Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Fluorinated boron subphthalocyanines: Lewis acid based templating chemistry facilitates random halide exchange, and fluoride versus chloride affects the basic photophysical properties and the solid-state arrangement.

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Supporting Information

EXPERIMENTAL.

General

Solvents were purchased from Caledon Laboratories Ltd. (Ontario, Canada) and used as received. Reagents were purchased from a selection of suppliers: TCI America (tetrafluorophthalonitrile, 4,5-difluorophthalonitrile), Sigma Aldrich (Boron trichloride in 1M Heptane and boron trifluoride diethyl etherate). Chloro-hexachloro boron subphthalocyanine (Cl-Cl_6BsubPc)[1] and chloro-dodecachloro boron subphthalocyanine (Cl-Cl_{12}BsubPc)[2] were prepared using literature methods. High pressure liquid chromatography (HPLC) analysis was conducted using a Waters 2695 separation module with a Waters 2998 photodiode array fitted with a SunFire™ C18 3.5 μm 3.0 x 150 mm column. HPLC grade acetonitrile and distilled in glass N,N-dimethylformamide were used as the mobile phase eluted at 0.6 mL/min at a composition of 80:20 (v:v). HPLC was used to monitor each reaction. Ultraviolet-visible (UV-Vis) spectroscopy was enabled by a PerkinElmer Lambda 1050 using PerkinElmer quartz cuvette with 10 mm path length. Photoluminescence spectra was measured using a PerkinElmer LS 55 in toluene at room temperature by excitation at 540 nm. The fluorescence quantum yields (Φ) were calculated using the formula[3]: $\Phi = \Phi_R (I/I_R)(OD_R/OD)(n^2/n_R^2)$, where *I* is the integrated fluorescence intensity, *OD* is the optical density (*i.e.* absorbance), and *n* is the refractive index of the solvent, toluene for this study. The subscript R is the reference fluorophore, F_5PhO-BsubPc, with a reported $\Phi = 0.42$[4] in toluene at room temperature. This is an adapted standard operating procedure from literature[3] and utilized for BsubPcs.[4, 5] Low resolution mass spectra (LRMS) and high-resolution spectra (HRMS) were collected using Waters GC Premier and time-of-flight spectrometer with an electron ionization source (TOF-EI MS). Nuclear magnetic resonance (NMR) spectra were collected from a Bruker Avance III 400 MHz system. ^{1}H NMR spectra were referenced to the deuterated solvent peak

($CDCl_3$, δ_H = 7.26 ppm) and ^{19}F NMR spectra were shifted by that same ppm difference. Thermogravimetric analysis (TGA) was run on TA Instrument Q50 under nitrogen and a heating rate of 5°C min^{-1}. All x-ray crystal structure data was collected using a Bruker Kappa APEX DUO CCD diffractometer. Bond lengths, and other points of data were noted, calculated and measured using Mercury CSD 3.9.

Chloro-hexafluoro boron subphthalocyanine (Cl_mF_n-F_6BsubPc).

4,5-Difluorophthalonitrile (2.0233 g, 12.3 mmol, 3 eq) was added in a round bottom flask that contained 1,2-dichlorobenzene (54 mL) and was fitted with a condenser while being held under a constant pressure of argon gas. BCl_3 (1.0 M in heptane, 30 mL, 29.7 mmol, 7.23 eq) was added to the stirring mixture. The resulting slurry was heated and the heptane was removed through distillation using a short-path condenser. The round bottom flask was then heated at reflux (180 °C) for 26 hours. The mixture was cooled and the solvent was removed by a rotary evaporator. The solid was dried in a vacuum oven at 80 °C. The solid was further purified by train sublimation (38% yield, 99% pure by HPLC). ^1H NMR (400 MHz, $CDCl_3$): δ 8.63 (t, $J_{H\text{-}F}$ = 8 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -128.56 (1.00, t, J = 8.0 Hz), -129.06 (0.02, t, J = 8.1 Hz). HRMS EI calcd [M^+] 538.0334, found 538.0305. UV/Vis λ_{max} (CH_2Cl_2): 560 nm. Elemental Analysis calcd C 53.52, H 1.12, N 15.60; found C 53.88, H 0.99, N 15.32. TGA 5% degradation temperature: 353 °C.

Chloro-dodecafluoro boron subphthalocyanine (Cl_mF_n-F_{12}BsubPc).

Tetrafluorophthalonitrile (2.586 g, 4.80 mmol, 3 eq) was added in a round bottom flask that contained 1,2-dichlorobenzene (77.5 mL) and was fitted with a condenser while being held under

a constant pressure of argon gas. BCl_3 (1.0 M in heptane, 31 mL, 31.1 mmol, 7.23 eq) was added to the stirring mixture. The resulting slurry was heated, and the heptane was removed through distillation using a short-path condenser. The round bottom flask was then heated at reflux (180 °C) for 26 hours. The mixture was cooled and the solvent was removed by rotary evaporator. The solid was dried in a vacuum oven at 80 °C. The solid was further purified by train sublimation (28% yield, 97% pure by HPLC). ^{19}F NMR (377 MHz, $CDCl_3$) δ -136.07 (1.00, m, 6F), -136.41 (0.02, m), δ -146.56(1.02, m, 6F), -149.93 (0.05, m). HRMS EI calcd [M^+] 645.9769, found 645.9766 . UV/Vis λ_{max} (CH_2Cl_2): 580 nm. Elemental Analysis calcd C 44.59, N 13.00; found C 44.78, N 12.81. Crystals of suitable quantity for X-ray diffraction were grown by train sublimation. TGA 5% degradation temperature: 339 °C.

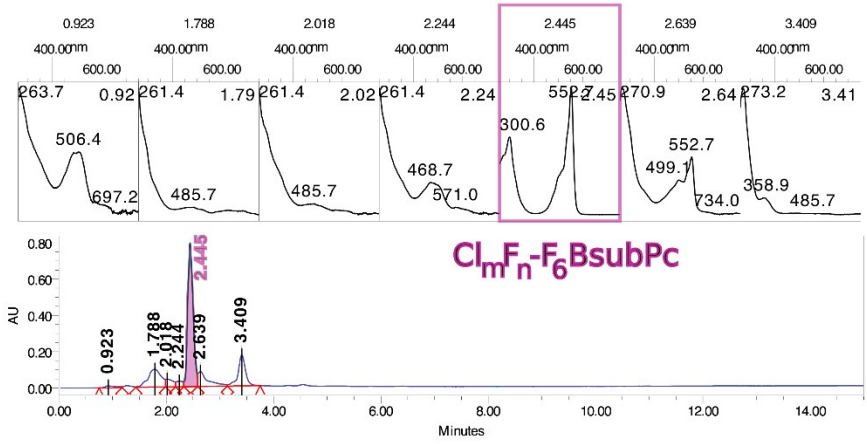
Fluoro-hexafluoro boron subphthalocyanine (F-F_6BsubPc).

Cl-F_6BsubPc (0.560 g, 1.04 mmol, 1 eq) was added to a round bottom flask containing toluene (6.7 mL). To the stirring solution was added boron trifluoride diethyl etherate (BF_3•OEt_2), 1.28 mL, 10.4 mmol, 10 eq). The resulting mixture was allowed to reflux under argon for 1.5 hours. The solvent, excess boron trifluoride diethyl etherate and other volatiles were removed through distillation using a short-path condenser. After cooling to room temperature, the solid was dried in a vacuum oven at 80 °C. The solid was further purified by train sublimation (28% yield, >99% pure by HPLC).^1H NMR (400 MHz, $CDCl_3$) δ 8.64 (t, J = 8.0 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -129.06 (t, J = 8.0 Hz, 6F), -156.71 (m, 1F). HRMS EI calcd [M^+] 522.0630, found 522.0646. UV/Vis λ_{max} (CH_2Cl_2): 555 nm. Elemental Analysis calcd C 53.52, H 1.12, N 15.60; found C 55.78, H 0.91, N 15.83. Crystals of suitable quantity for X-ray diffraction were grown by train sublimation. TGA 5% degradation temperature: 352 °C.

Fluoro-dodecafluoro boron subphthalocyanine (F-F_{12}BsubPc).

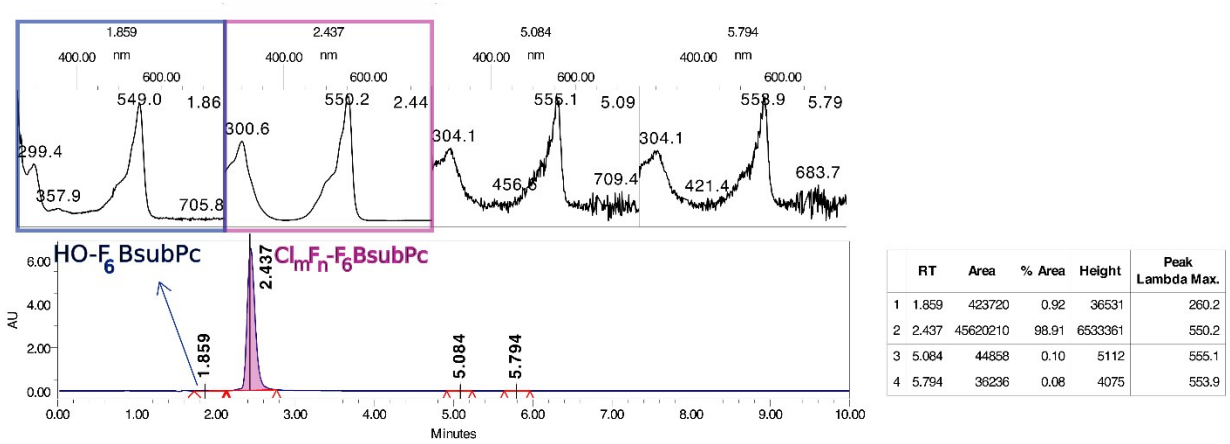
Cl-F_{12}BsubPc (0.695 g, 1.07 mmol, 1 eq) was added to a round bottom flask containing toluene (6.9 mL). To the stirring solution was added boron trifluoride diethyl etherate (BF_3•OEt_2), 1.3 mL, 10.75 mmol, 10 eq). The resulting mixture was allowed to reflux under argon for 7 hours. The solvent, excess boron trifluoride diethyl etherate and other volatiles were removed through distillation using a short-path condenser. After cooling to room temperature, the solid was dried in a vacuum oven at 80 °C. The solid was further purified by train sublimation (18% yield, >99% pure by HPLC). ^{19}F NMR (377 MHz, $CDCl_3$) δ -136.38 (m, *6F*), δ -147.01 (m, *6F*), δ -155.04 (dd, $J_{F\text{-}B}$ = 58.5, 28.6 Hz, 1F). HRMS EI calcd [M^+] 630.0064, found 630.0054. UV/Vis λ_{max} (CH_2Cl_2): 580 nm. Elemental Analysis calcd C 45.75, N 13.34; found C 44.78, N 12.81. Crystals of suitable quantity for X-ray diffraction were grown by train sublimation. TGA 5% degradation temperature: 321 °C.

CHARACTERIZATION OF FLUORINATED BSUBPCS.



	RT	Area	% Area	Height	Peak Lambda Max.
1	0.923	143394	1.35	10217	263.7
2	1.788	1686679	15.85	98199	261.4
3	2.018	413974	3.89	42779	261.4
4	2.244	261080	2.45	30160	261.4
5	2.445	5458081	51.29	791898	552.7
6	2.639	1058514	9.95	82142	270.9
7	3.409	1619046	15.22	170640	273.2

Figure S1. HPLC-UV/Vis trace (maxplot) of the Cl_mF_n-F_6BsubPc crude product using Jones et al[6] procedure, depicting a series of other non-BsubPc components. Note, the hydroxy derivative is a known by-product generated as the sample goes through the HPLC column.



	RT	Area	% Area	Height	Peak Lambda Max.
1	1.859	423720	0.92	36531	260.2
2	2.437	45620210	98.91	6533361	550.2
3	5.084	44858	0.10	5112	555.1
4	5.794	36236	0.08	4075	553.9

Figure S2. HPLC-UV/Vis trace (560-590 nm plot) of the Cl_mF_n-F_6BsubPc crude product using our established procedure, depicting Cl-F_6BsuPc at 98.9%. Note, the hydroxy derivative is a known by-product generated as the sample goes through the HPLC column.

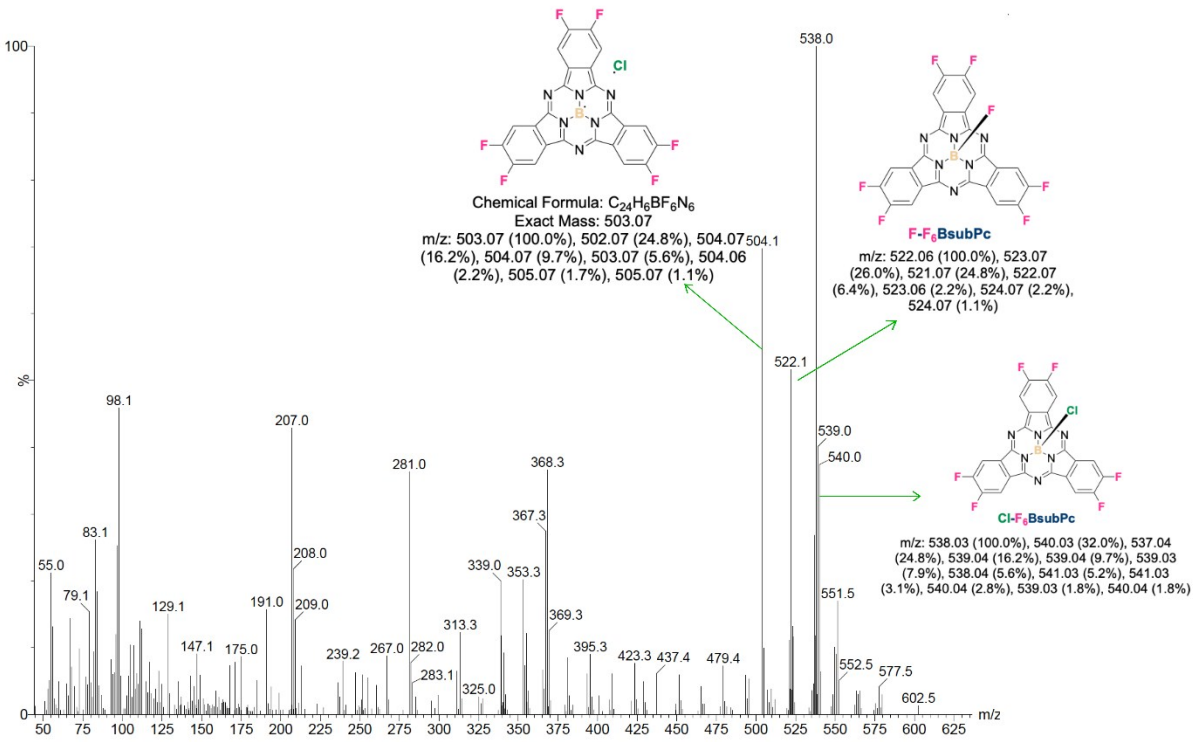


Figure S3. Mass spectrum of Cl_mF_n-F_6BsubPc crude product (depicting the presence of it and F-F_6BsubPc impurity)

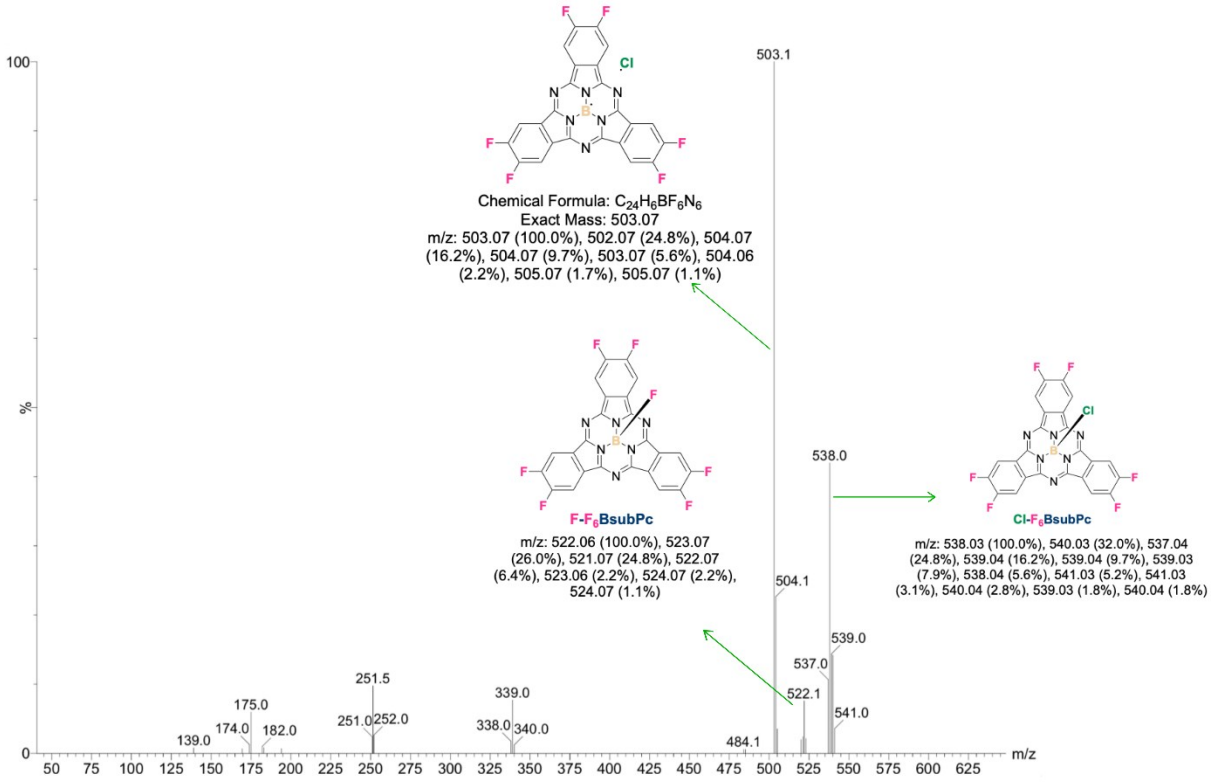


Figure S4. Mass spectrum of doubly sublimed Cl_mF_n-F_6BsubPc (depicting the presence of it and F-F_6BsubPc impurity)

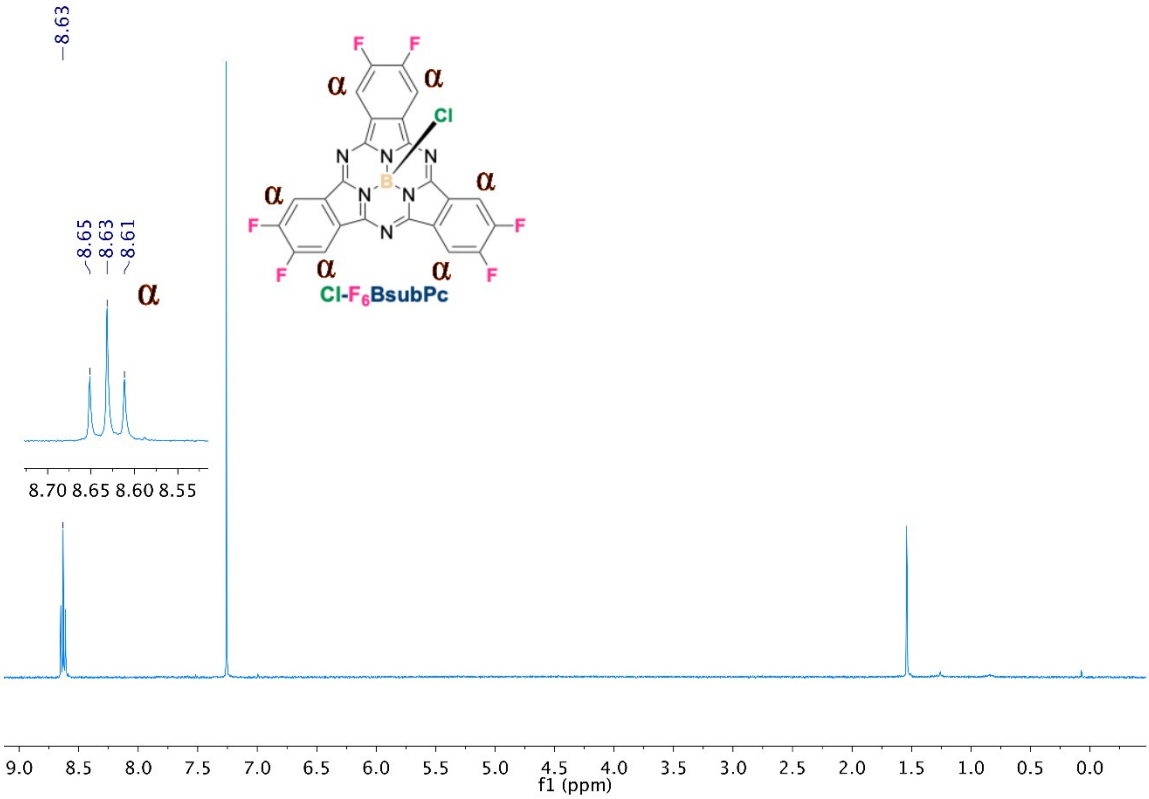


Figure S5. ^{1}H NMR of Cl_mF_n-F_6BsubPc (depicting the presence of it and F-F_6BsubPc impurity)

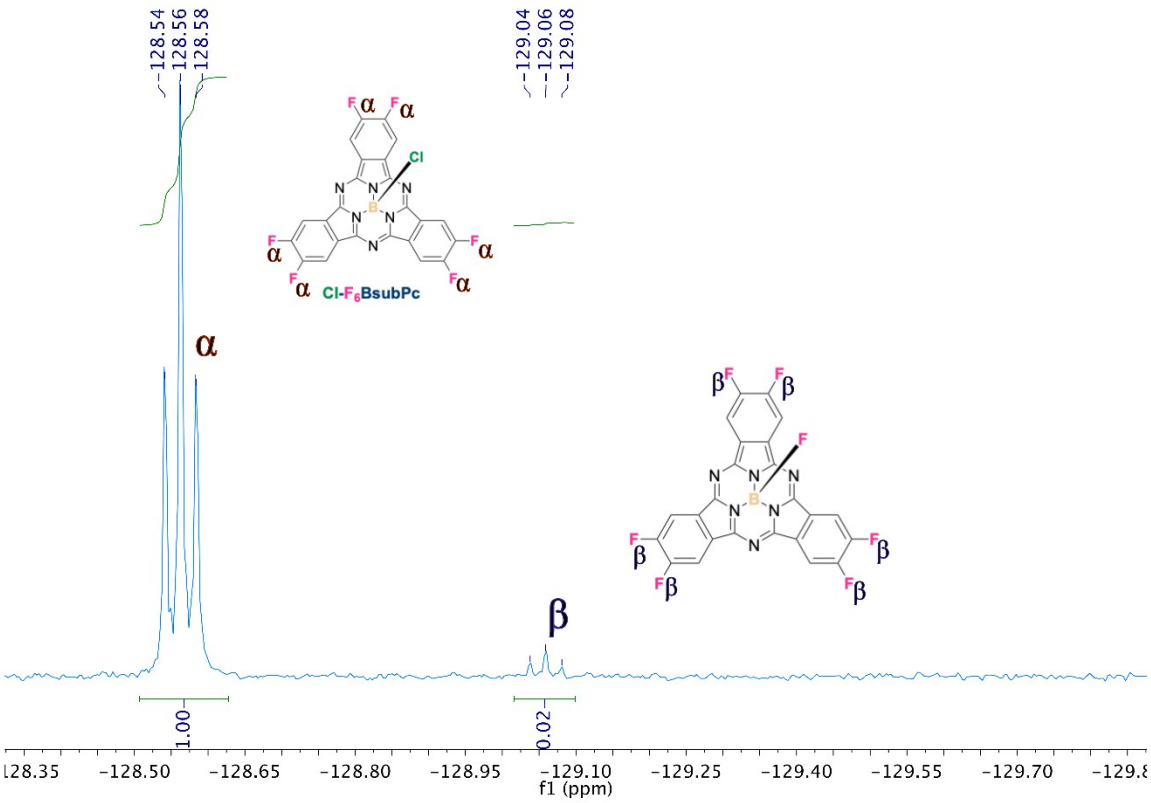
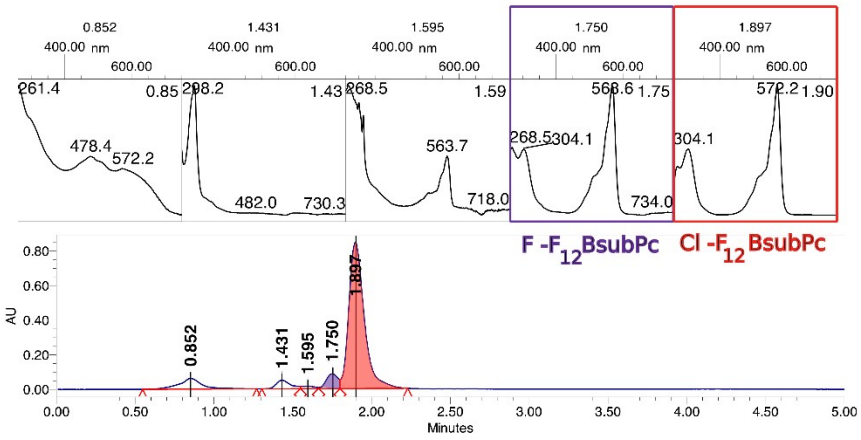
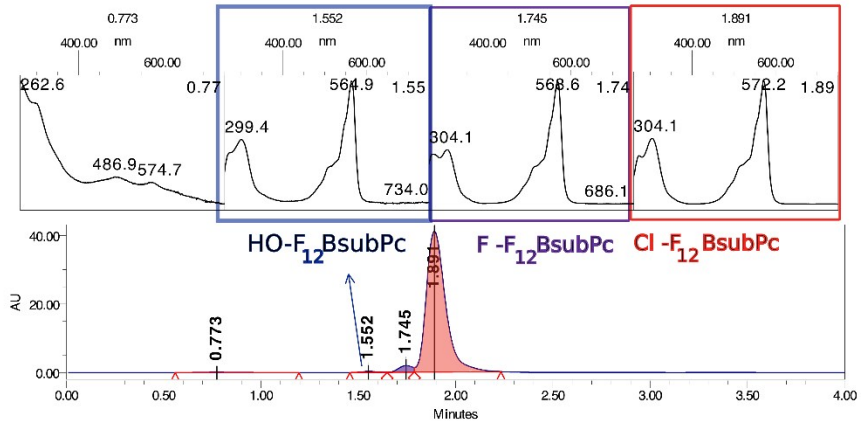


Figure S6. ^{19}F NMR of Cl_mF_n-F_6BsubPc (depicting the presence of it and F-F_6BsubPc impurity)



	RT	Area	%Area	Height	Peak Lambda Max.
1	0.852	632890	8.85	62295	261.4
2	1.431	303272	4.24	48874	298.2
3	1.595	81337	1.14	14236	268.5
4	1.750	432851	6.05	84706	568.6
5	1.897	5703638	79.73	843616	572.2

Figure S7. HPLC-UV/Vis trace (maxplot) of the Cl_mF_n-F_{12}BsubPc crude product, depicting the presence of it and F-F_{12}BsubPc impurity.



	RT	Area	% Area	Height	Peak Lambda Max.
1	0.773	1052555	0.36	93361	262.6
2	1.552	1533697	0.52	277608	564.9
3	1.745	9283152	3.17	1922818	568.6
4	1.891	280724378	95.94	41014931	572.2

Figure S8. HPLC-UV/Vis trace (maxplot) of the sublimed Cl_mF_n-F_{12}BsubPc, depicting the persistence of the F-F_{12}BsubPc impurity. Note, the hydroxy derivative is a known by-product generated as the sample goes through the HPLC column.

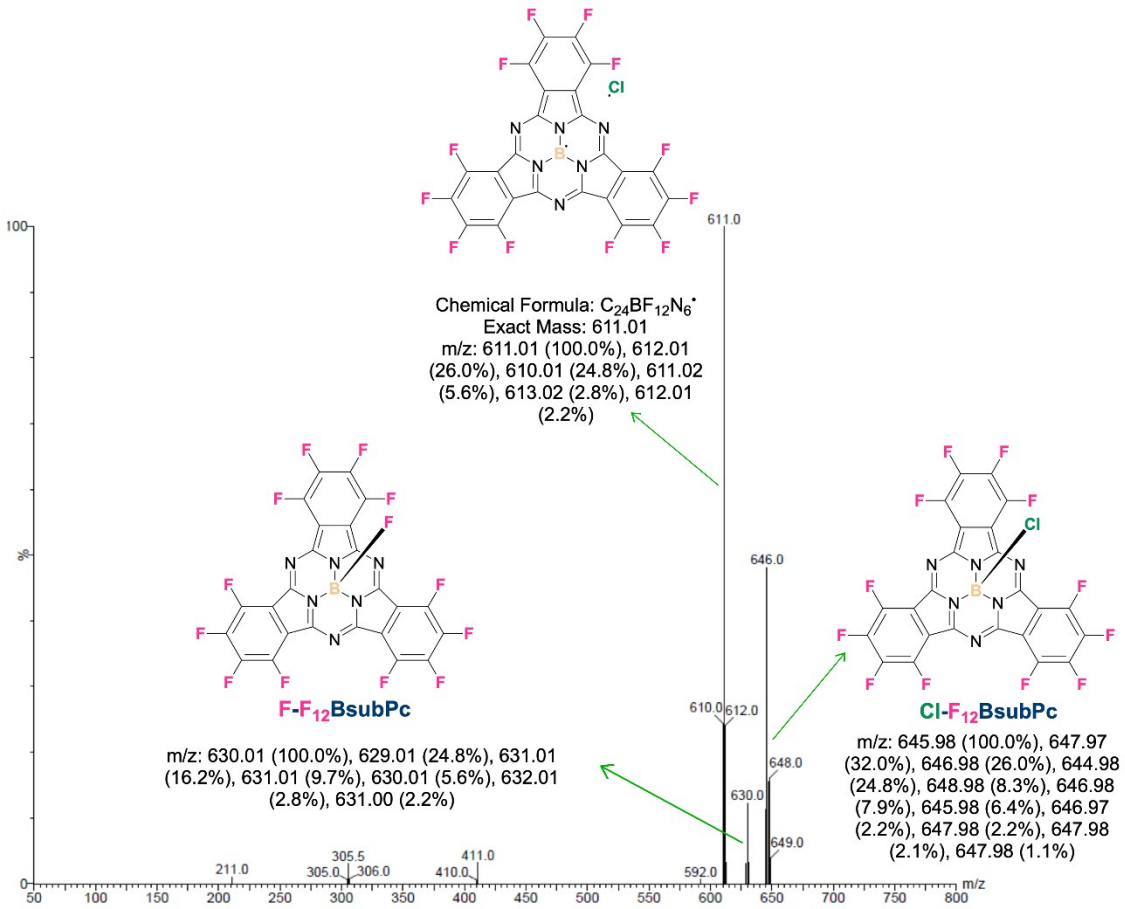


Figure S9. Mass spectrum of doubly sublimed Cl_mF_n-F_{12}BsubPc (depicting the presence of it and F-F_{12}BsubPc impurity).

