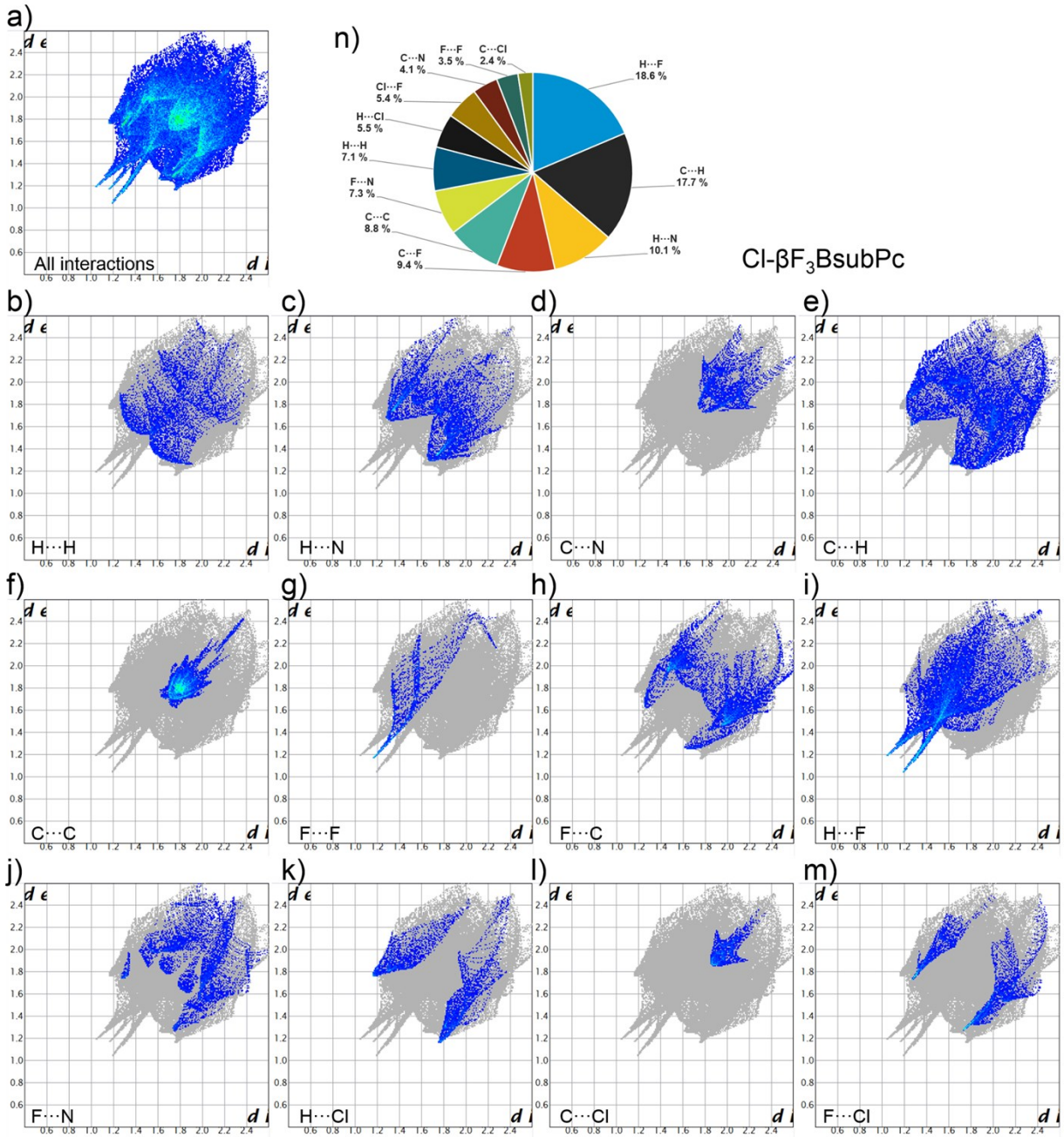


Figure S8. Summary of close contacts in the Cl-βF$_3$BsubPc crystal. (a)-(m) Fingerprint plots of $d_{external}$ (d_e) vs. $d_{internal}$ (d_i) showing instances of each interaction type from low occurrence (blue) to high occurrence (red). (n) Pie chart summarizing percentage contributions from each interaction type.

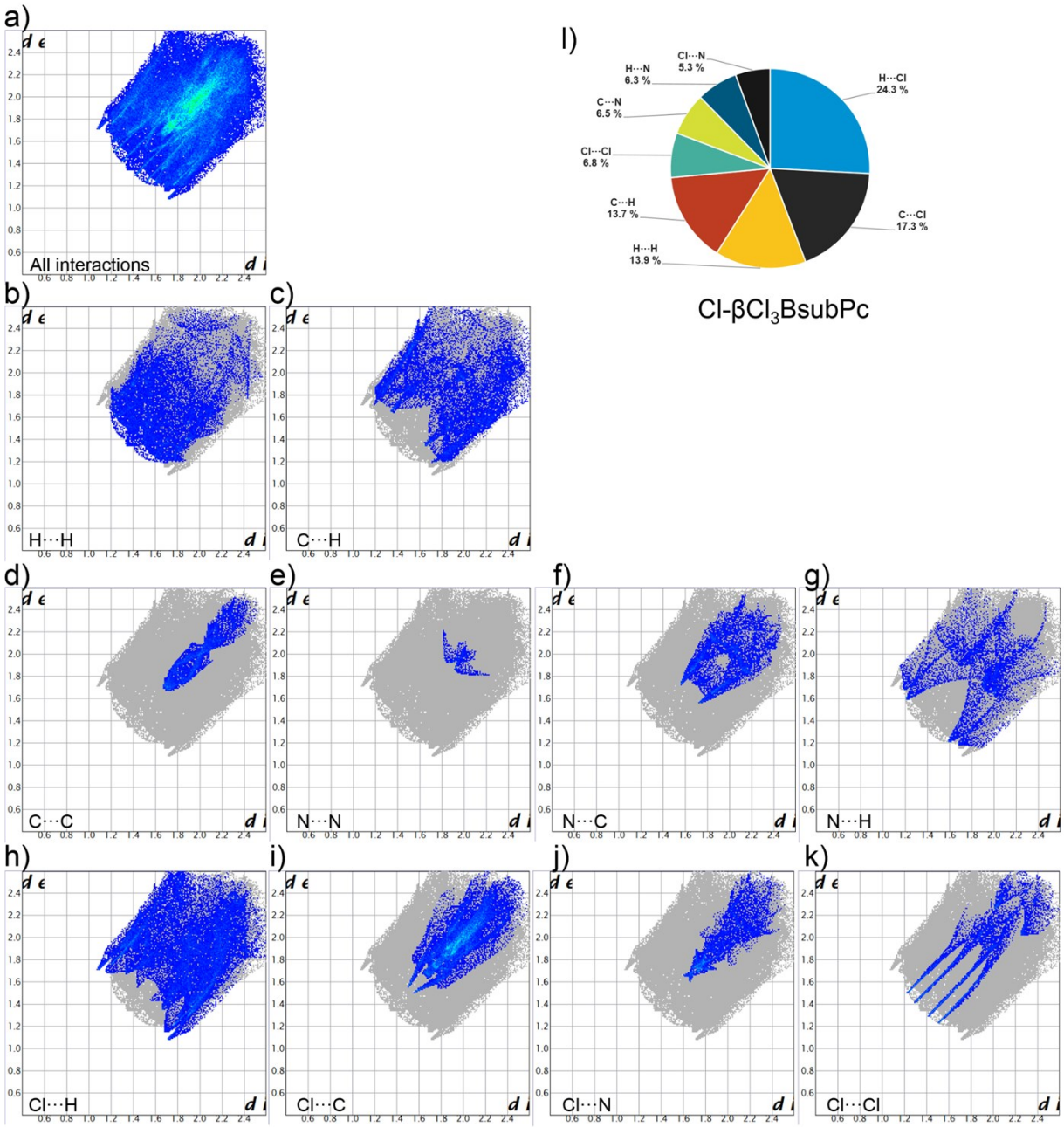


Figure S9. Summary of close contacts in the Cl-βCl$_3$BsubPc crystal. (a)-(k) Fingerprint plots of $d_{external}$ (d_e) vs. $d_{internal}$ (d_i) showing instances of each interaction type from low occurrence (blue) to high occurrence (red). (l) Pie chart summarizing percentage contributions from each interaction type.

Cyclic Voltammetry

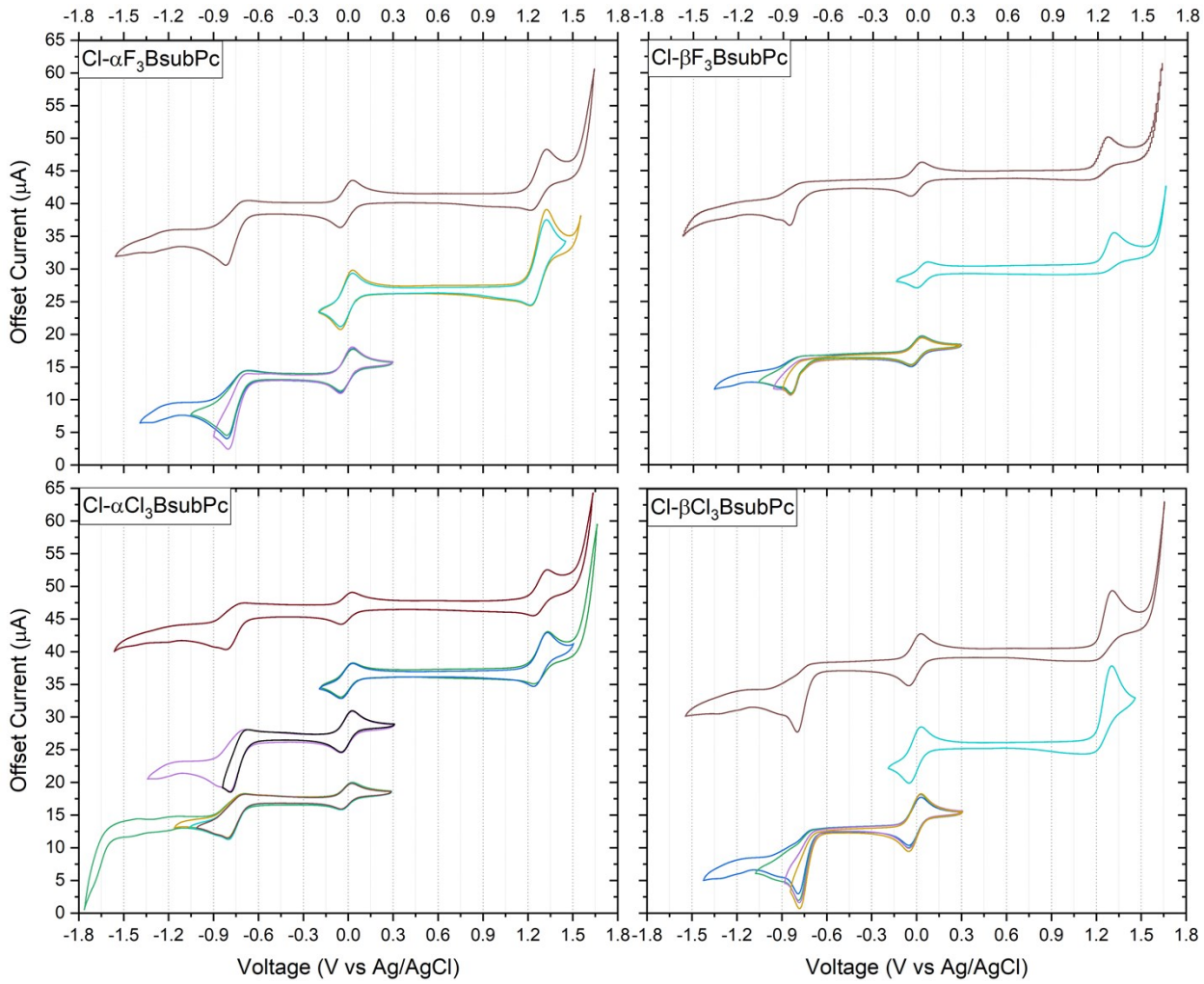


Figure S10. Cyclic voltammograms (CV) of Cl-αF_3BsubPc, Cl-βF_3BsubP, Cl-αCl_3BsubPc and Cl-βCl_3BsubPc (nitrogen degassed dichloromethane as the solvent, scan rate 100 mV/s, decamethylferrocene ($E_{1/2,red}$ = -0.012 V vs Ag/AgCl) as the internal reference, 0.1M tetrabutylammonium perchlorate as the electrolyte, at room temperature. Multiple scans with various switching potentials were taken for each BsubPc in attempts to isolate each reductive or oxidative reaction and study the possibility of reversibility of each chemical reaction.