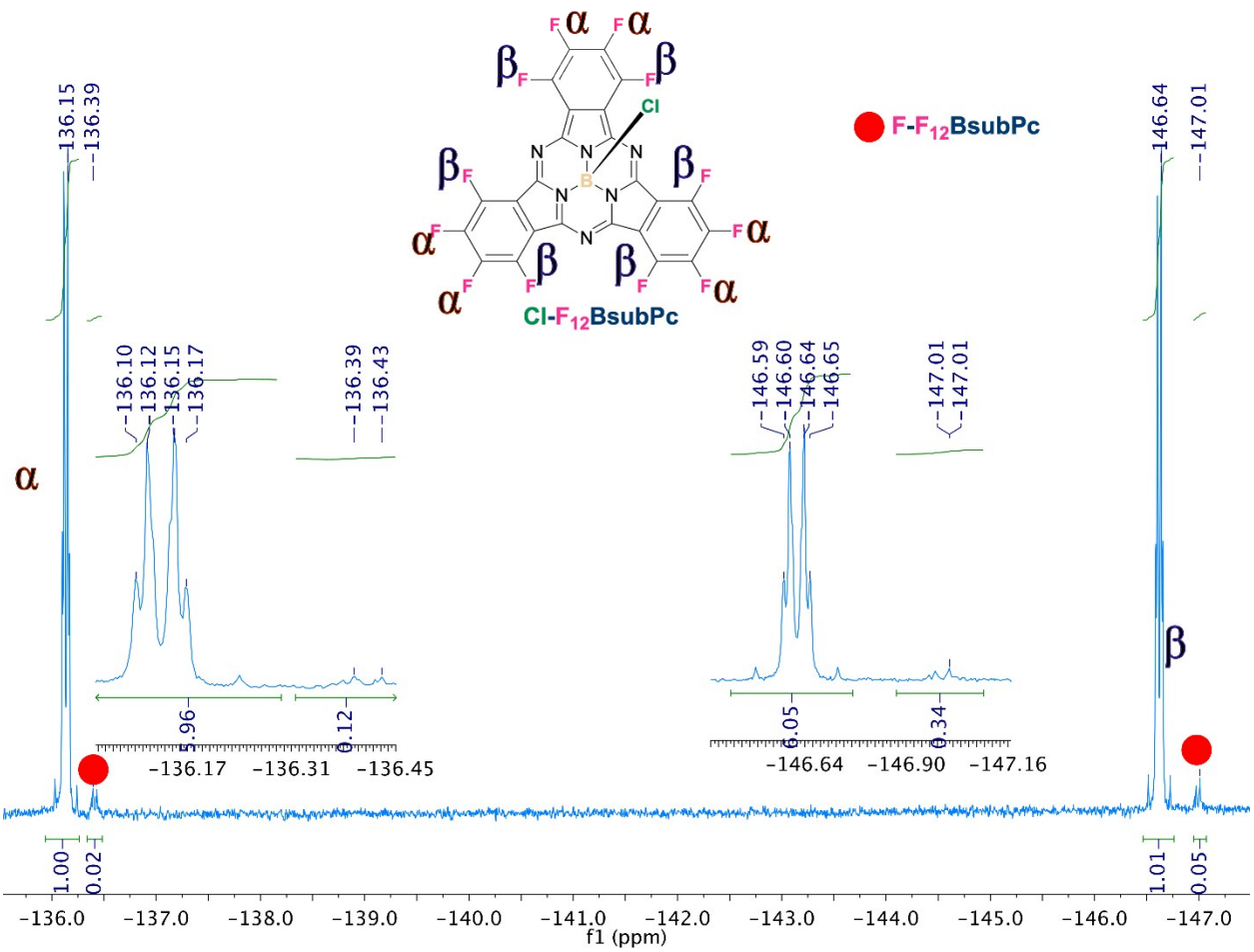
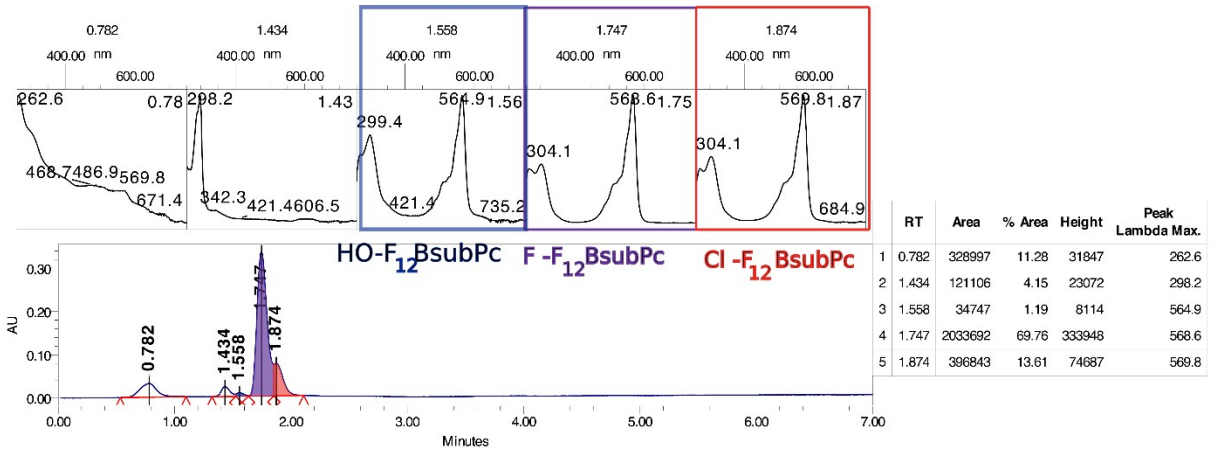


Figure S10. ^{19}F NMR of doubly sublimed Cl_mF_n-F_{12}BsubPc (depicting the presence of it and F-F_{12}BsubPc impurity).



	RT	Area	% Area	Height	Peak Lambda Max.
1	0.782	328997	11.28	31847	262.6
2	1.434	121106	4.15	23072	298.2
3	1.558	34747	1.19	8114	564.9
4	1.747	2033692	69.76	333948	568.6
5	1.874	396843	13.61	74687	569.8

Figure S11. HPLC-UV/Vis trace (maxplot) of the Cl_mF_n-F_{12}BsubPc crude product after a scaled-up reaction, depicting the dominance of F-F_{12}BsubPc instead. This is show the random axially fluorination of the BsubPc using tetrafluorophthalonitrile. Note, the hydroxy derivative is a known by-product generated as the sample goes through the HPLC column.

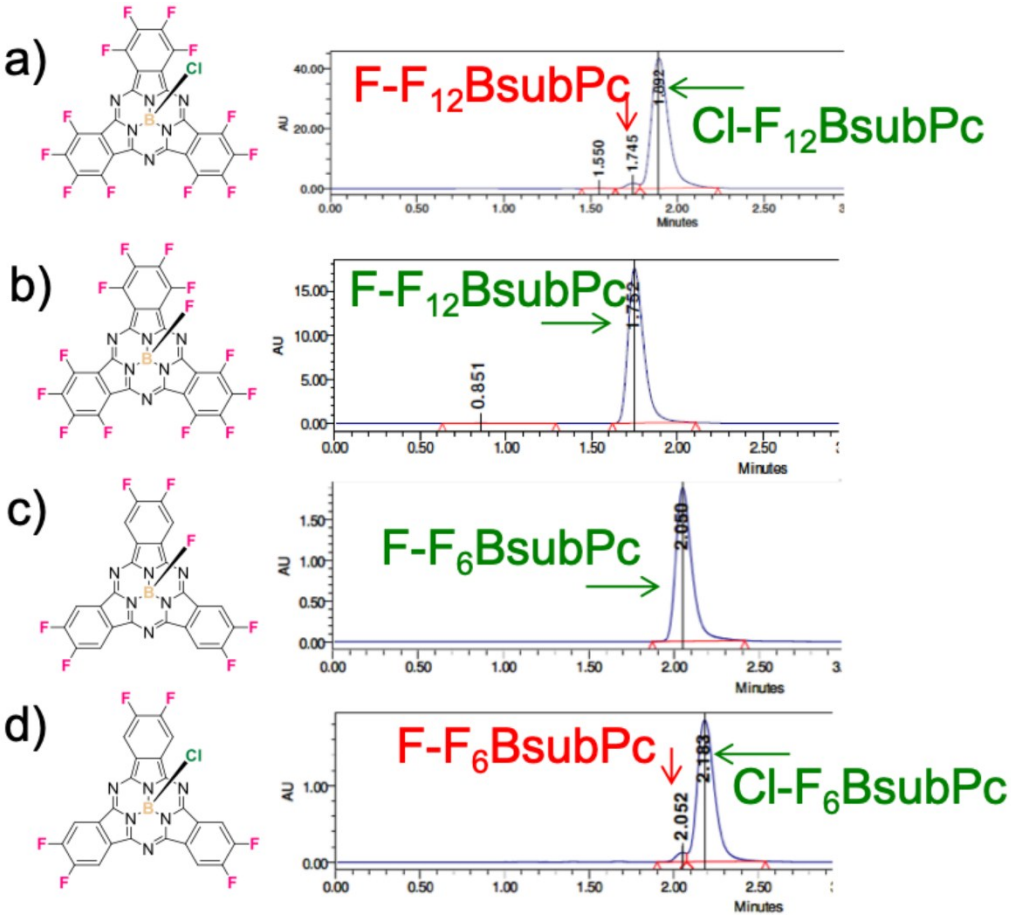


Figure S12. HPLC traces of all four peripherally fluorinated following double train sublimation.

Table S1. X-ray diffraction experimental details for single crystals of chlorinated and fluorinated BsubPcs as part of this study. Also included is two previously published single crystal results as points of comparison.

	Cl-F_6BsubPc	**Cl-F_6BsubPc**	**Cl-F_6BsubPc**	**Cl-F_{12}BsubPc**	**Cl-F_{12}BsubPc**	**F-F_6BsubPc**	**F-F_{12}BsubPc**	**F-F_{12}BsubPc**
Crystal growth method	Train sublimation	solvent/vapour diffusion (Benzene/heptane)	solvent/vapour diffusion (Benzene/methanol)	Train sublimation	Slow evaporation (toluene)	Train sublimation	Train sublimation	Slow evaporation (chloroform)
Identification code	d1770a_a	d1640	d1641	d17163_a	Literature	d17132twin5	d17130	Literature
CCDC	1945786	1945789	1945788	1945784	OFUTUE	1945783	1945787	YIYHUK
Source	This study	This study	This study	This study	Durfee et al.[7]	This study	This study	Torres et al.[8]
Empirical formula	C_{24} H_6 B Cl F_6 N_6	C_{24} H_6 B Cl F_6 N_6	C_{24} H_6 B Cl F_6 N_6	C_{24} B Cl F_{12} N_6	C_{24} B Cl F_{12} N_6	C_{24} H_6 B F_7 N_6	C_{24} B F_{13} N_6	C_{24} B F_{13} N_6
Formula weight	538.61	538.61	538.61	646.56		522.16	630.11	
Temperature	149(2) K	147(2) K	147(2) K	150(2) K		150(2) K	150(2) K	
Wavelength	1.54178 Å	1.54178 Å	1.54178 Å	1.54178 Å		1.54178 Å	1.54178 Å	
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic		Monoclinic	Orthorhombic	
Space group	Pbca	Pbca	Pbca	$P2_1/c$	$P2_1/c$	$P2_1/m$	$P2_12_12_1$	$P2_12_12_1$
Unit cell dimensions	a = 13.4808(7) Å	a = 13.4684(5) Å	a = 13.4953(4) Å	a = 11.2770(2) Å	a = 11.2997(11) Å	a = 13.1545(4) Å	a = 11.5570(3) Å	a = 11.5346(2) Å
	b = 13.4532(8) Å	b = 13.4295(5) Å	b = 13.4233(4) Å	b = 10.5657(2) Å	b = 10.6022(11) Å	b = 19.3823(6) Å	b = 22.1670(6) Å	b = 22.1148(6) Å
	c = 23.0190(12) Å	c = 23.0284(8) Å	c = 23.0059(7) Å	c = 19.0940(4) Å	c = 19.1563(19) Å	c = 13.5266(4) Å	c = 26.3618(7) Å	c = 26.3004(5) Å
	a= 90°.	a= 90°.	a= 90°.	a= 90°.	a= 90°.	a= 90°.	a= 90°.	a= 90°.
	b= 90°.	b= 90°.	b= 90°.	b= 95.436(1)°.	b= 95.507(1)°.	b= 117.621(2)°.	b= 90°.	b= 90°.
	g = 90°.	g = 90°.	g = 90°.	g = 90°.	g = 90°.	g = 90°.	g = 90°.	g = 90°.
Volume	4174.7(4) $Å^3$	4165.2(3) $Å^3$	4167.6(2) $Å^3$	2264.81(8) $Å^3$	2284.36 $Å^3$	3055.75(17) $Å^3$	6753.5(3) $Å^3$	6708.85 $Å^3$
Z	8	8	8	4	4	6	12	12
Density (calculated)	1.714 Mg/m^3	1.718 Mg/m^3	1.717 Mg/m^3	1.896 Mg/m^3		1.702 Mg/m^3	1.859 Mg/m^3	
Absorption coefficient	2.389 mm^{-1}	2.395 mm^{-1}	2.394 mm^{-1}	2.729 mm^{-1}		1.321 mm^{-1}	1.726 mm^{-1}	
F(000)	2144	2144	2144	1264		1560	3696	

Crystal size	0.110 x 0.040 x 0.030 mm^3	0.290 x 0.130 x 0.015 mm^3	0.200 x 0.180 x 0.010 mm^3	0.090 x 0.040 x 0.030 mm^3		0.080 x 0.040 x 0.010 mm^3	0.040 x 0.030 x 0.020 mm^3	
Theta range for data collection	3.840 to 66.909°.	3.839 to 67.633°.	3.843 to 67.356°.	3.938 to 67.206°.		3.688 to 67.241°.	2.604 to 67.250°.	
Index ranges	-16<=h<=15, -15<=k<=15, -27<=l<=27	-15<=h<=14, -15<=k<=16, -27<=l<=27	-16<=h<=16, -15<=k<=15, -27<=l<=27	-13<=h<=13, -12<=k<=12, -22<=l<=22		-15<=h<=13, 0<=k<=23, 0<=l<=16	-13<=h<=13, -26<=k<=26, -31<=l<=31	
Reflections collected	77749	106939	77485	45198		118237	148198	
Independent reflections	3699 [R(int) = 0.0675]	3720 [R(int) = 0.0444]	3708 [R(int) = 0.0620]	4031 [R(int) = 0.0565]		5714 [R(int) = 0.1421]	11988 [R(int) = 0.0875]	
Completeness to theta = 66.909°	99.70%	99.10%	99.20%	99.20%		99.40%	99.30%	
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents		Semi-empirical from equivalents	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6497	0.7529 and 0.5929	0.7529 and 0.6167	0.7529 and 0.6507		0.7529 and 0.5584	0.7529 and 0.6851	
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2		Full-matrix least-squares on F2	Full-matrix least-squares on F2	
Data / restraints / parameters	3699 / 0 / 343	3720 / 0 / 343	3708 / 0 / 343	4031 / 0 / 397		5714 / 513 / 533	11988 / 0 / 1190	
Goodness-of-fit on F2	1.04	1.038	1.034	1.043		1.017	1.03	
Final R indices [I>2sigma(I)]	R1 = 0.0294, wR2 = 0.0736	R1 = 0.0312, wR2 = 0.0831	R1 = 0.0355, wR2 = 0.0931	R1 = 0.0310, wR2 = 0.0760		R1 = 0.0696, wR2 = 0.1533	R1 = 0.0358, wR2 = 0.0811	
R indices (all data)	R1 = 0.0340, wR2 = 0.0771	R1 = 0.0337, wR2 = 0.0856	R1 = 0.0417, wR2 = 0.0976	R1 = 0.0392, wR2 = 0.0805		R1 = 0.1858, wR2 = 0.2188	R1 = 0.0465, wR2 = 0.0875	
Absolute structure parameter	-	-	-	-		-	0.11(4)	
Extinction coefficient	n/a	n/a	n/a	n/a		n/a	0.00044(4)	
Largest diff. peak and hole	0.237 and -0.328 e.Å-3	0.246 and -0.399 e.Å-3	0.393 and -0.484 e.Å-3	0.265 and -0.299 e.Å-3		0.296 and -0.310 e.Å-3	0.241 and -0.233 e.Å-3	

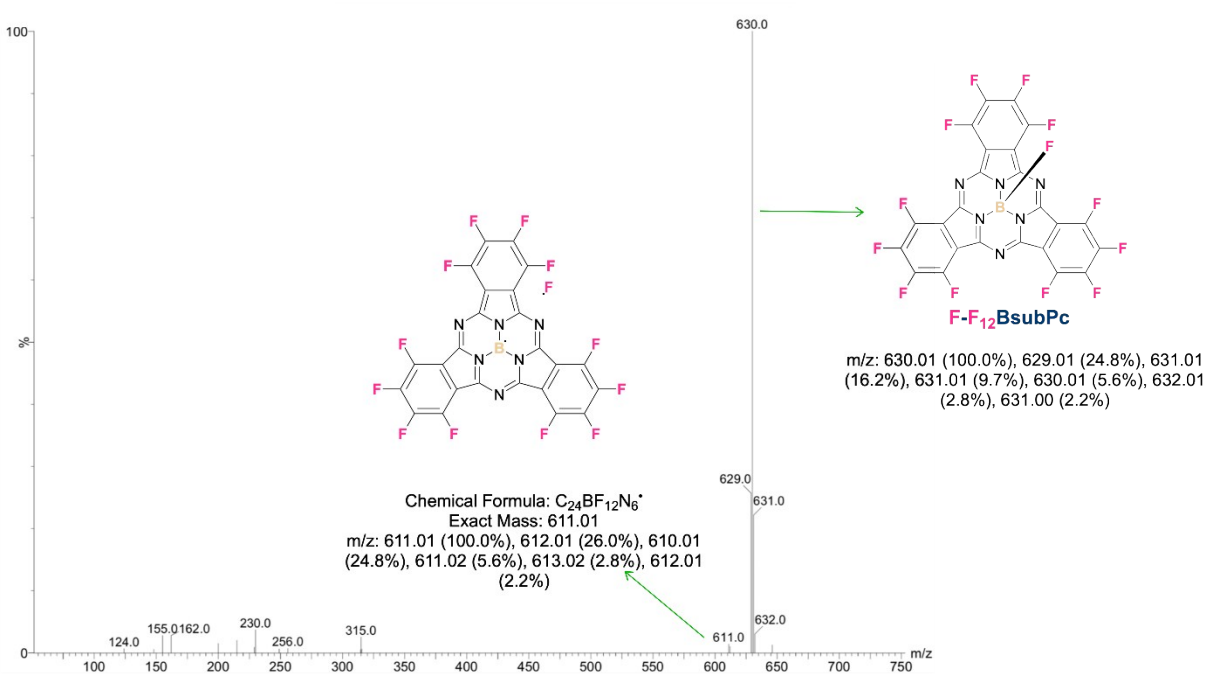


Figure S13. Mass spectrum of sublimed F-F_{12}BsubPc

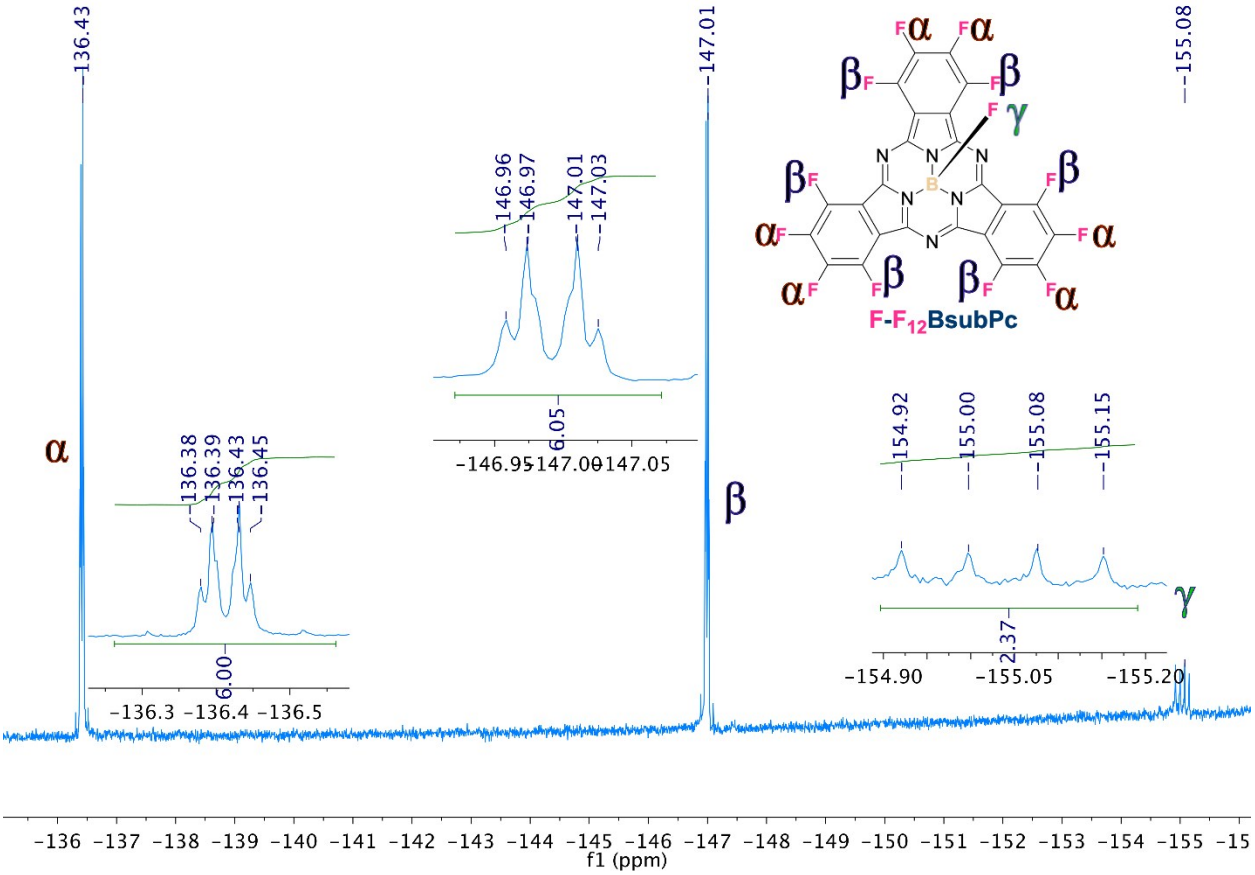


Figure S14. ^{19}F NMR of F-F$_{12}$BsubPc

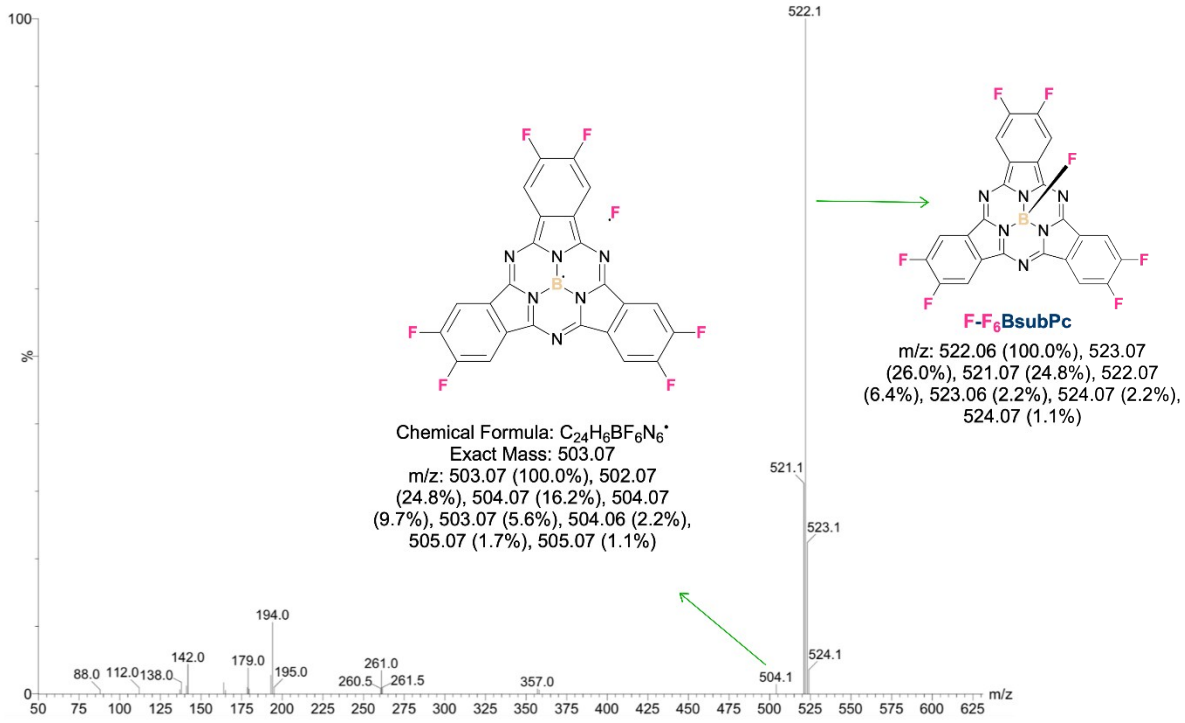


Figure S15. Mass spectrum of sublimed F-F_6BsubPc

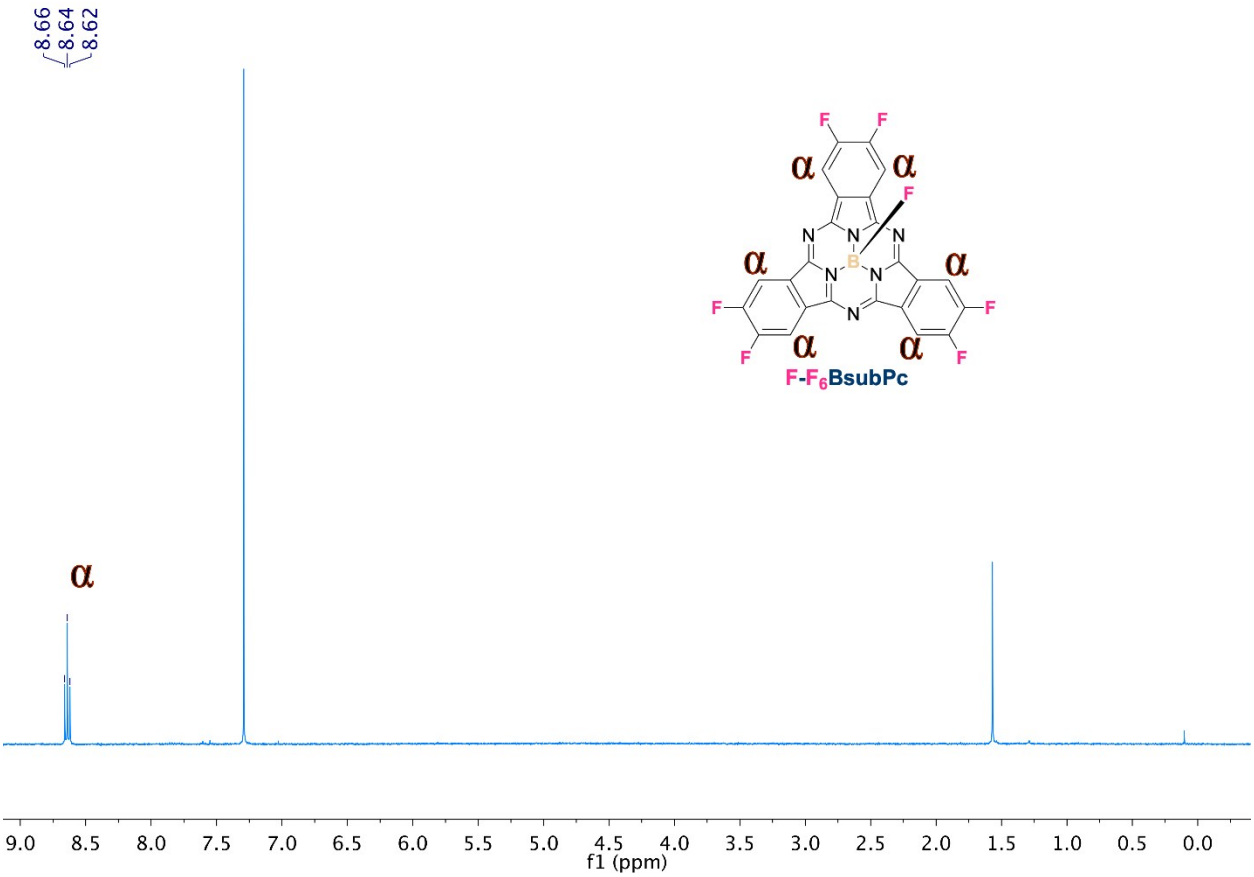


Figure S16. ^{1}H NMR of F-F$_6$BsubPc

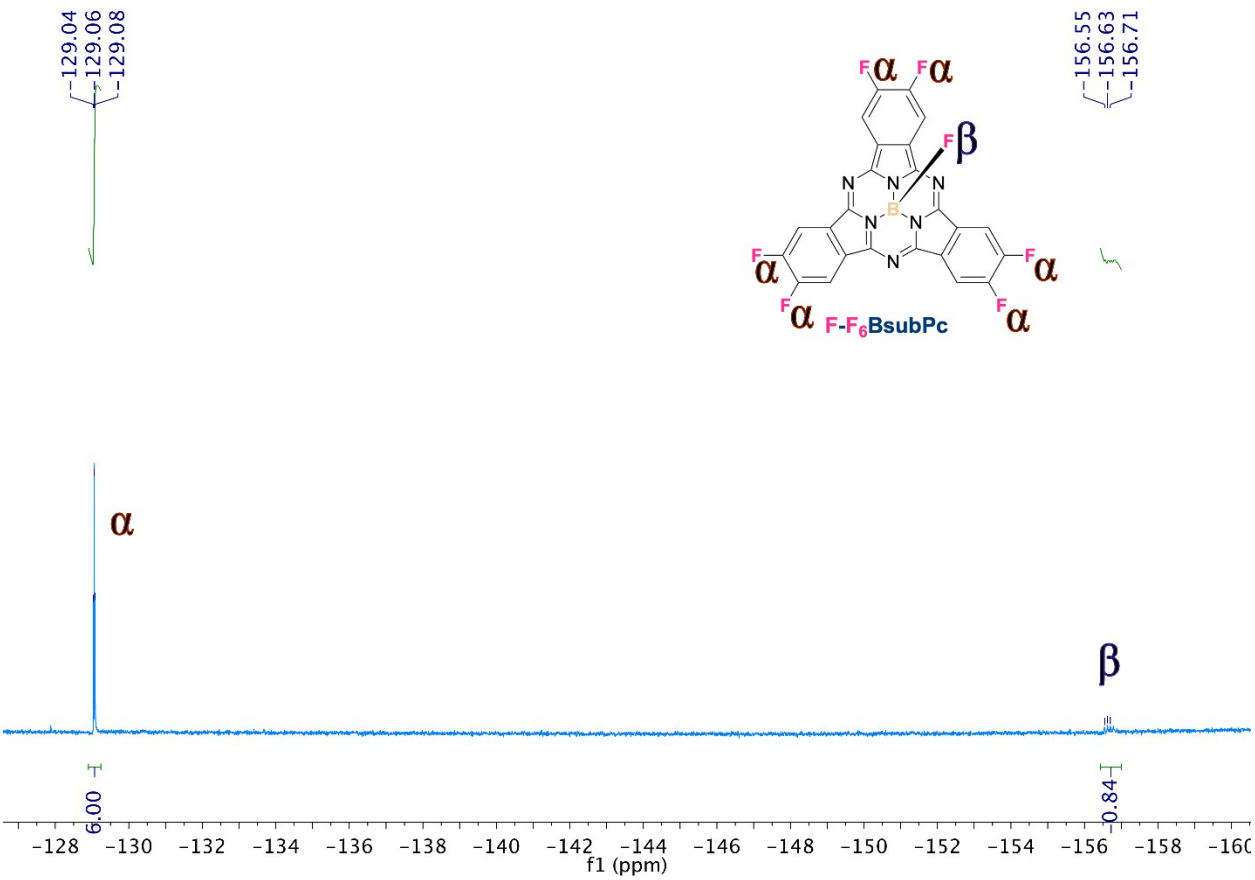


Figure S17. ^{19}F NMR of F-F_6BsubPc

SINGLE-CRYSTAL CRYSTALLOGRAPHIC DATA OF FLUORINATED BSUBPCS.