UV-Vis Spectrum of OPV Irradiation Lamp

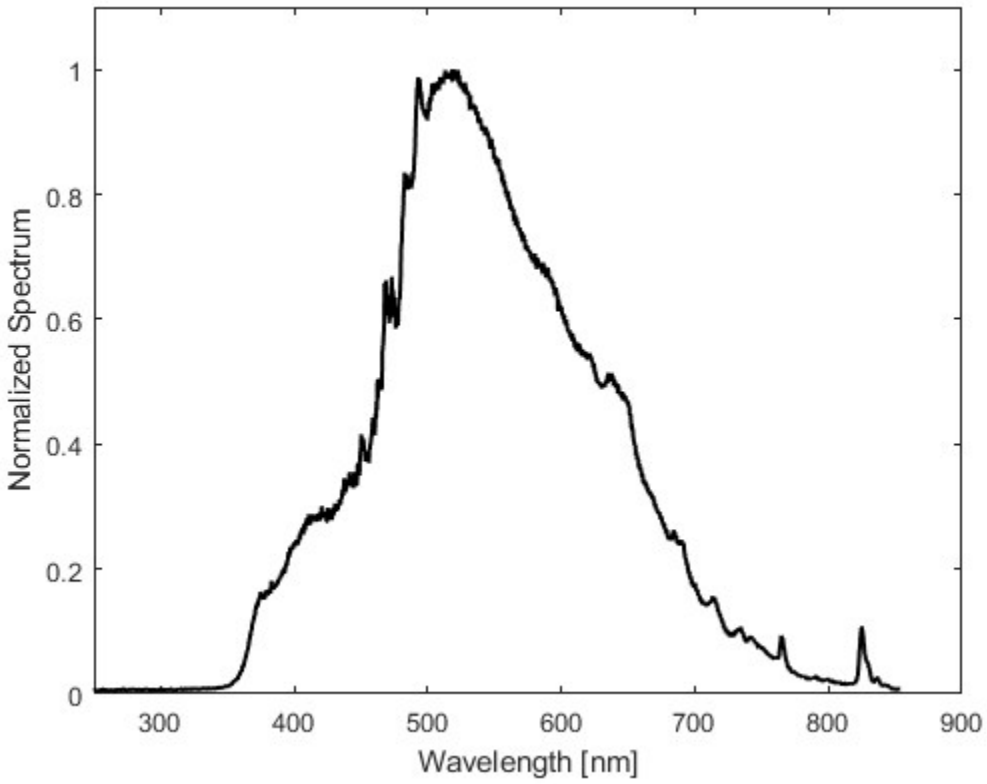


Figure S11. UV-Vis spectrum of the excitation light (lamp: 100 W Xe arc lamp (Oriel) after passing through the filter (AM1.5G standard filter) in the Bender laboratory glovebox set up.

X-Ray Diffraction – Crystallographic Data

Table S2. Crystal data and structure refinement for **Cl-αCl$_3$BsubPc**.

Identification code	**Cl-αCl$_3$BsubPc**	
CCDC deposition number	2051784	
Empirical formula	C24 H8.07 B Cl3.90 N6	
Formula weight	529.63	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/m	
Unit cell dimensions	a = 22.9423(9) Å	α= 90°.
	b = 15.4999(6) Å	β= 114.218(1)°.
	c = 16.4607(6) Å	γ = 90°.
Volume	5338.3(4) Å^3	
Z	8	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.457 mm^{-1}	
F(000)	2123	
Crystal size	0.140 x 0.110 x 0.110 mm^3	
Theta range for data collection	1.356 to 27.534°.	
Index ranges	-22<=h<=29, -20<=k<=20, -21<=l<=17	
Reflections collected	46518	
Independent reflections	6375 [R(int) = 0.0494]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6806	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6375 / 0 / 361	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0609, wR2 = 0.1665	
R indices (all data)	R1 = 0.1138, wR2 = 0.2063	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.758 and -0.383 e.Å^{-3}	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-αCl$_3$BsubPc**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1A)	7650(1)	5000	1996(1)	42(1)
C(3A)	7121(2)	3013(3)	-1359(2)	65(1)
C(6A)	6410(2)	2119(3)	-579(3)	64(1)
C(11A)	4990(2)	4075(3)	1364(2)	59(1)
Cl(2A)	7592(1)	3508(1)	-1776(1)	76(1)
Cl(3A)	6030(3)	1524(3)	-167(4)	97(2)
Cl(4A)	5063(1)	3003(2)	1547(1)	74(1)
C(3C)	7121(2)	3013(3)	-1359(2)	65(1)
C(6C)	6410(2)	2119(3)	-579(3)	64(1)
C(11C)	4990(2)	4075(3)	1364(2)	59(1)
N(1A)	7256(2)	5000	-602(2)	50(1)
N(2A)	6895(1)	4240(2)	357(2)	40(1)
N(3A)	6121(1)	3507(2)	713(2)	45(1)
N(4A)	6315(2)	5000	1011(2)	37(1)
C(1A)	7110(2)	4260(2)	-300(2)	45(1)
C(2A)	6987(2)	3405(2)	-688(2)	50(1)
C(4A)	6908(2)	2196(3)	-1621(3)	76(1)
C(5A)	6558(2)	1750(3)	-1247(3)	76(1)
C(7A)	6630(2)	2945(2)	-297(2)	49(1)
C(8A)	6544(2)	3527(2)	341(2)	44(1)
C(9A)	5990(1)	4262(2)	1000(2)	40(1)
C(10A)	5448(2)	4543(2)	1185(2)	44(1)
C(12A)	4549(2)	4544(3)	1555(2)	66(1)
B(1A)	6923(2)	5000	911(3)	37(1)
Cl(1B)	6626(1)	5000	3131(1)	49(1)
C(3B)	7955(3)	6998(5)	6496(3)	128(3)
C(6B)	6791(4)	7921(4)	5607(4)	116(3)
C(11B)	4276(2)	5921(4)	3671(3)	92(2)
Cl(2B)	8594(1)	6641(2)	7008(2)	105(2)
Cl(3B)	6288(2)	8470(2)	5245(3)	105(2)
Cl(4B)	4225(1)	6902(2)	3559(2)	96(1)

C(3D)	7955(3)	6998(5)	6496(3)	128(3)
C(6D)	6791(4)	7921(4)	5607(4)	116(3)
C(11D)	4276(2)	5921(4)	3671(3)	92(2)
N(1B)	7670(2)	5000	5745(3)	70(1)
N(2B)	6774(1)	5760(2)	4738(2)	50(1)
N(3B)	5782(2)	6485(2)	4300(2)	60(1)
N(4B)	5822(2)	5000	4019(2)	46(1)
C(1B)	7363(2)	5736(3)	5433(2)	62(1)
C(2B)	7442(3)	6611(4)	5798(3)	84(2)
C(4B)	7877(5)	7817(6)	6733(5)	155(5)
C(5B)	7307(6)	8282(5)	6288(6)	167(5)
C(7B)	6863(3)	7060(3)	5353(3)	77(1)
C(8B)	6417(2)	6479(2)	4707(2)	58(1)
C(9B)	5490(2)	5736(3)	4010(2)	54(1)
C(10B)	4845(2)	5448(3)	3819(2)	64(1)
C(12B)	3739(2)	5458(4)	3513(3)	108(3)
B(1B)	6498(3)	5000	4172(3)	44(1)

Table S4. Bond lengths [Å] and angles [°] for **Cl-αCl$_3$BsubPc**.

Cl(1A)-B(1A)	1.877(5)
C(3A)-C(4A)	1.362(6)
C(3A)-C(2A)	1.401(5)
C(3A)-Cl(2A)	1.686(5)
C(6A)-C(7A)	1.385(5)
C(6A)-C(5A)	1.400(6)
C(6A)-Cl(3A)	1.599(7)
C(11A)-C(12A)	1.384(5)
C(11A)-C(10A)	1.403(5)
C(11A)-Cl(4A)	1.684(5)
C(3C)-C(4A)	1.362(6)
C(3C)-C(2A)	1.401(5)
C(3C)-H(3CA)	0.9500
C(6C)-C(7A)	1.385(5)
C(6C)-C(5A)	1.400(6)
C(6C)-H(6CA)	0.9500
C(11C)-C(12A)	1.384(5)
C(11C)-C(10A)	1.403(5)
N(1A)-C(1A)#1	1.345(4)
N(1A)-C(1A)	1.345(4)
N(2A)-C(8A)	1.361(4)
N(2A)-C(1A)	1.362(4)
N(2A)-B(1A)	1.475(4)
N(3A)-C(9A)	1.341(4)
N(3A)-C(8A)	1.343(4)
N(4A)-C(9A)	1.362(3)
N(4A)-C(9A)#1	1.362(3)
N(4A)-B(1A)	1.470(6)
C(1A)-C(2A)	1.448(5)
C(2A)-C(7A)	1.422(5)
C(4A)-C(5A)	1.381(7)
C(4A)-H(4A)	0.9500
C(5A)-H(5A)	0.9500
C(7A)-C(8A)	1.459(4)

C(9A)-C(10A)	1.463(4)
C(10A)-C(10A)#1	1.418(7)
C(12A)-C(12A)#1	1.412(9)
C(12A)-H(12A)	0.9500
Cl(1B)-B(1B)	1.852(5)
C(3B)-C(4B)	1.361(11)
C(3B)-C(2B)	1.398(7)
C(3B)-Cl(2B)	1.468(9)
C(6B)-Cl(3B)	1.359(9)
C(6B)-C(5B)	1.372(11)
C(6B)-C(7B)	1.428(8)
C(11B)-C(12B)	1.356(7)
C(11B)-C(10B)	1.427(6)
C(11B)-Cl(4B)	1.531(7)
C(3D)-C(4B)	1.361(11)
C(3D)-C(2B)	1.398(7)
C(3D)-H(3D)	0.9500
C(6D)-C(5B)	1.372(11)
C(6D)-C(7B)	1.428(8)
C(6D)-H(6D)	0.9500
C(11D)-C(12B)	1.356(7)
C(11D)-C(10B)	1.427(6)
N(1B)-C(1B)#1	1.327(5)
N(1B)-C(1B)	1.327(5)
N(2B)-C(1B)	1.367(5)
N(2B)-C(8B)	1.371(5)
N(2B)-B(1B)	1.474(4)
N(3B)-C(9B)	1.328(5)
N(3B)-C(8B)	1.330(5)
N(4B)-C(9B)#1	1.369(4)
N(4B)-C(9B)	1.369(4)
N(4B)-B(1B)	1.466(7)
C(1B)-C(2B)	1.464(6)
C(2B)-C(7B)	1.411(7)
C(4B)-C(5B)	1.407(13)
C(4B)-H(4B)	0.9500

C(5B)-H(5B)	0.9500
C(7B)-C(8B)	1.447(6)
C(9B)-C(10B)	1.450(5)
C(10B)-C(10B)#1	1.390(9)
C(12B)-C(12B)#1	1.421(12)
C(12B)-H(12B)	0.9500

C(4A)-C(3A)-C(2A)	119.1(4)
C(4A)-C(3A)-Cl(2A)	120.1(3)
C(2A)-C(3A)-Cl(2A)	120.6(4)
C(7A)-C(6A)-C(5A)	118.0(4)
C(7A)-C(6A)-Cl(3A)	125.4(4)
C(5A)-C(6A)-Cl(3A)	116.6(4)
C(12A)-C(11A)-C(10A)	117.2(4)
C(12A)-C(11A)-Cl(4A)	120.4(3)
C(10A)-C(11A)-Cl(4A)	121.3(3)
C(4A)-C(3C)-C(2A)	119.1(4)
C(4A)-C(3C)-H(3CA)	120.4
C(2A)-C(3C)-H(3CA)	120.4
C(7A)-C(6C)-C(5A)	118.0(4)
C(7A)-C(6C)-H(6CA)	121.0
C(5A)-C(6C)-H(6CA)	121.0
C(12A)-C(11C)-C(10A)	117.2(4)
C(1A)#1-N(1A)-C(1A)	116.9(4)
C(8A)-N(2A)-C(1A)	114.1(3)
C(8A)-N(2A)-B(1A)	122.4(3)
C(1A)-N(2A)-B(1A)	122.3(3)
C(9A)-N(3A)-C(8A)	116.6(3)
C(9A)-N(4A)-C(9A)#1	114.3(4)
C(9A)-N(4A)-B(1A)	122.56(18)
C(9A)#1-N(4A)-B(1A)	122.57(18)
N(1A)-C(1A)-N(2A)	122.6(3)
N(1A)-C(1A)-C(2A)	130.6(3)
N(2A)-C(1A)-C(2A)	105.0(3)
C(3C)-C(2A)-C(7A)	119.5(4)
C(3A)-C(2A)-C(7A)	119.5(4)

C(3C)-C(2A)-C(1A)	132.7(4)
C(3A)-C(2A)-C(1A)	132.7(4)
C(7A)-C(2A)-C(1A)	107.7(3)
C(3C)-C(4A)-C(5A)	121.5(4)
C(3A)-C(4A)-C(5A)	121.5(4)
C(3A)-C(4A)-H(4A)	119.2
C(5A)-C(4A)-H(4A)	119.2
C(4A)-C(5A)-C(6A)	121.2(4)
C(4A)-C(5A)-C(6C)	121.2(4)
C(4A)-C(5A)-H(5A)	119.4
C(6A)-C(5A)-H(5A)	119.4
C(6C)-C(7A)-C(2A)	120.7(3)
C(6A)-C(7A)-C(2A)	120.7(3)
C(6C)-C(7A)-C(8A)	132.4(4)
C(6A)-C(7A)-C(8A)	132.4(4)
C(2A)-C(7A)-C(8A)	106.8(3)
N(3A)-C(8A)-N(2A)	122.9(3)
N(3A)-C(8A)-C(7A)	130.6(3)
N(2A)-C(8A)-C(7A)	105.2(3)
N(3A)-C(9A)-N(4A)	122.5(3)
N(3A)-C(9A)-C(10A)	131.7(3)
N(4A)-C(9A)-C(10A)	104.8(3)
C(11A)-C(10A)-C(10A)#1	121.1(2)
C(11C)-C(10A)-C(9A)	131.6(3)
C(11A)-C(10A)-C(9A)	131.6(3)
C(10A)#1-C(10A)-C(9A)	107.31(18)
C(11A)-C(12A)-C(12A)#1	121.7(2)
C(11A)-C(12A)-H(12A)	119.1
C(12A)#1-C(12A)-H(12A)	119.1
N(4A)-B(1A)-N(2A)	105.4(3)
N(4A)-B(1A)-N(2A)#1	105.4(3)
N(2A)-B(1A)-N(2A)#1	106.0(3)
N(4A)-B(1A)-Cl(1A)	114.0(3)
N(2A)-B(1A)-Cl(1A)	112.6(2)
N(2A)#1-B(1A)-Cl(1A)	112.6(2)
C(4B)-C(3B)-C(2B)	118.1(8)

C(4B)-C(3B)-Cl(2B)	113.8(6)
C(2B)-C(3B)-Cl(2B)	128.1(7)
Cl(3B)-C(6B)-C(5B)	113.3(7)
Cl(3B)-C(6B)-C(7B)	129.5(6)
C(5B)-C(6B)-C(7B)	117.1(8)
C(12B)-C(11B)-C(10B)	117.2(6)
C(12B)-C(11B)-Cl(4B)	118.9(4)
C(10B)-C(11B)-Cl(4B)	123.4(4)
C(4B)-C(3D)-C(2B)	118.1(8)
C(4B)-C(3D)-H(3D)	121.0
C(2B)-C(3D)-H(3D)	121.0
C(5B)-C(6D)-C(7B)	117.1(8)
C(5B)-C(6D)-H(6D)	121.4
C(7B)-C(6D)-H(6D)	121.4
C(12B)-C(11D)-C(10B)	117.2(6)
C(1B)#1-N(1B)-C(1B)	118.4(5)
C(1B)-N(2B)-C(8B)	115.1(3)
C(1B)-N(2B)-B(1B)	121.9(3)
C(8B)-N(2B)-B(1B)	122.1(3)
C(9B)-N(3B)-C(8B)	117.5(3)
C(9B)#1-N(4B)-C(9B)	112.9(4)
C(9B)#1-N(4B)-B(1B)	123.2(2)
C(9B)-N(4B)-B(1B)	123.2(2)
N(1B)-C(1B)-N(2B)	122.2(4)
N(1B)-C(1B)-C(2B)	132.8(4)
N(2B)-C(1B)-C(2B)	103.4(4)
C(3D)-C(2B)-C(7B)	120.7(6)
C(3B)-C(2B)-C(7B)	120.7(6)
C(3D)-C(2B)-C(1B)	131.0(7)
C(3B)-C(2B)-C(1B)	131.0(7)
C(7B)-C(2B)-C(1B)	108.2(4)
C(3D)-C(4B)-C(5B)	122.1(8)
C(3B)-C(4B)-C(5B)	122.1(8)
C(3B)-C(4B)-H(4B)	118.9
C(5B)-C(4B)-H(4B)	118.9
C(6D)-C(5B)-C(4B)	121.5(8)

C(6B)-C(5B)-C(4B)	121.5(8)
C(6B)-C(5B)-H(5B)	119.2
C(4B)-C(5B)-H(5B)	119.2
C(2B)-C(7B)-C(6B)	120.4(5)
C(2B)-C(7B)-C(6D)	120.4(5)
C(2B)-C(7B)-C(8B)	107.8(4)
C(6B)-C(7B)-C(8B)	131.7(6)
C(6D)-C(7B)-C(8B)	131.7(6)
N(3B)-C(8B)-N(2B)	122.6(3)
N(3B)-C(8B)-C(7B)	131.6(4)
N(2B)-C(8B)-C(7B)	104.3(4)
N(3B)-C(9B)-N(4B)	121.9(3)
N(3B)-C(9B)-C(10B)	131.8(3)
N(4B)-C(9B)-C(10B)	105.1(3)
C(10B)#1-C(10B)-C(11B)	120.8(3)
C(10B)#1-C(10B)-C(11D)	120.8(3)
C(10B)#1-C(10B)-C(9B)	107.9(2)
C(11B)-C(10B)-C(9B)	131.2(4)
C(11D)-C(10B)-C(9B)	131.2(4)
C(11D)-C(12B)-C(12B)#1	121.9(3)
C(11B)-C(12B)-C(12B)#1	121.9(3)
C(11B)-C(12B)-H(12B)	119.0
C(12B)#1-C(12B)-H(12B)	119.0
N(4B)-B(1B)-N(2B)	105.0(3)
N(4B)-B(1B)-N(2B)#1	105.0(3)
N(2B)-B(1B)-N(2B)#1	106.1(4)
N(4B)-B(1B)-Cl(1B)	113.5(3)
N(2B)-B(1B)-Cl(1B)	113.3(2)
N(2B)#1-B(1B)-Cl(1B)	113.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-αCl$_3$BsubPc**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1A)	44(1)	50(1)	30(1)	0	14(1)	0
C(3A)	63(2)	85(3)	41(2)	-11(2)	14(2)	28(2)
C(6A)	68(2)	53(2)	54(2)	-9(2)	7(2)	14(2)
C(11A)	45(2)	96(3)	36(2)	10(2)	16(1)	-10(2)
Cl(2A)	77(1)	117(1)	41(1)	-1(1)	33(1)	35(1)
Cl(3A)	146(5)	57(3)	91(4)	-12(2)	54(3)	-23(3)
Cl(4A)	55(1)	93(2)	67(1)	25(1)	17(1)	-18(1)
C(3C)	63(2)	85(3)	41(2)	-11(2)	14(2)	28(2)
C(6C)	68(2)	53(2)	54(2)	-9(2)	7(2)	14(2)
C(11C)	45(2)	96(3)	36(2)	10(2)	16(1)	-10(2)
N(1A)	42(2)	75(3)	34(2)	0	18(2)	0
N(2A)	42(1)	47(2)	30(1)	-1(1)	16(1)	4(1)
N(3A)	54(2)	43(2)	36(1)	2(1)	18(1)	-1(1)
N(4A)	43(2)	44(2)	28(2)	0	16(2)	0
C(1A)	39(2)	65(2)	29(1)	-2(1)	13(1)	8(2)
C(2A)	49(2)	62(2)	36(2)	-4(2)	13(1)	18(2)
C(4A)	80(3)	90(3)	47(2)	-17(2)	14(2)	36(3)
C(5A)	82(3)	61(3)	58(2)	-21(2)	2(2)	24(2)
C(7A)	51(2)	48(2)	38(2)	-6(1)	9(1)	10(2)
C(8A)	48(2)	46(2)	32(2)	0(1)	10(1)	3(2)
C(9A)	42(2)	47(2)	30(1)	3(1)	14(1)	-5(1)
C(10A)	39(2)	65(2)	28(1)	1(1)	13(1)	-3(1)
C(12A)	41(2)	124(3)	34(2)	6(2)	17(1)	-10(2)
B(1A)	43(3)	41(3)	31(2)	0	19(2)	0
Cl(1B)	62(1)	59(1)	30(1)	0	24(1)	0
C(3B)	147(6)	203(7)	59(3)	-53(4)	67(4)	-116(5)
C(6B)	214(7)	94(4)	104(4)	-44(4)	128(5)	-69(5)
C(11B)	70(3)	173(6)	41(2)	23(3)	33(2)	29(3)
Cl(2B)	65(2)	196(4)	47(1)	-20(2)	17(1)	-46(2)
Cl(3B)	173(4)	55(2)	140(3)	-15(2)	117(3)	-2(2)
Cl(4B)	98(2)	138(3)	72(2)	43(2)	54(1)	65(2)

C(3D)	147(6)	203(7)	59(3)	-53(4)	67(4)	-116(5)
C(6D)	214(7)	94(4)	104(4)	-44(4)	128(5)	-69(5)
C(11D)	70(3)	173(6)	41(2)	23(3)	33(2)	29(3)
N(1B)	57(3)	123(5)	34(2)	0	23(2)	0
N(2B)	58(2)	65(2)	32(1)	-6(1)	24(1)	-10(2)
N(3B)	87(3)	57(2)	52(2)	10(2)	44(2)	12(2)
N(4B)	54(2)	54(2)	31(2)	0	19(2)	0
C(1B)	61(2)	98(3)	40(2)	-12(2)	32(2)	-21(2)
C(2B)	112(4)	111(4)	48(2)	-36(2)	54(3)	-66(3)
C(4B)	258(11)	162(9)	89(5)	-78(5)	116(7)	-152(8)
C(5B)	347(15)	106(6)	141(8)	-75(5)	197(10)	-125(8)
C(7B)	123(4)	76(3)	63(3)	-26(2)	69(3)	-44(3)
C(8B)	96(3)	47(2)	48(2)	-5(2)	49(2)	-9(2)
C(9B)	67(2)	65(2)	36(2)	10(2)	29(2)	16(2)
C(10B)	55(2)	108(3)	34(2)	11(2)	24(2)	14(2)
C(12B)	56(2)	229(8)	43(2)	16(3)	25(2)	27(3)
B(1B)	56(3)	51(3)	31(2)	0	23(2)	0

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **Cl-αCl$_3$BsubPc**.

	x	y	z	U(eq)
H(3CA)	7357	3313	-1628	78
H(6CA)	6167	1812	-326	77
H(4A)	7003	1927	-2072	91
H(5A)	6415	1182	-1447	91
H(12A)	4238	4246	1690	79
H(3D)	8346	6698	6795	154
H(6D)	6402	8230	5317	140
H(4B)	8218	8083	7215	186
H(5B)	7279	8859	6462	200
H(12B)	3351	5756	3399	129

Table S7. Torsion angles [°] for **Cl-αCl$_3$BsubPc**.

C(1A)#1-N(1A)-C(1A)-N(2A)	-7.6(6)
C(1A)#1-N(1A)-C(1A)-C(2A)	155.3(3)
C(8A)-N(2A)-C(1A)-N(1A)	155.5(3)
B(1A)-N(2A)-C(1A)-N(1A)	-12.3(5)
C(8A)-N(2A)-C(1A)-C(2A)	-11.1(3)
B(1A)-N(2A)-C(1A)-C(2A)	-178.9(3)
C(4A)-C(3C)-C(2A)-C(7A)	-0.3(5)
C(4A)-C(3C)-C(2A)-C(1A)	-176.1(4)
C(4A)-C(3A)-C(2A)-C(7A)	-0.3(5)
Cl(2A)-C(3A)-C(2A)-C(7A)	-175.0(3)
C(4A)-C(3A)-C(2A)-C(1A)	-176.1(4)
Cl(2A)-C(3A)-C(2A)-C(1A)	9.2(5)
N(1A)-C(1A)-C(2A)-C(3C)	17.8(6)
N(2A)-C(1A)-C(2A)-C(3C)	-177.1(4)
N(1A)-C(1A)-C(2A)-C(3A)	17.8(6)
N(2A)-C(1A)-C(2A)-C(3A)	-177.1(4)
N(1A)-C(1A)-C(2A)-C(7A)	-158.4(4)
N(2A)-C(1A)-C(2A)-C(7A)	6.8(3)
C(2A)-C(3C)-C(4A)-C(5A)	0.7(6)
C(2A)-C(3A)-C(4A)-C(5A)	0.7(6)
Cl(2A)-C(3A)-C(4A)-C(5A)	175.4(3)
C(3A)-C(4A)-C(5A)-C(6A)	-0.3(6)
C(3C)-C(4A)-C(5A)-C(6C)	-0.3(6)
C(7A)-C(6A)-C(5A)-C(4A)	-0.5(6)
Cl(3A)-C(6A)-C(5A)-C(4A)	-177.4(4)
C(7A)-C(6C)-C(5A)-C(4A)	-0.5(6)
C(5A)-C(6C)-C(7A)-C(2A)	0.9(5)
C(5A)-C(6C)-C(7A)-C(8A)	176.9(4)
C(5A)-C(6A)-C(7A)-C(2A)	0.9(5)
Cl(3A)-C(6A)-C(7A)-C(2A)	177.5(4)
C(5A)-C(6A)-C(7A)-C(8A)	176.9(4)
Cl(3A)-C(6A)-C(7A)-C(8A)	-6.5(6)
C(3C)-C(2A)-C(7A)-C(6C)	-0.5(5)
C(1A)-C(2A)-C(7A)-C(6C)	176.3(3)