Table S2. Crystal data and structure refinement for **Cl-F_6BsubPc (grown by train sublimation)**

Empirical formula	C24 H6 B Cl F6 N6	
Formula weight	538.61	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 13.4587(11) Å	a= 90°.
	b = 13.4298(11) Å	b= 90°.
	c = 22.9739(18) Å	g = 90°.
Volume	4152.5(6) Å^3	
Z	8	
Density (calculated)	1.723 Mg/m^3	
Absorption coefficient	0.268 mm^{-1}	
F(000)	2144	
Crystal size	0.120 x 0.110 x 0.100 mm^3	
Theta range for data collection	1.773 to 27.712°.	
Index ranges	-17<=h<=17, -17<=k<=16, -30<=l<=26	
Reflections collected	24657	
Independent reflections	4807 [R(int) = 0.0940]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6862	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4807 / 0 / 343	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.0866	
R indices (all data)	R1 = 0.1078, wR2 = 0.1049	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.308 and -0.389 e.Å^{-3}	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-F_6BsubPc (grown by train sublimation)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6366(1)	5517(1)	2597(1)	25(1)
F(1)	1717(1)	4576(1)	335(1)	29(1)
F(2)	1998(1)	2698(1)	645(1)	32(1)
F(3)	4024(1)	787(1)	4507(1)	45(1)
F(4)	4272(1)	2116(1)	5339(1)	38(1)
F(5)	2698(1)	9066(1)	4517(1)	35(1)
F(6)	2213(1)	9654(1)	3450(1)	33(1)
N(1)	4448(2)	4890(2)	2293(1)	16(1)
N(2)	4390(2)	3184(2)	2570(1)	18(1)
N(3)	4971(2)	4412(2)	3232(1)	16(1)
N(4)	4677(2)	5529(2)	4016(1)	21(1)
N(5)	4531(2)	6071(2)	3038(1)	17(1)
N(6)	3678(2)	6466(2)	2166(1)	18(1)
C(1)	3875(2)	5541(2)	1979(1)	17(1)
C(2)	3373(2)	4937(2)	1545(1)	18(1)
C(3)	2742(2)	5175(2)	1088(1)	21(1)
C(4)	2313(2)	4400(2)	795(1)	21(1)
C(5)	2460(2)	3411(2)	960(1)	23(1)
C(6)	3078(2)	3155(2)	1405(1)	22(1)
C(7)	3561(2)	3928(2)	1690(1)	17(1)
C(8)	4212(2)	3917(2)	2190(1)	17(1)
C(9)	4713(2)	3454(2)	3098(1)	18(1)
C(10)	4616(2)	2936(2)	3649(1)	19(1)
C(11)	4359(2)	1955(2)	3771(1)	23(1)
C(12)	4256(2)	1721(2)	4347(1)	28(1)
C(13)	4379(2)	2428(2)	4785(1)	25(1)
C(14)	4596(2)	3400(2)	4676(1)	24(1)
C(15)	4724(2)	3658(2)	4093(1)	19(1)
C(16)	4863(2)	4612(2)	3814(1)	19(1)
C(17)	4445(2)	6226(2)	3622(1)	19(1)

C(18)	3876(2)	7143(2)	3679(1)	20(1)
C(19)	3557(2)	7672(2)	4166(1)	22(1)
C(20)	3009(2)	8510(2)	4068(1)	24(1)
C(21)	2751(2)	8808(2)	3507(1)	24(1)
C(22)	3008(2)	8277(2)	3024(1)	22(1)
C(23)	3583(2)	7433(2)	3112(1)	18(1)
C(24)	3956(2)	6690(2)	2710(1)	18(1)
B(1)	5063(2)	5209(2)	2796(1)	18(1)

Table S4. Bond lengths [Å] and angles [°] for **Cl-F_6BsubPc (grown by train sublimation**.

Cl(1)-B(1)	1.858(3)
F(1)-C(4)	1.349(3)
F(2)-C(5)	1.352(3)
F(3)-C(12)	1.344(3)
F(4)-C(13)	1.347(3)
F(5)-C(20)	1.342(3)
F(6)-C(21)	1.355(3)
N(1)-C(8)	1.365(3)
N(1)-C(1)	1.371(3)
N(1)-B(1)	1.484(4)
N(2)-C(8)	1.337(3)
N(2)-C(9)	1.339(3)
N(3)-C(9)	1.366(3)
N(3)-C(16)	1.373(3)
N(3)-B(1)	1.471(4)
N(4)-C(17)	1.338(3)
N(4)-C(16)	1.339(3)
N(5)-C(24)	1.362(3)
N(5)-C(17)	1.363(3)
N(5)-B(1)	1.472(4)
N(6)-C(24)	1.340(3)
N(6)-C(1)	1.341(3)
C(1)-C(2)	1.452(4)
C(2)-C(3)	1.388(3)
C(2)-C(7)	1.419(4)
C(3)-C(4)	1.367(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.394(4)
C(5)-C(6)	1.362(4)
C(6)-C(7)	1.389(4)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.444(3)
C(9)-C(10)	1.452(4)
C(10)-C(11)	1.391(4)

C(10)-C(15)	1.414(4)
C(11)-C(12)	1.367(4)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.394(4)
C(13)-C(14)	1.362(4)
C(14)-C(15)	1.394(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.444(4)
C(17)-C(18)	1.455(4)
C(18)-C(19)	1.393(4)
C(18)-C(23)	1.415(4)
C(19)-C(20)	1.364(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.393(4)
C(21)-C(22)	1.364(4)
C(22)-C(23)	1.387(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.450(4)
C(8)-N(1)-C(1)	112.8(2)
C(8)-N(1)-B(1)	122.7(2)
C(1)-N(1)-B(1)	122.6(2)
C(8)-N(2)-C(9)	116.8(2)
C(9)-N(3)-C(16)	112.1(2)
C(9)-N(3)-B(1)	123.6(2)
C(16)-N(3)-B(1)	122.0(2)
C(17)-N(4)-C(16)	117.0(2)
C(24)-N(5)-C(17)	113.7(2)
C(24)-N(5)-B(1)	123.2(2)
C(17)-N(5)-B(1)	122.3(2)
C(24)-N(6)-C(1)	116.9(2)
N(6)-C(1)-N(1)	122.2(2)
N(6)-C(1)-C(2)	130.2(2)
N(1)-C(1)-C(2)	105.5(2)
C(3)-C(2)-C(7)	120.4(2)
C(3)-C(2)-C(1)	132.5(3)
C(7)-C(2)-C(1)	106.8(2)

C(4)-C(3)-C(2)	117.1(2)
C(4)-C(3)-H(3A)	121.5
C(2)-C(3)-H(3A)	121.5
F(1)-C(4)-C(3)	120.2(2)
F(1)-C(4)-C(5)	117.7(2)
C(3)-C(4)-C(5)	122.1(2)
F(2)-C(5)-C(6)	120.2(3)
F(2)-C(5)-C(4)	117.6(2)
C(6)-C(5)-C(4)	122.1(2)
C(5)-C(6)-C(7)	116.8(3)
C(5)-C(6)-H(6A)	121.6
C(7)-C(6)-H(6A)	121.6
C(6)-C(7)-C(2)	121.3(2)
C(6)-C(7)-C(8)	130.6(3)
C(2)-C(7)-C(8)	107.7(2)
N(2)-C(8)-N(1)	123.3(2)
N(2)-C(8)-C(7)	129.4(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)	129.2(2)
N(3)-C(9)-C(10)	106.1(2)
C(11)-C(10)-C(15)	122.1(2)
C(11)-C(10)-C(9)	130.7(3)
C(15)-C(10)-C(9)	106.9(2)
C(12)-C(11)-C(10)	115.9(3)
C(12)-C(11)-H(11A)	122.0
C(10)-C(11)-H(11A)	122.0
F(3)-C(12)-C(11)	120.1(3)
F(3)-C(12)-C(13)	117.8(3)
C(11)-C(12)-C(13)	122.1(3)
F(4)-C(13)-C(14)	119.7(3)
F(4)-C(13)-C(12)	117.3(3)
C(14)-C(13)-C(12)	123.0(3)
C(13)-C(14)-C(15)	116.3(3)
C(13)-C(14)-H(14A)	121.9
C(15)-C(14)-H(14A)	121.9

C(14)-C(15)-C(10)	120.6(3)
C(14)-C(15)-C(16)	131.5(3)
C(10)-C(15)-C(16)	107.6(2)
N(4)-C(16)-N(3)	122.5(2)
N(4)-C(16)-C(15)	129.6(2)
N(3)-C(16)-C(15)	105.8(2)
N(4)-C(17)-N(5)	122.6(2)
N(4)-C(17)-C(18)	130.8(2)
N(5)-C(17)-C(18)	105.2(2)
C(19)-C(18)-C(23)	120.8(2)
C(19)-C(18)-C(17)	131.7(3)
C(23)-C(18)-C(17)	107.3(2)
C(20)-C(19)-C(18)	117.0(3)
C(20)-C(19)-H(19A)	121.5
C(18)-C(19)-H(19A)	121.5
F(5)-C(20)-C(19)	120.1(3)
F(5)-C(20)-C(21)	118.3(2)
C(19)-C(20)-C(21)	121.7(3)
F(6)-C(21)-C(22)	119.7(3)
F(6)-C(21)-C(20)	117.6(2)
C(22)-C(21)-C(20)	122.6(3)
C(21)-C(22)-C(23)	116.6(3)
C(21)-C(22)-H(22A)	121.7
C(23)-C(22)-H(22A)	121.7
C(22)-C(23)-C(18)	121.1(2)
C(22)-C(23)-C(24)	131.4(3)
C(18)-C(23)-C(24)	107.4(2)
N(6)-C(24)-N(5)	122.5(2)
N(6)-C(24)-C(23)	130.7(2)
N(5)-C(24)-C(23)	105.4(2)
N(3)-B(1)-N(5)	105.9(2)
N(3)-B(1)-N(1)	105.8(2)
N(5)-B(1)-N(1)	104.5(2)
N(3)-B(1)-Cl(1)	114.14(19)
N(5)-B(1)-Cl(1)	112.1(2)
N(1)-B(1)-Cl(1)	113.6(2)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for for **Cl-F_6BsubPc (grown by train sublimation**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	18(1)	28(1)	28(1)	2(1)	1(1)	0(1)
F(1)	30(1)	37(1)	21(1)	2(1)	-9(1)	-4(1)
F(2)	39(1)	28(1)	30(1)	-8(1)	-13(1)	-4(1)
F(3)	66(1)	31(1)	36(1)	11(1)	0(1)	-20(1)
F(4)	46(1)	46(1)	21(1)	8(1)	3(1)	-12(1)
F(5)	36(1)	32(1)	37(1)	-13(1)	11(1)	4(1)
F(6)	29(1)	24(1)	45(1)	0(1)	7(1)	10(1)
N(1)	15(1)	18(1)	15(1)	-1(1)	0(1)	1(1)
N(2)	18(1)	18(1)	18(1)	-2(1)	2(1)	4(1)
N(3)	17(1)	17(1)	15(1)	-1(1)	0(1)	0(1)
N(4)	21(1)	19(1)	22(1)	-2(1)	-2(1)	-2(1)
N(5)	16(1)	17(1)	17(1)	-3(1)	-1(1)	-2(1)
N(6)	17(1)	16(1)	20(1)	1(1)	2(1)	-4(1)
C(1)	16(1)	21(1)	14(1)	3(1)	3(1)	-1(1)
C(2)	16(1)	23(2)	16(1)	-2(1)	4(1)	-2(1)
C(3)	20(1)	24(2)	18(1)	2(1)	2(1)	2(1)
C(4)	17(1)	33(2)	12(1)	1(1)	-2(1)	0(1)
C(5)	24(2)	26(2)	18(1)	-9(1)	2(1)	-6(1)
C(6)	24(1)	21(2)	20(1)	-2(1)	1(1)	1(1)
C(7)	18(1)	21(2)	12(1)	-2(1)	3(1)	1(1)
C(8)	16(1)	17(1)	17(1)	-3(1)	4(1)	4(1)
C(9)	18(1)	17(2)	18(2)	-3(1)	2(1)	4(1)
C(10)	16(1)	22(2)	18(1)	0(1)	-1(1)	5(1)
C(11)	22(2)	25(2)	23(2)	0(1)	0(1)	2(1)
C(12)	27(2)	26(2)	30(2)	10(2)	1(1)	-4(1)
C(13)	24(2)	34(2)	16(2)	7(1)	0(1)	-3(1)
C(14)	19(1)	31(2)	20(2)	-2(1)	-3(1)	2(1)
C(15)	16(1)	22(2)	19(1)	2(1)	-1(1)	2(1)
C(16)	16(1)	23(2)	17(1)	-2(1)	-2(1)	1(1)
C(17)	19(1)	18(2)	19(1)	-4(1)	-2(1)	-3(1)

C(18)	18(1)	16(1)	25(2)	-3(1)	2(1)	-2(1)
C(19)	22(2)	23(2)	22(2)	-3(1)	0(1)	-4(1)
C(20)	22(2)	22(2)	29(2)	-10(1)	5(1)	-2(1)
C(21)	17(1)	18(2)	36(2)	-2(1)	2(1)	3(1)
C(22)	17(1)	20(2)	29(2)	-1(1)	1(1)	-2(1)
C(23)	15(1)	15(1)	25(2)	-2(1)	-1(1)	-4(1)
C(24)	16(1)	16(1)	22(2)	0(1)	-1(1)	-4(1)
B(1)	17(2)	20(2)	18(2)	1(1)	-2(1)	-1(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **Cl-F_6BsubPc (grown by train sublimation**.

	x	y	z	U(eq)
H(3A)	2613	5847	983	25
H(6A)	3173	2480	1515	26
H(11A)	4261	1476	3472	28
H(14A)	4658	3876	4980	28
H(19A)	3715	7458	4549	27
H(22A)	2802	8474	2645	27

Table S7. Torsion angles [°] for **Cl-F$_6$BsubPc (grown by train sublimation**.

C(24)-N(6)-C(1)-N(1)	-8.5(4)
C(24)-N(6)-C(1)-C(2)	152.5(3)
C(8)-N(1)-C(1)-N(6)	152.1(2)
B(1)-N(1)-C(1)-N(6)	-13.1(4)
C(8)-N(1)-C(1)-C(2)	-12.9(3)
B(1)-N(1)-C(1)-C(2)	-178.1(2)
N(6)-C(1)-C(2)-C(3)	20.5(5)
N(1)-C(1)-C(2)-C(3)	-176.2(3)
N(6)-C(1)-C(2)-C(7)	-154.2(3)
N(1)-C(1)-C(2)-C(7)	9.1(3)
C(7)-C(2)-C(3)-C(4)	0.7(4)
C(1)-C(2)-C(3)-C(4)	-173.4(3)
C(2)-C(3)-C(4)-F(1)	-177.9(2)
C(2)-C(3)-C(4)-C(5)	2.8(4)
F(1)-C(4)-C(5)-F(2)	0.2(4)
C(3)-C(4)-C(5)-F(2)	179.6(2)
F(1)-C(4)-C(5)-C(6)	177.5(2)
C(3)-C(4)-C(5)-C(6)	-3.1(4)
F(2)-C(5)-C(6)-C(7)	177.0(2)
C(4)-C(5)-C(6)-C(7)	-0.2(4)
C(5)-C(6)-C(7)-C(2)	3.6(4)
C(5)-C(6)-C(7)-C(8)	176.4(3)
C(3)-C(2)-C(7)-C(6)	-4.0(4)
C(1)-C(2)-C(7)-C(6)	171.5(2)
C(3)-C(2)-C(7)-C(8)	-178.2(2)
C(1)-C(2)-C(7)-C(8)	-2.7(3)
C(9)-N(2)-C(8)-N(1)	7.6(4)
C(9)-N(2)-C(8)-C(7)	-155.7(3)
C(1)-N(1)-C(8)-N(2)	-155.5(2)
B(1)-N(1)-C(8)-N(2)	9.7(4)
C(1)-N(1)-C(8)-C(7)	11.2(3)
B(1)-N(1)-C(8)-C(7)	176.4(2)
C(6)-C(7)-C(8)-N(2)	-12.6(5)
C(2)-C(7)-C(8)-N(2)	160.8(3)

C(6)-C(7)-C(8)-N(1)	-178.2(3)
C(2)-C(7)-C(8)-N(1)	-4.8(3)
C(8)-N(2)-C(9)-N(3)	-7.9(4)
C(8)-N(2)-C(9)-C(10)	154.0(3)
C(16)-N(3)-C(9)-N(2)	153.7(2)
B(1)-N(3)-C(9)-N(2)	-9.3(4)
C(16)-N(3)-C(9)-C(10)	-11.8(3)
B(1)-N(3)-C(9)-C(10)	-174.8(2)
N(2)-C(9)-C(10)-C(11)	15.2(5)
N(3)-C(9)-C(10)-C(11)	179.3(3)
N(2)-C(9)-C(10)-C(15)	-158.1(3)
N(3)-C(9)-C(10)-C(15)	6.0(3)
C(15)-C(10)-C(11)-C(12)	-2.5(4)
C(9)-C(10)-C(11)-C(12)	-174.9(3)
C(10)-C(11)-C(12)-F(3)	-179.0(2)
C(10)-C(11)-C(12)-C(13)	1.4(4)
F(3)-C(12)-C(13)-F(4)	1.1(4)
C(11)-C(12)-C(13)-F(4)	-179.3(2)
F(3)-C(12)-C(13)-C(14)	-178.8(3)
C(11)-C(12)-C(13)-C(14)	0.8(4)
F(4)-C(13)-C(14)-C(15)	178.2(2)
C(12)-C(13)-C(14)-C(15)	-1.9(4)
C(13)-C(14)-C(15)-C(10)	0.8(4)
C(13)-C(14)-C(15)-C(16)	173.3(3)
C(11)-C(10)-C(15)-C(14)	1.4(4)
C(9)-C(10)-C(15)-C(14)	175.4(2)
C(11)-C(10)-C(15)-C(16)	-172.7(2)
C(9)-C(10)-C(15)-C(16)	1.3(3)
C(17)-N(4)-C(16)-N(3)	10.1(4)
C(17)-N(4)-C(16)-C(15)	-151.0(3)
C(9)-N(3)-C(16)-N(4)	-152.4(2)
B(1)-N(3)-C(16)-N(4)	10.9(4)
C(9)-N(3)-C(16)-C(15)	12.5(3)
B(1)-N(3)-C(16)-C(15)	175.9(2)
C(14)-C(15)-C(16)-N(4)	-17.9(5)
C(10)-C(15)-C(16)-N(4)	155.4(3)

C(14)-C(15)-C(16)-N(3)	178.6(3)
C(10)-C(15)-C(16)-N(3)	-8.1(3)
C(16)-N(4)-C(17)-N(5)	-9.5(4)
C(16)-N(4)-C(17)-C(18)	154.9(3)
C(24)-N(5)-C(17)-N(4)	158.1(2)
B(1)-N(5)-C(17)-N(4)	-12.2(4)
C(24)-N(5)-C(17)-C(18)	-9.7(3)
B(1)-N(5)-C(17)-C(18)	-180.0(2)
N(4)-C(17)-C(18)-C(19)	13.7(5)
N(5)-C(17)-C(18)-C(19)	-179.9(3)
N(4)-C(17)-C(18)-C(23)	-161.4(3)
N(5)-C(17)-C(18)-C(23)	5.0(3)
C(23)-C(18)-C(19)-C(20)	-4.1(4)
C(17)-C(18)-C(19)-C(20)	-178.7(3)
C(18)-C(19)-C(20)-F(5)	-178.5(2)
C(18)-C(19)-C(20)-C(21)	2.0(4)
F(5)-C(20)-C(21)-F(6)	1.1(4)
C(19)-C(20)-C(21)-F(6)	-179.5(2)
F(5)-C(20)-C(21)-C(22)	-178.1(2)
C(19)-C(20)-C(21)-C(22)	1.4(4)
F(6)-C(21)-C(22)-C(23)	178.2(2)
C(20)-C(21)-C(22)-C(23)	-2.7(4)
C(21)-C(22)-C(23)-C(18)	0.6(4)
C(21)-C(22)-C(23)-C(24)	177.6(3)
C(19)-C(18)-C(23)-C(22)	2.9(4)
C(17)-C(18)-C(23)-C(22)	178.6(2)
C(19)-C(18)-C(23)-C(24)	-174.8(2)
C(17)-C(18)-C(23)-C(24)	0.9(3)
C(1)-N(6)-C(24)-N(5)	8.9(4)
C(1)-N(6)-C(24)-C(23)	-155.7(3)
C(17)-N(5)-C(24)-N(6)	-157.6(2)
B(1)-N(5)-C(24)-N(6)	12.6(4)
C(17)-N(5)-C(24)-C(23)	10.3(3)
B(1)-N(5)-C(24)-C(23)	-179.5(2)
C(22)-C(23)-C(24)-N(6)	-17.4(5)
C(18)-C(23)-C(24)-N(6)	160.0(3)

C(22)-C(23)-C(24)-N(5)	176.1(3)
C(18)-C(23)-C(24)-N(5)	-6.5(3)
C(9)-N(3)-B(1)-N(5)	133.4(2)
C(16)-N(3)-B(1)-N(5)	-28.0(3)
C(9)-N(3)-B(1)-N(1)	22.9(3)
C(16)-N(3)-B(1)-N(1)	-138.6(2)
C(9)-N(3)-B(1)-Cl(1)	-102.8(3)
C(16)-N(3)-B(1)-Cl(1)	95.8(3)
C(24)-N(5)-B(1)-N(3)	-140.6(2)
C(17)-N(5)-B(1)-N(3)	28.7(3)
C(24)-N(5)-B(1)-N(1)	-29.1(3)
C(17)-N(5)-B(1)-N(1)	140.2(2)
C(24)-N(5)-B(1)-Cl(1)	94.3(3)
C(17)-N(5)-B(1)-Cl(1)	-96.4(3)
C(8)-N(1)-B(1)-N(3)	-22.9(3)
C(1)-N(1)-B(1)-N(3)	140.8(2)
C(8)-N(1)-B(1)-N(5)	-134.5(2)
C(1)-N(1)-B(1)-N(5)	29.3(3)
C(8)-N(1)-B(1)-Cl(1)	103.0(3)
C(1)-N(1)-B(1)-Cl(1)	-93.2(3)

Symmetry transformations used to generate equivalent atoms:

Table S8. Crystal data and structure refinement for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**

Empirical formula	C24 H6 B Cl F6 N6	
Formula weight	538.61	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 13.4684(5) Å	a= 90°.
	b = 13.4295(5) Å	b= 90°.
	c = 23.0284(8) Å	g = 90°.
Volume	4165.2(3) $Å^3$	
Z	8	
Density (calculated)	1.718 Mg/m^3	
Absorption coefficient	2.395 mm^{-1}	
F(000)	2144	
Crystal size	0.290 x 0.130 x 0.015 mm^3	
Theta range for data collection	3.839 to 67.633°.	
Index ranges	-15<=h<=14, -15<=k<=16, -27<=l<=27	
Reflections collected	106939	
Independent reflections	3720 [R(int) = 0.0444]	
Completeness to theta = 67.633°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.5929	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3720 / 0 / 343	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0831	
R indices (all data)	R1 = 0.0337, wR2 = 0.0856	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.246 and -0.399 $e.Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6367(1)	5521(1)	7402(1)	26(1)
F(1)	1719(1)	4573(1)	9665(1)	31(1)
F(2)	2002(1)	2694(1)	9356(1)	34(1)
F(3)	4036(1)	777(1)	5494(1)	46(1)
F(4)	4280(1)	2108(1)	4660(1)	40(1)
F(5)	2689(1)	9072(1)	5484(1)	36(1)
F(6)	2210(1)	9659(1)	6549(1)	35(1)
N(1)	4448(1)	4889(1)	7706(1)	18(1)
N(2)	4396(1)	3183(1)	7430(1)	20(1)
N(3)	4972(1)	4411(1)	6765(1)	19(1)
N(4)	4675(1)	5533(1)	5983(1)	21(1)
N(5)	4532(1)	6075(1)	6960(1)	19(1)
N(6)	3677(1)	6469(1)	7834(1)	19(1)
C(1)	3876(1)	5542(1)	8020(1)	18(1)
C(2)	3377(1)	4935(1)	8455(1)	20(1)
C(3)	2740(1)	5177(1)	8913(1)	22(1)
C(4)	2313(1)	4398(1)	9206(1)	23(1)
C(5)	2467(1)	3406(1)	9044(1)	24(1)
C(6)	3081(1)	3145(1)	8596(1)	22(1)
C(7)	3566(1)	3924(1)	8312(1)	18(1)
C(8)	4216(1)	3915(1)	7811(1)	18(1)
C(9)	4716(1)	3454(1)	6902(1)	19(1)
C(10)	4619(1)	2935(1)	6353(1)	21(1)
C(11)	4362(1)	1951(1)	6227(1)	25(1)
C(12)	4265(1)	1712(1)	5653(1)	30(1)
C(13)	4388(1)	2420(1)	5212(1)	28(1)
C(14)	4601(1)	3397(1)	5324(1)	25(1)
C(15)	4725(1)	3655(1)	5906(1)	21(1)
C(16)	4866(1)	4615(1)	6186(1)	20(1)
C(17)	4442(1)	6231(1)	6376(1)	20(1)

C(18)	3874(1)	7147(1)	6320(1)	21(1)
C(19)	3555(1)	7672(1)	5831(1)	25(1)
C(20)	3003(1)	8515(1)	5931(1)	27(1)
C(21)	2743(1)	8818(1)	6492(1)	26(1)
C(22)	3002(1)	8283(1)	6976(1)	24(1)
C(23)	3579(1)	7438(1)	6886(1)	21(1)
C(24)	3956(1)	6691(1)	7289(1)	19(1)
B(1)	5067(1)	5211(1)	7206(1)	19(1)

Table S10. Bond lengths [Å] and angles [°] for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**.

Cl(1)-B(1)	1.8552(19)
F(1)-C(4)	1.3462(19)
F(2)-C(5)	1.3509(19)
F(3)-C(12)	1.343(2)
F(4)-C(13)	1.347(2)
F(5)-C(20)	1.3412(19)
F(6)-C(21)	1.346(2)
N(1)-C(8)	1.366(2)
N(1)-C(1)	1.371(2)
N(1)-B(1)	1.486(2)
N(2)-C(8)	1.339(2)
N(2)-C(9)	1.339(2)
N(3)-C(9)	1.367(2)
N(3)-C(16)	1.369(2)
N(3)-B(1)	1.484(2)
N(4)-C(17)	1.341(2)
N(4)-C(16)	1.343(2)
N(5)-C(24)	1.364(2)
N(5)-C(17)	1.366(2)
N(5)-B(1)	1.479(2)
N(6)-C(24)	1.343(2)
N(6)-C(1)	1.344(2)
C(1)-C(2)	1.457(2)
C(2)-C(3)	1.397(2)
C(2)-C(7)	1.420(2)
C(3)-C(4)	1.371(2)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.398(3)
C(5)-C(6)	1.368(2)
C(6)-C(7)	1.396(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.449(2)
C(9)-C(10)	1.450(2)

C(10)-C(11)	1.396(2)
C(10)-C(15)	1.419(2)
C(11)-C(12)	1.367(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.401(3)
C(13)-C(14)	1.367(3)
C(14)-C(15)	1.394(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.453(2)
C(17)-C(18)	1.455(2)
C(18)-C(19)	1.395(2)
C(18)-C(23)	1.417(2)
C(19)-C(20)	1.373(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.398(3)
C(21)-C(22)	1.372(2)
C(22)-C(23)	1.391(2)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.459(2)

C(8)-N(1)-C(1)	113.03(14)
C(8)-N(1)-B(1)	122.87(13)
C(1)-N(1)-B(1)	122.48(13)
C(8)-N(2)-C(9)	116.95(14)
C(9)-N(3)-C(16)	112.76(14)
C(9)-N(3)-B(1)	122.95(13)
C(16)-N(3)-B(1)	122.05(14)
C(17)-N(4)-C(16)	116.81(14)
C(24)-N(5)-C(17)	113.82(14)
C(24)-N(5)-B(1)	122.67(13)
C(17)-N(5)-B(1)	122.72(14)
C(24)-N(6)-C(1)	116.54(14)
N(6)-C(1)-N(1)	122.48(14)
N(6)-C(1)-C(2)	130.18(15)
N(1)-C(1)-C(2)	105.30(14)
C(3)-C(2)-C(7)	120.53(15)

C(3)-C(2)-C(1)	132.27(16)
C(7)-C(2)-C(1)	106.96(14)
C(4)-C(3)-C(2)	116.81(16)
C(4)-C(3)-H(3A)	121.6
C(2)-C(3)-H(3A)	121.6
F(1)-C(4)-C(3)	120.15(16)
F(1)-C(4)-C(5)	117.64(15)
C(3)-C(4)-C(5)	122.21(15)
F(2)-C(5)-C(6)	119.98(16)
F(2)-C(5)-C(4)	117.64(15)
C(6)-C(5)-C(4)	122.37(15)
C(5)-C(6)-C(7)	116.35(16)
C(5)-C(6)-H(6A)	121.8
C(7)-C(6)-H(6A)	121.8
C(6)-C(7)-C(2)	121.55(15)
C(6)-C(7)-C(8)	130.56(15)
C(2)-C(7)-C(8)	107.53(14)
N(2)-C(8)-N(1)	123.12(14)
N(2)-C(8)-C(7)	129.52(15)
N(1)-C(8)-C(7)	105.70(13)
N(2)-C(9)-N(3)	123.06(14)
N(2)-C(9)-C(10)	129.23(15)
N(3)-C(9)-C(10)	105.80(13)
C(11)-C(10)-C(15)	121.31(15)
C(11)-C(10)-C(9)	131.11(15)
C(15)-C(10)-C(9)	107.24(14)
C(12)-C(11)-C(10)	116.54(16)
C(12)-C(11)-H(11A)	121.7
C(10)-C(11)-H(11A)	121.7
F(3)-C(12)-C(11)	120.36(17)
F(3)-C(12)-C(13)	117.64(16)
C(11)-C(12)-C(13)	122.00(16)
F(4)-C(13)-C(14)	119.92(17)
F(4)-C(13)-C(12)	117.45(16)
C(14)-C(13)-C(12)	122.63(16)
C(13)-C(14)-C(15)	116.48(16)

C(13)-C(14)-H(14A)	121.8
C(15)-C(14)-H(14A)	121.8
C(14)-C(15)-C(10)	120.97(16)
C(14)-C(15)-C(16)	131.52(16)
C(10)-C(15)-C(16)	107.22(14)
N(4)-C(16)-N(3)	122.89(15)
N(4)-C(16)-C(15)	129.39(15)
N(3)-C(16)-C(15)	105.54(13)
N(4)-C(17)-N(5)	122.49(15)
N(4)-C(17)-C(18)	130.83(15)
N(5)-C(17)-C(18)	105.33(14)
C(19)-C(18)-C(23)	121.05(16)
C(19)-C(18)-C(17)	131.43(16)
C(23)-C(18)-C(17)	107.32(14)
C(20)-C(19)-C(18)	116.66(17)
C(20)-C(19)-H(19A)	121.7
C(18)-C(19)-H(19A)	121.7
F(5)-C(20)-C(19)	120.12(16)
F(5)-C(20)-C(21)	117.95(16)
C(19)-C(20)-C(21)	121.93(16)
F(6)-C(21)-C(22)	119.66(17)
F(6)-C(21)-C(20)	117.95(15)
C(22)-C(21)-C(20)	122.38(16)
C(21)-C(22)-C(23)	116.56(16)
C(21)-C(22)-H(22A)	121.7
C(23)-C(22)-H(22A)	121.7
C(22)-C(23)-C(18)	121.26(15)
C(22)-C(23)-C(24)	131.28(16)
C(18)-C(23)-C(24)	107.41(14)
N(6)-C(24)-N(5)	122.93(14)
N(6)-C(24)-C(23)	130.61(15)
N(5)-C(24)-C(23)	105.09(14)
N(5)-B(1)-N(3)	105.30(13)
N(5)-B(1)-N(1)	104.57(13)
N(3)-B(1)-N(1)	105.77(13)
N(5)-B(1)-Cl(1)	112.12(12)

N(3)-B(1)-Cl(1)	114.20(12)
N(1)-B(1)-Cl(1)	114.02(12)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	20(1)	29(1)	28(1)	-1(1)	-1(1)	0(1)
F(1)	31(1)	40(1)	22(1)	-2(1)	9(1)	-3(1)
F(2)	41(1)	31(1)	30(1)	9(1)	12(1)	-5(1)
F(3)	68(1)	33(1)	37(1)	-12(1)	0(1)	-19(1)
F(4)	47(1)	51(1)	21(1)	-11(1)	-3(1)	-13(1)
F(5)	36(1)	33(1)	39(1)	15(1)	-10(1)	4(1)
F(6)	30(1)	26(1)	49(1)	2(1)	-7(1)	10(1)
N(1)	18(1)	20(1)	16(1)	1(1)	-1(1)	0(1)
N(2)	21(1)	20(1)	18(1)	2(1)	-1(1)	4(1)
N(3)	20(1)	19(1)	16(1)	1(1)	1(1)	1(1)
N(4)	23(1)	22(1)	19(1)	3(1)	3(1)	0(1)
N(5)	19(1)	17(1)	19(1)	1(1)	1(1)	-1(1)
N(6)	19(1)	19(1)	20(1)	-1(1)	-1(1)	-2(1)
C(1)	18(1)	20(1)	17(1)	-2(1)	-2(1)	-1(1)
C(2)	20(1)	24(1)	15(1)	1(1)	-4(1)	-1(1)
C(3)	22(1)	25(1)	18(1)	-2(1)	-1(1)	0(1)
C(4)	20(1)	35(1)	15(1)	0(1)	1(1)	0(1)
C(5)	26(1)	28(1)	19(1)	7(1)	1(1)	-4(1)
C(6)	26(1)	23(1)	18(1)	3(1)	-2(1)	0(1)
C(7)	19(1)	22(1)	14(1)	1(1)	-3(1)	0(1)
C(8)	19(1)	19(1)	18(1)	3(1)	-4(1)	1(1)
C(9)	18(1)	19(1)	19(1)	1(1)	-2(1)	3(1)
C(10)	19(1)	23(1)	19(1)	-1(1)	1(1)	2(1)
C(11)	26(1)	24(1)	24(1)	-1(1)	0(1)	-1(1)
C(12)	31(1)	26(1)	31(1)	-8(1)	0(1)	-7(1)
C(13)	25(1)	39(1)	19(1)	-8(1)	-2(1)	-4(1)
C(14)	21(1)	34(1)	19(1)	0(1)	0(1)	0(1)
C(15)	19(1)	25(1)	19(1)	0(1)	1(1)	2(1)
C(16)	19(1)	25(1)	17(1)	1(1)	2(1)	1(1)
C(17)	20(1)	22(1)	19(1)	4(1)	2(1)	-2(1)

C(18)	20(1)	21(1)	24(1)	4(1)	-1(1)	-3(1)
C(19)	25(1)	25(1)	26(1)	6(1)	-1(1)	-3(1)
C(20)	22(1)	25(1)	32(1)	11(1)	-7(1)	-3(1)
C(21)	18(1)	19(1)	41(1)	3(1)	-4(1)	2(1)
C(22)	18(1)	22(1)	31(1)	0(1)	-1(1)	-2(1)
C(23)	18(1)	18(1)	25(1)	2(1)	-1(1)	-2(1)
C(24)	16(1)	18(1)	22(1)	-1(1)	0(1)	-3(1)
B(1)	17(1)	20(1)	19(1)	1(1)	0(1)	0(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**.

	x	y	z	U(eq)
H(3A)	2610	5849	9017	26
H(6A)	3172	2470	8484	27
H(11A)	4261	1473	6525	30
H(14A)	4661	3874	5022	30
H(19A)	3711	7458	5449	30
H(22A)	2798	8479	7354	28

Table S13. Torsion angles [°] for **Cl-F$_6$BsubPc (grown from solvent/vapour diffusion: benzene-heptane)**.

C(24)-N(6)-C(1)-N(1)	8.5(2)
C(24)-N(6)-C(1)-C(2)	-152.78(16)
C(8)-N(1)-C(1)-N(6)	-152.39(15)
B(1)-N(1)-C(1)-N(6)	13.4(2)
C(8)-N(1)-C(1)-C(2)	12.88(17)
B(1)-N(1)-C(1)-C(2)	178.71(14)
N(6)-C(1)-C(2)-C(3)	-19.7(3)
N(1)-C(1)-C(2)-C(3)	176.57(17)
N(6)-C(1)-C(2)-C(7)	154.53(16)
N(1)-C(1)-C(2)-C(7)	-9.17(17)
C(7)-C(2)-C(3)-C(4)	-0.5(2)
C(1)-C(2)-C(3)-C(4)	173.13(17)
C(2)-C(3)-C(4)-F(1)	177.69(14)
C(2)-C(3)-C(4)-C(5)	-2.7(2)
F(1)-C(4)-C(5)-F(2)	0.5(2)
C(3)-C(4)-C(5)-F(2)	-179.14(15)
F(1)-C(4)-C(5)-C(6)	-177.91(15)
C(3)-C(4)-C(5)-C(6)	2.4(3)
F(2)-C(5)-C(6)-C(7)	-177.27(15)
C(4)-C(5)-C(6)-C(7)	1.1(3)
C(5)-C(6)-C(7)-C(2)	-4.3(2)
C(5)-C(6)-C(7)-C(8)	-176.48(16)
C(3)-C(2)-C(7)-C(6)	4.1(2)
C(1)-C(2)-C(7)-C(6)	-170.99(15)
C(3)-C(2)-C(7)-C(8)	177.88(14)
C(1)-C(2)-C(7)-C(8)	2.82(17)
C(9)-N(2)-C(8)-N(1)	-7.5(2)
C(9)-N(2)-C(8)-C(7)	155.70(16)
C(1)-N(1)-C(8)-N(2)	155.42(15)
B(1)-N(1)-C(8)-N(2)	-10.3(2)
C(1)-N(1)-C(8)-C(7)	-11.17(18)
B(1)-N(1)-C(8)-C(7)	-176.94(14)
C(6)-C(7)-C(8)-N(2)	12.3(3)

C(2)-C(7)-C(8)-N(2)	-160.78(16)
C(6)-C(7)-C(8)-N(1)	177.69(16)
C(2)-C(7)-C(8)-N(1)	4.64(17)
C(8)-N(2)-C(9)-N(3)	7.9(2)
C(8)-N(2)-C(9)-C(10)	-154.06(16)
C(16)-N(3)-C(9)-N(2)	-153.75(15)
B(1)-N(3)-C(9)-N(2)	9.5(2)
C(16)-N(3)-C(9)-C(10)	11.81(18)
B(1)-N(3)-C(9)-C(10)	175.08(14)
N(2)-C(9)-C(10)-C(11)	-14.9(3)
N(3)-C(9)-C(10)-C(11)	-179.21(17)
N(2)-C(9)-C(10)-C(15)	158.28(16)
N(3)-C(9)-C(10)-C(15)	-6.07(18)
C(15)-C(10)-C(11)-C(12)	2.9(3)
C(9)-C(10)-C(11)-C(12)	175.25(17)
C(10)-C(11)-C(12)-F(3)	178.94(16)
C(10)-C(11)-C(12)-C(13)	-1.8(3)
F(3)-C(12)-C(13)-F(4)	-1.0(3)
C(11)-C(12)-C(13)-F(4)	179.75(17)
F(3)-C(12)-C(13)-C(14)	178.58(17)
C(11)-C(12)-C(13)-C(14)	-0.7(3)
F(4)-C(13)-C(14)-C(15)	-178.45(16)
C(12)-C(13)-C(14)-C(15)	2.0(3)
C(13)-C(14)-C(15)-C(10)	-0.8(2)
C(13)-C(14)-C(15)-C(16)	-173.75(18)
C(11)-C(10)-C(15)-C(14)	-1.7(3)
C(9)-C(10)-C(15)-C(14)	-175.62(15)
C(11)-C(10)-C(15)-C(16)	172.78(16)
C(9)-C(10)-C(15)-C(16)	-1.17(18)
C(17)-N(4)-C(16)-N(3)	-9.8(2)
C(17)-N(4)-C(16)-C(15)	150.91(17)
C(9)-N(3)-C(16)-N(4)	152.12(16)
B(1)-N(3)-C(16)-N(4)	-11.3(2)
C(9)-N(3)-C(16)-C(15)	-12.51(18)
B(1)-N(3)-C(16)-C(15)	-175.95(14)
C(14)-C(15)-C(16)-N(4)	18.3(3)

C(10)-C(15)-C(16)-N(4)	-155.31(17)
C(14)-C(15)-C(16)-N(3)	-178.41(17)
C(10)-C(15)-C(16)-N(3)	7.96(18)
C(16)-N(4)-C(17)-N(5)	9.5(2)
C(16)-N(4)-C(17)-C(18)	-155.23(17)
C(24)-N(5)-C(17)-N(4)	-158.04(15)
B(1)-N(5)-C(17)-N(4)	12.0(2)
C(24)-N(5)-C(17)-C(18)	10.05(18)
B(1)-N(5)-C(17)-C(18)	-179.89(14)
N(4)-C(17)-C(18)-C(19)	-13.4(3)
N(5)-C(17)-C(18)-C(19)	179.94(17)
N(4)-C(17)-C(18)-C(23)	161.44(17)
N(5)-C(17)-C(18)-C(23)	-5.26(18)
C(23)-C(18)-C(19)-C(20)	4.3(2)
C(17)-C(18)-C(19)-C(20)	178.50(17)
C(18)-C(19)-C(20)-F(5)	178.42(15)
C(18)-C(19)-C(20)-C(21)	-2.0(3)
F(5)-C(20)-C(21)-F(6)	-1.1(2)
C(19)-C(20)-C(21)-F(6)	179.29(15)
F(5)-C(20)-C(21)-C(22)	177.98(15)
C(19)-C(20)-C(21)-C(22)	-1.6(3)
F(6)-C(21)-C(22)-C(23)	-178.12(14)
C(20)-C(21)-C(22)-C(23)	2.8(3)
C(21)-C(22)-C(23)-C(18)	-0.4(2)
C(21)-C(22)-C(23)-C(24)	-177.78(17)
C(19)-C(18)-C(23)-C(22)	-3.2(3)
C(17)-C(18)-C(23)-C(22)	-178.63(15)
C(19)-C(18)-C(23)-C(24)	174.72(15)
C(17)-C(18)-C(23)-C(24)	-0.72(18)
C(1)-N(6)-C(24)-N(5)	-9.0(2)
C(1)-N(6)-C(24)-C(23)	155.59(16)
C(17)-N(5)-C(24)-N(6)	157.48(15)
B(1)-N(5)-C(24)-N(6)	-12.6(2)
C(17)-N(5)-C(24)-C(23)	-10.47(18)
B(1)-N(5)-C(24)-C(23)	179.46(14)
C(22)-C(23)-C(24)-N(6)	17.4(3)

C(18)-C(23)-C(24)-N(6)	-160.21(16)
C(22)-C(23)-C(24)-N(5)	-175.95(17)
C(18)-C(23)-C(24)-N(5)	6.43(17)
C(24)-N(5)-B(1)-N(3)	140.66(15)
C(17)-N(5)-B(1)-N(3)	-28.5(2)
C(24)-N(5)-B(1)-N(1)	29.4(2)
C(17)-N(5)-B(1)-N(1)	-139.76(15)
C(24)-N(5)-B(1)-Cl(1)	-94.59(16)
C(17)-N(5)-B(1)-Cl(1)	96.22(16)
C(9)-N(3)-B(1)-N(5)	-133.70(15)
C(16)-N(3)-B(1)-N(5)	28.0(2)
C(9)-N(3)-B(1)-N(1)	-23.3(2)
C(16)-N(3)-B(1)-N(1)	138.42(15)
C(9)-N(3)-B(1)-Cl(1)	102.87(16)
C(16)-N(3)-B(1)-Cl(1)	-95.38(16)
C(8)-N(1)-B(1)-N(5)	134.62(15)
C(1)-N(1)-B(1)-N(5)	-29.8(2)
C(8)-N(1)-B(1)-N(3)	23.7(2)
C(1)-N(1)-B(1)-N(3)	-140.72(14)
C(8)-N(1)-B(1)-Cl(1)	-102.59(16)
C(1)-N(1)-B(1)-Cl(1)	92.97(16)

Symmetry transformations used to generate equivalent atoms:

Table S14. Crystal data and structure refinement for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**

Empirical formula	C24 H6 B Cl F6 N6	
Formula weight	538.61	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 13.4953(4) Å	a= 90°.
	b = 13.4233(4) Å	b= 90°.
	c = 23.0059(7) Å	g = 90°.
Volume	4167.6(2) $Å^3$	
Z	8	
Density (calculated)	1.717 Mg/m^3	
Absorption coefficient	2.394 mm^{-1}	
F(000)	2144	
Crystal size	0.200 x 0.180 x 0.010 mm^3	
Theta range for data collection	3.843 to 67.356°.	
Index ranges	-16<=h<=16, -15<=k<=15, -27<=l<=27	
Reflections collected	77485	
Independent reflections	3708 [R(int) = 0.0620]	
Completeness to theta = 67.356°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6167	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3708 / 0 / 343	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0931	
R indices (all data)	R1 = 0.0417, wR2 = 0.0976	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.393 and -0.484 e.$Å^{-3}$	

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6366(1)	5519(1)	7400(1)	32(1)
F(1)	1997(1)	2691(1)	9356(1)	39(1)
F(2)	1719(1)	4571(1)	9666(1)	35(1)
F(3)	2208(1)	9655(1)	6554(1)	39(1)
F(4)	2690(1)	9069(1)	5486(1)	40(1)
F(5)	4280(1)	2111(1)	4659(1)	44(1)
F(6)	4033(1)	777(1)	5492(1)	51(1)
N(1)	4446(1)	4886(1)	7710(1)	22(1)
N(2)	3680(1)	6467(1)	7838(1)	24(1)
N(3)	4534(1)	6073(1)	6964(1)	23(1)
N(4)	4675(1)	5532(1)	5985(1)	26(1)
N(5)	4969(1)	4409(1)	6768(1)	23(1)
N(6)	4390(1)	3180(1)	7430(1)	24(1)
C(1)	4212(1)	3912(1)	7813(1)	22(1)
C(2)	3564(2)	3919(2)	8313(1)	23(1)
C(3)	3077(2)	3143(2)	8597(1)	27(1)
C(4)	2464(2)	3403(2)	9044(1)	28(1)
C(5)	2313(2)	4395(2)	9207(1)	27(1)
C(6)	2742(2)	5173(2)	8916(1)	26(1)
C(7)	3379(2)	4931(2)	8457(1)	24(1)
C(8)	3876(2)	5538(1)	8023(1)	23(1)
C(9)	3957(1)	6690(1)	7293(1)	23(1)
C(10)	3584(1)	7437(2)	6889(1)	25(1)
C(11)	3004(2)	8281(2)	6978(1)	28(1)
C(12)	2746(2)	8814(2)	6496(1)	30(1)
C(13)	3004(2)	8513(2)	5934(1)	30(1)
C(14)	3559(2)	7671(2)	5834(1)	29(1)
C(15)	3875(2)	7147(2)	6323(1)	26(1)
C(16)	4444(2)	6230(2)	6380(1)	24(1)
C(17)	4863(2)	4614(2)	6188(1)	24(1)

C(18)	4722(2)	3654(2)	5907(1)	25(1)
C(19)	4600(2)	3397(2)	5326(1)	28(1)
C(20)	4386(2)	2422(2)	5211(1)	32(1)
C(21)	4262(2)	1712(2)	5654(1)	34(1)
C(22)	4357(2)	1950(2)	6227(1)	28(1)
C(23)	4616(1)	2933(2)	6354(1)	24(1)
C(24)	4712(1)	3451(1)	6904(1)	23(1)
B(1)	5064(2)	5207(2)	7209(1)	24(1)

Table S16. Bond lengths [Å] and angles [°] for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**.

Cl(1)-B(1)	1.859(2)
F(1)-C(4)	1.350(2)
F(2)-C(5)	1.347(2)
F(3)-C(12)	1.349(2)
F(4)-C(13)	1.340(2)
F(5)-C(20)	1.345(2)
F(6)-C(21)	1.345(3)
N(1)-C(1)	1.367(3)
N(1)-C(8)	1.371(3)
N(1)-B(1)	1.485(3)
N(2)-C(9)	1.341(3)
N(2)-C(8)	1.345(3)
N(3)-C(16)	1.365(3)
N(3)-C(9)	1.366(3)
N(3)-B(1)	1.477(3)
N(4)-C(16)	1.341(3)
N(4)-C(17)	1.342(3)
N(5)-C(24)	1.369(3)
N(5)-C(17)	1.369(3)
N(5)-B(1)	1.481(3)
N(6)-C(24)	1.337(3)
N(6)-C(1)	1.339(3)
C(1)-C(2)	1.446(3)
C(2)-C(3)	1.395(3)
C(2)-C(7)	1.421(3)
C(3)-C(4)	1.366(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.398(3)
C(5)-C(6)	1.370(3)
C(6)-C(7)	1.399(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.453(3)
C(9)-C(10)	1.458(3)

C(10)-C(11)	1.392(3)
C(10)-C(15)	1.414(3)
C(11)-C(12)	1.366(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.398(3)
C(13)-C(14)	1.375(3)
C(14)-C(15)	1.393(3)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.457(3)
C(17)-C(18)	1.454(3)
C(18)-C(19)	1.391(3)
C(18)-C(23)	1.419(3)
C(19)-C(20)	1.365(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.404(3)
C(21)-C(22)	1.364(3)
C(22)-C(23)	1.396(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.450(3)

C(1)-N(1)-C(8)	112.95(17)
C(1)-N(1)-B(1)	122.78(17)
C(8)-N(1)-B(1)	122.59(17)
C(9)-N(2)-C(8)	116.60(17)
C(16)-N(3)-C(9)	113.74(16)
C(16)-N(3)-B(1)	122.69(17)
C(9)-N(3)-B(1)	122.72(17)
C(16)-N(4)-C(17)	116.80(17)
C(24)-N(5)-C(17)	112.68(17)
C(24)-N(5)-B(1)	122.98(17)
C(17)-N(5)-B(1)	122.07(17)
C(24)-N(6)-C(1)	116.99(17)
N(6)-C(1)-N(1)	123.13(18)
N(6)-C(1)-C(2)	129.49(18)
N(1)-C(1)-C(2)	105.73(16)
C(3)-C(2)-C(7)	121.48(19)

C(3)-C(2)-C(1)	130.74(19)
C(7)-C(2)-C(1)	107.42(17)
C(4)-C(3)-C(2)	116.54(19)
C(4)-C(3)-H(3A)	121.7
C(2)-C(3)-H(3A)	121.7
F(1)-C(4)-C(3)	120.06(19)
F(1)-C(4)-C(5)	117.62(18)
C(3)-C(4)-C(5)	122.29(19)
F(2)-C(5)-C(6)	120.14(19)
F(2)-C(5)-C(4)	117.64(18)
C(6)-C(5)-C(4)	122.21(19)
C(5)-C(6)-C(7)	116.88(19)
C(5)-C(6)-H(6A)	121.6
C(7)-C(6)-H(6A)	121.6
C(6)-C(7)-C(2)	120.43(19)
C(6)-C(7)-C(8)	132.22(19)
C(2)-C(7)-C(8)	107.10(17)
N(2)-C(8)-N(1)	122.36(18)
N(2)-C(8)-C(7)	130.34(18)
N(1)-C(8)-C(7)	105.29(17)
N(2)-C(9)-N(3)	122.91(18)
N(2)-C(9)-C(10)	130.72(18)
N(3)-C(9)-C(10)	105.04(17)
C(11)-C(10)-C(15)	121.08(19)
C(11)-C(10)-C(9)	131.29(19)
C(15)-C(10)-C(9)	107.57(17)
C(12)-C(11)-C(10)	116.7(2)
C(12)-C(11)-H(11A)	121.7
C(10)-C(11)-H(11A)	121.7
F(3)-C(12)-C(11)	119.7(2)
F(3)-C(12)-C(13)	117.79(19)
C(11)-C(12)-C(13)	122.47(19)
F(4)-C(13)-C(14)	120.1(2)
F(4)-C(13)-C(12)	118.11(19)
C(14)-C(13)-C(12)	121.81(19)
C(13)-C(14)-C(15)	116.6(2)

C(13)-C(14)-H(14A)	121.7
C(15)-C(14)-H(14A)	121.7
C(14)-C(15)-C(10)	121.24(19)
C(14)-C(15)-C(16)	131.3(2)
C(10)-C(15)-C(16)	107.25(17)
N(4)-C(16)-N(3)	122.51(18)
N(4)-C(16)-C(15)	130.71(18)
N(3)-C(16)-C(15)	105.37(17)
N(4)-C(17)-N(5)	122.87(18)
N(4)-C(17)-C(18)	129.38(18)
N(5)-C(17)-C(18)	105.61(16)
C(19)-C(18)-C(23)	120.99(19)
C(19)-C(18)-C(17)	131.54(19)
C(23)-C(18)-C(17)	107.18(17)
C(20)-C(19)-C(18)	116.6(2)
C(20)-C(19)-H(19A)	121.7
C(18)-C(19)-H(19A)	121.7
F(5)-C(20)-C(19)	120.1(2)
F(5)-C(20)-C(21)	117.5(2)
C(19)-C(20)-C(21)	122.4(2)
F(6)-C(21)-C(22)	120.5(2)
F(6)-C(21)-C(20)	117.39(19)
C(22)-C(21)-C(20)	122.1(2)
C(21)-C(22)-C(23)	116.5(2)
C(21)-C(22)-H(22A)	121.7
C(23)-C(22)-H(22A)	121.7
C(22)-C(23)-C(18)	121.30(19)
C(22)-C(23)-C(24)	131.09(19)
C(18)-C(23)-C(24)	107.25(17)
N(6)-C(24)-N(5)	123.04(18)
N(6)-C(24)-C(23)	129.20(18)
N(5)-C(24)-C(23)	105.81(16)
N(3)-B(1)-N(5)	105.45(17)
N(3)-B(1)-N(1)	104.65(17)
N(5)-B(1)-N(1)	105.88(16)
N(3)-B(1)-Cl(1)	111.73(14)

N(5)-B(1)-Cl(1)	113.97(15)
N(1)-B(1)-Cl(1)	114.32(15)

Symmetry transformations used to generate equivalent atoms:

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	28(1)	33(1)	34(1)	-1(1)	-1(1)	1(1)
F(1)	49(1)	33(1)	34(1)	9(1)	12(1)	-4(1)
F(2)	38(1)	42(1)	26(1)	-2(1)	8(1)	-3(1)
F(3)	35(1)	28(1)	54(1)	2(1)	-7(1)	10(1)
F(4)	41(1)	36(1)	45(1)	16(1)	-10(1)	4(1)
F(5)	52(1)	55(1)	26(1)	-10(1)	-3(1)	-14(1)
F(6)	75(1)	36(1)	41(1)	-12(1)	0(1)	-20(1)
N(1)	25(1)	21(1)	21(1)	0(1)	-2(1)	1(1)
N(2)	26(1)	22(1)	25(1)	-1(1)	-2(1)	-1(1)
N(3)	24(1)	20(1)	25(1)	1(1)	1(1)	-1(1)
N(4)	28(1)	24(1)	25(1)	3(1)	3(1)	0(1)
N(5)	25(1)	21(1)	22(1)	0(1)	1(1)	1(1)
N(6)	27(1)	22(1)	22(1)	2(1)	-2(1)	3(1)
C(1)	26(1)	20(1)	21(1)	2(1)	-5(1)	2(1)
C(2)	27(1)	24(1)	18(1)	2(1)	-5(1)	0(1)
C(3)	33(1)	24(1)	23(1)	3(1)	-3(1)	1(1)
C(4)	33(1)	29(1)	22(1)	8(1)	-1(1)	-4(1)
C(5)	27(1)	37(1)	17(1)	0(1)	0(1)	1(1)
C(6)	30(1)	27(1)	23(1)	-2(1)	-2(1)	1(1)
C(7)	28(1)	25(1)	20(1)	0(1)	-5(1)	-1(1)
C(8)	25(1)	22(1)	21(1)	-2(1)	-3(1)	-1(1)
C(9)	22(1)	21(1)	26(1)	-1(1)	0(1)	-3(1)
C(10)	22(1)	20(1)	31(1)	3(1)	0(1)	-2(1)
C(11)	22(1)	24(1)	36(1)	0(1)	-1(1)	-3(1)
C(12)	23(1)	20(1)	45(1)	3(1)	-4(1)	1(1)
C(13)	27(1)	28(1)	37(1)	11(1)	-6(1)	-3(1)
C(14)	29(1)	27(1)	30(1)	6(1)	0(1)	-2(1)
C(15)	25(1)	22(1)	30(1)	3(1)	0(1)	-3(1)
C(16)	25(1)	24(1)	24(1)	4(1)	2(1)	-2(1)
C(17)	24(1)	26(1)	22(1)	1(1)	3(1)	1(1)

C(18)	23(1)	28(1)	24(1)	1(1)	1(1)	3(1)
C(19)	26(1)	36(1)	24(1)	1(1)	1(1)	1(1)
C(20)	30(1)	43(1)	23(1)	-8(1)	-2(1)	-4(1)
C(21)	37(1)	28(1)	36(1)	-8(1)	0(1)	-7(1)
C(22)	32(1)	26(1)	27(1)	0(1)	0(1)	-1(1)
C(23)	24(1)	25(1)	24(1)	0(1)	0(1)	3(1)
C(24)	24(1)	21(1)	24(1)	1(1)	-3(1)	4(1)
B(1)	24(1)	23(1)	24(1)	-1(1)	-1(1)	-1(1)

Table S18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**.

	x	y	z	U(eq)
H(3A)	3167	2467	8485	32
H(6A)	2613	5846	9020	32
H(11A)	2799	8477	7357	33
H(14A)	3718	7458	5452	35
H(19A)	4661	3876	5023	34
H(22A)	4252	1472	6525	34

Table S19. Torsion angles [°] for **Cl-F_6BsubPc (grown from solvent/vapour diffusion: benzene-methanol)**.

C(24)-N(6)-C(1)-N(1)	-7.4(3)
C(24)-N(6)-C(1)-C(2)	155.8(2)
C(8)-N(1)-C(1)-N(6)	155.34(18)
B(1)-N(1)-C(1)-N(6)	-10.2(3)
C(8)-N(1)-C(1)-C(2)	-11.3(2)
B(1)-N(1)-C(1)-C(2)	-176.82(17)
N(6)-C(1)-C(2)-C(3)	12.3(4)
N(1)-C(1)-C(2)-C(3)	177.7(2)
N(6)-C(1)-C(2)-C(7)	-160.78(19)
N(1)-C(1)-C(2)-C(7)	4.7(2)
C(7)-C(2)-C(3)-C(4)	-4.1(3)
C(1)-C(2)-C(3)-C(4)	-176.3(2)
C(2)-C(3)-C(4)-F(1)	-177.25(18)
C(2)-C(3)-C(4)-C(5)	1.0(3)
F(1)-C(4)-C(5)-F(2)	0.4(3)
C(3)-C(4)-C(5)-F(2)	-177.86(18)
F(1)-C(4)-C(5)-C(6)	-179.21(18)
C(3)-C(4)-C(5)-C(6)	2.5(3)
F(2)-C(5)-C(6)-C(7)	177.70(18)
C(4)-C(5)-C(6)-C(7)	-2.7(3)
C(5)-C(6)-C(7)-C(2)	-0.5(3)
C(5)-C(6)-C(7)-C(8)	173.0(2)
C(3)-C(2)-C(7)-C(6)	4.0(3)
C(1)-C(2)-C(7)-C(6)	177.78(17)
C(3)-C(2)-C(7)-C(8)	-170.94(18)
C(1)-C(2)-C(7)-C(8)	2.9(2)
C(9)-N(2)-C(8)-N(1)	8.7(3)
C(9)-N(2)-C(8)-C(7)	-152.7(2)
C(1)-N(1)-C(8)-N(2)	-152.36(18)
B(1)-N(1)-C(8)-N(2)	13.2(3)
C(1)-N(1)-C(8)-C(7)	13.0(2)
B(1)-N(1)-C(8)-C(7)	178.59(17)
C(6)-C(7)-C(8)-N(2)	-19.6(4)

C(2)-C(7)-C(8)-N(2)	154.5(2)
C(6)-C(7)-C(8)-N(1)	176.6(2)
C(2)-C(7)-C(8)-N(1)	-9.3(2)
C(8)-N(2)-C(9)-N(3)	-9.3(3)
C(8)-N(2)-C(9)-C(10)	155.5(2)
C(16)-N(3)-C(9)-N(2)	157.52(18)
B(1)-N(3)-C(9)-N(2)	-12.2(3)
C(16)-N(3)-C(9)-C(10)	-10.6(2)
B(1)-N(3)-C(9)-C(10)	179.72(17)
N(2)-C(9)-C(10)-C(11)	17.0(4)
N(3)-C(9)-C(10)-C(11)	-176.2(2)
N(2)-C(9)-C(10)-C(15)	-160.1(2)
N(3)-C(9)-C(10)-C(15)	6.7(2)
C(15)-C(10)-C(11)-C(12)	-0.7(3)
C(9)-C(10)-C(11)-C(12)	-177.5(2)
C(10)-C(11)-C(12)-F(3)	-178.16(17)
C(10)-C(11)-C(12)-C(13)	2.9(3)
F(3)-C(12)-C(13)-F(4)	-1.1(3)
C(11)-C(12)-C(13)-F(4)	177.91(19)
F(3)-C(12)-C(13)-C(14)	179.38(18)
C(11)-C(12)-C(13)-C(14)	-1.7(3)
F(4)-C(13)-C(14)-C(15)	178.61(18)
C(12)-C(13)-C(14)-C(15)	-1.8(3)
C(13)-C(14)-C(15)-C(10)	3.9(3)
C(13)-C(14)-C(15)-C(16)	178.5(2)
C(11)-C(10)-C(15)-C(14)	-2.7(3)
C(9)-C(10)-C(15)-C(14)	174.69(18)
C(11)-C(10)-C(15)-C(16)	-178.44(18)
C(9)-C(10)-C(15)-C(16)	-1.0(2)
C(17)-N(4)-C(16)-N(3)	9.5(3)
C(17)-N(4)-C(16)-C(15)	-154.9(2)
C(9)-N(3)-C(16)-N(4)	-157.79(18)
B(1)-N(3)-C(16)-N(4)	11.9(3)
C(9)-N(3)-C(16)-C(15)	10.0(2)
B(1)-N(3)-C(16)-C(15)	179.70(17)
C(14)-C(15)-C(16)-N(4)	-13.8(4)