C(3A)-C(2A)-C(7A)-C(6A)	-0.5(5)
C(1A)-C(2A)-C(7A)-C(6A)	176.3(3)
C(3C)-C(2A)-C(7A)-C(8A)	-177.5(3)
C(3A)-C(2A)-C(7A)-C(8A)	-177.5(3)
C(1A)-C(2A)-C(7A)-C(8A)	-0.7(3)
C(9A)-N(3A)-C(8A)-N(2A)	8.9(4)
C(9A)-N(3A)-C(8A)-C(7A)	-155.5(3)
C(1A)-N(2A)-C(8A)-N(3A)	-157.1(3)
B(1A)-N(2A)-C(8A)-N(3A)	10.7(5)
C(1A)-N(2A)-C(8A)-C(7A)	10.7(3)
B(1A)-N(2A)-C(8A)-C(7A)	178.5(3)
C(6C)-C(7A)-C(8A)-N(3A)	-15.6(6)
C(6A)-C(7A)-C(8A)-N(3A)	-15.6(6)
C(2A)-C(7A)-C(8A)-N(3A)	160.8(3)
C(6C)-C(7A)-C(8A)-N(2A)	177.9(3)
C(6A)-C(7A)-C(8A)-N(2A)	177.9(3)
C(2A)-C(7A)-C(8A)-N(2A)	-5.6(3)
C(8A)-N(3A)-C(9A)-N(4A)	-7.0(4)
C(8A)-N(3A)-C(9A)-C(10A)	159.3(3)
C(9A)#1-N(4A)-C(9A)-N(3A)	157.0(2)
B(1A)-N(4A)-C(9A)-N(3A)	-14.6(5)
C(9A)#1-N(4A)-C(9A)-C(10A)	-12.5(4)
B(1A)-N(4A)-C(9A)-C(10A)	175.9(3)
C(12A)-C(11C)-C(10A)-C(10A)#1	-1.1(4)
C(12A)-C(11C)-C(10A)-C(9A)	177.0(3)
C(12A)-C(11A)-C(10A)-C(10A)#1	-1.1(4)
Cl(4A)-C(11A)-C(10A)-C(10A)#1	-168.85(17)
C(12A)-C(11A)-C(10A)-C(9A)	177.0(3)
Cl(4A)-C(11A)-C(10A)-C(9A)	9.3(5)
N(3A)-C(9A)-C(10A)-C(11C)	20.6(5)
N(4A)-C(9A)-C(10A)-C(11C)	-171.2(3)
N(3A)-C(9A)-C(10A)-C(11A)	20.6(5)
N(4A)-C(9A)-C(10A)-C(11A)	-171.2(3)
N(3A)-C(9A)-C(10A)-C(10A)#1	-161.1(3)
N(4A)-C(9A)-C(10A)-C(10A)#1	7.1(2)
C(10A)-C(11C)-C(12A)-C(12A)#1	1.2(4)

C(10A)-C(11A)-C(12A)-C(12A)#1	1.2(4)
Cl(4A)-C(11A)-C(12A)-C(12A)#1	168.98(16)
C(9A)-N(4A)-B(1A)-N(2A)	29.5(4)
C(9A)#1-N(4A)-B(1A)-N(2A)	-141.4(3)
C(9A)-N(4A)-B(1A)-N(2A)#1	141.4(3)
C(9A)#1-N(4A)-B(1A)-N(2A)#1	-29.5(4)
C(9A)-N(4A)-B(1A)-Cl(1A)	-94.5(3)
C(9A)#1-N(4A)-B(1A)-Cl(1A)	94.5(3)
C(8A)-N(2A)-B(1A)-N(4A)	-27.6(4)
C(1A)-N(2A)-B(1A)-N(4A)	139.2(3)
C(8A)-N(2A)-B(1A)-N(2A)#1	-139.1(3)
C(1A)-N(2A)-B(1A)-N(2A)#1	27.7(5)
C(8A)-N(2A)-B(1A)-Cl(1A)	97.3(3)
C(1A)-N(2A)-B(1A)-Cl(1A)	-95.9(3)
C(1B)#1-N(1B)-C(1B)-N(2B)	-7.2(7)
C(1B)#1-N(1B)-C(1B)-C(2B)	155.7(3)
C(8B)-N(2B)-C(1B)-N(1B)	155.9(4)
B(1B)-N(2B)-C(1B)-N(1B)	-12.9(5)
C(8B)-N(2B)-C(1B)-C(2B)	-11.3(4)
B(1B)-N(2B)-C(1B)-C(2B)	179.9(3)
C(4B)-C(3D)-C(2B)-C(7B)	0.2(7)
C(4B)-C(3D)-C(2B)-C(1B)	-175.4(5)
C(4B)-C(3B)-C(2B)-C(7B)	0.2(7)
Cl(2B)-C(3B)-C(2B)-C(7B)	-177.7(4)
C(4B)-C(3B)-C(2B)-C(1B)	-175.4(5)
Cl(2B)-C(3B)-C(2B)-C(1B)	6.6(7)
N(1B)-C(1B)-C(2B)-C(3D)	17.4(7)
N(2B)-C(1B)-C(2B)-C(3D)	-177.5(4)
N(1B)-C(1B)-C(2B)-C(3B)	17.4(7)
N(2B)-C(1B)-C(2B)-C(3B)	-177.5(4)
N(1B)-C(1B)-C(2B)-C(7B)	-158.7(4)
N(2B)-C(1B)-C(2B)-C(7B)	6.5(4)
C(2B)-C(3D)-C(4B)-C(5B)	-1.4(10)
C(2B)-C(3B)-C(4B)-C(5B)	-1.4(10)
Cl(2B)-C(3B)-C(4B)-C(5B)	176.8(6)
C(7B)-C(6D)-C(5B)-C(4B)	-1.7(9)

Cl(3B)-C(6B)-C(5B)-C(4B)	-178.8(6)
C(7B)-C(6B)-C(5B)-C(4B)	-1.7(9)
C(3D)-C(4B)-C(5B)-C(6D)	2.2(12)
C(3B)-C(4B)-C(5B)-C(6B)	2.2(12)
C(3B)-C(2B)-C(7B)-C(6B)	0.2(6)
C(1B)-C(2B)-C(7B)-C(6B)	176.8(3)
C(3D)-C(2B)-C(7B)-C(6D)	0.2(6)
C(1B)-C(2B)-C(7B)-C(6D)	176.8(3)
C(3D)-C(2B)-C(7B)-C(8B)	-176.7(3)
C(3B)-C(2B)-C(7B)-C(8B)	-176.7(3)
C(1B)-C(2B)-C(7B)-C(8B)	-0.1(4)
Cl(3B)-C(6B)-C(7B)-C(2B)	177.1(4)
C(5B)-C(6B)-C(7B)-C(2B)	0.5(6)
Cl(3B)-C(6B)-C(7B)-C(8B)	-6.9(7)
C(5B)-C(6B)-C(7B)-C(8B)	176.5(4)
C(5B)-C(6D)-C(7B)-C(2B)	0.5(6)
C(5B)-C(6D)-C(7B)-C(8B)	176.5(4)
C(9B)-N(3B)-C(8B)-N(2B)	8.2(5)
C(9B)-N(3B)-C(8B)-C(7B)	-155.2(4)
C(1B)-N(2B)-C(8B)-N(3B)	-155.9(3)
B(1B)-N(2B)-C(8B)-N(3B)	12.9(5)
C(1B)-N(2B)-C(8B)-C(7B)	11.4(4)
B(1B)-N(2B)-C(8B)-C(7B)	-179.8(3)
C(2B)-C(7B)-C(8B)-N(3B)	159.3(4)
C(6B)-C(7B)-C(8B)-N(3B)	-17.1(7)
C(6D)-C(7B)-C(8B)-N(3B)	-17.1(7)
C(2B)-C(7B)-C(8B)-N(2B)	-6.3(4)
C(6B)-C(7B)-C(8B)-N(2B)	177.3(4)
C(6D)-C(7B)-C(8B)-N(2B)	177.3(4)
C(8B)-N(3B)-C(9B)-N(4B)	-8.4(5)
C(8B)-N(3B)-C(9B)-C(10B)	156.6(3)
C(9B)#1-N(4B)-C(9B)-N(3B)	157.8(2)
B(1B)-N(4B)-C(9B)-N(3B)	-12.7(5)
C(9B)#1-N(4B)-C(9B)-C(10B)	-10.8(5)
B(1B)-N(4B)-C(9B)-C(10B)	178.8(3)
C(12B)-C(11B)-C(10B)-C(10B)#1	-1.4(4)

Cl(4B)-C(11B)-C(10B)-C(10B)#1	-172.9(2)
C(12B)-C(11B)-C(10B)-C(9B)	-179.5(3)
Cl(4B)-C(11B)-C(10B)-C(9B)	8.9(6)
C(12B)-C(11D)-C(10B)-C(10B)#1	-1.4(4)
C(12B)-C(11D)-C(10B)-C(9B)	-179.5(3)
N(3B)-C(9B)-C(10B)-C(10B)#1	-160.7(3)
N(4B)-C(9B)-C(10B)-C(10B)#1	6.2(3)
N(3B)-C(9B)-C(10B)-C(11B)	17.6(6)
N(4B)-C(9B)-C(10B)-C(11B)	-175.5(4)
N(3B)-C(9B)-C(10B)-C(11D)	17.6(6)
N(4B)-C(9B)-C(10B)-C(11D)	-175.5(4)
C(10B)-C(11D)-C(12B)-C(12B)#1	1.4(4)
C(10B)-C(11B)-C(12B)-C(12B)#1	1.4(4)
Cl(4B)-C(11B)-C(12B)-C(12B)#1	173.33(19)
C(9B)#1-N(4B)-B(1B)-N(2B)	-140.5(3)
C(9B)-N(4B)-B(1B)-N(2B)	28.9(5)
C(9B)#1-N(4B)-B(1B)-N(2B)#1	-28.9(5)
C(9B)-N(4B)-B(1B)-N(2B)#1	140.5(3)
C(9B)#1-N(4B)-B(1B)-Cl(1B)	95.3(3)
C(9B)-N(4B)-B(1B)-Cl(1B)	-95.3(3)
C(1B)-N(2B)-B(1B)-N(4B)	139.2(3)
C(8B)-N(2B)-B(1B)-N(4B)	-28.8(4)
C(1B)-N(2B)-B(1B)-N(2B)#1	28.4(5)
C(8B)-N(2B)-B(1B)-N(2B)#1	-139.6(3)
C(1B)-N(2B)-B(1B)-Cl(1B)	-96.4(3)
C(8B)-N(2B)-B(1B)-Cl(1B)	95.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z

Table S8. Crystal data and structure refinement for **Cl-βCl$_3$BsubPc**.

Identification code	**Cl-βCl$_3$BsubPc**	
CCDC deposition number	2051785	
Empirical formula	C24 H9.11 B Cl3.89 N6	
Formula weight	530.19	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.1595(6) Å	α= 90°.
	b = 10.3924(4) Å	β= 102.519(4)°.
	c = 19.5637(8) Å	γ = 90°.
Volume	2214.94(18) Å^3	
Z	4	
Density (calculated)	1.590 Mg/m^3	
Absorption coefficient	4.969 mm^{-1}	
F(000)	1065	
Crystal size	0.100 x 0.030 x 0.010 mm^3	
Theta range for data collection	4.058 to 67.985°.	
Index ranges	-13<=h<=13, -12<=k<=12, -23<=l<=23	
Reflections collected	30857	
Independent reflections	4019 [R(int) = 0.0993]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7530 and 0.6155	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4019 / 0 / 340	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0779, wR2 = 0.1858	
R indices (all data)	R1 = 0.1089, wR2 = 0.2072	
Extinction coefficient	0.0015(3)	
Largest diff. peak and hole	0.776 and -0.842 e.Å^{-3}	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-βCl$_3$BsubPc**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4726(1)	9253(1)	2927(1)	62(1)
Cl(2)	9914(6)	3225(6)	4667(4)	103(3)
Cl(3)	8256(2)	2970(2)	5532(1)	86(1)
Cl(4)	-536(2)	3173(2)	2661(2)	74(1)
Cl(5)	-1182(5)	3775(5)	1584(4)	128(3)
Cl(6)	8451(3)	6319(3)	-184(1)	140(2)
N(1)	5775(4)	6812(3)	3215(2)	47(1)
N(2)	4239(4)	5733(4)	3665(2)	55(1)
N(3)	3741(4)	6812(4)	2572(2)	54(1)
N(4)	3397(5)	6853(4)	1327(3)	71(1)
N(5)	5335(4)	7398(4)	2022(2)	57(1)
N(6)	7373(4)	6822(4)	2584(2)	56(1)
C(1)	6958(5)	6564(4)	3160(3)	51(1)
C(2)	7465(5)	5733(5)	3741(3)	54(1)
C(3)	8615(5)	5145(6)	3928(3)	67(2)
C(4)	8791(6)	4271(6)	4470(3)	76(2)
C(5)	7884(6)	4018(5)	4836(3)	69(2)
C(4A)	8791(6)	4271(6)	4470(3)	76(2)
C(5A)	7884(6)	4018(5)	4836(3)	69(2)
C(6)	6741(5)	4589(5)	4655(3)	61(1)
C(7)	6528(5)	5435(4)	4095(2)	52(1)
C(8)	5416(5)	6043(4)	3704(2)	50(1)
C(9)	3425(5)	6050(5)	3076(3)	58(1)
C(10)	2258(5)	5485(5)	2740(4)	72(2)
C(11)	1488(5)	4648(6)	3002(5)	88(2)
C(12)	461(7)	4217(7)	2490(7)	116(4)
C(13)	221(8)	4580(9)	1783(7)	122(4)
C(12A)	461(7)	4217(7)	2490(7)	116(4)
C(13A)	221(8)	4580(9)	1783(7)	122(4)
C(14)	981(6)	5369(7)	1560(5)	101(3)
C(15)	2002(5)	5832(6)	2024(4)	78(2)

C(16)	3021(5)	6611(5)	1918(3)	64(1)
C(17)	4577(6)	7151(5)	1388(3)	64(2)
C(18)	5360(7)	6986(5)	900(3)	70(2)
C(19)	5102(8)	6712(5)	174(3)	85(2)
C(20)	6086(10)	6497(6)	-139(4)	96(3)
C(21)	7281(10)	6538(6)	255(4)	96(3)
C(21A)	7281(10)	6538(6)	255(4)	96(3)
C(22)	7568(7)	6771(5)	965(3)	79(2)
C(23)	6575(6)	7006(5)	1282(3)	65(2)
C(24)	6543(6)	7156(5)	2015(3)	59(1)
B(1)	4896(5)	7528(5)	2675(3)	51(1)

Table S10. Bond lengths [Å] and angles [°] for **Cl-βCl$_3$BsubPc**.