C(10)-C(15)-C(16)-N(4)	161.3(2)
C(14)-C(15)-C(16)-N(3)	179.8(2)
C(10)-C(15)-C(16)-N(3)	-5.1(2)
C(16)-N(4)-C(17)-N(5)	-9.8(3)
C(16)-N(4)-C(17)-C(18)	151.1(2)
C(24)-N(5)-C(17)-N(4)	152.19(19)
B(1)-N(5)-C(17)-N(4)	-11.2(3)
C(24)-N(5)-C(17)-C(18)	-12.6(2)
B(1)-N(5)-C(17)-C(18)	-175.92(17)
N(4)-C(17)-C(18)-C(19)	18.3(4)
N(5)-C(17)-C(18)-C(19)	-178.3(2)
N(4)-C(17)-C(18)-C(23)	-155.4(2)
N(5)-C(17)-C(18)-C(23)	8.0(2)
C(23)-C(18)-C(19)-C(20)	-0.8(3)
C(17)-C(18)-C(19)-C(20)	-173.8(2)
C(18)-C(19)-C(20)-F(5)	-178.43(19)
C(18)-C(19)-C(20)-C(21)	2.1(3)
F(5)-C(20)-C(21)-F(6)	-0.9(3)
C(19)-C(20)-C(21)-F(6)	178.7(2)
F(5)-C(20)-C(21)-C(22)	179.8(2)
C(19)-C(20)-C(21)-C(22)	-0.7(4)
F(6)-C(21)-C(22)-C(23)	178.7(2)
C(20)-C(21)-C(22)-C(23)	-2.0(3)
C(21)-C(22)-C(23)-C(18)	3.2(3)
C(21)-C(22)-C(23)-C(24)	175.3(2)
C(19)-C(18)-C(23)-C(22)	-1.9(3)
C(17)-C(18)-C(23)-C(22)	172.63(19)
C(19)-C(18)-C(23)-C(24)	-175.67(18)
C(17)-C(18)-C(23)-C(24)	-1.2(2)
C(1)-N(6)-C(24)-N(5)	7.7(3)
C(1)-N(6)-C(24)-C(23)	-154.1(2)
C(17)-N(5)-C(24)-N(6)	-153.56(19)
B(1)-N(5)-C(24)-N(6)	9.6(3)
C(17)-N(5)-C(24)-C(23)	11.9(2)
B(1)-N(5)-C(24)-C(23)	175.05(17)
C(22)-C(23)-C(24)-N(6)	-14.9(4)

C(18)-C(23)-C(24)-N(6)	158.1(2)
C(22)-C(23)-C(24)-N(5)	-179.1(2)
C(18)-C(23)-C(24)-N(5)	-6.1(2)
C(16)-N(3)-B(1)-N(5)	-28.3(2)
C(9)-N(3)-B(1)-N(5)	140.47(18)
C(16)-N(3)-B(1)-N(1)	-139.76(18)
C(9)-N(3)-B(1)-N(1)	29.0(2)
C(16)-N(3)-B(1)-Cl(1)	96.0(2)
C(9)-N(3)-B(1)-Cl(1)	-95.2(2)
C(24)-N(5)-B(1)-N(3)	-133.82(18)
C(17)-N(5)-B(1)-N(3)	27.8(2)
C(24)-N(5)-B(1)-N(1)	-23.2(2)
C(17)-N(5)-B(1)-N(1)	138.39(18)
C(24)-N(5)-B(1)-Cl(1)	103.28(19)
C(17)-N(5)-B(1)-Cl(1)	-95.1(2)
C(1)-N(1)-B(1)-N(3)	134.65(18)
C(8)-N(1)-B(1)-N(3)	-29.5(2)
C(1)-N(1)-B(1)-N(5)	23.5(2)
C(8)-N(1)-B(1)-N(5)	-140.67(18)
C(1)-N(1)-B(1)-Cl(1)	-102.80(19)
C(8)-N(1)-B(1)-Cl(1)	93.0(2)

Symmetry transformations used to generate equivalent atoms:

Table S20. Crystal data and structure refinement for **F-F_6BsubPc (grown by train sublimation)**

Empirical formula	C24 H6 B F7 N6	
Formula weight	522.16	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/m$	
Unit cell dimensions	a = 13.1545(4) Å	a= 90°.
	b = 19.3823(6) Å	b= 117.621(2)°.
	c = 13.5266(4) Å	g = 90°.
Volume	3055.75(17) $Å^3$	
Z	6	
Density (calculated)	1.702 Mg/m^3	
Absorption coefficient	1.321 mm^{-1}	
F(000)	1560	
Crystal size	0.080 x 0.040 x 0.010 mm^3	
Theta range for data collection	3.688 to 67.241°.	
Index ranges	-15<=h<=13, 0<=k<=23, 0<=l<=16	
Reflections collected	118237	
Independent reflections	5714 [R(int) = 0.1421]	
Completeness to theta = 67.241°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.5584	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5714 / 513 / 533	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0696, wR2 = 0.1533	
R indices (all data)	R1 = 0.1858, wR2 = 0.2188	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.296 and -0.310 e.$Å^{-3}$	

Table S21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **F-F_6BsubPc (grown by train sublimation)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1A)	-1202(6)	2500	9044(6)	34(2)
F(2A)	1191(5)	4862(3)	5652(5)	55(2)
F(3A)	2055(5)	5550(3)	7561(5)	47(2)
F(4A)	4759(5)	3193(3)	14464(4)	58(2)
N(1A)	-188(8)	2500	6865(8)	25(2)
N(2A)	41(6)	3104(3)	8489(5)	23(1)
N(3A)	1287(6)	3685(3)	10187(5)	22(1)
N(4A)	830(8)	2500	10229(8)	23(2)
C(1A)	-53(7)	3067(4)	7433(6)	26(2)
C(2A)	366(7)	3747(4)	7281(7)	28(2)
C(3A)	462(7)	3974(5)	6333(7)	33(2)
C(4A)	1032(8)	4590(5)	6486(8)	35(2)
C(5A)	1474(9)	4959(4)	7476(9)	36(2)
C(6A)	1413(7)	4719(4)	8411(7)	30(2)
C(7A)	801(7)	4095(4)	8253(7)	24(2)
C(8A)	689(7)	3675(4)	9092(7)	24(2)
C(9A)	1397(7)	3068(4)	10735(6)	22(2)
C(10A)	2295(7)	2869(4)	11805(7)	27(2)
C(11A)	3149(7)	3236(5)	12706(6)	28(2)
C(12A)	3954(8)	2859(5)	13582(8)	41(2)
B(1A)	-134(12)	2500	9094(11)	23(2)
F(1C)	4542(5)	7500	966(5)	25(1)
F(2C)	2125(5)	5129(3)	4344(5)	52(2)
F(3C)	1275(5)	4453(3)	2444(6)	54(2)
F(4C)	-1434(5)	6818(3)	-4455(5)	60(2)
N(1C)	3519(9)	7500	3120(8)	30(2)
N(2C)	3284(5)	6884(3)	1499(5)	21(1)
N(3C)	2046(6)	6306(3)	-197(6)	25(2)
N(4C)	2525(8)	7500	-190(8)	22(2)
C(1C)	3383(7)	6894(4)	2544(7)	28(2)

C(2C)	2983(7)	6264(4)	2761(7)	27(2)
C(3C)	2852(8)	6000(5)	3662(8)	37(2)
C(4C)	2285(8)	5403(6)	3506(8)	41(2)
C(5C)	1819(8)	5042(5)	2510(9)	41(2)
C(6C)	1921(8)	5265(4)	1583(8)	37(2)
C(7C)	2511(8)	5892(5)	1718(8)	31(2)
C(8C)	2658(7)	6321(4)	912(7)	25(2)
C(9C)	1932(7)	6917(4)	-742(6)	22(2)
C(10C)	1019(7)	7137(4)	-1820(7)	26(2)
C(11C)	184(8)	6762(5)	-2701(8)	39(2)
C(12C)	-594(8)	7132(4)	-3546(8)	39(2)
B(1C)	3472(11)	7500	955(10)	21(2)
F(1B)	7886(5)	7500	963(5)	26(2)
F(2B)	5451(5)	9868(3)	4339(5)	54(2)
F(3B)	4618(5)	10570(3)	2447(6)	56(2)
F(4B)	1895(5)	8185(3)	-4448(5)	58(2)
N(1B)	6860(8)	7500	3117(8)	29(2)
N(2B)	6625(6)	8127(3)	1511(5)	24(1)
N(3B)	5398(6)	8669(4)	-198(6)	28(2)
N(4B)	5837(7)	7500	-199(7)	18(2)
C(1B)	6723(7)	8088(4)	2562(6)	24(2)
C(2B)	6318(8)	8744(4)	2755(8)	30(2)
C(3B)	6195(8)	8988(5)	3642(8)	36(2)
C(4B)	5614(9)	9617(5)	3508(9)	40(2)
C(5B)	5175(8)	9970(4)	2495(9)	38(2)
C(6B)	5287(8)	9739(4)	1614(8)	35(2)
C(7B)	5850(7)	9130(4)	1709(7)	28(2)
C(8B)	5995(7)	8659(4)	941(7)	24(2)
C(9B)	5269(7)	8099(4)	-729(6)	24(2)
C(10B)	4366(7)	7864(4)	-1802(7)	24(2)
C(11B)	3541(7)	8228(5)	-2684(7)	32(2)
C(12B)	2729(8)	7850(5)	-3565(8)	39(2)
B(1B)	6812(11)	7500	963(11)	22(2)

Table S22. Bond lengths [Å] and angles [°] for F-**F_6BsubPc (grown by train sublimation)**.

F(1A)-B(1A)	1.374(14)
F(2A)-C(4A)	1.346(10)
F(3A)-C(5A)	1.353(10)
F(4A)-C(12A)	1.339(10)
N(1A)-C(1A)	1.305(10)
N(1A)-C(1A)#1	1.305(10)
N(2A)-C(1A)	1.377(10)
N(2A)-C(8A)	1.404(10)
N(2A)-B(1A)	1.506(10)
N(3A)-C(8A)	1.317(10)
N(3A)-C(9A)	1.378(10)
N(4A)-C(9A)#1	1.328(10)
N(4A)-C(9A)	1.328(10)
N(4A)-B(1A)	1.470(16)
C(1A)-C(2A)	1.480(11)
C(2A)-C(7A)	1.346(12)
C(2A)-C(3A)	1.415(11)
C(3A)-C(4A)	1.374(13)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.385(14)
C(5A)-C(6A)	1.383(12)
C(6A)-C(7A)	1.414(11)
C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.460(11)
C(9A)-C(10A)	1.433(11)
C(10A)-C(11A)	1.408(11)
C(10A)-C(10A)#1	1.431(15)
C(11A)-C(12A)	1.377(12)
C(11A)-H(11A)	0.9500
C(12A)-C(12A)#1	1.391(19)
F(1C)-B(1C)	1.401(13)
F(2C)-C(4C)	1.354(10)
F(3C)-C(5C)	1.328(11)
F(4C)-C(12C)	1.358(10)

N(1C)-C(1C)	1.375(10)
N(1C)-C(1C)#2	1.375(10)
N(2C)-C(1C)	1.357(10)
N(2C)-C(8C)	1.376(11)
N(2C)-B(1C)	1.482(9)
N(3C)-C(8C)	1.334(10)
N(3C)-C(9C)	1.366(10)
N(4C)-C(9C)#2	1.380(9)
N(4C)-C(9C)	1.380(9)
N(4C)-B(1C)	1.470(15)
C(1C)-C(2C)	1.413(11)
C(2C)-C(3C)	1.404(12)
C(2C)-C(7C)	1.443(13)
C(3C)-C(4C)	1.338(14)
C(3C)-H(3CA)	0.9500
C(4C)-C(5C)	1.384(15)
C(5C)-C(6C)	1.391(13)
C(6C)-C(7C)	1.409(12)
C(6C)-H(6CA)	0.9500
C(7C)-C(8C)	1.452(11)
C(9C)-C(10C)	1.458(11)
C(10C)-C(11C)	1.392(12)
C(10C)-C(10C)#2	1.409(15)
C(11C)-C(12C)	1.335(13)
C(11C)-H(11C)	0.9500
C(12C)-C(12C)#2	1.426(17)
F(1B)-B(1B)	1.413(14)
F(2B)-C(4B)	1.331(10)
F(3B)-C(5B)	1.360(10)
F(4B)-C(12B)	1.355(10)
N(1B)-C(1B)	1.331(10)
N(1B)-C(1B)#2	1.331(10)
N(2B)-C(8B)	1.323(10)
N(2B)-C(1B)	1.368(10)
N(2B)-B(1B)	1.501(10)
N(3B)-C(9B)	1.286(10)

N(3B)-C(8B)	1.367(10)
N(4B)-C(9B)	1.387(9)
N(4B)-C(9B)#2	1.387(9)
N(4B)-B(1B)	1.499(15)
C(1B)-C(2B)	1.449(11)
C(2B)-C(3B)	1.367(12)
C(2B)-C(7B)	1.459(13)
C(3B)-C(4B)	1.406(13)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.394(14)
C(5B)-C(6B)	1.343(13)
C(6B)-C(7B)	1.369(12)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.461(10)
C(9B)-C(10B)	1.458(11)
C(10B)-C(11B)	1.379(11)
C(10B)-C(10B)#2	1.411(15)
C(11B)-C(12B)	1.385(12)
C(11B)-H(11B)	0.9500
C(12B)-C(12B)#2	1.356(18)

C(1A)-N(1A)-C(1A)#1	114.7(10)
C(1A)-N(2A)-C(8A)	112.5(6)
C(1A)-N(2A)-B(1A)	124.1(7)
C(8A)-N(2A)-B(1A)	120.1(7)
C(8A)-N(3A)-C(9A)	116.8(6)
C(9A)#1-N(4A)-C(9A)	112.0(10)
C(9A)#1-N(4A)-B(1A)	123.0(5)
C(9A)-N(4A)-B(1A)	123.0(5)
N(1A)-C(1A)-N(2A)	125.2(8)
N(1A)-C(1A)-C(2A)	128.8(7)
N(2A)-C(1A)-C(2A)	103.7(7)
C(7A)-C(2A)-C(3A)	123.6(8)
C(7A)-C(2A)-C(1A)	109.1(7)
C(3A)-C(2A)-C(1A)	126.7(8)
C(4A)-C(3A)-C(2A)	113.9(9)

C(4A)-C(3A)-H(3AA)	123.1
C(2A)-C(3A)-H(3AA)	123.1
F(2A)-C(4A)-C(3A)	120.0(9)
F(2A)-C(4A)-C(5A)	116.7(8)
C(3A)-C(4A)-C(5A)	123.3(8)
F(3A)-C(5A)-C(6A)	118.5(9)
F(3A)-C(5A)-C(4A)	119.1(8)
C(6A)-C(5A)-C(4A)	122.3(8)
C(5A)-C(6A)-C(7A)	114.8(8)
C(5A)-C(6A)-H(6AA)	122.6
C(7A)-C(6A)-H(6AA)	122.6
C(2A)-C(7A)-C(6A)	122.0(8)
C(2A)-C(7A)-C(8A)	109.2(7)
C(6A)-C(7A)-C(8A)	128.0(7)
N(3A)-C(8A)-N(2A)	123.4(7)
N(3A)-C(8A)-C(7A)	130.1(7)
N(2A)-C(8A)-C(7A)	103.9(7)
N(4A)-C(9A)-N(3A)	123.2(8)
N(4A)-C(9A)-C(10A)	107.5(7)
N(3A)-C(9A)-C(10A)	127.5(7)
C(11A)-C(10A)-C(10A)#1	120.3(5)
C(11A)-C(10A)-C(9A)	133.7(7)
C(10A)#1-C(10A)-C(9A)	105.6(4)
C(12A)-C(11A)-C(10A)	117.6(8)
C(12A)-C(11A)-H(11A)	121.2
C(10A)-C(11A)-H(11A)	121.2
F(4A)-C(12A)-C(11A)	119.0(8)
F(4A)-C(12A)-C(12A)#1	118.9(5)
C(11A)-C(12A)-C(12A)#1	122.1(5)
F(1A)-B(1A)-N(4A)	114.8(10)
F(1A)-B(1A)-N(2A)#1	112.5(7)
N(4A)-B(1A)-N(2A)#1	107.0(7)
F(1A)-B(1A)-N(2A)	112.5(7)
N(4A)-B(1A)-N(2A)	107.0(7)
N(2A)#1-B(1A)-N(2A)	102.0(9)
C(1C)-N(1C)-C(1C)#2	117.4(10)

C(1C)-N(2C)-C(8C)	110.8(7)
C(1C)-N(2C)-B(1C)	123.3(7)
C(8C)-N(2C)-B(1C)	123.0(7)
C(8C)-N(3C)-C(9C)	116.5(7)
C(9C)#2-N(4C)-C(9C)	110.0(10)
C(9C)#2-N(4C)-B(1C)	124.1(5)
C(9C)-N(4C)-B(1C)	124.1(5)
N(2C)-C(1C)-N(1C)	121.8(8)
N(2C)-C(1C)-C(2C)	109.8(7)
N(1C)-C(1C)-C(2C)	125.7(7)
C(3C)-C(2C)-C(1C)	134.7(9)
C(3C)-C(2C)-C(7C)	119.8(8)
C(1C)-C(2C)-C(7C)	105.1(7)
C(4C)-C(3C)-C(2C)	117.5(9)
C(4C)-C(3C)-H(3CA)	121.2
C(2C)-C(3C)-H(3CA)	121.2
C(3C)-C(4C)-F(2C)	119.9(10)
C(3C)-C(4C)-C(5C)	123.6(9)
F(2C)-C(4C)-C(5C)	116.4(9)
F(3C)-C(5C)-C(4C)	118.8(8)
F(3C)-C(5C)-C(6C)	118.8(10)
C(4C)-C(5C)-C(6C)	122.4(10)
C(5C)-C(6C)-C(7C)	115.5(10)
C(5C)-C(6C)-H(6CA)	122.3
C(7C)-C(6C)-H(6CA)	122.3
C(6C)-C(7C)-C(2C)	121.2(8)
C(6C)-C(7C)-C(8C)	130.8(9)
C(2C)-C(7C)-C(8C)	107.6(7)
N(3C)-C(8C)-N(2C)	123.7(7)
N(3C)-C(8C)-C(7C)	127.6(8)
N(2C)-C(8C)-C(7C)	105.8(7)
N(3C)-C(9C)-N(4C)	121.6(8)
N(3C)-C(9C)-C(10C)	128.8(7)
N(4C)-C(9C)-C(10C)	107.4(7)
C(11C)-C(10C)-C(10C)#2	121.4(5)
C(11C)-C(10C)-C(9C)	131.4(7)

C(10C)#2-C(10C)-C(9C)	107.0(4)
C(12C)-C(11C)-C(10C)	116.1(8)
C(12C)-C(11C)-H(11C)	121.9
C(10C)-C(11C)-H(11C)	121.9
C(11C)-C(12C)-F(4C)	120.9(8)
C(11C)-C(12C)-C(12C)#2	122.5(6)
F(4C)-C(12C)-C(12C)#2	116.7(4)
F(1C)-B(1C)-N(4C)	111.5(9)
F(1C)-B(1C)-N(2C)	113.1(6)
N(4C)-B(1C)-N(2C)	105.6(7)
F(1C)-B(1C)-N(2C)#2	113.1(6)
N(4C)-B(1C)-N(2C)#2	105.6(7)
N(2C)-B(1C)-N(2C)#2	107.3(9)
C(1B)-N(1B)-C(1B)#2	117.9(10)
C(8B)-N(2B)-C(1B)	112.3(7)
C(8B)-N(2B)-B(1B)	123.0(8)
C(1B)-N(2B)-B(1B)	120.7(7)
C(9B)-N(3B)-C(8B)	118.3(7)
C(9B)-N(4B)-C(9B)#2	113.7(10)
C(9B)-N(4B)-B(1B)	122.4(5)
C(9B)#2-N(4B)-B(1B)	122.4(5)
N(1B)-C(1B)-N(2B)	123.8(8)
N(1B)-C(1B)-C(2B)	128.0(7)
N(2B)-C(1B)-C(2B)	105.9(7)
C(3B)-C(2B)-C(1B)	131.6(9)
C(3B)-C(2B)-C(7B)	120.4(9)
C(1B)-C(2B)-C(7B)	107.4(7)
C(2B)-C(3B)-C(4B)	117.7(9)
C(2B)-C(3B)-H(3BA)	121.2
C(4B)-C(3B)-H(3BA)	121.2
F(2B)-C(4B)-C(5B)	119.8(9)
F(2B)-C(4B)-C(3B)	119.9(9)
C(5B)-C(4B)-C(3B)	120.3(8)
C(6B)-C(5B)-F(3B)	121.4(10)
C(6B)-C(5B)-C(4B)	122.9(9)
F(3B)-C(5B)-C(4B)	115.7(8)

C(5B)-C(6B)-C(7B)	118.7(10)
C(5B)-C(6B)-H(6BA)	120.6
C(7B)-C(6B)-H(6BA)	120.6
C(6B)-C(7B)-C(2B)	120.0(8)
C(6B)-C(7B)-C(8B)	135.7(8)
C(2B)-C(7B)-C(8B)	103.6(7)
N(2B)-C(8B)-N(3B)	123.1(7)
N(2B)-C(8B)-C(7B)	109.0(7)
N(3B)-C(8B)-C(7B)	126.6(7)
N(3B)-C(9B)-N(4B)	122.1(8)
N(3B)-C(9B)-C(10B)	131.3(7)
N(4B)-C(9B)-C(10B)	104.3(7)
C(11B)-C(10B)-C(10B)#2	120.8(5)
C(11B)-C(10B)-C(9B)	130.7(7)
C(10B)#2-C(10B)-C(9B)	108.2(4)
C(10B)-C(11B)-C(12B)	117.2(8)
C(10B)-C(11B)-H(11B)	121.4
C(12B)-C(11B)-H(11B)	121.4
F(4B)-C(12B)-C(12B)#2	118.6(5)
F(4B)-C(12B)-C(11B)	119.4(8)
C(12B)#2-C(12B)-C(11B)	122.0(5)
F(1B)-B(1B)-N(4B)	111.6(10)
F(1B)-B(1B)-N(2B)#2	113.1(6)
N(4B)-B(1B)-N(2B)#2	105.2(7)
F(1B)-B(1B)-N(2B)	113.1(6)
N(4B)-B(1B)-N(2B)	105.2(6)
N(2B)#2-B(1B)-N(2B)	108.1(10)

Symmetry transformations used to generate equivalent atoms:

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

Table S23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F-F_6BsubPc (grown by train sublimation)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1A)	21(4)	39(4)	47(4)	0	20(3)	0
F(2A)	64(4)	62(4)	53(4)	29(3)	38(3)	4(3)
F(3A)	58(4)	29(3)	64(4)	4(2)	36(3)	-12(2)
F(4A)	59(4)	62(4)	27(3)	-13(3)	-2(3)	-14(3)
N(1A)	15(5)	34(5)	17(4)	0	-1(4)	0
N(2A)	25(4)	17(3)	26(3)	4(2)	11(3)	4(3)
N(3A)	32(4)	15(3)	25(3)	0(2)	17(3)	1(3)
N(4A)	19(4)	23(4)	24(4)	0	9(3)	0
C(1A)	23(4)	29(4)	22(3)	-2(3)	6(3)	-7(3)
C(2A)	21(4)	32(4)	28(4)	5(3)	9(3)	3(3)
C(3A)	31(5)	34(4)	35(4)	13(3)	16(4)	10(4)
C(4A)	29(5)	46(5)	32(4)	16(3)	16(4)	9(4)
C(5A)	44(6)	18(4)	56(5)	5(3)	32(5)	2(4)
C(6A)	28(5)	27(4)	34(4)	0(3)	13(4)	0(3)
C(7A)	16(4)	22(3)	30(4)	1(3)	7(3)	2(3)
C(8A)	23(4)	21(4)	31(3)	0(3)	14(3)	1(3)
C(9A)	20(4)	21(3)	26(3)	5(3)	13(3)	7(3)
C(10A)	26(4)	21(4)	30(4)	-7(3)	9(3)	-9(3)
C(11A)	38(5)	34(4)	14(3)	-6(3)	14(3)	-8(4)
C(12A)	34(5)	56(6)	16(4)	-3(3)	-2(3)	-8(4)
B(1A)	22(5)	23(5)	24(5)	0	12(4)	0
F(1C)	19(3)	30(4)	27(3)	0	11(3)	0
F(2C)	59(4)	57(4)	57(4)	26(3)	43(3)	11(3)
F(3C)	62(4)	37(3)	85(5)	16(3)	52(4)	-2(3)
F(4C)	54(4)	49(4)	45(3)	-7(3)	-6(3)	-6(3)
N(1C)	31(6)	35(5)	28(5)	0	17(5)	0
N(2C)	9(3)	27(3)	25(3)	1(2)	5(2)	5(3)
N(3C)	26(4)	20(3)	30(3)	0(3)	13(3)	0(3)
N(4C)	20(4)	27(4)	21(4)	0	11(3)	0
C(1C)	24(4)	32(4)	33(4)	5(3)	18(3)	9(3)

C(2C)	20(4)	27(4)	33(4)	11(3)	12(3)	13(3)
C(3C)	33(5)	49(5)	33(4)	17(4)	18(4)	13(4)
C(4C)	33(5)	52(5)	44(4)	26(4)	22(4)	16(4)
C(5C)	32(5)	42(5)	56(5)	17(4)	26(4)	7(4)
C(6C)	42(6)	24(4)	53(5)	10(4)	30(5)	7(4)
C(7C)	35(5)	30(4)	36(4)	8(3)	23(4)	6(4)
C(8C)	26(4)	20(3)	33(3)	5(3)	17(3)	7(3)
C(9C)	20(4)	22(4)	28(3)	-2(3)	13(3)	-2(3)
C(10C)	30(4)	32(4)	22(3)	4(3)	17(3)	0(3)
C(11C)	37(5)	32(4)	45(4)	-3(4)	15(4)	0(4)
C(12C)	33(5)	32(5)	41(5)	-8(3)	7(4)	1(4)
B(1C)	16(5)	31(6)	18(5)	0	10(4)	0
F(1B)	18(3)	25(3)	36(4)	0	13(3)	0
F(2B)	55(4)	60(4)	60(4)	-30(3)	38(3)	-12(3)
F(3B)	72(4)	25(3)	94(5)	-19(3)	59(4)	-3(3)
F(4B)	37(3)	57(4)	45(3)	10(3)	-11(3)	9(3)
N(1B)	14(5)	41(5)	18(5)	0	-5(4)	0
N(2B)	22(4)	26(3)	26(3)	2(3)	12(3)	3(3)
N(3B)	23(4)	28(3)	33(3)	-1(3)	12(3)	-4(3)
N(4B)	13(4)	16(4)	23(4)	0	7(3)	0
C(1B)	15(4)	33(4)	19(3)	-7(3)	3(3)	-4(3)
C(2B)	25(5)	31(4)	39(4)	-7(3)	19(4)	-7(4)
C(3B)	36(5)	39(5)	35(4)	-8(4)	19(4)	-2(4)
C(4B)	45(6)	36(4)	57(5)	-23(4)	38(5)	-15(4)
C(5B)	41(5)	23(4)	62(5)	-19(3)	34(5)	-7(4)
C(6B)	35(5)	23(4)	54(5)	-5(4)	28(5)	-5(4)
C(7B)	25(5)	19(3)	41(4)	-16(3)	17(4)	-11(3)
C(8B)	15(4)	24(4)	28(3)	-5(3)	7(3)	-6(3)
C(9B)	25(4)	23(4)	23(3)	8(3)	9(3)	6(3)
C(10B)	20(4)	28(4)	21(3)	1(3)	7(3)	-4(3)
C(11B)	29(4)	31(4)	31(4)	4(3)	10(3)	0(4)
C(12B)	27(5)	47(6)	27(4)	3(3)	-1(3)	7(4)
B(1B)	11(5)	26(5)	22(5)	0	2(4)	0

Table S24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **F-F_6BsubPc (grown by train sublimation)**.

	x	y	z	U(eq)
H(3AA)	160	3723	5653	40
H(6AA)	1756	4956	9105	36
H(11A)	3168	3726	12710	33
H(3CA)	3155	6235	4356	45
H(6CA)	1613	5012	904	44
H(11C)	168	6272	-2700	47
H(3BA)	6492	8741	4326	43
H(6BA)	4981	9994	938	42
H(11B)	3529	8719	-2688	38

Table S25. Torsion angles [°] for **F-F$_6$BsubPc (grown by train sublimation)**.

C(1A)#1-N(1A)-C(1A)-N(2A)	-10.3(16)
C(1A)#1-N(1A)-C(1A)-C(2A)	149.8(6)
C(8A)-N(2A)-C(1A)-N(1A)	151.9(9)
B(1A)-N(2A)-C(1A)-N(1A)	-7.3(14)
C(8A)-N(2A)-C(1A)-C(2A)	-12.3(9)
B(1A)-N(2A)-C(1A)-C(2A)	-171.5(8)
N(1A)-C(1A)-C(2A)-C(7A)	-155.8(10)
N(2A)-C(1A)-C(2A)-C(7A)	7.6(9)
N(1A)-C(1A)-C(2A)-C(3A)	15.7(15)
N(2A)-C(1A)-C(2A)-C(3A)	179.1(8)
C(7A)-C(2A)-C(3A)-C(4A)	-0.7(13)
C(1A)-C(2A)-C(3A)-C(4A)	-171.1(8)
C(2A)-C(3A)-C(4A)-F(2A)	179.4(8)
C(2A)-C(3A)-C(4A)-C(5A)	0.0(13)
F(2A)-C(4A)-C(5A)-F(3A)	-1.6(13)
C(3A)-C(4A)-C(5A)-F(3A)	177.8(8)
F(2A)-C(4A)-C(5A)-C(6A)	-177.0(9)
C(3A)-C(4A)-C(5A)-C(6A)	2.5(15)
F(3A)-C(5A)-C(6A)-C(7A)	-179.3(7)
C(4A)-C(5A)-C(6A)-C(7A)	-4.0(14)
C(3A)-C(2A)-C(7A)-C(6A)	-1.0(14)
C(1A)-C(2A)-C(7A)-C(6A)	170.8(7)
C(3A)-C(2A)-C(7A)-C(8A)	-172.3(8)
C(1A)-C(2A)-C(7A)-C(8A)	-0.5(10)
C(5A)-C(6A)-C(7A)-C(2A)	3.3(12)
C(5A)-C(6A)-C(7A)-C(8A)	172.8(8)
C(9A)-N(3A)-C(8A)-N(2A)	9.1(11)
C(9A)-N(3A)-C(8A)-C(7A)	-149.6(8)
C(1A)-N(2A)-C(8A)-N(3A)	-151.3(7)
B(1A)-N(2A)-C(8A)-N(3A)	8.8(12)
C(1A)-N(2A)-C(8A)-C(7A)	12.1(9)
B(1A)-N(2A)-C(8A)-C(7A)	172.2(8)
C(2A)-C(7A)-C(8A)-N(3A)	155.1(8)
C(6A)-C(7A)-C(8A)-N(3A)	-15.5(14)

C(2A)-C(7A)-C(8A)-N(2A)	-6.7(9)
C(6A)-C(7A)-C(8A)-N(2A)	-177.3(8)
C(9A)#1-N(4A)-C(9A)-N(3A)	152.0(6)
B(1A)-N(4A)-C(9A)-N(3A)	-12.6(14)
C(9A)#1-N(4A)-C(9A)-C(10A)	-13.5(12)
B(1A)-N(4A)-C(9A)-C(10A)	-178.2(9)
C(8A)-N(3A)-C(9A)-N(4A)	-7.8(12)
C(8A)-N(3A)-C(9A)-C(10A)	154.8(8)
N(4A)-C(9A)-C(10A)-C(11A)	-178.9(9)
N(3A)-C(9A)-C(10A)-C(11A)	16.4(14)
N(4A)-C(9A)-C(10A)-C(10A)#1	7.8(7)
N(3A)-C(9A)-C(10A)-C(10A)#1	-156.9(6)
C(10A)#1-C(10A)-C(11A)-C(12A)	-1.3(9)
C(9A)-C(10A)-C(11A)-C(12A)	-173.9(9)
C(10A)-C(11A)-C(12A)-F(4A)	-178.4(8)
C(10A)-C(11A)-C(12A)-C(12A)#1	1.4(10)
C(9A)#1-N(4A)-B(1A)-F(1A)	98.5(9)
C(9A)-N(4A)-B(1A)-F(1A)	-98.5(9)
C(9A)#1-N(4A)-B(1A)-N(2A)#1	-27.1(13)
C(9A)-N(4A)-B(1A)-N(2A)#1	135.9(8)
C(9A)#1-N(4A)-B(1A)-N(2A)	-135.9(8)
C(9A)-N(4A)-B(1A)-N(2A)	27.1(13)
C(1A)-N(2A)-B(1A)-F(1A)	-100.2(9)
C(8A)-N(2A)-B(1A)-F(1A)	102.1(10)
C(1A)-N(2A)-B(1A)-N(4A)	132.8(8)
C(8A)-N(2A)-B(1A)-N(4A)	-24.9(11)
C(1A)-N(2A)-B(1A)-N(2A)#1	20.6(13)
C(8A)-N(2A)-B(1A)-N(2A)#1	-137.1(7)
C(8C)-N(2C)-C(1C)-N(1C)	-152.3(9)
B(1C)-N(2C)-C(1C)-N(1C)	8.8(13)
C(8C)-N(2C)-C(1C)-C(2C)	9.9(9)
B(1C)-N(2C)-C(1C)-C(2C)	171.0(8)
C(1C)#2-N(1C)-C(1C)-N(2C)	9.3(16)
C(1C)#2-N(1C)-C(1C)-C(2C)	-150.0(7)
N(2C)-C(1C)-C(2C)-C(3C)	-177.7(9)
N(1C)-C(1C)-C(2C)-C(3C)	-16.4(16)

N(2C)-C(1C)-C(2C)-C(7C)	-6.1(9)
N(1C)-C(1C)-C(2C)-C(7C)	155.3(10)
C(1C)-C(2C)-C(3C)-C(4C)	170.8(9)
C(7C)-C(2C)-C(3C)-C(4C)	0.1(13)
C(2C)-C(3C)-C(4C)-F(2C)	-179.4(8)
C(2C)-C(3C)-C(4C)-C(5C)	-0.6(14)
C(3C)-C(4C)-C(5C)-F(3C)	179.8(8)
F(2C)-C(4C)-C(5C)-F(3C)	-1.4(14)
C(3C)-C(4C)-C(5C)-C(6C)	1.2(16)
F(2C)-C(4C)-C(5C)-C(6C)	-180.0(8)
F(3C)-C(5C)-C(6C)-C(7C)	-179.8(8)
C(4C)-C(5C)-C(6C)-C(7C)	-1.2(14)
C(5C)-C(6C)-C(7C)-C(2C)	0.7(13)
C(5C)-C(6C)-C(7C)-C(8C)	-171.4(9)
C(3C)-C(2C)-C(7C)-C(6C)	-0.2(13)
C(1C)-C(2C)-C(7C)-C(6C)	-173.4(8)
C(3C)-C(2C)-C(7C)-C(8C)	173.5(7)
C(1C)-C(2C)-C(7C)-C(8C)	0.3(9)
C(9C)-N(3C)-C(8C)-N(2C)	-8.6(11)
C(9C)-N(3C)-C(8C)-C(7C)	149.2(8)
C(1C)-N(2C)-C(8C)-N(3C)	152.6(7)
B(1C)-N(2C)-C(8C)-N(3C)	-8.5(12)
C(1C)-N(2C)-C(8C)-C(7C)	-9.3(9)
B(1C)-N(2C)-C(8C)-C(7C)	-170.4(7)
C(6C)-C(7C)-C(8C)-N(3C)	17.3(15)
C(2C)-C(7C)-C(8C)-N(3C)	-155.6(8)
C(6C)-C(7C)-C(8C)-N(2C)	178.2(9)
C(2C)-C(7C)-C(8C)-N(2C)	5.3(9)
C(8C)-N(3C)-C(9C)-N(4C)	7.2(11)
C(8C)-N(3C)-C(9C)-C(10C)	-153.9(8)
C(9C)#2-N(4C)-C(9C)-N(3C)	-153.5(5)
B(1C)-N(4C)-C(9C)-N(3C)	11.7(13)
C(9C)#2-N(4C)-C(9C)-C(10C)	11.2(11)
B(1C)-N(4C)-C(9C)-C(10C)	176.3(8)
N(3C)-C(9C)-C(10C)-C(11C)	-17.5(14)
N(4C)-C(9C)-C(10C)-C(11C)	179.3(9)

N(3C)-C(9C)-C(10C)-C(10C)#2	156.5(7)
N(4C)-C(9C)-C(10C)-C(10C)#2	-6.7(6)
C(10C)#2-C(10C)-C(11C)-C(12C)	1.4(11)
C(9C)-C(10C)-C(11C)-C(12C)	174.7(8)
C(10C)-C(11C)-C(12C)-F(4C)	178.9(8)
C(10C)-C(11C)-C(12C)-C(12C)#2	-1.4(11)
C(9C)#2-N(4C)-B(1C)-F(1C)	-98.5(8)
C(9C)-N(4C)-B(1C)-F(1C)	98.4(8)
C(9C)#2-N(4C)-B(1C)-N(2C)	138.3(8)
C(9C)-N(4C)-B(1C)-N(2C)	-24.8(12)
C(9C)#2-N(4C)-B(1C)-N(2C)#2	24.8(12)
C(9C)-N(4C)-B(1C)-N(2C)#2	-138.3(8)
C(1C)-N(2C)-B(1C)-F(1C)	102.2(9)
C(8C)-N(2C)-B(1C)-F(1C)	-99.0(10)
C(1C)-N(2C)-B(1C)-N(4C)	-135.6(8)
C(8C)-N(2C)-B(1C)-N(4C)	23.2(10)
C(1C)-N(2C)-B(1C)-N(2C)#2	-23.3(13)
C(8C)-N(2C)-B(1C)-N(2C)#2	135.5(7)
C(1B)#2-N(1B)-C(1B)-N(2B)	-10.5(16)
C(1B)#2-N(1B)-C(1B)-C(2B)	149.6(7)
C(8B)-N(2B)-C(1B)-N(1B)	150.6(8)
B(1B)-N(2B)-C(1B)-N(1B)	-7.4(13)
C(8B)-N(2B)-C(1B)-C(2B)	-13.3(9)
B(1B)-N(2B)-C(1B)-C(2B)	-171.3(8)
N(1B)-C(1B)-C(2B)-C(3B)	15.3(16)
N(2B)-C(1B)-C(2B)-C(3B)	178.2(10)
N(1B)-C(1B)-C(2B)-C(7B)	-156.0(9)
N(2B)-C(1B)-C(2B)-C(7B)	6.9(9)
C(1B)-C(2B)-C(3B)-C(4B)	-170.7(9)
C(7B)-C(2B)-C(3B)-C(4B)	-0.3(13)
C(2B)-C(3B)-C(4B)-F(2B)	178.5(8)
C(2B)-C(3B)-C(4B)-C(5B)	0.6(14)
F(2B)-C(4B)-C(5B)-C(6B)	-178.6(8)
C(3B)-C(4B)-C(5B)-C(6B)	-0.6(15)
F(2B)-C(4B)-C(5B)-F(3B)	1.4(13)
C(3B)-C(4B)-C(5B)-F(3B)	179.4(8)

F(3B)-C(5B)-C(6B)-C(7B)	-179.6(8)
C(4B)-C(5B)-C(6B)-C(7B)	0.4(15)
C(5B)-C(6B)-C(7B)-C(2B)	-0.1(13)
C(5B)-C(6B)-C(7B)-C(8B)	168.2(9)
C(3B)-C(2B)-C(7B)-C(6B)	0.1(13)
C(1B)-C(2B)-C(7B)-C(6B)	172.6(7)
C(3B)-C(2B)-C(7B)-C(8B)	-171.5(8)
C(1B)-C(2B)-C(7B)-C(8B)	1.0(9)
C(1B)-N(2B)-C(8B)-N(3B)	-153.2(7)
B(1B)-N(2B)-C(8B)-N(3B)	4.2(12)
C(1B)-N(2B)-C(8B)-C(7B)	14.3(10)
B(1B)-N(2B)-C(8B)-C(7B)	171.7(7)
C(9B)-N(3B)-C(8B)-N(2B)	13.1(11)
C(9B)-N(3B)-C(8B)-C(7B)	-152.1(8)
C(6B)-C(7B)-C(8B)-N(2B)	-178.5(9)
C(2B)-C(7B)-C(8B)-N(2B)	-8.9(9)
C(6B)-C(7B)-C(8B)-N(3B)	-11.5(15)
C(2B)-C(7B)-C(8B)-N(3B)	158.0(8)
C(8B)-N(3B)-C(9B)-N(4B)	-8.6(12)
C(8B)-N(3B)-C(9B)-C(10B)	151.5(8)
C(9B)#2-N(4B)-C(9B)-N(3B)	153.6(6)
B(1B)-N(4B)-C(9B)-N(3B)	-12.7(14)
C(9B)#2-N(4B)-C(9B)-C(10B)	-11.1(11)
B(1B)-N(4B)-C(9B)-C(10B)	-177.4(9)
N(3B)-C(9B)-C(10B)-C(11B)	18.2(15)
N(4B)-C(9B)-C(10B)-C(11B)	-179.2(9)
N(3B)-C(9B)-C(10B)-C(10B)#2	-156.3(8)
N(4B)-C(9B)-C(10B)-C(10B)#2	6.4(7)
C(10B)#2-C(10B)-C(11B)-C(12B)	-0.7(10)
C(9B)-C(10B)-C(11B)-C(12B)	-174.5(8)
C(10B)-C(11B)-C(12B)-F(4B)	179.5(8)
C(10B)-C(11B)-C(12B)-C(12B)#2	0.7(10)
C(9B)-N(4B)-B(1B)-F(1B)	-97.5(8)
C(9B)#2-N(4B)-B(1B)-F(1B)	97.5(8)
C(9B)-N(4B)-B(1B)-N(2B)#2	139.5(8)
C(9B)#2-N(4B)-B(1B)-N(2B)#2	-25.6(12)

C(9B)-N(4B)-B(1B)-N(2B)	25.6(12)
C(9B)#2-N(4B)-B(1B)-N(2B)	-139.5(8)
C(8B)-N(2B)-B(1B)-F(1B)	100.6(10)
C(1B)-N(2B)-B(1B)-F(1B)	-103.7(9)
C(8B)-N(2B)-B(1B)-N(4B)	-21.4(11)
C(1B)-N(2B)-B(1B)-N(4B)	134.2(8)
C(8B)-N(2B)-B(1B)-N(2B)#2	-133.4(7)
C(1B)-N(2B)-B(1B)-N(2B)#2	22.2(13)

Symmetry transformations used to generate equivalent atoms:

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

Table S26. Crystal data and structure refinement for **Cl-F_{12}BsubPc (grown by train sublimation)**

Empirical formula	C24 B Cl F12 N6	
Formula weight	646.56	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.2770(2) Å	a= 90°.
	b = 10.5657(2) Å	b= 95.436(1)°.
	c = 19.0940(4) Å	g = 90°.
Volume	2264.81(8) $Å^3$	
Z	4	
Density (calculated)	1.896 Mg/m^3	
Absorption coefficient	2.729 mm^{-1}	
F(000)	1264	
Crystal size	0.090 x 0.040 x 0.030 mm^3	
Theta range for data collection	3.938 to 67.206°.	
Index ranges	-13<=h<=13, -12<=k<=12, -22<=l<=22	
Reflections collected	45198	
Independent reflections	4031 [R(int) = 0.0565]	
Completeness to theta = 67.206°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6507	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4031 / 0 / 397	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0310, wR2 = 0.0760	
R indices (all data)	R1 = 0.0392, wR2 = 0.0805	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.265 and -0.299 $e.Å^{-3}$	

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cl-F_{12}BsubPc (grown by train sublimation)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	5331(1)	9009(1)	2154(1)	22(1)
F(1)	8511(1)	4330(1)	1363(1)	26(1)
F(2)	10398(1)	3531(1)	2264(1)	35(1)
F(3)	10546(1)	4136(1)	3631(1)	35(1)
F(4)	8855(1)	5606(1)	4157(1)	27(1)
F(5)	5208(1)	6374(1)	5265(1)	24(1)
F(6)	3142(1)	6290(1)	5874(1)	26(1)
F(7)	1034(1)	6596(1)	5115(1)	29(1)
F(8)	904(1)	6844(1)	3694(1)	24(1)
F(9)	598(1)	5653(1)	1292(1)	29(1)
F(10)	418(1)	3850(1)	265(1)	35(1)
F(11)	2358(1)	3035(1)	-309(1)	34(1)
F(12)	4549(1)	3890(1)	152(1)	22(1)
N(1)	6152(1)	6585(1)	2496(1)	16(1)
N(2)	6206(1)	6616(1)	3744(1)	17(1)
N(3)	4439(1)	7174(1)	3029(1)	16(1)
N(4)	2534(1)	6756(1)	2427(1)	18(1)
N(5)	4287(1)	6632(1)	1825(1)	15(1)
N(6)	5904(1)	5510(1)	1399(1)	17(1)
C(1)	6572(2)	5856(2)	1987(1)	17(1)
C(2)	7694(2)	5349(2)	2307(1)	18(1)
C(3)	8572(2)	4621(2)	2047(1)	21(1)
C(4)	9523(2)	4218(2)	2503(1)	25(1)
C(5)	9601(2)	4534(2)	3211(1)	25(1)
C(6)	8745(2)	5272(2)	3481(1)	22(1)
C(7)	7787(2)	5686(2)	3032(1)	19(1)
C(8)	6725(2)	6401(2)	3150(1)	17(1)
C(9)	5044(2)	6903(2)	3665(1)	17(1)
C(10)	4134(2)	6764(2)	4151(1)	17(1)
C(11)	4174(2)	6524(2)	4866(1)	18(1)

C(12)	3124(2)	6464(2)	5178(1)	20(1)
C(13)	2025(2)	6600(2)	4784(1)	21(1)
C(14)	1967(2)	6753(2)	4068(1)	19(1)
C(15)	3009(2)	6854(2)	3746(1)	18(1)
C(16)	3237(2)	7012(2)	3018(1)	17(1)
C(17)	3090(2)	6486(2)	1856(1)	17(1)
C(18)	2690(2)	5696(2)	1258(1)	18(1)
C(19)	1575(2)	5235(2)	1016(1)	22(1)
C(20)	1479(2)	4337(2)	493(1)	24(1)
C(21)	2487(2)	3910(2)	196(1)	23(1)
C(22)	3599(2)	4367(2)	427(1)	19(1)
C(23)	3721(2)	5270(2)	953(1)	17(1)
C(24)	4748(2)	5836(2)	1358(1)	16(1)
B(1)	5042(2)	7330(2)	2378(1)	16(1)

Table S28. Bond lengths [Å] and angles [°] for **Cl-F_{12}BsubPc (grown by train sublimation)**.

Cl(1)-B(1)	1.861(2)
F(1)-C(3)	1.336(2)
F(2)-C(4)	1.339(2)
F(3)-C(5)	1.340(2)
F(4)-C(6)	1.334(2)
F(5)-C(11)	1.339(2)
F(6)-C(12)	1.340(2)
F(7)-C(13)	1.335(2)
F(8)-C(14)	1.339(2)
F(9)-C(19)	1.341(2)
F(10)-C(20)	1.337(2)
F(11)-C(21)	1.334(2)
F(12)-C(22)	1.336(2)
N(1)-C(1)	1.359(2)
N(1)-C(8)	1.365(2)
N(1)-B(1)	1.477(3)
N(2)-C(9)	1.340(2)
N(2)-C(8)	1.343(2)
N(3)-C(16)	1.364(2)
N(3)-C(9)	1.366(2)
N(3)-B(1)	1.482(3)
N(4)-C(17)	1.339(2)
N(4)-C(16)	1.344(2)
N(5)-C(24)	1.365(2)
N(5)-C(17)	1.366(2)
N(5)-B(1)	1.487(3)
N(6)-C(1)	1.343(2)
N(6)-C(24)	1.343(2)
C(1)-C(2)	1.454(3)
C(2)-C(3)	1.382(3)
C(2)-C(7)	1.424(3)
C(3)-C(4)	1.383(3)
C(4)-C(5)	1.387(3)
C(5)-C(6)	1.378(3)

C(6)-C(7)	1.385(3)
C(7)-C(8)	1.451(3)
C(9)-C(10)	1.454(3)
C(10)-C(11)	1.385(3)
C(10)-C(15)	1.425(3)
C(11)-C(12)	1.377(3)
C(12)-C(13)	1.394(3)
C(13)-C(14)	1.373(3)
C(14)-C(15)	1.380(3)
C(15)-C(16)	1.447(3)
C(17)-C(18)	1.451(3)
C(18)-C(19)	1.386(3)
C(18)-C(23)	1.422(3)
C(19)-C(20)	1.374(3)
C(20)-C(21)	1.392(3)
C(21)-C(22)	1.377(3)
C(22)-C(23)	1.382(3)
C(23)-C(24)	1.460(3)

C(1)-N(1)-C(8)	113.92(15)
C(1)-N(1)-B(1)	122.76(15)
C(8)-N(1)-B(1)	122.43(16)
C(9)-N(2)-C(8)	116.36(15)
C(16)-N(3)-C(9)	113.47(15)
C(16)-N(3)-B(1)	122.39(15)
C(9)-N(3)-B(1)	122.66(16)
C(17)-N(4)-C(16)	116.27(15)
C(24)-N(5)-C(17)	113.46(15)
C(24)-N(5)-B(1)	122.73(15)
C(17)-N(5)-B(1)	121.89(16)
C(1)-N(6)-C(24)	116.28(16)
N(6)-C(1)-N(1)	123.07(16)
N(6)-C(1)-C(2)	130.39(17)
N(1)-C(1)-C(2)	104.93(15)
C(3)-C(2)-C(7)	119.98(17)
C(3)-C(2)-C(1)	132.70(18)

C(7)-C(2)-C(1)	107.26(16)
F(1)-C(3)-C(2)	120.45(17)
F(1)-C(3)-C(4)	120.63(17)
C(2)-C(3)-C(4)	118.91(18)
F(2)-C(4)-C(3)	120.30(19)
F(2)-C(4)-C(5)	118.77(18)
C(3)-C(4)-C(5)	120.92(18)
F(3)-C(5)-C(6)	120.01(19)
F(3)-C(5)-C(4)	118.77(18)
C(6)-C(5)-C(4)	121.20(18)
F(4)-C(6)-C(5)	120.49(17)
F(4)-C(6)-C(7)	120.76(18)
C(5)-C(6)-C(7)	118.73(18)
C(6)-C(7)-C(2)	120.25(18)
C(6)-C(7)-C(8)	132.47(18)
C(2)-C(7)-C(8)	107.19(16)
N(2)-C(8)-N(1)	122.79(16)
N(2)-C(8)-C(7)	130.60(17)
N(1)-C(8)-C(7)	104.98(16)
N(2)-C(9)-N(3)	123.15(17)
N(2)-C(9)-C(10)	130.40(17)
N(3)-C(9)-C(10)	105.41(15)
C(11)-C(10)-C(15)	119.43(17)
C(11)-C(10)-C(9)	133.44(17)
C(15)-C(10)-C(9)	107.06(16)
F(5)-C(11)-C(12)	119.14(17)
F(5)-C(11)-C(10)	121.84(17)
C(12)-C(11)-C(10)	119.01(17)
F(6)-C(12)-C(11)	120.16(17)
F(6)-C(12)-C(13)	118.53(17)
C(11)-C(12)-C(13)	121.30(18)
F(7)-C(13)-C(14)	120.62(17)
F(7)-C(13)-C(12)	119.03(17)
C(14)-C(13)-C(12)	120.34(18)
F(8)-C(14)-C(13)	119.69(17)
F(8)-C(14)-C(15)	120.93(17)

C(13)-C(14)-C(15)	119.34(17)
C(14)-C(15)-C(10)	120.37(17)
C(14)-C(15)-C(16)	132.28(17)
C(10)-C(15)-C(16)	107.33(16)
N(4)-C(16)-N(3)	122.96(16)
N(4)-C(16)-C(15)	129.70(17)
N(3)-C(16)-C(15)	105.50(15)
N(4)-C(17)-N(5)	123.46(16)
N(4)-C(17)-C(18)	128.99(17)
N(5)-C(17)-C(18)	105.43(16)
C(19)-C(18)-C(23)	120.21(17)
C(19)-C(18)-C(17)	131.94(18)
C(23)-C(18)-C(17)	107.43(16)
F(9)-C(19)-C(20)	120.15(17)
F(9)-C(19)-C(18)	120.45(17)
C(20)-C(19)-C(18)	119.40(18)
F(10)-C(20)-C(19)	120.59(18)
F(10)-C(20)-C(21)	118.80(18)
C(19)-C(20)-C(21)	120.61(18)
F(11)-C(21)-C(22)	120.54(18)
F(11)-C(21)-C(20)	118.84(17)
C(22)-C(21)-C(20)	120.61(18)
F(12)-C(22)-C(21)	118.80(17)
F(12)-C(22)-C(23)	121.20(17)
C(21)-C(22)-C(23)	119.96(18)
C(22)-C(23)-C(18)	119.18(17)
C(22)-C(23)-C(24)	133.41(18)
C(18)-C(23)-C(24)	106.97(15)
N(6)-C(24)-N(5)	123.28(16)
N(6)-C(24)-C(23)	130.00(17)
N(5)-C(24)-C(23)	105.44(15)
N(1)-B(1)-N(3)	105.22(15)
N(1)-B(1)-N(5)	105.31(15)
N(3)-B(1)-N(5)	105.20(15)
N(1)-B(1)-Cl(1)	112.27(14)
N(3)-B(1)-Cl(1)	113.78(13)

N(5)-B(1)-Cl(1)	114.22(13)

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Cl-F_{12}BsubPc (grown by train sublimation)**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	28(1)	14(1)	24(1)	1(1)	2(1)	-1(1)
F(1)	22(1)	27(1)	29(1)	-9(1)	3(1)	0(1)
F(2)	21(1)	36(1)	47(1)	-9(1)	-1(1)	12(1)
F(3)	22(1)	38(1)	43(1)	4(1)	-10(1)	8(1)
F(4)	23(1)	34(1)	23(1)	3(1)	-5(1)	-2(1)
F(5)	24(1)	26(1)	19(1)	2(1)	-4(1)	-2(1)
F(6)	34(1)	30(1)	15(1)	2(1)	4(1)	-3(1)
F(7)	25(1)	35(1)	27(1)	6(1)	11(1)	2(1)
F(8)	17(1)	27(1)	26(1)	2(1)	0(1)	-1(1)
F(9)	17(1)	40(1)	31(1)	-4(1)	2(1)	-3(1)
F(10)	24(1)	41(1)	39(1)	-9(1)	-7(1)	-12(1)
F(11)	39(1)	30(1)	31(1)	-14(1)	-4(1)	-6(1)
F(12)	28(1)	19(1)	20(1)	-3(1)	3(1)	3(1)
N(1)	16(1)	15(1)	16(1)	0(1)	0(1)	-2(1)
N(2)	18(1)	16(1)	17(1)	-1(1)	0(1)	-2(1)
N(3)	17(1)	14(1)	16(1)	-2(1)	0(1)	1(1)
N(4)	18(1)	17(1)	17(1)	0(1)	-1(1)	2(1)
N(5)	16(1)	15(1)	14(1)	1(1)	-1(1)	1(1)
N(6)	17(1)	16(1)	17(1)	0(1)	1(1)	-1(1)
C(1)	17(1)	15(1)	19(1)	1(1)	3(1)	-2(1)
C(2)	15(1)	16(1)	23(1)	1(1)	1(1)	-3(1)
C(3)	18(1)	19(1)	26(1)	-2(1)	2(1)	-4(1)
C(4)	15(1)	20(1)	40(1)	-3(1)	2(1)	3(1)
C(5)	16(1)	23(1)	35(1)	5(1)	-6(1)	1(1)
C(6)	19(1)	23(1)	23(1)	3(1)	-2(1)	-4(1)
C(7)	16(1)	18(1)	23(1)	2(1)	1(1)	-4(1)
C(8)	17(1)	16(1)	19(1)	0(1)	-1(1)	-4(1)
C(9)	21(1)	14(1)	16(1)	-2(1)	-1(1)	-2(1)
C(10)	20(1)	13(1)	18(1)	-3(1)	1(1)	1(1)
C(11)	21(1)	15(1)	18(1)	-1(1)	-3(1)	-1(1)

C(12)	29(1)	17(1)	15(1)	1(1)	2(1)	-3(1)
C(13)	21(1)	17(1)	24(1)	1(1)	8(1)	-1(1)
C(14)	18(1)	16(1)	22(1)	-1(1)	-1(1)	-1(1)
C(15)	20(1)	14(1)	18(1)	-2(1)	1(1)	0(1)
C(16)	18(1)	14(1)	17(1)	0(1)	1(1)	1(1)
C(17)	17(1)	15(1)	18(1)	2(1)	-1(1)	1(1)
C(18)	19(1)	17(1)	16(1)	2(1)	-2(1)	1(1)
C(19)	18(1)	26(1)	20(1)	2(1)	0(1)	0(1)
C(20)	20(1)	26(1)	25(1)	-1(1)	-5(1)	-7(1)
C(21)	31(1)	18(1)	20(1)	-3(1)	-4(1)	-3(1)
C(22)	24(1)	16(1)	18(1)	1(1)	1(1)	3(1)
C(23)	20(1)	16(1)	14(1)	2(1)	0(1)	0(1)
C(24)	19(1)	15(1)	13(1)	1(1)	2(1)	0(1)
B(1)	19(1)	15(1)	16(1)	0(1)	1(1)	-1(1)

Table S30. Torsion angles [°] for **Cl-F_{12}BsubPc (grown by train sublimation)**

C(24)-N(6)-C(1)-N(1)	-5.3(3)
C(24)-N(6)-C(1)-C(2)	157.95(18)
C(8)-N(1)-C(1)-N(6)	153.43(17)
B(1)-N(1)-C(1)-N(6)	-16.0(3)
C(8)-N(1)-C(1)-C(2)	-13.5(2)
B(1)-N(1)-C(1)-C(2)	177.14(16)
N(6)-C(1)-C(2)-C(3)	19.4(3)
N(1)-C(1)-C(2)-C(3)	-175.02(19)
N(6)-C(1)-C(2)-C(7)	-157.68(18)
N(1)-C(1)-C(2)-C(7)	7.86(19)
C(7)-C(2)-C(3)-F(1)	-178.07(16)
C(1)-C(2)-C(3)-F(1)	5.1(3)
C(7)-C(2)-C(3)-C(4)	0.8(3)
C(1)-C(2)-C(3)-C(4)	-176.06(19)
F(1)-C(3)-C(4)-F(2)	0.1(3)
C(2)-C(3)-C(4)-F(2)	-178.76(17)
F(1)-C(3)-C(4)-C(5)	178.95(17)
C(2)-C(3)-C(4)-C(5)	0.1(3)
F(2)-C(4)-C(5)-F(3)	-0.2(3)
C(3)-C(4)-C(5)-F(3)	-179.12(18)
F(2)-C(4)-C(5)-C(6)	177.96(18)
C(3)-C(4)-C(5)-C(6)	-0.9(3)
F(3)-C(5)-C(6)-F(4)	0.7(3)
C(4)-C(5)-C(6)-F(4)	-177.49(18)
F(3)-C(5)-C(6)-C(7)	178.99(17)
C(4)-C(5)-C(6)-C(7)	0.8(3)
F(4)-C(6)-C(7)-C(2)	178.38(16)
C(5)-C(6)-C(7)-C(2)	0.1(3)
F(4)-C(6)-C(7)-C(8)	-5.5(3)
C(5)-C(6)-C(7)-C(8)	176.20(19)
C(3)-C(2)-C(7)-C(6)	-0.9(3)
C(1)-C(2)-C(7)-C(6)	176.69(16)
C(3)-C(2)-C(7)-C(8)	-177.88(16)
C(1)-C(2)-C(7)-C(8)	-0.3(2)

C(9)-N(2)-C(8)-N(1)	6.6(3)
C(9)-N(2)-C(8)-C(7)	-156.58(18)
C(1)-N(1)-C(8)-N(2)	-153.57(17)
B(1)-N(1)-C(8)-N(2)	15.9(3)
C(1)-N(1)-C(8)-C(7)	13.3(2)
B(1)-N(1)-C(8)-C(7)	-177.29(16)
C(6)-C(7)-C(8)-N(2)	-18.4(3)
C(2)-C(7)-C(8)-N(2)	158.10(18)
C(6)-C(7)-C(8)-N(1)	176.20(19)
C(2)-C(7)-C(8)-N(1)	-7.30(19)
C(8)-N(2)-C(9)-N(3)	-10.6(3)
C(8)-N(2)-C(9)-C(10)	156.00(18)
C(16)-N(3)-C(9)-N(2)	158.69(17)
B(1)-N(3)-C(9)-N(2)	-7.7(3)
C(16)-N(3)-C(9)-C(10)	-10.7(2)
B(1)-N(3)-C(9)-C(10)	-177.14(15)
N(2)-C(9)-C(10)-C(11)	13.6(3)
N(3)-C(9)-C(10)-C(11)	-178.08(19)
N(2)-C(9)-C(10)-C(15)	-163.17(18)
N(3)-C(9)-C(10)-C(15)	5.19(19)
C(15)-C(10)-C(11)-F(5)	176.89(16)
C(9)-C(10)-C(11)-F(5)	0.5(3)
C(15)-C(10)-C(11)-C(12)	-4.4(3)
C(9)-C(10)-C(11)-C(12)	179.20(19)
F(5)-C(11)-C(12)-F(6)	1.8(3)
C(10)-C(11)-C(12)-F(6)	-176.97(16)
F(5)-C(11)-C(12)-C(13)	-179.25(16)
C(10)-C(11)-C(12)-C(13)	2.0(3)
F(6)-C(12)-C(13)-F(7)	2.2(3)
C(11)-C(12)-C(13)-F(7)	-176.75(17)
F(6)-C(12)-C(13)-C(14)	-178.64(17)
C(11)-C(12)-C(13)-C(14)	2.4(3)
F(7)-C(13)-C(14)-F(8)	-2.9(3)
C(12)-C(13)-C(14)-F(8)	177.98(16)
F(7)-C(13)-C(14)-C(15)	174.91(17)
C(12)-C(13)-C(14)-C(15)	-4.2(3)

F(8)-C(14)-C(15)-C(10)	179.53(15)
C(13)-C(14)-C(15)-C(10)	1.8(3)
F(8)-C(14)-C(15)-C(16)	-2.6(3)
C(13)-C(14)-C(15)-C(16)	179.64(19)
C(11)-C(10)-C(15)-C(14)	2.6(3)
C(9)-C(10)-C(15)-C(14)	179.86(16)
C(11)-C(10)-C(15)-C(16)	-175.79(16)
C(9)-C(10)-C(15)-C(16)	1.5(2)
C(17)-N(4)-C(16)-N(3)	9.2(2)
C(17)-N(4)-C(16)-C(15)	-153.03(19)
C(9)-N(3)-C(16)-N(4)	-154.26(17)
B(1)-N(3)-C(16)-N(4)	12.2(3)
C(9)-N(3)-C(16)-C(15)	11.7(2)
B(1)-N(3)-C(16)-C(15)	178.12(15)
C(14)-C(15)-C(16)-N(4)	-21.1(3)
C(10)-C(15)-C(16)-N(4)	157.00(18)
C(14)-C(15)-C(16)-N(3)	174.29(19)
C(10)-C(15)-C(16)-N(3)	-7.62(19)
C(16)-N(4)-C(17)-N(5)	-9.4(3)
C(16)-N(4)-C(17)-C(18)	151.52(18)
C(24)-N(5)-C(17)-N(4)	152.87(17)
B(1)-N(5)-C(17)-N(4)	-11.7(3)
C(24)-N(5)-C(17)-C(18)	-11.9(2)
B(1)-N(5)-C(17)-C(18)	-176.46(16)
N(4)-C(17)-C(18)-C(19)	16.6(3)
N(5)-C(17)-C(18)-C(19)	-179.87(19)
N(4)-C(17)-C(18)-C(23)	-155.79(18)
N(5)-C(17)-C(18)-C(23)	7.79(19)
C(23)-C(18)-C(19)-F(9)	-178.65(16)
C(17)-C(18)-C(19)-F(9)	9.8(3)
C(23)-C(18)-C(19)-C(20)	1.7(3)
C(17)-C(18)-C(19)-C(20)	-169.79(19)
F(9)-C(19)-C(20)-F(10)	-1.6(3)
C(18)-C(19)-C(20)-F(10)	178.05(17)
F(9)-C(19)-C(20)-C(21)	179.09(18)
C(18)-C(19)-C(20)-C(21)	-1.3(3)