Cl(1)-B(1)	1.879(5)
Cl(2)-C(4)	1.640(8)
Cl(3)-C(5)	1.722(6)
Cl(4)-C(12)	1.639(8)
Cl(4)-Cl(5)	2.167(7)
Cl(5)-C(13)	1.744(10)
Cl(6)-C(21)	1.725(8)
N(1)-C(1)	1.371(6)
N(1)-C(8)	1.372(6)
N(1)-B(1)	1.477(7)
N(2)-C(8)	1.339(6)
N(2)-C(9)	1.345(7)
N(3)-C(9)	1.369(7)
N(3)-C(16)	1.372(7)
N(3)-B(1)	1.464(7)
N(4)-C(17)	1.332(8)
N(4)-C(16)	1.337(8)
N(5)-C(17)	1.365(7)
N(5)-C(24)	1.374(7)
N(5)-B(1)	1.471(7)
N(6)-C(24)	1.331(7)
N(6)-C(1)	1.335(6)
C(1)-C(2)	1.442(7)
C(2)-C(3)	1.397(7)
C(2)-C(7)	1.408(7)
C(3)-C(4A)	1.378(9)
C(3)-C(4)	1.378(9)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.385(9)
C(5)-C(6)	1.382(8)
C(4A)-C(5A)	1.385(9)
C(4A)-H(4A)	0.9500
C(5A)-C(6)	1.382(8)
C(5A)-H(5A)	0.9500

C(6)-C(7)	1.385(7)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.453(7)
C(9)-C(10)	1.449(8)
C(10)-C(11)	1.396(9)
C(10)-C(15)	1.416(10)
C(11)-C(12A)	1.420(12)
C(11)-C(12)	1.420(12)
C(11)-H(11)	0.9500
C(12)-C(13)	1.404(15)
C(13)-C(14)	1.320(14)
C(12A)-C(13A)	1.404(15)
C(12A)-H(12A)	0.9500
C(13A)-C(14)	1.320(14)
C(13A)-H(13A)	0.9500
C(14)-C(15)	1.380(9)
C(14)-H(14)	0.9500
C(15)-C(16)	1.446(9)
C(17)-C(18)	1.439(8)
C(18)-C(23)	1.400(9)
C(18)-C(19)	1.414(8)
C(19)-C(20)	1.387(11)
C(19)-H(19A)	0.9500
C(20)-C(21A)	1.388(12)
C(20)-C(21)	1.388(12)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.377(9)
C(21A)-C(22)	1.377(9)
C(21A)-H(21A)	0.9500
C(22)-C(23)	1.404(9)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.452(7)

C(12)-Cl(4)-Cl(5)	73.1(5)
C(13)-Cl(5)-Cl(4)	80.1(5)
C(1)-N(1)-C(8)	112.1(4)

C(1)-N(1)-B(1)	122.7(4)
C(8)-N(1)-B(1)	122.9(4)
C(8)-N(2)-C(9)	117.5(4)
C(9)-N(3)-C(16)	113.1(5)
C(9)-N(3)-B(1)	123.5(4)
C(16)-N(3)-B(1)	121.8(5)
C(17)-N(4)-C(16)	117.1(5)
C(17)-N(5)-C(24)	112.0(5)
C(17)-N(5)-B(1)	123.2(5)
C(24)-N(5)-B(1)	122.5(4)
C(24)-N(6)-C(1)	116.9(5)
N(6)-C(1)-N(1)	123.0(5)
N(6)-C(1)-C(2)	129.5(5)
N(1)-C(1)-C(2)	105.7(4)
C(3)-C(2)-C(7)	120.8(5)
C(3)-C(2)-C(1)	130.6(5)
C(7)-C(2)-C(1)	108.2(4)
C(4A)-C(3)-C(2)	117.4(6)
C(4)-C(3)-C(2)	117.4(6)
C(4)-C(3)-H(3A)	121.3
C(2)-C(3)-H(3A)	121.3
C(3)-C(4)-C(5)	121.6(6)
C(3)-C(4)-Cl(2)	126.3(6)
C(5)-C(4)-Cl(2)	111.1(6)
C(6)-C(5)-C(4)	121.6(5)
C(6)-C(5)-Cl(3)	121.7(5)
C(4)-C(5)-Cl(3)	116.8(5)
C(3)-C(4A)-C(5A)	121.6(6)
C(3)-C(4A)-H(4A)	119.2
C(5A)-C(4A)-H(4A)	119.2
C(6)-C(5A)-C(4A)	121.6(5)
C(6)-C(5A)-H(5A)	119.2
C(4A)-C(5A)-H(5A)	119.2
C(5A)-C(6)-C(7)	117.8(5)
C(5)-C(6)-C(7)	117.8(5)
C(5)-C(6)-H(6A)	121.1

C(7)-C(6)-H(6A)	121.1
C(6)-C(7)-C(2)	120.7(5)
C(6)-C(7)-C(8)	132.3(5)
C(2)-C(7)-C(8)	106.6(4)
N(2)-C(8)-N(1)	122.1(4)
N(2)-C(8)-C(7)	129.9(4)
N(1)-C(8)-C(7)	106.0(4)
N(2)-C(9)-N(3)	121.8(5)
N(2)-C(9)-C(10)	131.5(5)
N(3)-C(9)-C(10)	104.7(5)
C(11)-C(10)-C(15)	120.9(6)
C(11)-C(10)-C(9)	130.6(7)
C(15)-C(10)-C(9)	108.3(5)
C(10)-C(11)-C(12A)	113.8(8)
C(10)-C(11)-C(12)	113.8(8)
C(10)-C(11)-H(11)	123.1
C(12)-C(11)-H(11)	123.1
C(13)-C(12)-C(11)	124.3(8)
C(13)-C(12)-Cl(4)	112.7(8)
C(11)-C(12)-Cl(4)	122.9(10)
C(14)-C(13)-C(12)	119.6(8)
C(14)-C(13)-Cl(5)	146.6(10)
C(12)-C(13)-Cl(5)	93.5(9)
C(13A)-C(12A)-C(11)	124.3(8)
C(13A)-C(12A)-H(12A)	117.9
C(11)-C(12A)-H(12A)	117.9
C(14)-C(13A)-C(12A)	119.6(8)
C(14)-C(13A)-H(13A)	120.2
C(12A)-C(13A)-H(13A)	120.2
C(13A)-C(14)-C(15)	119.9(10)
C(13)-C(14)-C(15)	119.9(10)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(10)	121.5(7)
C(14)-C(15)-C(16)	131.6(8)
C(10)-C(15)-C(16)	106.7(5)

N(4)-C(16)-N(3)	123.2(5)
N(4)-C(16)-C(15)	129.3(5)
N(3)-C(16)-C(15)	105.8(5)
N(4)-C(17)-N(5)	122.1(5)
N(4)-C(17)-C(18)	130.0(5)
N(5)-C(17)-C(18)	106.2(6)
C(23)-C(18)-C(19)	120.1(6)
C(23)-C(18)-C(17)	107.5(5)
C(19)-C(18)-C(17)	132.1(7)
C(20)-C(19)-C(18)	117.8(8)
C(20)-C(19)-H(19A)	121.1
C(18)-C(19)-H(19A)	121.1
C(19)-C(20)-C(21A)	120.5(6)
C(19)-C(20)-C(21)	120.5(6)
C(19)-C(20)-H(20A)	119.7
C(21)-C(20)-H(20A)	119.7
C(22)-C(21)-C(20)	123.3(8)
C(22)-C(21)-Cl(6)	119.3(8)
C(20)-C(21)-Cl(6)	117.4(6)
C(22)-C(21A)-C(20)	123.3(8)
C(22)-C(21A)-H(21A)	118.3
C(20)-C(21A)-H(21A)	118.3
C(21A)-C(22)-C(23)	116.3(8)
C(21)-C(22)-C(23)	116.3(8)
C(21)-C(22)-H(22A)	121.9
C(23)-C(22)-H(22A)	121.9
C(18)-C(23)-C(22)	121.9(6)
C(18)-C(23)-C(24)	107.5(5)
C(22)-C(23)-C(24)	130.3(6)
N(6)-C(24)-N(5)	123.1(5)
N(6)-C(24)-C(23)	129.6(5)
N(5)-C(24)-C(23)	105.3(5)
N(3)-B(1)-N(5)	106.4(4)
N(3)-B(1)-N(1)	105.7(4)
N(5)-B(1)-N(1)	106.3(4)
N(3)-B(1)-Cl(1)	112.6(4)

N(5)-B(1)-Cl(1)	112.8(3)
N(1)-B(1)-Cl(1)	112.5(4)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-βCl$_3$BsubPc**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	86(1)	33(1)	65(1)	-3(1)	13(1)	2(1)
Cl(2)	99(5)	72(4)	110(5)	-13(3)	-36(4)	16(3)
Cl(3)	98(2)	74(2)	75(2)	9(1)	-3(1)	30(1)
Cl(4)	70(2)	60(2)	101(2)	-11(1)	37(1)	-26(1)
Cl(5)	85(3)	99(4)	179(6)	30(3)	-21(3)	-30(3)
Cl(6)	242(4)	118(2)	89(2)	20(1)	101(2)	57(2)
N(1)	55(2)	35(2)	50(2)	-2(2)	12(2)	-3(2)
N(2)	59(3)	40(2)	69(3)	-2(2)	22(2)	-1(2)
N(3)	56(2)	40(2)	64(3)	-2(2)	7(2)	2(2)
N(4)	88(4)	50(3)	64(3)	-4(2)	-6(3)	13(2)
N(5)	80(3)	34(2)	54(2)	1(2)	11(2)	-2(2)
N(6)	66(3)	49(2)	56(2)	-6(2)	21(2)	-7(2)
C(1)	54(3)	41(2)	58(3)	-6(2)	14(2)	-3(2)
C(2)	61(3)	49(3)	52(3)	-7(2)	8(2)	0(2)
C(3)	59(3)	71(4)	67(3)	-13(3)	7(3)	8(3)
C(4)	86(4)	74(4)	62(3)	-8(3)	2(3)	23(3)
C(5)	90(4)	51(3)	57(3)	-5(2)	-6(3)	17(3)
C(4A)	86(4)	74(4)	62(3)	-8(3)	2(3)	23(3)
C(5A)	90(4)	51(3)	57(3)	-5(2)	-6(3)	17(3)
C(6)	81(4)	45(3)	54(3)	-5(2)	12(3)	0(3)
C(7)	62(3)	41(2)	51(3)	-5(2)	11(2)	3(2)
C(8)	61(3)	37(2)	54(3)	-2(2)	20(2)	3(2)
C(9)	60(3)	37(2)	78(4)	-9(2)	18(3)	0(2)
C(10)	54(3)	42(3)	122(5)	-18(3)	25(3)	0(2)
C(11)	55(3)	48(3)	168(7)	-20(4)	37(4)	0(3)
C(12)	51(4)	57(4)	246(12)	-54(6)	43(6)	-15(3)
C(13)	73(5)	79(5)	198(11)	-55(7)	-8(6)	9(4)
C(12A)	51(4)	57(4)	246(12)	-54(6)	43(6)	-15(3)
C(13A)	73(5)	79(5)	198(11)	-55(7)	-8(6)	9(4)
C(14)	60(4)	76(4)	152(7)	-47(5)	-9(4)	2(4)
C(15)	57(3)	61(3)	106(5)	-24(3)	-9(3)	9(3)

C(16)	62(3)	45(3)	78(4)	-11(3)	-6(3)	7(2)
C(17)	95(5)	36(2)	55(3)	2(2)	1(3)	7(3)
C(18)	127(6)	36(3)	50(3)	4(2)	24(3)	3(3)
C(19)	154(7)	39(3)	58(3)	0(2)	12(4)	4(3)
C(20)	198(9)	44(3)	55(4)	0(3)	46(5)	8(4)
C(21)	179(9)	56(4)	65(4)	5(3)	54(5)	10(4)
C(21A)	179(9)	56(4)	65(4)	5(3)	54(5)	10(4)
C(22)	129(6)	49(3)	68(4)	3(3)	43(4)	3(3)
C(23)	108(5)	38(3)	55(3)	0(2)	29(3)	-1(3)
C(24)	79(4)	38(2)	63(3)	2(2)	24(3)	-7(2)
B(1)	59(3)	35(3)	56(3)	0(2)	8(3)	0(2)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **Cl-βCl$_3$BsubPc**.

	x	y	z	U(eq)
H(3A)	9251	5340	3691	80
H(4A)	9553	3830	4596	92
H(5A)	8053	3439	5221	83
H(6A)	6122	4408	4907	73
H(11)	1636	4389	3479	106
H(12A)	-100	3647	2637	140
H(13A)	-484	4259	1466	147
H(14)	825	5618	1082	121
H(19A)	4281	6677	-90	102
H(20A)	5942	6321	-626	115
H(21A)	7934	6398	22	115
H(22A)	8392	6771	1225	94

Table S13. Torsion angles [°] for **Cl-βCl$_3$BsubPc**.

C(24)-N(6)-C(1)-N(1)	-9.9(7)
C(24)-N(6)-C(1)-C(2)	152.7(5)
C(8)-N(1)-C(1)-N(6)	155.7(4)
B(1)-N(1)-C(1)-N(6)	-7.6(7)
C(8)-N(1)-C(1)-C(2)	-10.5(5)
B(1)-N(1)-C(1)-C(2)	-173.7(4)
N(6)-C(1)-C(2)-C(3)	12.4(9)
N(1)-C(1)-C(2)-C(3)	177.3(5)
N(6)-C(1)-C(2)-C(7)	-160.5(5)
N(1)-C(1)-C(2)-C(7)	4.4(5)
C(7)-C(2)-C(3)-C(4A)	-0.2(8)
C(1)-C(2)-C(3)-C(4A)	-172.4(5)
C(7)-C(2)-C(3)-C(4)	-0.2(8)
C(1)-C(2)-C(3)-C(4)	-172.4(5)
C(2)-C(3)-C(4)-C(5)	-2.5(9)
C(2)-C(3)-C(4)-Cl(2)	164.9(5)
C(3)-C(4)-C(5)-C(6)	2.9(9)
Cl(2)-C(4)-C(5)-C(6)	-166.3(5)
C(3)-C(4)-C(5)-Cl(3)	-176.6(5)
Cl(2)-C(4)-C(5)-Cl(3)	14.3(7)
C(2)-C(3)-C(4A)-C(5A)	-2.5(9)
C(3)-C(4A)-C(5A)-C(6)	2.9(9)
C(4A)-C(5A)-C(6)-C(7)	-0.4(8)
C(4)-C(5)-C(6)-C(7)	-0.4(8)
Cl(3)-C(5)-C(6)-C(7)	179.0(4)
C(5A)-C(6)-C(7)-C(2)	-2.3(7)
C(5)-C(6)-C(7)-C(2)	-2.3(7)
C(5A)-C(6)-C(7)-C(8)	169.5(5)
C(5)-C(6)-C(7)-C(8)	169.5(5)
C(3)-C(2)-C(7)-C(6)	2.6(7)
C(1)-C(2)-C(7)-C(6)	176.4(4)
C(3)-C(2)-C(7)-C(8)	-171.1(4)
C(1)-C(2)-C(7)-C(8)	2.7(5)
C(9)-N(2)-C(8)-N(1)	9.2(6)

C(9)-N(2)-C(8)-C(7)	-152.2(5)
C(1)-N(1)-C(8)-N(2)	-153.1(4)
B(1)-N(1)-C(8)-N(2)	10.1(7)
C(1)-N(1)-C(8)-C(7)	12.2(5)
B(1)-N(1)-C(8)-C(7)	175.4(4)
C(6)-C(7)-C(8)-N(2)	-17.7(9)
C(2)-C(7)-C(8)-N(2)	154.9(5)
C(6)-C(7)-C(8)-N(1)	178.6(5)
C(2)-C(7)-C(8)-N(1)	-8.8(5)
C(8)-N(2)-C(9)-N(3)	-8.8(7)
C(8)-N(2)-C(9)-C(10)	152.9(5)
C(16)-N(3)-C(9)-N(2)	154.5(5)
B(1)-N(3)-C(9)-N(2)	-11.2(7)
C(16)-N(3)-C(9)-C(10)	-11.3(6)
B(1)-N(3)-C(9)-C(10)	-177.1(4)
N(2)-C(9)-C(10)-C(11)	17.4(10)
N(3)-C(9)-C(10)-C(11)	-178.7(5)
N(2)-C(9)-C(10)-C(15)	-157.5(5)
N(3)-C(9)-C(10)-C(15)	6.4(6)
C(15)-C(10)-C(11)-C(12A)	-0.6(8)
C(9)-C(10)-C(11)-C(12A)	-174.9(6)
C(15)-C(10)-C(11)-C(12)	-0.6(8)
C(9)-C(10)-C(11)-C(12)	-174.9(6)
C(10)-C(11)-C(12)-C(13)	0.2(10)
C(10)-C(11)-C(12)-Cl(4)	176.8(5)
Cl(5)-Cl(4)-C(12)-C(13)	-6.6(6)
Cl(5)-Cl(4)-C(12)-C(11)	176.5(7)
C(11)-C(12)-C(13)-C(14)	0.1(13)
Cl(4)-C(12)-C(13)-C(14)	-176.8(6)
C(11)-C(12)-C(13)-Cl(5)	-175.3(6)
Cl(4)-C(12)-C(13)-Cl(5)	7.8(7)
Cl(4)-Cl(5)-C(13)-C(14)	-178.2(13)
Cl(4)-Cl(5)-C(13)-C(12)	-5.5(5)
C(10)-C(11)-C(12A)-C(13A)	0.2(10)
C(11)-C(12A)-C(13A)-C(14)	0.1(13)
C(12A)-C(13A)-C(14)-C(15)	-0.1(12)

C(12)-C(13)-C(14)-C(15)	-0.1(12)
Cl(5)-C(13)-C(14)-C(15)	171.5(10)
C(13A)-C(14)-C(15)-C(10)	-0.3(10)
C(13)-C(14)-C(15)-C(10)	-0.3(10)
C(13A)-C(14)-C(15)-C(16)	174.5(7)
C(13)-C(14)-C(15)-C(16)	174.5(7)
C(11)-C(10)-C(15)-C(14)	0.7(9)
C(9)-C(10)-C(15)-C(14)	176.1(5)
C(11)-C(10)-C(15)-C(16)	-175.2(5)
C(9)-C(10)-C(15)-C(16)	0.2(6)
C(17)-N(4)-C(16)-N(3)	8.4(7)
C(17)-N(4)-C(16)-C(15)	-154.3(5)
C(9)-N(3)-C(16)-N(4)	-154.6(5)
B(1)-N(3)-C(16)-N(4)	11.5(7)
C(9)-N(3)-C(16)-C(15)	11.6(6)
B(1)-N(3)-C(16)-C(15)	177.6(4)
C(14)-C(15)-C(16)-N(4)	-17.1(10)
C(10)-C(15)-C(16)-N(4)	158.3(5)
C(14)-C(15)-C(16)-N(3)	177.9(6)
C(10)-C(15)-C(16)-N(3)	-6.8(6)
C(16)-N(4)-C(17)-N(5)	-9.9(7)
C(16)-N(4)-C(17)-C(18)	153.4(5)
C(24)-N(5)-C(17)-N(4)	154.7(5)
B(1)-N(5)-C(17)-N(4)	-8.5(7)
C(24)-N(5)-C(17)-C(18)	-12.0(5)
B(1)-N(5)-C(17)-C(18)	-175.2(4)
N(4)-C(17)-C(18)-C(23)	-159.1(5)
N(5)-C(17)-C(18)-C(23)	6.2(5)
N(4)-C(17)-C(18)-C(19)	14.5(9)
N(5)-C(17)-C(18)-C(19)	179.8(5)
C(23)-C(18)-C(19)-C(20)	-1.4(8)
C(17)-C(18)-C(19)-C(20)	-174.3(5)
C(18)-C(19)-C(20)-C(21A)	0.7(9)
C(18)-C(19)-C(20)-C(21)	0.7(9)
C(19)-C(20)-C(21)-C(22)	0.9(10)
C(19)-C(20)-C(21)-Cl(6)	-177.6(5)

C(19)-C(20)-C(21A)-C(22)	0.9(10)
C(20)-C(21A)-C(22)-C(23)	-1.7(9)
C(20)-C(21)-C(22)-C(23)	-1.7(9)
Cl(6)-C(21)-C(22)-C(23)	176.8(4)
C(19)-C(18)-C(23)-C(22)	0.5(8)
C(17)-C(18)-C(23)-C(22)	175.0(5)
C(19)-C(18)-C(23)-C(24)	-173.2(5)
C(17)-C(18)-C(23)-C(24)	1.3(5)
C(21A)-C(22)-C(23)-C(18)	1.0(8)
C(21)-C(22)-C(23)-C(18)	1.0(8)
C(21A)-C(22)-C(23)-C(24)	173.2(5)
C(21)-C(22)-C(23)-C(24)	173.2(5)
C(1)-N(6)-C(24)-N(5)	8.3(7)
C(1)-N(6)-C(24)-C(23)	-152.9(5)
C(17)-N(5)-C(24)-N(6)	-152.4(5)
B(1)-N(5)-C(24)-N(6)	10.9(7)
C(17)-N(5)-C(24)-C(23)	12.7(5)
B(1)-N(5)-C(24)-C(23)	176.0(4)
C(18)-C(23)-C(24)-N(6)	155.6(5)
C(22)-C(23)-C(24)-N(6)	-17.5(9)
C(18)-C(23)-C(24)-N(5)	-8.2(5)
C(22)-C(23)-C(24)-N(5)	178.7(5)
C(9)-N(3)-B(1)-N(5)	138.9(4)
C(16)-N(3)-B(1)-N(5)	-25.7(6)
C(9)-N(3)-B(1)-N(1)	26.2(6)
C(16)-N(3)-B(1)-N(1)	-138.4(4)
C(9)-N(3)-B(1)-Cl(1)	-97.0(5)
C(16)-N(3)-B(1)-Cl(1)	98.4(5)
C(17)-N(5)-B(1)-N(3)	24.6(6)
C(24)-N(5)-B(1)-N(3)	-136.8(4)
C(17)-N(5)-B(1)-N(1)	136.9(4)
C(24)-N(5)-B(1)-N(1)	-24.6(6)
C(17)-N(5)-B(1)-Cl(1)	-99.4(5)
C(24)-N(5)-B(1)-Cl(1)	99.2(5)
C(1)-N(1)-B(1)-N(3)	135.8(4)
C(8)-N(1)-B(1)-N(3)	-25.6(6)

C(1)-N(1)-B(1)-N(5)	23.0(6)
C(8)-N(1)-B(1)-N(5)	-138.4(4)
C(1)-N(1)-B(1)-Cl(1)	-100.9(5)
C(8)-N(1)-B(1)-Cl(1)	97.7(5)

Symmetry transformations used to generate equivalent atoms:

Table S14. Crystal data and structure refinement for **Cl-αF$_3$BsubPc**.

Identification code	**Cl-αF$_3$BsubPc**	
CCDC deposition number	2051782	
Empirical formula	C24 H9 B Cl F3 N6	
Formula weight	484.63	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 12.3458(6) Å	α= 90°.
	b = 15.1437(7) Å	β= 90°.
	c = 10.3431(5) Å	γ = 90°.
Volume	1933.76(16) Å^3	
Z	4	
Density (calculated)	1.665 Mg/m^3	
Absorption coefficient	2.271 mm^{-1}	
F(000)	976	
Crystal size	0.140 x 0.130 x 0.120 mm^3	
Theta range for data collection	5.178 to 67.263°.	
Index ranges	-14<=h<=14, -17<=k<=18, -12<=l<=12	
Reflections collected	26520	
Independent reflections	1795 [R(int) = 0.0552]	
Completeness to theta = 67.263°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6666	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1795 / 0 / 179	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0836	
R indices (all data)	R1 = 0.0397, wR2 = 0.0871	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.194 and -0.235 e.Å^{-3}	

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-αF$_3$BsubPc**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8243(1)	7500	7408(1)	34(1)
C(3)	10417(2)	5440(1)	3174(2)	37(1)
F(1)	11324(1)	5840(1)	3009(1)	39(1)
C(3A)	10417(2)	5440(1)	3174(2)	37(1)
C(6)	8493(2)	4521(1)	3598(2)	39(1)
C(6A)	8493(2)	4521(1)	3598(2)	39(1)
F(2)	7745(3)	4101(3)	3810(4)	42(1)
C(11)	4255(2)	6571(2)	4398(2)	54(1)
C(11A)	4255(2)	6571(2)	4398(2)	54(1)
F(3)	4166(2)	5823(2)	4397(2)	42(1)
N(1)	9980(2)	7500	4107(2)	29(1)
N(2)	8463(1)	6725(1)	4955(1)	28(1)
N(3)	6781(1)	5968(1)	4784(1)	33(1)
N(4)	6840(2)	7500	5286(2)	29(1)
C(1)	9447(1)	6743(1)	4347(2)	28(1)
C(2)	9589(2)	5857(1)	3832(2)	30(1)
C(4)	10311(2)	4585(1)	2748(2)	42(1)
C(5)	9349(2)	4127(1)	2966(2)	42(1)
C(7)	8607(2)	5382(1)	4041(2)	31(1)
C(8)	7865(2)	5984(1)	4688(2)	30(1)
C(9)	6288(2)	6739(1)	4999(2)	33(1)
C(10)	5187(2)	7030(2)	4713(2)	38(1)
C(12)	3332(2)	7042(2)	4090(2)	65(1)
B(1)	8004(2)	7500	5618(3)	28(1)

Table S16. Bond lengths [Å] and angles [°] for **Cl-αF$_3$BsubPc**.