F(10)-C(20)-C(21)-F(11)	0.5(3)
C(19)-C(20)-C(21)-F(11)	179.86(18)
F(10)-C(20)-C(21)-C(22)	-178.57(17)
C(19)-C(20)-C(21)-C(22)	0.8(3)
F(11)-C(21)-C(22)-F(12)	-2.2(3)
C(20)-C(21)-C(22)-F(12)	176.89(17)
F(11)-C(21)-C(22)-C(23)	-179.77(17)
C(20)-C(21)-C(22)-C(23)	-0.7(3)
F(12)-C(22)-C(23)-C(18)	-176.41(16)
C(21)-C(22)-C(23)-C(18)	1.1(3)
F(12)-C(22)-C(23)-C(24)	-5.2(3)
C(21)-C(22)-C(23)-C(24)	172.36(19)
C(19)-C(18)-C(23)-C(22)	-1.7(3)
C(17)-C(18)-C(23)-C(22)	171.74(16)
C(19)-C(18)-C(23)-C(24)	-175.01(17)
C(17)-C(18)-C(23)-C(24)	-1.6(2)
C(1)-N(6)-C(24)-N(5)	9.6(3)
C(1)-N(6)-C(24)-C(23)	-155.53(18)
C(17)-N(5)-C(24)-N(6)	-157.36(17)
B(1)-N(5)-C(24)-N(6)	7.1(3)
C(17)-N(5)-C(24)-C(23)	10.9(2)
B(1)-N(5)-C(24)-C(23)	175.32(15)
C(22)-C(23)-C(24)-N(6)	-10.1(3)
C(18)-C(23)-C(24)-N(6)	161.93(18)
C(22)-C(23)-C(24)-N(5)	-177.19(19)
C(18)-C(23)-C(24)-N(5)	-5.20(19)
C(1)-N(1)-B(1)-N(3)	139.04(16)
C(8)-N(1)-B(1)-N(3)	-29.5(2)
C(1)-N(1)-B(1)-N(5)	28.2(2)
C(8)-N(1)-B(1)-N(5)	-140.33(16)
C(1)-N(1)-B(1)-Cl(1)	-96.69(18)
C(8)-N(1)-B(1)-Cl(1)	94.79(18)
C(16)-N(3)-B(1)-N(1)	-139.62(16)
C(9)-N(3)-B(1)-N(1)	25.6(2)
C(16)-N(3)-B(1)-N(5)	-28.7(2)
C(9)-N(3)-B(1)-N(5)	136.54(16)

C(16)-N(3)-B(1)-Cl(1)	97.08(18)
C(9)-N(3)-B(1)-Cl(1)	-97.71(18)
C(24)-N(5)-B(1)-N(1)	-23.9(2)
C(17)-N(5)-B(1)-N(1)	139.25(16)
C(24)-N(5)-B(1)-N(3)	-134.80(17)
C(17)-N(5)-B(1)-N(3)	28.4(2)
C(24)-N(5)-B(1)-Cl(1)	99.72(18)
C(17)-N(5)-B(1)-Cl(1)	-97.11(18)

Symmetry transformations used to generate equivalent atoms:

Table S31. Crystal data and structure refinement for **F-F_{12}BsubPc (grown by train sublimation)**

Identification code	d17130	
Empirical formula	C24 B F13 N6	
Formula weight	630.11	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 11.5570(3) Å	a= 90°.
	b = 22.1670(6) Å	b= 90°.
	c = 26.3618(7) Å	g = 90°.
Volume	6753.5(3) Å^3	
Z	12	
Density (calculated)	1.859 Mg/m^3	
Absorption coefficient	1.726 mm^{-1}	
F(000)	3696	
Crystal size	0.040 x 0.030 x 0.020 mm^3	
Theta range for data collection	2.604 to 67.250°.	
Index ranges	-13<=h<=13, -26<=k<=26, -31<=l<=31	
Reflections collected	148198	
Independent reflections	11988 [R(int) = 0.0875]	
Completeness to theta = 67.250°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6851	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11988 / 0 / 1190	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0811	
R indices (all data)	R1 = 0.0465, wR2 = 0.0875	
Absolute structure parameter	0.11(4)	
Extinction coefficient	0.00044(4)	
Largest diff. peak and hole	0.241 and -0.233 e.Å^{-3}	

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **F-F_{12}BsubPc (grown by train sublimation)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2277(3)	-602(2)	9565(1)	23(1)
C(2)	626(3)	-65(2)	9725(1)	22(1)
C(3)	756(3)	941(2)	9882(1)	22(1)
C(4)	2496(3)	1426(2)	9834(1)	22(1)
C(5)	4129(3)	902(2)	9641(1)	22(1)
C(6)	4014(3)	-118(2)	9528(1)	24(1)
C(7)	4243(4)	-740(2)	9663(2)	24(1)
C(8)	3164(3)	-1044(2)	9684(2)	24(1)
C(9)	-386(3)	102(2)	10022(1)	23(1)
C(10)	-289(3)	728(2)	10123(2)	25(1)
C(11)	3467(3)	1770(2)	10021(1)	22(1)
C(12)	4487(3)	1447(2)	9898(1)	22(1)
C(13)	5241(4)	-1042(2)	9804(2)	29(1)
C(14)	5176(4)	-1633(2)	9953(2)	35(1)
C(15)	4116(4)	-1930(2)	9967(2)	35(1)
C(16)	3112(4)	-1638(2)	9839(2)	29(1)
C(17)	-1287(4)	-234(2)	10219(2)	26(1)
C(18)	-2089(4)	52(2)	10517(2)	29(1)
C(19)	-1991(4)	658(2)	10631(2)	29(1)
C(20)	-1104(4)	1000(2)	10437(2)	28(1)
C(21)	3554(3)	2294(2)	10309(1)	22(1)
C(22)	4625(4)	2492(2)	10457(1)	24(1)
C(23)	5617(3)	2168(2)	10346(1)	23(1)
C(24)	5552(3)	1646(2)	10066(1)	23(1)
N(1)	2857(3)	-88(1)	9424(1)	22(1)
N(2)	1146(3)	-606(2)	9680(1)	24(1)
N(3)	1164(3)	465(1)	9605(1)	21(1)
N(4)	1383(3)	1441(1)	9974(1)	23(1)
N(5)	2964(3)	964(1)	9555(1)	21(1)
N(6)	4682(3)	372(1)	9599(1)	22(1)

B(1)	2259(4)	490(2)	9307(2)	21(1)
F(1)	2097(2)	588(1)	8791(1)	28(1)
F(2)	6279(2)	-768(1)	9785(1)	37(1)
F(3)	6134(3)	-1937(1)	10074(1)	54(1)
F(4)	4098(3)	-2515(1)	10097(1)	52(1)
F(5)	2102(2)	-1934(1)	9858(1)	40(1)
F(6)	-1384(2)	-827(1)	10118(1)	33(1)
F(7)	-2989(2)	-255(1)	10713(1)	39(1)
F(8)	-2796(2)	914(1)	10929(1)	39(1)
F(9)	-1043(2)	1592(1)	10547(1)	38(1)
F(10)	2607(2)	2605(1)	10447(1)	30(1)
F(11)	4719(2)	3008(1)	10724(1)	30(1)
F(12)	6636(2)	2358(1)	10528(1)	29(1)
F(13)	6518(2)	1335(1)	9960(1)	28(1)
C(25)	4018(3)	-534(2)	6418(1)	24(1)
C(26)	4068(3)	419(2)	6092(1)	23(1)
C(27)	2401(4)	973(2)	6028(2)	27(1)
C(28)	684(4)	562(2)	6284(1)	27(1)
C(29)	624(4)	-397(2)	6596(1)	25(1)
C(30)	2303(3)	-935(2)	6677(1)	22(1)
C(31)	3213(3)	-1257(2)	6943(2)	25(1)
C(32)	4282(4)	-1002(2)	6783(1)	25(1)
C(33)	4394(4)	1056(2)	6081(1)	25(1)
C(34)	3349(4)	1397(2)	6044(2)	27(1)
C(35)	-360(4)	512(2)	6589(2)	29(1)
C(36)	-412(3)	-91(2)	6771(1)	27(1)
C(37)	3219(4)	-1698(2)	7317(2)	28(1)
C(38)	4247(4)	-1890(2)	7516(2)	34(1)
C(39)	5287(4)	-1631(2)	7366(2)	33(1)
C(40)	5313(4)	-1193(2)	6997(2)	28(1)
C(41)	5443(4)	1350(2)	6129(2)	29(1)
C(42)	5469(4)	1967(2)	6126(2)	34(1)
C(43)	4452(5)	2298(2)	6100(2)	37(1)
C(44)	3403(4)	2018(2)	6063(2)	34(1)
C(45)	-1186(4)	927(2)	6741(2)	33(1)
C(46)	-2066(4)	740(2)	7052(2)	38(1)

C(47)	-2140(4)	146(2)	7218(2)	36(1)
C(48)	-1316(4)	-270(2)	7083(2)	31(1)
N(7)	2850(3)	-575(1)	6334(1)	22(1)
N(8)	4653(3)	-54(2)	6272(1)	24(1)
N(9)	2904(3)	413(1)	5996(1)	22(1)
N(10)	1281(3)	1051(2)	6141(1)	29(1)
N(11)	1128(3)	-10(2)	6261(1)	24(1)
N(12)	1170(3)	-877(2)	6790(1)	26(1)
B(2)	2224(4)	-154(2)	5991(2)	22(1)
F(14)	2057(2)	-387(1)	5505(1)	29(1)
F(15)	2231(2)	-1949(1)	7483(1)	36(1)
F(16)	4269(3)	-2328(1)	7864(1)	49(1)
F(17)	6268(2)	-1826(1)	7582(1)	50(1)
F(18)	6323(2)	-958(1)	6849(1)	36(1)
F(19)	6435(2)	1042(1)	6169(1)	35(1)
F(20)	6486(3)	2256(1)	6151(1)	47(1)
F(21)	4519(3)	2904(1)	6112(1)	51(1)
F(22)	2434(3)	2354(1)	6033(1)	47(1)
F(23)	-1144(2)	1504(1)	6582(1)	46(1)
F(24)	-2889(2)	1135(1)	7201(1)	49(1)
F(25)	-3034(2)	-10(2)	7514(1)	48(1)
F(26)	-1390(2)	-836(1)	7254(1)	38(1)
C(49)	2584(3)	-478(2)	8054(2)	25(1)
C(50)	4304(4)	25(2)	8117(1)	26(1)
C(51)	4333(4)	1051(2)	8053(2)	26(1)
C(52)	2664(4)	1566(2)	7911(2)	26(1)
C(53)	951(3)	1065(2)	7812(1)	24(1)
C(54)	913(3)	39(2)	7902(1)	23(1)
C(55)	5342(4)	235(2)	8373(2)	28(1)
C(56)	5361(4)	873(2)	8333(2)	28(1)
C(57)	1739(4)	1986(2)	8033(2)	26(1)
C(58)	670(4)	1676(2)	7961(2)	25(1)
C(59)	598(4)	-519(2)	8152(2)	24(1)
C(60)	1637(4)	-840(2)	8246(2)	26(1)
C(61)	6176(4)	-67(2)	8651(2)	31(1)
C(62)	7032(4)	266(2)	8882(2)	34(1)

C(63)	7067(4)	894(2)	8838(2)	37(1)
C(64)	6226(4)	1195(2)	8573(2)	34(1)
C(65)	1726(4)	2556(2)	8248(2)	27(1)
C(66)	693(4)	2819(2)	8375(2)	27(1)
C(67)	-341(4)	2519(2)	8297(2)	26(1)
C(68)	-363(3)	1950(2)	8091(1)	24(1)
C(69)	-443(4)	-739(2)	8333(2)	29(1)
C(70)	-459(4)	-1275(2)	8596(2)	36(1)
C(71)	555(4)	-1593(2)	8683(2)	37(1)
C(72)	1601(4)	-1377(2)	8514(2)	31(1)
N(13)	2122(3)	1062(2)	7729(1)	24(1)
N(14)	320(3)	562(2)	7871(1)	24(1)
N(15)	2078(3)	-2(2)	7809(1)	23(1)
N(16)	3707(3)	-488(2)	8179(1)	27(1)
N(17)	3849(3)	522(2)	7886(1)	24(1)
N(18)	3775(3)	1583(2)	8041(1)	28(1)
B(3)	2758(4)	507(2)	7586(2)	24(1)
F(27)	2925(2)	446(1)	7067(1)	31(1)
F(28)	2715(2)	2850(1)	8354(1)	36(1)
F(29)	673(2)	3362(1)	8598(1)	34(1)
F(30)	-1334(2)	2774(1)	8457(1)	32(1)
F(31)	-1377(2)	1662(1)	8034(1)	32(1)
F(32)	-1432(2)	-440(1)	8250(1)	34(1)
F(33)	-1462(2)	-1495(1)	8767(1)	52(1)
F(34)	499(3)	-2115(1)	8936(1)	54(1)
F(35)	2571(2)	-1688(1)	8611(1)	39(1)
F(36)	6165(2)	-668(1)	8693(1)	39(1)
F(37)	7852(2)	-10(1)	9158(1)	46(1)
F(38)	7934(2)	1187(1)	9066(1)	47(1)
F(39)	6271(2)	1803(1)	8549(1)	45(1)

Table S33. Bond lengths [Å] and angles [°] for **F-F_{12}BsubPc (grown by train sublimation)**.

C(1)-N(2)	1.342(5)
C(1)-N(1)	1.373(5)
C(1)-C(8)	1.453(6)
C(2)-N(2)	1.348(5)
C(2)-N(3)	1.365(5)
C(2)-C(9)	1.455(5)
C(3)-N(4)	1.345(5)
C(3)-N(3)	1.368(5)
C(3)-C(10)	1.445(6)
C(4)-N(4)	1.338(5)
C(4)-N(5)	1.373(5)
C(4)-C(11)	1.443(6)
C(5)-N(6)	1.340(5)
C(5)-N(5)	1.373(5)
C(5)-C(12)	1.448(6)
C(6)-N(6)	1.347(5)
C(6)-N(1)	1.366(5)
C(6)-C(7)	1.449(6)
C(7)-C(13)	1.385(6)
C(7)-C(8)	1.418(6)
C(8)-C(16)	1.380(6)
C(9)-C(17)	1.382(6)
C(9)-C(10)	1.418(6)
C(10)-C(20)	1.391(6)
C(11)-C(21)	1.391(5)
C(11)-C(12)	1.416(5)
C(12)-C(24)	1.379(6)
C(13)-F(2)	1.346(5)
C(13)-C(14)	1.368(6)
C(14)-F(3)	1.334(5)
C(14)-C(15)	1.392(7)
C(15)-F(4)	1.341(5)
C(15)-C(16)	1.371(6)
C(16)-F(5)	1.338(5)

C(17)-F(6)	1.346(5)
C(17)-C(18)	1.370(6)
C(18)-F(7)	1.346(5)
C(18)-C(19)	1.383(6)
C(19)-F(8)	1.343(5)
C(19)-C(20)	1.372(6)
C(20)-F(9)	1.346(5)
C(21)-F(10)	1.343(4)
C(21)-C(22)	1.370(6)
C(22)-F(11)	1.346(4)
C(22)-C(23)	1.385(6)
C(23)-F(12)	1.340(5)
C(23)-C(24)	1.374(5)
C(24)-F(13)	1.342(4)
N(1)-B(1)	1.489(5)
N(3)-B(1)	1.490(5)
N(5)-B(1)	1.480(6)
B(1)-F(1)	1.390(5)
C(25)-N(8)	1.348(5)
C(25)-N(7)	1.371(5)
C(25)-C(32)	1.447(6)
C(26)-N(8)	1.335(5)
C(26)-N(9)	1.369(5)
C(26)-C(33)	1.463(6)
C(27)-N(10)	1.339(5)
C(27)-N(9)	1.372(5)
C(27)-C(34)	1.445(6)
C(28)-N(10)	1.339(6)
C(28)-N(11)	1.370(5)
C(28)-C(35)	1.454(6)
C(29)-N(12)	1.339(5)
C(29)-N(11)	1.361(5)
C(29)-C(36)	1.452(6)
C(30)-N(12)	1.348(5)
C(30)-N(7)	1.362(5)
C(30)-C(31)	1.452(6)

C(31)-C(37)	1.388(6)
C(31)-C(32)	1.423(6)
C(32)-C(40)	1.385(6)
C(33)-C(41)	1.382(6)
C(33)-C(34)	1.428(6)
C(34)-C(44)	1.379(6)
C(35)-C(45)	1.385(6)
C(35)-C(36)	1.421(6)
C(36)-C(48)	1.388(6)
C(37)-F(15)	1.343(5)
C(37)-C(38)	1.367(6)
C(38)-F(16)	1.336(5)
C(38)-C(39)	1.390(7)
C(39)-F(17)	1.341(5)
C(39)-C(40)	1.374(6)
C(40)-F(18)	1.337(5)
C(41)-F(19)	1.339(5)
C(41)-C(42)	1.368(6)
C(42)-F(20)	1.340(5)
C(42)-C(43)	1.387(7)
C(43)-F(21)	1.346(5)
C(43)-C(44)	1.365(7)
C(44)-F(22)	1.346(5)
C(45)-F(23)	1.347(5)
C(45)-C(46)	1.371(7)
C(46)-F(24)	1.351(5)
C(46)-C(47)	1.392(7)
C(47)-F(25)	1.339(5)
C(47)-C(48)	1.372(6)
C(48)-F(26)	1.337(5)
N(7)-B(2)	1.487(5)
N(9)-B(2)	1.482(6)
N(11)-B(2)	1.487(5)
B(2)-F(14)	1.395(5)
C(49)-N(16)	1.339(5)
C(49)-N(15)	1.368(5)

C(49)-C(60)	1.449(6)
C(50)-N(16)	1.341(6)
C(50)-N(17)	1.364(5)
C(50)-C(55)	1.453(6)
C(51)-N(18)	1.345(5)
C(51)-N(17)	1.372(5)
C(51)-C(56)	1.454(6)
C(52)-N(18)	1.330(5)
C(52)-N(13)	1.365(5)
C(52)-C(57)	1.454(6)
C(53)-N(14)	1.342(5)
C(53)-N(13)	1.370(5)
C(53)-C(58)	1.446(6)
C(54)-N(14)	1.349(5)
C(54)-N(15)	1.371(5)
C(54)-C(59)	1.448(6)
C(55)-C(61)	1.383(6)
C(55)-C(56)	1.419(6)
C(56)-C(64)	1.381(6)
C(57)-C(65)	1.386(6)
C(57)-C(58)	1.426(6)
C(58)-C(68)	1.383(6)
C(59)-C(69)	1.382(6)
C(59)-C(60)	1.418(6)
C(60)-C(72)	1.383(6)
C(61)-F(36)	1.337(5)
C(61)-C(62)	1.377(6)
C(62)-F(37)	1.341(5)
C(62)-C(63)	1.397(7)
C(63)-F(38)	1.337(5)
C(63)-C(64)	1.372(7)
C(64)-F(39)	1.349(5)
C(65)-F(28)	1.344(5)
C(65)-C(66)	1.369(6)
C(66)-F(29)	1.340(5)
C(66)-C(67)	1.383(6)

C(67)-F(30)	1.347(5)
C(67)-C(68)	1.373(6)
C(68)-F(31)	1.343(5)
C(69)-F(32)	1.339(5)
C(69)-C(70)	1.378(6)
C(70)-F(33)	1.334(5)
C(70)-C(71)	1.387(7)
C(71)-F(34)	1.337(5)
C(71)-C(72)	1.374(7)
C(72)-F(35)	1.340(5)
N(13)-B(3)	1.484(6)
N(15)-B(3)	1.495(6)
N(17)-B(3)	1.489(6)
B(3)-F(27)	1.388(5)

N(2)-C(1)-N(1)	123.0(4)
N(2)-C(1)-C(8)	129.3(4)
N(1)-C(1)-C(8)	105.8(3)
N(2)-C(2)-N(3)	122.9(3)
N(2)-C(2)-C(9)	129.1(4)
N(3)-C(2)-C(9)	105.8(3)
N(4)-C(3)-N(3)	123.1(3)
N(4)-C(3)-C(10)	129.9(3)
N(3)-C(3)-C(10)	105.6(3)
N(4)-C(4)-N(5)	122.9(4)
N(4)-C(4)-C(11)	129.9(4)
N(5)-C(4)-C(11)	105.7(3)
N(6)-C(5)-N(5)	122.8(4)
N(6)-C(5)-C(12)	129.3(4)
N(5)-C(5)-C(12)	105.9(3)
N(6)-C(6)-N(1)	123.4(4)
N(6)-C(6)-C(7)	129.0(4)
N(1)-C(6)-C(7)	105.9(3)
C(13)-C(7)-C(8)	119.5(4)
C(13)-C(7)-C(6)	132.7(4)
C(8)-C(7)-C(6)	107.5(3)

C(16)-C(8)-C(7)	120.2(4)
C(16)-C(8)-C(1)	132.6(4)
C(7)-C(8)-C(1)	107.0(3)
C(17)-C(9)-C(10)	121.1(4)
C(17)-C(9)-C(2)	132.2(4)
C(10)-C(9)-C(2)	106.6(3)
C(20)-C(10)-C(9)	118.9(4)
C(20)-C(10)-C(3)	133.3(4)
C(9)-C(10)-C(3)	107.7(3)
C(21)-C(11)-C(12)	119.1(4)
C(21)-C(11)-C(4)	133.1(4)
C(12)-C(11)-C(4)	107.6(3)
C(24)-C(12)-C(11)	120.5(4)
C(24)-C(12)-C(5)	132.2(4)
C(11)-C(12)-C(5)	107.0(3)
F(2)-C(13)-C(14)	119.5(4)
F(2)-C(13)-C(7)	120.9(4)
C(14)-C(13)-C(7)	119.6(4)
F(3)-C(14)-C(13)	120.4(4)
F(3)-C(14)-C(15)	119.0(4)
C(13)-C(14)-C(15)	120.6(4)
F(4)-C(15)-C(16)	120.4(4)
F(4)-C(15)-C(14)	118.6(4)
C(16)-C(15)-C(14)	121.0(4)
F(5)-C(16)-C(15)	119.9(4)
F(5)-C(16)-C(8)	121.1(4)
C(15)-C(16)-C(8)	119.1(4)
F(6)-C(17)-C(18)	120.6(4)
F(6)-C(17)-C(9)	121.0(4)
C(18)-C(17)-C(9)	118.4(4)
F(7)-C(18)-C(17)	120.6(4)
F(7)-C(18)-C(19)	118.1(4)
C(17)-C(18)-C(19)	121.3(4)
F(8)-C(19)-C(20)	120.2(4)
F(8)-C(19)-C(18)	118.7(4)
C(20)-C(19)-C(18)	121.1(4)

F(9)-C(20)-C(19)	119.7(4)
F(9)-C(20)-C(10)	121.0(4)
C(19)-C(20)-C(10)	119.2(4)
F(10)-C(21)-C(22)	119.7(3)
F(10)-C(21)-C(11)	121.2(4)
C(22)-C(21)-C(11)	119.2(4)
F(11)-C(22)-C(21)	119.6(4)
F(11)-C(22)-C(23)	119.0(4)
C(21)-C(22)-C(23)	121.4(3)
F(12)-C(23)-C(24)	120.4(4)
F(12)-C(23)-C(22)	119.2(3)
C(24)-C(23)-C(22)	120.4(4)
F(13)-C(24)-C(23)	119.9(3)
F(13)-C(24)-C(12)	120.8(3)
C(23)-C(24)-C(12)	119.3(4)
C(6)-N(1)-C(1)	112.6(3)
C(6)-N(1)-B(1)	122.5(3)
C(1)-N(1)-B(1)	122.9(3)
C(1)-N(2)-C(2)	116.5(3)
C(2)-N(3)-C(3)	112.6(3)
C(2)-N(3)-B(1)	122.8(3)
C(3)-N(3)-B(1)	123.0(3)
C(4)-N(4)-C(3)	116.7(3)
C(5)-N(5)-C(4)	111.9(3)
C(5)-N(5)-B(1)	122.8(3)
C(4)-N(5)-B(1)	123.3(3)
C(5)-N(6)-C(6)	116.4(3)
F(1)-B(1)-N(5)	113.3(3)
F(1)-B(1)-N(1)	113.5(3)
N(5)-B(1)-N(1)	105.3(3)
F(1)-B(1)-N(3)	114.0(3)
N(5)-B(1)-N(3)	105.2(3)
N(1)-B(1)-N(3)	104.6(3)
N(8)-C(25)-N(7)	122.8(4)
N(8)-C(25)-C(32)	129.8(4)
N(7)-C(25)-C(32)	105.5(3)

N(8)-C(26)-N(9)	123.8(4)
N(8)-C(26)-C(33)	129.5(4)
N(9)-C(26)-C(33)	105.0(3)
N(10)-C(27)-N(9)	122.7(4)
N(10)-C(27)-C(34)	130.0(4)
N(9)-C(27)-C(34)	105.6(3)
N(10)-C(28)-N(11)	123.0(4)
N(10)-C(28)-C(35)	130.2(4)
N(11)-C(28)-C(35)	105.4(4)
N(12)-C(29)-N(11)	123.1(4)
N(12)-C(29)-C(36)	129.7(4)
N(11)-C(29)-C(36)	105.3(4)
N(12)-C(30)-N(7)	122.8(4)
N(12)-C(30)-C(31)	130.0(4)
N(7)-C(30)-C(31)	105.8(3)
C(37)-C(31)-C(32)	119.1(4)
C(37)-C(31)-C(30)	133.9(4)
C(32)-C(31)-C(30)	106.9(3)
C(40)-C(32)-C(31)	120.3(4)
C(40)-C(32)-C(25)	132.2(4)
C(31)-C(32)-C(25)	107.4(3)
C(41)-C(33)-C(34)	119.9(4)
C(41)-C(33)-C(26)	132.8(4)
C(34)-C(33)-C(26)	107.1(3)
C(44)-C(34)-C(33)	119.2(4)
C(44)-C(34)-C(27)	133.3(4)
C(33)-C(34)-C(27)	107.4(3)
C(45)-C(35)-C(36)	119.8(4)
C(45)-C(35)-C(28)	133.0(4)
C(36)-C(35)-C(28)	107.1(3)
C(48)-C(36)-C(35)	120.1(4)
C(48)-C(36)-C(29)	132.5(4)
C(35)-C(36)-C(29)	107.3(4)
F(15)-C(37)-C(38)	119.0(4)
F(15)-C(37)-C(31)	121.2(4)
C(38)-C(37)-C(31)	119.8(4)

F(16)-C(38)-C(37)	120.5(4)
F(16)-C(38)-C(39)	118.6(4)
C(37)-C(38)-C(39)	120.9(4)
F(17)-C(39)-C(40)	120.7(4)
F(17)-C(39)-C(38)	118.5(4)
C(40)-C(39)-C(38)	120.8(4)
F(18)-C(40)-C(39)	120.1(4)
F(18)-C(40)-C(32)	120.8(4)
C(39)-C(40)-C(32)	119.1(4)
F(19)-C(41)-C(42)	119.5(4)
F(19)-C(41)-C(33)	121.2(4)
C(42)-C(41)-C(33)	119.4(4)
F(20)-C(42)-C(41)	119.8(4)
F(20)-C(42)-C(43)	119.5(4)
C(41)-C(42)-C(43)	120.7(4)
F(21)-C(43)-C(44)	120.4(4)
F(21)-C(43)-C(42)	118.5(4)
C(44)-C(43)-C(42)	121.1(4)
F(22)-C(44)-C(43)	119.5(4)
F(22)-C(44)-C(34)	120.8(4)
C(43)-C(44)-C(34)	119.7(4)
F(23)-C(45)-C(46)	119.9(4)
F(23)-C(45)-C(35)	121.1(4)
C(46)-C(45)-C(35)	119.0(4)
F(24)-C(46)-C(45)	120.0(5)
F(24)-C(46)-C(47)	118.6(4)
C(45)-C(46)-C(47)	121.3(4)
F(25)-C(47)-C(48)	120.9(4)
F(25)-C(47)-C(46)	118.4(4)
C(48)-C(47)-C(46)	120.7(4)
F(26)-C(48)-C(47)	119.9(4)
F(26)-C(48)-C(36)	121.1(4)
C(47)-C(48)-C(36)	119.0(4)
C(30)-N(7)-C(25)	112.8(3)
C(30)-N(7)-B(2)	123.0(3)
C(25)-N(7)-B(2)	122.4(3)

C(26)-N(8)-C(25)	116.4(3)
C(26)-N(9)-C(27)	113.4(3)
C(26)-N(9)-B(2)	122.0(3)
C(27)-N(9)-B(2)	122.8(3)
C(27)-N(10)-C(28)	117.1(3)
C(29)-N(11)-C(28)	113.2(3)
C(29)-N(11)-B(2)	122.7(3)
C(28)-N(11)-B(2)	122.6(3)
C(29)-N(12)-C(30)	116.6(3)
F(14)-B(2)-N(9)	113.3(3)
F(14)-B(2)-N(7)	113.0(3)
N(9)-B(2)-N(7)	105.7(3)
F(14)-B(2)-N(11)	113.6(3)
N(9)-B(2)-N(11)	105.4(3)
N(7)-B(2)-N(11)	105.0(3)
N(16)-C(49)-N(15)	122.9(4)
N(16)-C(49)-C(60)	129.5(4)
N(15)-C(49)-C(60)	105.6(3)
N(16)-C(50)-N(17)	122.7(4)
N(16)-C(50)-C(55)	129.8(4)
N(17)-C(50)-C(55)	105.5(4)
N(18)-C(51)-N(17)	123.1(4)
N(18)-C(51)-C(56)	130.0(4)
N(17)-C(51)-C(56)	105.4(4)
N(18)-C(52)-N(13)	123.9(4)
N(18)-C(52)-C(57)	129.4(4)
N(13)-C(52)-C(57)	105.3(3)
N(14)-C(53)-N(13)	123.5(4)
N(14)-C(53)-C(58)	128.7(4)
N(13)-C(53)-C(58)	105.6(3)
N(14)-C(54)-N(15)	122.9(4)
N(14)-C(54)-C(59)	129.4(4)
N(15)-C(54)-C(59)	105.8(3)
C(61)-C(55)-C(56)	120.7(4)
C(61)-C(55)-C(50)	131.8(4)
C(56)-C(55)-C(50)	107.3(4)

C(64)-C(56)-C(55)	119.6(4)
C(64)-C(56)-C(51)	133.1(4)
C(55)-C(56)-C(51)	107.1(4)
C(65)-C(57)-C(58)	119.0(4)
C(65)-C(57)-C(52)	133.1(4)
C(58)-C(57)-C(52)	107.4(3)
C(68)-C(58)-C(57)	120.2(4)
C(68)-C(58)-C(53)	132.3(4)
C(57)-C(58)-C(53)	107.0(4)
C(69)-C(59)-C(60)	120.0(4)
C(69)-C(59)-C(54)	132.5(4)
C(60)-C(59)-C(54)	107.2(4)
C(72)-C(60)-C(59)	119.7(4)
C(72)-C(60)-C(49)	132.6(4)
C(59)-C(60)-C(49)	107.5(3)
F(36)-C(61)-C(62)	120.2(4)
F(36)-C(61)-C(55)	121.3(4)
C(62)-C(61)-C(55)	118.5(4)
F(37)-C(62)-C(61)	120.3(4)
F(37)-C(62)-C(63)	118.6(4)
C(61)-C(62)-C(63)	121.2(4)
F(38)-C(63)-C(64)	121.5(4)
F(38)-C(63)-C(62)	118.0(4)
C(64)-C(63)-C(62)	120.5(4)
F(39)-C(64)-C(63)	118.9(4)
F(39)-C(64)-C(56)	121.5(4)
C(63)-C(64)-C(56)	119.6(4)
F(28)-C(65)-C(66)	119.0(4)
F(28)-C(65)-C(57)	121.1(4)
C(66)-C(65)-C(57)	119.8(4)
F(29)-C(66)-C(65)	120.3(4)
F(29)-C(66)-C(67)	118.8(4)
C(65)-C(66)-C(67)	120.9(4)
F(30)-C(67)-C(68)	119.6(4)
F(30)-C(67)-C(66)	119.2(4)
C(68)-C(67)-C(66)	121.1(4)