Cl(1)-B(1)	1.875(3)
C(3)-F(1)	1.285(2)
C(3)-C(4)	1.375(3)
C(3)-C(2)	1.380(3)
C(3A)-C(4)	1.375(3)
C(3A)-C(2)	1.380(3)
C(3A)-H(3A)	0.9500
C(6)-C(5)	1.379(3)
C(6)-C(7)	1.389(3)
C(6)-H(6)	0.9500
C(6A)-F(2)	1.142(5)
C(6A)-C(5)	1.379(3)
C(6A)-C(7)	1.389(3)
C(11)-F(3)	1.138(3)
C(11)-C(12)	1.381(4)
C(11)-C(10)	1.384(3)
C(11A)-C(12)	1.381(4)
C(11A)-C(10)	1.384(3)
C(11A)-H(11A)	0.9500
N(1)-C(1)	1.345(2)
N(1)-C(1)#1	1.345(2)
N(2)-C(1)	1.368(2)
N(2)-C(8)	1.371(2)
N(2)-B(1)	1.472(2)
N(3)-C(9)	1.336(2)
N(3)-C(8)	1.342(2)
N(4)-C(9)#1	1.371(2)
N(4)-C(9)	1.371(2)
N(4)-B(1)	1.478(3)
C(1)-C(2)	1.454(3)
C(2)-C(7)	1.426(3)
C(4)-C(5)	1.393(3)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500

C(7)-C(8)	1.455(3)
C(9)-C(10)	1.459(3)
C(10)-C(10)#1	1.423(4)
C(12)-C(12)#1	1.388(6)
C(12)-H(12)	0.9500

F(1)-C(3)-C(4)	118.96(18)
F(1)-C(3)-C(2)	119.74(18)
C(4)-C(3)-C(2)	121.2(2)
C(4)-C(3A)-C(2)	121.2(2)
C(4)-C(3A)-H(3A)	119.4
C(2)-C(3A)-H(3A)	119.4
C(5)-C(6)-C(7)	119.0(2)
C(5)-C(6)-H(6)	120.5
C(7)-C(6)-H(6)	120.5
F(2)-C(6A)-C(5)	118.0(3)
F(2)-C(6A)-C(7)	122.8(3)
C(5)-C(6A)-C(7)	119.0(2)
F(3)-C(11)-C(12)	115.7(2)
F(3)-C(11)-C(10)	125.5(3)
C(12)-C(11)-C(10)	118.8(3)
C(12)-C(11A)-C(10)	118.8(3)
C(12)-C(11A)-H(11A)	120.6
C(10)-C(11A)-H(11A)	120.6
C(1)-N(1)-C(1)#1	117.0(2)
C(1)-N(2)-C(8)	113.64(15)
C(1)-N(2)-B(1)	122.72(16)
C(8)-N(2)-B(1)	122.60(16)
C(9)-N(3)-C(8)	116.81(16)
C(9)#1-N(4)-C(9)	114.4(2)
C(9)#1-N(4)-B(1)	122.23(11)
C(9)-N(4)-B(1)	122.24(11)
N(1)-C(1)-N(2)	122.39(16)
N(1)-C(1)-C(2)	131.29(16)
N(2)-C(1)-C(2)	104.92(15)
C(3A)-C(2)-C(7)	118.29(17)

C(3)-C(2)-C(7)	118.29(17)
C(3A)-C(2)-C(1)	133.74(18)
C(3)-C(2)-C(1)	133.74(18)
C(7)-C(2)-C(1)	107.88(15)
C(3A)-C(4)-C(5)	119.84(19)
C(3)-C(4)-C(5)	119.84(19)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(6A)-C(5)-C(4)	121.02(19)
C(6)-C(5)-C(4)	121.02(19)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(6A)-C(7)-C(2)	120.62(18)
C(6)-C(7)-C(2)	120.62(18)
C(6A)-C(7)-C(8)	132.54(18)
C(6)-C(7)-C(8)	132.54(18)
C(2)-C(7)-C(8)	106.78(15)
N(3)-C(8)-N(2)	122.46(17)
N(3)-C(8)-C(7)	130.51(17)
N(2)-C(8)-C(7)	105.50(15)
N(3)-C(9)-N(4)	122.97(16)
N(3)-C(9)-C(10)	130.93(17)
N(4)-C(9)-C(10)	104.63(17)
C(11)-C(10)-C(10)#1	120.15(16)
C(11A)-C(10)-C(9)	132.1(2)
C(11)-C(10)-C(9)	132.1(2)
C(10)#1-C(10)-C(9)	107.59(11)
C(11A)-C(12)-C(12)#1	121.05(17)
C(11)-C(12)-C(12)#1	121.05(17)
C(11)-C(12)-H(12)	119.5
C(12)#1-C(12)-H(12)	119.5
N(2)#1-B(1)-N(2)	105.6(2)
N(2)#1-B(1)-N(4)	105.45(15)
N(2)-B(1)-N(4)	105.45(15)
N(2)#1-B(1)-Cl(1)	113.53(13)
N(2)-B(1)-Cl(1)	113.53(13)

N(4)-B(1)-Cl(1)	112.51(18)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-αF$_3$BsubPc**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	46(1)	36(1)	21(1)	0	-2(1)	0
C(3)	36(1)	49(1)	25(1)	-3(1)	-6(1)	10(1)
F(1)	31(1)	52(1)	36(1)	-4(1)	4(1)	-1(1)
C(3A)	36(1)	49(1)	25(1)	-3(1)	-6(1)	10(1)
C(6)	55(1)	37(1)	26(1)	-2(1)	-9(1)	2(1)
C(6A)	55(1)	37(1)	26(1)	-2(1)	-9(1)	2(1)
F(2)	41(2)	36(2)	48(3)	-7(2)	3(2)	-14(2)
C(11)	35(1)	99(2)	28(1)	-6(1)	7(1)	-18(1)
C(11A)	35(1)	99(2)	28(1)	-6(1)	7(1)	-18(1)
F(3)	39(1)	44(1)	44(1)	-5(1)	6(1)	-14(1)
N(1)	28(1)	36(1)	23(1)	0	-4(1)	0
N(2)	30(1)	32(1)	21(1)	-1(1)	0(1)	0(1)
N(3)	35(1)	41(1)	24(1)	-1(1)	3(1)	-6(1)
N(4)	28(1)	38(1)	22(1)	0	2(1)	0
C(1)	28(1)	36(1)	20(1)	-1(1)	-4(1)	1(1)
C(2)	35(1)	36(1)	20(1)	-2(1)	-6(1)	4(1)
C(4)	51(1)	50(1)	25(1)	-8(1)	-8(1)	20(1)
C(5)	61(1)	39(1)	27(1)	-8(1)	-13(1)	11(1)
C(7)	38(1)	35(1)	21(1)	0(1)	-5(1)	2(1)
C(8)	35(1)	34(1)	20(1)	0(1)	-1(1)	-3(1)
C(9)	33(1)	44(1)	21(1)	-1(1)	4(1)	-6(1)
C(10)	29(1)	64(1)	21(1)	-2(1)	6(1)	-3(1)
C(12)	28(1)	134(2)	34(1)	-4(1)	2(1)	-15(1)
B(1)	32(1)	34(2)	20(1)	0	-1(1)	0

Table S18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **Cl-αF$_3$BsubPc**

	x	y	z	U(eq)
H(3A)	11072	5750	3014	44
H(6)	7834	4209	3728	47
H(11A)	4250	5944	4393	64
H(4)	10892	4306	2305	50
H(5)	9282	3535	2675	51
H(12)	2686	6733	3876	78

Table S19. Torsion angles [°] for **Cl-αF$_3$BsubPc**.

C(1)#1-N(1)-C(1)-N(2)	-7.9(3)
C(1)#1-N(1)-C(1)-C(2)	156.45(13)
C(8)-N(2)-C(1)-N(1)	156.38(17)
B(1)-N(2)-C(1)-N(1)	-12.2(3)
C(8)-N(2)-C(1)-C(2)	-11.50(18)
B(1)-N(2)-C(1)-C(2)	179.89(17)
C(4)-C(3A)-C(2)-C(7)	-1.1(3)
C(4)-C(3A)-C(2)-C(1)	-177.29(18)
F(1)-C(3)-C(2)-C(7)	-177.63(16)
C(4)-C(3)-C(2)-C(7)	-1.1(3)
F(1)-C(3)-C(2)-C(1)	6.2(3)
C(4)-C(3)-C(2)-C(1)	-177.29(18)
N(1)-C(1)-C(2)-C(3A)	16.8(3)
N(2)-C(1)-C(2)-C(3A)	-176.89(18)
N(1)-C(1)-C(2)-C(3)	16.8(3)
N(2)-C(1)-C(2)-C(3)	-176.89(18)
N(1)-C(1)-C(2)-C(7)	-159.75(19)
N(2)-C(1)-C(2)-C(7)	6.60(17)
C(2)-C(3A)-C(4)-C(5)	0.7(3)
F(1)-C(3)-C(4)-C(5)	177.27(17)
C(2)-C(3)-C(4)-C(5)	0.7(3)
F(2)-C(6A)-C(5)-C(4)	-176.0(3)
C(7)-C(6A)-C(5)-C(4)	-1.2(3)
C(7)-C(6)-C(5)-C(4)	-1.2(3)
C(3A)-C(4)-C(5)-C(6A)	0.5(3)
C(3)-C(4)-C(5)-C(6)	0.5(3)
F(2)-C(6A)-C(7)-C(2)	175.3(3)
C(5)-C(6A)-C(7)-C(2)	0.8(3)
F(2)-C(6A)-C(7)-C(8)	-8.0(4)
C(5)-C(6A)-C(7)-C(8)	177.55(18)
C(5)-C(6)-C(7)-C(2)	0.8(3)
C(5)-C(6)-C(7)-C(8)	177.55(18)
C(3A)-C(2)-C(7)-C(6A)	0.3(2)
C(1)-C(2)-C(7)-C(6A)	177.44(15)

C(3)-C(2)-C(7)-C(6)	0.3(2)
C(1)-C(2)-C(7)-C(6)	177.44(15)
C(3A)-C(2)-C(7)-C(8)	-177.17(15)
C(3)-C(2)-C(7)-C(8)	-177.17(15)
C(1)-C(2)-C(7)-C(8)	-0.04(18)
C(9)-N(3)-C(8)-N(2)	8.0(2)
C(9)-N(3)-C(8)-C(7)	-155.73(18)
C(1)-N(2)-C(8)-N(3)	-155.70(16)
B(1)-N(2)-C(8)-N(3)	12.9(3)
C(1)-N(2)-C(8)-C(7)	11.55(19)
B(1)-N(2)-C(8)-C(7)	-179.82(16)
C(6A)-C(7)-C(8)-N(3)	-17.8(3)
C(6)-C(7)-C(8)-N(3)	-17.8(3)
C(2)-C(7)-C(8)-N(3)	159.27(18)
C(6A)-C(7)-C(8)-N(2)	176.39(18)
C(6)-C(7)-C(8)-N(2)	176.39(18)
C(2)-C(7)-C(8)-N(2)	-6.55(18)
C(8)-N(3)-C(9)-N(4)	-8.6(3)
C(8)-N(3)-C(9)-C(10)	155.30(18)
C(9)#1-N(4)-C(9)-N(3)	156.44(12)
B(1)-N(4)-C(9)-N(3)	-11.6(3)
C(9)#1-N(4)-C(9)-C(10)	-11.1(3)
B(1)-N(4)-C(9)-C(10)	-179.10(19)
C(12)-C(11A)-C(10)-C(10)#1	-0.2(2)
C(12)-C(11A)-C(10)-C(9)	-175.70(18)
F(3)-C(11)-C(10)-C(10)#1	-178.2(2)
C(12)-C(11)-C(10)-C(10)#1	-0.2(2)
F(3)-C(11)-C(10)-C(9)	6.3(4)
C(12)-C(11)-C(10)-C(9)	-175.70(18)
N(3)-C(9)-C(10)-C(11A)	16.1(3)
N(4)-C(9)-C(10)-C(11A)	-177.83(19)
N(3)-C(9)-C(10)-C(11)	16.1(3)
N(4)-C(9)-C(10)-C(11)	-177.83(19)
N(3)-C(9)-C(10)-C(10)#1	-159.85(16)
N(4)-C(9)-C(10)-C(10)#1	6.27(14)
C(10)-C(11A)-C(12)-C(12)#1	0.2(2)

F(3)-C(11)-C(12)-C(12)#1	178.42(17)
C(10)-C(11)-C(12)-C(12)#1	0.2(2)
C(1)-N(2)-B(1)-N(2)#1	27.7(3)
C(8)-N(2)-B(1)-N(2)#1	-139.86(15)
C(1)-N(2)-B(1)-N(4)	139.11(16)
C(8)-N(2)-B(1)-N(4)	-28.5(2)
C(1)-N(2)-B(1)-Cl(1)	-97.29(18)
C(8)-N(2)-B(1)-Cl(1)	95.1(2)
C(9)#1-N(4)-B(1)-N(2)#1	-27.8(3)
C(9)-N(4)-B(1)-N(2)#1	139.29(17)
C(9)#1-N(4)-B(1)-N(2)	-139.29(17)
C(9)-N(4)-B(1)-N(2)	27.8(3)
C(9)#1-N(4)-B(1)-Cl(1)	96.46(18)
C(9)-N(4)-B(1)-Cl(1)	-96.46(18)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Table S20. Crystal data and structure refinement for **Cl-βF$_3$BsubPc**.

Identification code	d1802_a	
CCDC deposition number	2051783	
Empirical formula	C24 H9 B Cl F3 N6	
Formula weight	484.63	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 12.6548(9) Å	α= 90°.
	b = 15.1757(11) Å	β= 90°.
	c = 10.1016(7) Å	γ = 90°.
Volume	1940.0(2) Å^3	
Z	4	
Density (calculated)	1.659 Mg/m^3	
Absorption coefficient	2.263 mm^{-1}	
F(000)	976	
Crystal size	0.180 x 0.170 x 0.160 mm^3	
Theta range for data collection	5.260 to 67.100°.	
Index ranges	-14<=h<=15, -14<=k<=17, -12<=l<=11	
Reflections collected	9460	
Independent reflections	1776 [R(int) = 0.0425]	
Completeness to theta = 67.100°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6229	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1776 / 0 / 179	
Goodness-of-fit on F^2	1.173	
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1198	
R indices (all data)	R1 = 0.0577, wR2 = 0.1223	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.453 and -0.478 e.Å^{-3}	

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-βF$_3$BsubPc**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	7991(1)	7500	7468(1)	41(1)
F(1)	10856(2)	4223(2)	2244(3)	45(1)
C(4)	10118(3)	4619(2)	2855(3)	36(1)
C(4A)	10118(3)	4619(2)	2855(3)	36(1)
F(2)	9303(3)	3269(3)	2755(4)	36(1)
C(5)	9195(3)	4143(2)	3060(3)	35(1)
C(5A)	9195(3)	4143(2)	3060(3)	35(1)
C(12)	3261(2)	7039(3)	3921(3)	42(1)
C(12A)	3261(2)	7039(3)	3921(3)	42(1)
F(3)	2380(3)	6654(3)	3520(4)	58(1)
N(1)	9738(3)	7500	4177(3)	28(1)
N(2)	8233(2)	6727(2)	4985(2)	28(1)
N(3)	6598(2)	5972(2)	4741(2)	32(1)
N(4)	6643(3)	7500	5261(3)	29(1)
C(1)	9208(2)	6748(2)	4406(3)	27(1)
C(2)	9373(2)	5863(2)	3891(3)	28(1)
C(3)	10229(2)	5480(2)	3252(3)	30(1)
C(6)	8320(2)	4520(2)	3639(3)	33(1)
C(7)	8412(2)	5388(2)	4070(3)	29(1)
C(8)	7664(2)	5985(2)	4687(3)	30(1)
C(9)	6106(2)	6746(2)	4944(3)	30(1)
C(10)	5041(2)	7031(2)	4622(3)	33(1)
C(11)	4135(2)	6557(3)	4268(3)	36(1)
B(1)	7767(4)	7500	5647(5)	28(1)

Table S22. Bond lengths [Å] and angles [°] for **Cl-βF$_3$BsubPc**.

Cl(1)-B(1)	1.862(5)
F(1)-C(4)	1.270(4)
C(4)-C(3)	1.373(4)
C(4)-C(5)	1.389(5)
C(4A)-C(3)	1.373(4)
C(4A)-C(5A)	1.389(5)
C(4A)-H(4A)	0.9500
F(2)-C(5)	1.369(5)
C(5)-C(6)	1.377(4)
C(5A)-C(6)	1.377(4)
C(5A)-H(5A)	0.9500
C(12)-C(11)	1.373(5)
C(12)-C(12)#1	1.398(8)
C(12)-H(12)	0.9500
C(12A)-F(3)	1.323(5)
C(12A)-C(11)	1.373(5)
N(1)-C(1)#1	1.343(3)
N(1)-C(1)	1.343(3)
N(2)-C(1)	1.366(4)
N(2)-C(8)	1.371(4)
N(2)-B(1)	1.474(4)
N(3)-C(9)	1.344(4)
N(3)-C(8)	1.350(4)
N(4)-C(9)#1	1.369(3)
N(4)-C(9)	1.369(3)
N(4)-B(1)	1.475(6)
C(1)-C(2)	1.456(4)
C(2)-C(3)	1.389(4)
C(2)-C(7)	1.424(4)
C(3)-H(3A)	0.9500
C(6)-C(7)	1.393(4)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.450(4)
C(9)-C(10)	1.453(4)

C(10)-C(11)	1.399(4)
C(10)-C(10)#1	1.424(7)
C(11)-H(11)	0.9500

F(1)-C(4)-C(3)	121.2(3)
F(1)-C(4)-C(5)	116.4(3)
C(3)-C(4)-C(5)	122.5(3)
C(3)-C(4A)-C(5A)	122.5(3)
C(3)-C(4A)-H(4A)	118.8
C(5A)-C(4A)-H(4A)	118.8
F(2)-C(5)-C(6)	125.4(3)
F(2)-C(5)-C(4)	112.7(3)
C(6)-C(5)-C(4)	121.6(3)
C(6)-C(5A)-C(4A)	121.6(3)
C(6)-C(5A)-H(5A)	119.2
C(4A)-C(5A)-H(5A)	119.2
C(11)-C(12)-C(12)#1	122.3(2)
C(11)-C(12)-H(12)	118.9
C(12)#1-C(12)-H(12)	118.9
F(3)-C(12A)-C(11)	121.4(4)
C(1)#1-N(1)-C(1)	116.2(3)
C(1)-N(2)-C(8)	113.6(2)
C(1)-N(2)-B(1)	122.5(3)
C(8)-N(2)-B(1)	122.9(3)
C(9)-N(3)-C(8)	117.2(3)
C(9)#1-N(4)-C(9)	113.5(3)
C(9)#1-N(4)-B(1)	122.70(18)
C(9)-N(4)-B(1)	122.70(18)
N(1)-C(1)-N(2)	123.1(3)
N(1)-C(1)-C(2)	130.6(3)
N(2)-C(1)-C(2)	105.1(2)
C(3)-C(2)-C(7)	120.9(3)
C(3)-C(2)-C(1)	131.6(3)
C(7)-C(2)-C(1)	107.4(3)
C(4A)-C(3)-C(2)	117.0(3)
C(4)-C(3)-C(2)	117.0(3)

C(4)-C(3)-H(3A)	121.5
C(2)-C(3)-H(3A)	121.5
C(5A)-C(6)-C(7)	117.3(3)
C(5)-C(6)-C(7)	117.3(3)
C(5)-C(6)-H(6A)	121.3
C(7)-C(6)-H(6A)	121.3
C(6)-C(7)-C(2)	120.7(3)
C(6)-C(7)-C(8)	132.1(3)
C(2)-C(7)-C(8)	107.2(3)
N(3)-C(8)-N(2)	121.8(3)
N(3)-C(8)-C(7)	131.4(3)
N(2)-C(8)-C(7)	105.3(2)
N(3)-C(9)-N(4)	122.4(3)
N(3)-C(9)-C(10)	130.9(3)
N(4)-C(9)-C(10)	105.3(3)
C(11)-C(10)-C(10)#1	120.9(2)
C(11)-C(10)-C(9)	131.6(3)
C(10)#1-C(10)-C(9)	107.33(18)
C(12A)-C(11)-C(10)	116.8(3)
C(12)-C(11)-C(10)	116.8(3)
C(12)-C(11)-H(11)	121.6
C(10)-C(11)-H(11)	121.6
N(2)-B(1)-N(2)#1	105.6(4)
N(2)-B(1)-N(4)	105.4(2)
N(2)#1-B(1)-N(4)	105.4(2)
N(2)-B(1)-Cl(1)	112.8(2)
N(2)#1-B(1)-Cl(1)	112.8(2)
N(4)-B(1)-Cl(1)	114.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Table S23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-βF$_3$BsubPc**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	44(1)	50(1)	27(1)	0	-4(1)	0
F(1)	34(2)	40(2)	60(2)	-6(2)	11(2)	9(2)
C(4)	46(2)	36(2)	26(2)	-1(1)	-1(1)	6(2)
C(4A)	46(2)	36(2)	26(2)	-1(1)	-1(1)	6(2)
F(2)	38(2)	28(2)	41(3)	-12(2)	-2(2)	-2(2)
C(5)	51(2)	26(2)	28(2)	-3(1)	-4(1)	4(2)
C(5A)	51(2)	26(2)	28(2)	-3(1)	-4(1)	4(2)
C(12)	25(2)	69(2)	32(2)	-3(2)	3(1)	-5(2)
C(12A)	25(2)	69(2)	32(2)	-3(2)	3(1)	-5(2)
F(3)	25(2)	79(3)	69(3)	-16(3)	-1(2)	-13(2)
N(1)	29(2)	29(2)	25(2)	0	-6(1)	0
N(2)	29(1)	29(1)	25(1)	-1(1)	-3(1)	-2(1)
N(3)	31(1)	39(2)	25(1)	-1(1)	0(1)	-5(1)
N(4)	29(2)	36(2)	21(2)	0	-2(1)	0
C(1)	26(1)	30(2)	24(1)	2(1)	-5(1)	-2(1)
C(2)	31(2)	31(2)	22(1)	2(1)	-7(1)	1(1)
C(3)	31(2)	32(2)	27(1)	4(1)	-4(1)	1(1)
C(6)	39(2)	34(2)	26(1)	-2(1)	-5(1)	-5(1)
C(7)	33(2)	32(2)	21(1)	1(1)	-4(1)	-2(1)
C(8)	35(2)	34(2)	21(1)	2(1)	-3(1)	-5(1)
C(9)	34(2)	35(2)	20(1)	-1(1)	1(1)	-4(1)
C(10)	30(2)	48(2)	20(1)	0(1)	3(1)	1(1)
C(11)	30(2)	53(2)	26(1)	-6(2)	6(1)	-4(2)
B(1)	31(2)	31(3)	22(2)	0	-4(2)	0

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **Cl-βF$_3$BsubPc**.

	x	y	z	U(eq)
H(4A)	10695	4339	2425	43
H(5A)	9166	3543	2794	42
H(12)	2634	6737	3672	51
H(3A)	10862	5799	3095	36
H(6A)	7679	4201	3740	40
H(11)	4126	5931	4267	44

Table S25. Torsion angles [°] for **Cl-βF$_3$BsubPc**.

F(1)-C(4)-C(5)-F(2)	10.2(5)
C(3)-C(4)-C(5)-F(2)	-171.6(3)
F(1)-C(4)-C(5)-C(6)	-176.0(3)
C(3)-C(4)-C(5)-C(6)	2.1(5)
C(3)-C(4A)-C(5A)-C(6)	2.1(5)
C(1)#1-N(1)-C(1)-N(2)	-7.5(5)
C(1)#1-N(1)-C(1)-C(2)	157.4(2)
C(8)-N(2)-C(1)-N(1)	156.4(3)
B(1)-N(2)-C(1)-N(1)	-12.4(4)
C(8)-N(2)-C(1)-C(2)	-11.9(3)
B(1)-N(2)-C(1)-C(2)	179.4(3)
N(1)-C(1)-C(2)-C(3)	15.8(5)
N(2)-C(1)-C(2)-C(3)	-177.2(3)
N(1)-C(1)-C(2)-C(7)	-160.4(3)
N(2)-C(1)-C(2)-C(7)	6.6(3)
C(5A)-C(4A)-C(3)-C(2)	0.8(4)
F(1)-C(4)-C(3)-C(2)	178.8(3)
C(5)-C(4)-C(3)-C(2)	0.8(4)
C(7)-C(2)-C(3)-C(4A)	-2.6(4)
C(1)-C(2)-C(3)-C(4A)	-178.4(3)
C(7)-C(2)-C(3)-C(4)	-2.6(4)
C(1)-C(2)-C(3)-C(4)	-178.4(3)
C(4A)-C(5A)-C(6)-C(7)	-2.9(4)
F(2)-C(5)-C(6)-C(7)	170.0(3)
C(4)-C(5)-C(6)-C(7)	-2.9(4)
C(5A)-C(6)-C(7)-C(2)	1.1(4)
C(5)-C(6)-C(7)-C(2)	1.1(4)
C(5A)-C(6)-C(7)-C(8)	178.7(3)
C(5)-C(6)-C(7)-C(8)	178.7(3)
C(3)-C(2)-C(7)-C(6)	1.7(4)
C(1)-C(2)-C(7)-C(6)	178.4(2)
C(3)-C(2)-C(7)-C(8)	-176.4(2)
C(1)-C(2)-C(7)-C(8)	0.3(3)
C(9)-N(3)-C(8)-N(2)	7.9(4)

C(9)-N(3)-C(8)-C(7)	-156.2(3)
C(1)-N(2)-C(8)-N(3)	-155.6(3)
B(1)-N(2)-C(8)-N(3)	13.1(4)
C(1)-N(2)-C(8)-C(7)	12.1(3)
B(1)-N(2)-C(8)-C(7)	-179.2(3)
C(6)-C(7)-C(8)-N(3)	-18.9(5)
C(2)-C(7)-C(8)-N(3)	158.9(3)
C(6)-C(7)-C(8)-N(2)	175.1(3)
C(2)-C(7)-C(8)-N(2)	-7.1(3)
C(8)-N(3)-C(9)-N(4)	-8.6(4)
C(8)-N(3)-C(9)-C(10)	156.2(3)
C(9)#1-N(4)-C(9)-N(3)	156.6(2)
B(1)-N(4)-C(9)-N(3)	-11.6(5)
C(9)#1-N(4)-C(9)-C(10)	-11.6(4)
B(1)-N(4)-C(9)-C(10)	-179.8(3)
N(3)-C(9)-C(10)-C(11)	15.5(5)
N(4)-C(9)-C(10)-C(11)	-177.8(3)
N(3)-C(9)-C(10)-C(10)#1	-160.1(3)
N(4)-C(9)-C(10)-C(10)#1	6.6(2)
F(3)-C(12A)-C(11)-C(10)	177.3(3)
C(12)#1-C(12)-C(11)-C(10)	-0.2(3)
C(10)#1-C(10)-C(11)-C(12A)	0.2(3)
C(9)-C(10)-C(11)-C(12A)	-174.9(3)
C(10)#1-C(10)-C(11)-C(12)	0.2(3)
C(9)-C(10)-C(11)-C(12)	-174.9(3)
C(1)-N(2)-B(1)-N(2)#1	27.8(5)
C(8)-N(2)-B(1)-N(2)#1	-140.0(2)
C(1)-N(2)-B(1)-N(4)	139.1(3)
C(8)-N(2)-B(1)-N(4)	-28.6(4)
C(1)-N(2)-B(1)-Cl(1)	-95.8(3)
C(8)-N(2)-B(1)-Cl(1)	96.5(3)
C(9)#1-N(4)-B(1)-N(2)	-139.3(3)
C(9)-N(4)-B(1)-N(2)	27.9(4)
C(9)#1-N(4)-B(1)-N(2)#1	-27.9(4)
C(9)-N(4)-B(1)-N(2)#1	139.3(3)
C(9)#1-N(4)-B(1)-Cl(1)	96.4(3)

C(9)-N(4)-B(1)-Cl(1)	-96.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z