F(31)-C(68)-C(67)	119.8(4)
F(31)-C(68)-C(58)	121.1(4)
C(67)-C(68)-C(58)	119.1(4)
F(32)-C(69)-C(70)	119.8(4)
F(32)-C(69)-C(59)	120.9(4)
C(70)-C(69)-C(59)	119.3(4)
F(33)-C(70)-C(69)	119.8(4)
F(33)-C(70)-C(71)	119.6(4)
C(69)-C(70)-C(71)	120.6(4)
F(34)-C(71)-C(72)	120.4(4)
F(34)-C(71)-C(70)	118.7(4)
C(72)-C(71)-C(70)	120.9(4)
F(35)-C(72)-C(71)	119.6(4)
F(35)-C(72)-C(60)	121.0(4)
C(71)-C(72)-C(60)	119.4(4)
C(52)-N(13)-C(53)	113.2(3)
C(52)-N(13)-B(3)	122.7(4)
C(53)-N(13)-B(3)	122.2(4)
C(53)-N(14)-C(54)	116.5(3)
C(49)-N(15)-C(54)	112.7(3)
C(49)-N(15)-B(3)	122.9(4)
C(54)-N(15)-B(3)	122.5(4)
C(49)-N(16)-C(50)	117.1(4)
C(50)-N(17)-C(51)	112.9(3)
C(50)-N(17)-B(3)	123.1(3)
C(51)-N(17)-B(3)	122.4(3)
C(52)-N(18)-C(51)	116.4(4)
F(27)-B(3)-N(13)	113.6(3)
F(27)-B(3)-N(17)	114.1(4)
N(13)-B(3)-N(17)	105.4(3)
F(27)-B(3)-N(15)	112.8(3)
N(13)-B(3)-N(15)	105.4(3)
N(17)-B(3)-N(15)	104.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S34 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F-F_{12}BsubPc (grown by train sublimation)**. 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}
C(1)	25(2)	23(2)	21(2)	-2(2)	1(2)	-2(2)
C(2)	23(2)	26(2)	17(2)	-1(2)	-1(2)	-1(2)
C(3)	21(2)	25(2)	20(2)	-1(2)	-2(2)	4(2)
C(4)	24(2)	22(2)	20(2)	1(2)	2(2)	4(2)
C(5)	20(2)	26(2)	20(2)	1(2)	3(2)	2(2)
C(6)	25(2)	25(2)	23(2)	-3(2)	2(2)	3(2)
C(7)	26(2)	23(2)	24(2)	-2(2)	2(2)	4(2)
C(8)	27(2)	22(2)	24(2)	-2(2)	4(2)	2(2)
C(9)	19(2)	30(2)	20(2)	1(2)	-2(2)	2(2)
C(10)	21(2)	30(2)	23(2)	2(2)	1(2)	3(2)
C(11)	21(2)	22(2)	23(2)	1(2)	0(2)	2(2)
C(12)	24(2)	22(2)	19(2)	2(2)	1(2)	2(2)
C(13)	27(2)	31(2)	28(2)	-4(2)	0(2)	5(2)
C(14)	36(3)	30(2)	39(3)	2(2)	-4(2)	14(2)
C(15)	47(3)	22(2)	35(2)	3(2)	2(2)	7(2)
C(16)	33(2)	25(2)	30(2)	-1(2)	4(2)	-1(2)
C(17)	23(2)	33(2)	22(2)	2(2)	-3(2)	-2(2)
C(18)	20(2)	42(3)	25(2)	6(2)	4(2)	-1(2)
C(19)	19(2)	44(3)	23(2)	1(2)	7(2)	10(2)
C(20)	26(2)	31(2)	29(2)	2(2)	-1(2)	6(2)
C(21)	23(2)	23(2)	22(2)	0(2)	1(2)	6(2)
C(22)	30(2)	21(2)	20(2)	-3(2)	1(2)	-2(2)
C(23)	24(2)	24(2)	22(2)	2(2)	-4(2)	-1(2)
C(24)	18(2)	27(2)	24(2)	-1(2)	2(2)	2(2)
N(1)	24(2)	22(2)	18(2)	-2(1)	2(1)	2(2)
N(2)	22(2)	27(2)	23(2)	-2(1)	-1(1)	-1(2)
N(3)	20(2)	25(2)	19(2)	0(1)	0(1)	2(1)
N(4)	21(2)	24(2)	23(2)	1(1)	-1(1)	4(1)
N(5)	21(2)	22(2)	19(2)	0(1)	1(1)	1(1)
N(6)	25(2)	21(2)	21(2)	-2(1)	3(1)	0(1)

B(1)	22(2)	26(2)	15(2)	-2(2)	-1(2)	2(2)
F(1)	32(1)	35(1)	16(1)	1(1)	0(1)	1(1)
F(2)	26(1)	39(1)	46(2)	-4(1)	-4(1)	5(1)
F(3)	47(2)	42(2)	72(2)	7(1)	-9(2)	20(1)
F(4)	67(2)	26(1)	62(2)	11(1)	1(2)	9(1)
F(5)	44(2)	29(1)	48(2)	1(1)	6(1)	-6(1)
F(6)	28(1)	36(1)	34(1)	2(1)	2(1)	-5(1)
F(7)	25(1)	56(2)	35(1)	6(1)	9(1)	-4(1)
F(8)	29(1)	54(2)	35(1)	1(1)	11(1)	11(1)
F(9)	35(1)	34(1)	44(2)	-4(1)	8(1)	10(1)
F(10)	28(1)	28(1)	33(1)	-6(1)	-2(1)	8(1)
F(11)	37(1)	26(1)	26(1)	-6(1)	-1(1)	-1(1)
F(12)	24(1)	33(1)	30(1)	-1(1)	-4(1)	-5(1)
F(13)	20(1)	30(1)	34(1)	-1(1)	2(1)	4(1)
C(25)	21(2)	28(2)	21(2)	-2(2)	2(2)	-1(2)
C(26)	24(2)	26(2)	19(2)	-2(2)	3(2)	1(2)
C(27)	30(2)	29(2)	21(2)	1(2)	-2(2)	5(2)
C(28)	25(2)	34(2)	21(2)	-6(2)	-5(2)	5(2)
C(29)	24(2)	32(2)	19(2)	-5(2)	1(2)	-4(2)
C(30)	24(2)	23(2)	19(2)	-3(2)	0(2)	-5(2)
C(31)	28(2)	24(2)	22(2)	-2(2)	-1(2)	-2(2)
C(32)	25(2)	27(2)	22(2)	-2(2)	-1(2)	2(2)
C(33)	29(2)	27(2)	20(2)	1(2)	2(2)	-4(2)
C(34)	35(2)	24(2)	23(2)	2(2)	0(2)	0(2)
C(35)	22(2)	41(2)	24(2)	-8(2)	-3(2)	6(2)
C(36)	19(2)	42(2)	20(2)	-7(2)	-2(2)	1(2)
C(37)	32(2)	31(2)	23(2)	0(2)	3(2)	0(2)
C(38)	41(3)	36(2)	24(2)	6(2)	-1(2)	6(2)
C(39)	28(2)	43(3)	28(2)	0(2)	-4(2)	12(2)
C(40)	25(2)	31(2)	29(2)	-4(2)	0(2)	2(2)
C(41)	29(2)	33(2)	27(2)	-2(2)	2(2)	-2(2)
C(42)	39(3)	33(2)	32(2)	-2(2)	1(2)	-12(2)
C(43)	57(3)	24(2)	30(2)	2(2)	2(2)	-9(2)
C(44)	42(3)	29(2)	30(2)	2(2)	-1(2)	8(2)
C(45)	28(2)	39(3)	32(2)	-6(2)	-5(2)	10(2)
C(46)	24(2)	58(3)	33(2)	-16(2)	-3(2)	17(2)

C(47)	18(2)	63(3)	26(2)	-7(2)	0(2)	3(2)
C(48)	21(2)	46(3)	26(2)	-6(2)	-1(2)	-3(2)
N(7)	21(2)	26(2)	20(2)	-4(1)	-1(1)	0(1)
N(8)	25(2)	25(2)	22(2)	-2(1)	4(1)	1(1)
N(9)	24(2)	26(2)	17(2)	-1(1)	0(1)	1(2)
N(10)	29(2)	32(2)	25(2)	1(2)	-2(2)	6(2)
N(11)	22(2)	30(2)	19(2)	-4(1)	-3(1)	1(1)
N(12)	23(2)	31(2)	24(2)	-5(1)	-1(1)	-1(2)
B(2)	22(2)	28(2)	15(2)	-5(2)	-2(2)	1(2)
F(14)	32(1)	38(1)	18(1)	-7(1)	-3(1)	0(1)
F(15)	37(1)	40(1)	30(1)	6(1)	3(1)	-6(1)
F(16)	56(2)	53(2)	37(2)	21(1)	1(1)	10(1)
F(17)	36(2)	69(2)	44(2)	11(1)	-8(1)	15(1)
F(18)	21(1)	42(1)	46(2)	2(1)	-1(1)	1(1)
F(19)	29(1)	40(1)	35(1)	-6(1)	-1(1)	-4(1)
F(20)	51(2)	41(2)	50(2)	-5(1)	4(1)	-19(1)
F(21)	74(2)	24(1)	54(2)	2(1)	5(2)	-8(1)
F(22)	56(2)	30(1)	54(2)	4(1)	-2(1)	11(1)
F(23)	39(2)	48(2)	51(2)	-5(1)	-3(1)	16(1)
F(24)	33(2)	70(2)	44(2)	-15(1)	1(1)	21(2)
F(25)	27(1)	82(2)	35(1)	-9(1)	9(1)	3(1)
F(26)	28(1)	53(2)	34(1)	-4(1)	4(1)	-6(1)
C(49)	25(2)	28(2)	23(2)	-5(2)	-2(2)	6(2)
C(50)	22(2)	35(2)	20(2)	-5(2)	0(2)	5(2)
C(51)	23(2)	33(2)	22(2)	-5(2)	5(2)	-2(2)
C(52)	26(2)	30(2)	23(2)	-1(2)	3(2)	-3(2)
C(53)	24(2)	27(2)	20(2)	-1(2)	-2(2)	1(2)
C(54)	20(2)	29(2)	20(2)	-3(2)	-4(2)	3(2)
C(55)	20(2)	41(2)	22(2)	-5(2)	4(2)	1(2)
C(56)	20(2)	39(2)	25(2)	-6(2)	1(2)	-1(2)
C(57)	27(2)	27(2)	25(2)	1(2)	0(2)	1(2)
C(58)	29(2)	23(2)	23(2)	-2(2)	-3(2)	-1(2)
C(59)	25(2)	24(2)	25(2)	-6(2)	-2(2)	-1(2)
C(60)	27(2)	26(2)	24(2)	-5(2)	-3(2)	1(2)
C(61)	23(2)	46(3)	22(2)	-4(2)	3(2)	5(2)
C(62)	21(2)	57(3)	24(2)	-3(2)	-4(2)	3(2)

C(63)	19(2)	62(3)	30(2)	-14(2)	1(2)	-9(2)
C(64)	22(2)	44(3)	35(2)	-11(2)	5(2)	-6(2)
C(65)	30(2)	26(2)	26(2)	1(2)	-4(2)	-6(2)
C(66)	38(2)	22(2)	22(2)	-2(2)	-2(2)	4(2)
C(67)	26(2)	30(2)	22(2)	0(2)	-2(2)	6(2)
C(68)	23(2)	28(2)	23(2)	1(2)	-3(2)	0(2)
C(69)	24(2)	32(2)	30(2)	-4(2)	-3(2)	1(2)
C(70)	32(2)	36(2)	42(3)	3(2)	4(2)	-8(2)
C(71)	42(3)	28(2)	40(3)	5(2)	1(2)	-4(2)
C(72)	32(2)	30(2)	32(2)	-2(2)	-6(2)	6(2)
N(13)	24(2)	28(2)	20(2)	-3(1)	1(1)	-1(2)
N(14)	24(2)	24(2)	23(2)	-2(1)	-4(1)	-1(2)
N(15)	24(2)	27(2)	17(2)	-5(1)	-2(1)	1(2)
N(16)	25(2)	32(2)	23(2)	-4(1)	0(1)	3(2)
N(17)	22(2)	31(2)	20(2)	-2(1)	1(1)	0(2)
N(18)	24(2)	32(2)	28(2)	-1(1)	2(2)	-3(2)
B(3)	25(2)	30(2)	16(2)	-4(2)	1(2)	1(2)
F(27)	34(1)	41(1)	18(1)	-4(1)	1(1)	1(1)
F(28)	34(1)	31(1)	43(1)	-3(1)	1(1)	-10(1)
F(29)	45(2)	23(1)	35(1)	-5(1)	-6(1)	4(1)
F(30)	33(1)	31(1)	32(1)	-2(1)	-1(1)	11(1)
F(31)	24(1)	35(1)	38(1)	-2(1)	-2(1)	-1(1)
F(32)	25(1)	40(1)	38(1)	-2(1)	3(1)	1(1)
F(33)	40(2)	48(2)	68(2)	14(2)	12(2)	-9(1)
F(34)	63(2)	36(2)	63(2)	20(1)	0(2)	-4(1)
F(35)	42(2)	34(1)	43(1)	3(1)	-8(1)	11(1)
F(36)	31(1)	50(2)	36(1)	1(1)	-5(1)	4(1)
F(37)	29(1)	76(2)	32(1)	-1(1)	-8(1)	4(2)
F(38)	28(1)	70(2)	42(2)	-16(1)	-6(1)	-11(1)
F(39)	32(1)	46(2)	58(2)	-14(1)	-1(1)	-10(1)

Table S35. Torsion angles [°] for **F-F_{12}BsubPc (grown by train sublimation)**.

N(6)-C(6)-C(7)-C(13)	-14.7(7)
N(1)-C(6)-C(7)-C(13)	180.0(4)
N(6)-C(6)-C(7)-C(8)	159.2(4)
N(1)-C(6)-C(7)-C(8)	-6.1(4)
C(13)-C(7)-C(8)-C(16)	-0.7(6)
C(6)-C(7)-C(8)-C(16)	-175.5(4)
C(13)-C(7)-C(8)-C(1)	174.4(4)
C(6)-C(7)-C(8)-C(1)	-0.4(4)
N(2)-C(1)-C(8)-C(16)	16.7(7)
N(1)-C(1)-C(8)-C(16)	-179.0(4)
N(2)-C(1)-C(8)-C(7)	-157.6(4)
N(1)-C(1)-C(8)-C(7)	6.8(4)
N(2)-C(2)-C(9)-C(17)	-21.2(7)
N(3)-C(2)-C(9)-C(17)	175.5(4)
N(2)-C(2)-C(9)-C(10)	154.9(4)
N(3)-C(2)-C(9)-C(10)	-8.5(4)
C(17)-C(9)-C(10)-C(20)	1.6(6)
C(2)-C(9)-C(10)-C(20)	-175.0(4)
C(17)-C(9)-C(10)-C(3)	177.7(4)
C(2)-C(9)-C(10)-C(3)	1.1(4)
N(4)-C(3)-C(10)-C(20)	15.3(7)
N(3)-C(3)-C(10)-C(20)	-178.1(4)
N(4)-C(3)-C(10)-C(9)	-160.1(4)
N(3)-C(3)-C(10)-C(9)	6.6(4)
N(4)-C(4)-C(11)-C(21)	-16.2(7)
N(5)-C(4)-C(11)-C(21)	177.7(4)
N(4)-C(4)-C(11)-C(12)	158.6(4)
N(5)-C(4)-C(11)-C(12)	-7.5(4)
C(21)-C(11)-C(12)-C(24)	0.8(6)
C(4)-C(11)-C(12)-C(24)	-174.9(4)
C(21)-C(11)-C(12)-C(5)	174.9(3)
C(4)-C(11)-C(12)-C(5)	-0.7(4)
N(6)-C(5)-C(12)-C(24)	17.9(7)
N(5)-C(5)-C(12)-C(24)	-178.1(4)

N(6)-C(5)-C(12)-C(11)	-155.3(4)
N(5)-C(5)-C(12)-C(11)	8.7(4)
C(8)-C(7)-C(13)-F(2)	179.5(3)
C(6)-C(7)-C(13)-F(2)	-7.2(7)
C(8)-C(7)-C(13)-C(14)	1.2(6)
C(6)-C(7)-C(13)-C(14)	174.5(4)
F(2)-C(13)-C(14)-F(3)	-0.6(6)
C(7)-C(13)-C(14)-F(3)	177.7(4)
F(2)-C(13)-C(14)-C(15)	-178.9(4)
C(7)-C(13)-C(14)-C(15)	-0.5(7)
F(3)-C(14)-C(15)-F(4)	-0.8(7)
C(13)-C(14)-C(15)-F(4)	177.5(4)
F(3)-C(14)-C(15)-C(16)	-179.0(4)
C(13)-C(14)-C(15)-C(16)	-0.7(7)
F(4)-C(15)-C(16)-F(5)	2.1(6)
C(14)-C(15)-C(16)-F(5)	-179.7(4)
F(4)-C(15)-C(16)-C(8)	-177.0(4)
C(14)-C(15)-C(16)-C(8)	1.2(7)
C(7)-C(8)-C(16)-F(5)	-179.5(4)
C(1)-C(8)-C(16)-F(5)	6.8(7)
C(7)-C(8)-C(16)-C(15)	-0.5(6)
C(1)-C(8)-C(16)-C(15)	-174.2(4)
C(10)-C(9)-C(17)-F(6)	179.3(3)
C(2)-C(9)-C(17)-F(6)	-5.1(7)
C(10)-C(9)-C(17)-C(18)	0.1(6)
C(2)-C(9)-C(17)-C(18)	175.6(4)
F(6)-C(17)-C(18)-F(7)	0.0(6)
C(9)-C(17)-C(18)-F(7)	179.3(4)
F(6)-C(17)-C(18)-C(19)	178.9(4)
C(9)-C(17)-C(18)-C(19)	-1.8(6)
F(7)-C(18)-C(19)-F(8)	-0.3(6)
C(17)-C(18)-C(19)-F(8)	-179.2(4)
F(7)-C(18)-C(19)-C(20)	-179.1(4)
C(17)-C(18)-C(19)-C(20)	2.0(6)
F(8)-C(19)-C(20)-F(9)	-0.1(6)
C(18)-C(19)-C(20)-F(9)	178.7(4)

F(8)-C(19)-C(20)-C(10)	-179.1(4)
C(18)-C(19)-C(20)-C(10)	-0.3(6)
C(9)-C(10)-C(20)-F(9)	179.6(4)
C(3)-C(10)-C(20)-F(9)	4.6(7)
C(9)-C(10)-C(20)-C(19)	-1.4(6)
C(3)-C(10)-C(20)-C(19)	-176.4(4)
C(12)-C(11)-C(21)-F(10)	-178.0(3)
C(4)-C(11)-C(21)-F(10)	-3.7(7)
C(12)-C(11)-C(21)-C(22)	1.4(6)
C(4)-C(11)-C(21)-C(22)	175.7(4)
F(10)-C(21)-C(22)-F(11)	-2.4(5)
C(11)-C(21)-C(22)-F(11)	178.2(3)
F(10)-C(21)-C(22)-C(23)	176.4(4)
C(11)-C(21)-C(22)-C(23)	-3.0(6)
F(11)-C(22)-C(23)-F(12)	3.3(5)
C(21)-C(22)-C(23)-F(12)	-175.5(3)
F(11)-C(22)-C(23)-C(24)	-178.7(3)
C(21)-C(22)-C(23)-C(24)	2.5(6)
F(12)-C(23)-C(24)-F(13)	-2.2(5)
C(22)-C(23)-C(24)-F(13)	179.9(3)
F(12)-C(23)-C(24)-C(12)	177.7(3)
C(22)-C(23)-C(24)-C(12)	-0.3(6)
C(11)-C(12)-C(24)-F(13)	178.5(3)
C(5)-C(12)-C(24)-F(13)	6.1(6)
C(11)-C(12)-C(24)-C(23)	-1.3(6)
C(5)-C(12)-C(24)-C(23)	-173.8(4)
N(6)-C(6)-N(1)-C(1)	-155.4(4)
C(7)-C(6)-N(1)-C(1)	11.0(4)
N(6)-C(6)-N(1)-B(1)	8.8(6)
C(7)-C(6)-N(1)-B(1)	175.2(3)
N(2)-C(1)-N(1)-C(6)	154.3(4)
C(8)-C(1)-N(1)-C(6)	-11.3(4)
N(2)-C(1)-N(1)-B(1)	-9.8(6)
C(8)-C(1)-N(1)-B(1)	-175.4(3)
N(1)-C(1)-N(2)-C(2)	-9.5(5)
C(8)-C(1)-N(2)-C(2)	152.5(4)

N(3)-C(2)-N(2)-C(1)	7.3(5)
C(9)-C(2)-N(2)-C(1)	-153.5(4)
N(2)-C(2)-N(3)-C(3)	-151.2(4)
C(9)-C(2)-N(3)-C(3)	13.4(4)
N(2)-C(2)-N(3)-B(1)	14.4(5)
C(9)-C(2)-N(3)-B(1)	179.0(3)
N(4)-C(3)-N(3)-C(2)	155.2(4)
C(10)-C(3)-N(3)-C(2)	-12.6(4)
N(4)-C(3)-N(3)-B(1)	-10.4(6)
C(10)-C(3)-N(3)-B(1)	-178.2(3)
N(5)-C(4)-N(4)-C(3)	7.9(5)
C(11)-C(4)-N(4)-C(3)	-156.1(4)
N(3)-C(3)-N(4)-C(4)	-8.0(5)
C(10)-C(3)-N(4)-C(4)	156.6(4)
N(6)-C(5)-N(5)-C(4)	151.2(4)
C(12)-C(5)-N(5)-C(4)	-14.1(4)
N(6)-C(5)-N(5)-B(1)	-13.3(6)
C(12)-C(5)-N(5)-B(1)	-178.6(3)
N(4)-C(4)-N(5)-C(5)	-153.6(4)
C(11)-C(4)-N(5)-C(5)	13.7(4)
N(4)-C(4)-N(5)-B(1)	10.8(6)
C(11)-C(4)-N(5)-B(1)	178.1(3)
N(5)-C(5)-N(6)-C(6)	-7.8(5)
C(12)-C(5)-N(6)-C(6)	153.8(4)
N(1)-C(6)-N(6)-C(5)	10.0(5)
C(7)-C(6)-N(6)-C(5)	-153.1(4)
C(5)-N(5)-B(1)-F(1)	-97.0(4)
C(4)-N(5)-B(1)-F(1)	100.3(4)
C(5)-N(5)-B(1)-N(1)	27.6(5)
C(4)-N(5)-B(1)-N(1)	-135.1(3)
C(5)-N(5)-B(1)-N(3)	137.8(3)
C(4)-N(5)-B(1)-N(3)	-24.9(5)
C(6)-N(1)-B(1)-F(1)	99.1(4)
C(1)-N(1)-B(1)-F(1)	-98.3(4)
C(6)-N(1)-B(1)-N(5)	-25.4(5)
C(1)-N(1)-B(1)-N(5)	137.2(3)

C(6)-N(1)-B(1)-N(3)	-136.0(4)
C(1)-N(1)-B(1)-N(3)	26.6(5)
C(2)-N(3)-B(1)-F(1)	95.8(4)
C(3)-N(3)-B(1)-F(1)	-100.1(4)
C(2)-N(3)-B(1)-N(5)	-139.4(3)
C(3)-N(3)-B(1)-N(5)	24.7(5)
C(2)-N(3)-B(1)-N(1)	-28.8(5)
C(3)-N(3)-B(1)-N(1)	135.4(4)
N(12)-C(30)-C(31)-C(37)	16.2(7)
N(7)-C(30)-C(31)-C(37)	-177.0(4)
N(12)-C(30)-C(31)-C(32)	-159.0(4)
N(7)-C(30)-C(31)-C(32)	7.8(4)
C(37)-C(31)-C(32)-C(40)	0.0(6)
C(30)-C(31)-C(32)-C(40)	176.0(4)
C(37)-C(31)-C(32)-C(25)	-176.6(4)
C(30)-C(31)-C(32)-C(25)	-0.6(4)
N(8)-C(25)-C(32)-C(40)	-18.1(7)
N(7)-C(25)-C(32)-C(40)	177.2(4)
N(8)-C(25)-C(32)-C(31)	157.9(4)
N(7)-C(25)-C(32)-C(31)	-6.8(4)
N(8)-C(26)-C(33)-C(41)	18.0(7)
N(9)-C(26)-C(33)-C(41)	-176.9(4)
N(8)-C(26)-C(33)-C(34)	-157.4(4)
N(9)-C(26)-C(33)-C(34)	7.7(4)
C(41)-C(33)-C(34)-C(44)	-0.7(6)
C(26)-C(33)-C(34)-C(44)	175.4(4)
C(41)-C(33)-C(34)-C(27)	-176.6(4)
C(26)-C(33)-C(34)-C(27)	-0.5(4)
N(10)-C(27)-C(34)-C(44)	-16.9(8)
N(9)-C(27)-C(34)-C(44)	178.0(4)
N(10)-C(27)-C(34)-C(33)	158.2(4)
N(9)-C(27)-C(34)-C(33)	-6.9(4)
N(10)-C(28)-C(35)-C(45)	14.9(8)
N(11)-C(28)-C(35)-C(45)	-179.0(4)
N(10)-C(28)-C(35)-C(36)	-160.7(4)
N(11)-C(28)-C(35)-C(36)	5.4(4)

C(45)-C(35)-C(36)-C(48)	2.5(6)
C(28)-C(35)-C(36)-C(48)	178.8(4)
C(45)-C(35)-C(36)-C(29)	-173.8(4)
C(28)-C(35)-C(36)-C(29)	2.5(4)
N(12)-C(29)-C(36)-C(48)	-20.7(7)
N(11)-C(29)-C(36)-C(48)	174.8(4)
N(12)-C(29)-C(36)-C(35)	155.0(4)
N(11)-C(29)-C(36)-C(35)	-9.6(4)
C(32)-C(31)-C(37)-F(15)	179.5(4)
C(30)-C(31)-C(37)-F(15)	4.8(7)
C(32)-C(31)-C(37)-C(38)	-1.3(6)
C(30)-C(31)-C(37)-C(38)	-176.0(4)
F(15)-C(37)-C(38)-F(16)	1.4(6)
C(31)-C(37)-C(38)-F(16)	-177.9(4)
F(15)-C(37)-C(38)-C(39)	-178.2(4)
C(31)-C(37)-C(38)-C(39)	2.6(7)
F(16)-C(38)-C(39)-F(17)	-1.1(6)
C(37)-C(38)-C(39)-F(17)	178.5(4)
F(16)-C(38)-C(39)-C(40)	177.9(4)
C(37)-C(38)-C(39)-C(40)	-2.6(7)
F(17)-C(39)-C(40)-F(18)	0.4(6)
C(38)-C(39)-C(40)-F(18)	-178.6(4)
F(17)-C(39)-C(40)-C(32)	-179.8(4)
C(38)-C(39)-C(40)-C(32)	1.2(7)
C(31)-C(32)-C(40)-F(18)	179.8(4)
C(25)-C(32)-C(40)-F(18)	-4.5(7)
C(31)-C(32)-C(40)-C(39)	0.0(6)
C(25)-C(32)-C(40)-C(39)	175.7(4)
C(34)-C(33)-C(41)-F(19)	179.4(4)
C(26)-C(33)-C(41)-F(19)	4.4(7)
C(34)-C(33)-C(41)-C(42)	-2.0(6)
C(26)-C(33)-C(41)-C(42)	-176.9(4)
F(19)-C(41)-C(42)-F(20)	1.5(6)
C(33)-C(41)-C(42)-F(20)	-177.2(4)
F(19)-C(41)-C(42)-C(43)	-178.1(4)
C(33)-C(41)-C(42)-C(43)	3.2(7)

F(20)-C(42)-C(43)-F(21)	-1.5(6)
C(41)-C(42)-C(43)-F(21)	178.0(4)
F(20)-C(42)-C(43)-C(44)	178.6(4)
C(41)-C(42)-C(43)-C(44)	-1.9(7)
F(21)-C(43)-C(44)-F(22)	0.8(6)
C(42)-C(43)-C(44)-F(22)	-179.3(4)
F(21)-C(43)-C(44)-C(34)	179.3(4)
C(42)-C(43)-C(44)-C(34)	-0.8(7)
C(33)-C(34)-C(44)-F(22)	-179.5(4)
C(27)-C(34)-C(44)-F(22)	-4.8(7)
C(33)-C(34)-C(44)-C(43)	2.1(6)
C(27)-C(34)-C(44)-C(43)	176.7(4)
C(36)-C(35)-C(45)-F(23)	178.7(4)
C(28)-C(35)-C(45)-F(23)	3.6(7)
C(36)-C(35)-C(45)-C(46)	-2.2(6)
C(28)-C(35)-C(45)-C(46)	-177.3(4)
F(23)-C(45)-C(46)-F(24)	-0.2(6)
C(35)-C(45)-C(46)-F(24)	-179.3(4)
F(23)-C(45)-C(46)-C(47)	179.4(4)
C(35)-C(45)-C(46)-C(47)	0.2(7)
F(24)-C(46)-C(47)-F(25)	0.8(6)
C(45)-C(46)-C(47)-F(25)	-178.7(4)
F(24)-C(46)-C(47)-C(48)	-179.1(4)
C(45)-C(46)-C(47)-C(48)	1.4(7)
F(25)-C(47)-C(48)-F(26)	-1.0(6)
C(46)-C(47)-C(48)-F(26)	178.9(4)
F(25)-C(47)-C(48)-C(36)	179.1(4)
C(46)-C(47)-C(48)-C(36)	-1.0(6)
C(35)-C(36)-C(48)-F(26)	179.2(4)
C(29)-C(36)-C(48)-F(26)	-5.6(7)
C(35)-C(36)-C(48)-C(47)	-0.9(6)
C(29)-C(36)-C(48)-C(47)	174.3(4)
N(12)-C(30)-N(7)-C(25)	155.1(4)
C(31)-C(30)-N(7)-C(25)	-12.8(4)
N(12)-C(30)-N(7)-B(2)	-10.1(5)
C(31)-C(30)-N(7)-B(2)	-178.1(3)

N(8)-C(25)-N(7)-C(30)	-153.6(4)
C(32)-C(25)-N(7)-C(30)	12.4(4)
N(8)-C(25)-N(7)-B(2)	11.7(6)
C(32)-C(25)-N(7)-B(2)	177.8(3)
N(9)-C(26)-N(8)-C(25)	-7.9(5)
C(33)-C(26)-N(8)-C(25)	154.7(4)
N(7)-C(25)-N(8)-C(26)	7.8(5)
C(32)-C(25)-N(8)-C(26)	-154.6(4)
N(8)-C(26)-N(9)-C(27)	153.4(4)
C(33)-C(26)-N(9)-C(27)	-12.8(4)
N(8)-C(26)-N(9)-B(2)	-11.7(6)
C(33)-C(26)-N(9)-B(2)	-177.9(3)
N(10)-C(27)-N(9)-C(26)	-153.8(4)
C(34)-C(27)-N(9)-C(26)	12.6(4)
N(10)-C(27)-N(9)-B(2)	11.1(6)
C(34)-C(27)-N(9)-B(2)	177.6(3)
N(9)-C(27)-N(10)-C(28)	8.2(6)
C(34)-C(27)-N(10)-C(28)	-154.7(4)
N(11)-C(28)-N(10)-C(27)	-8.1(6)
C(35)-C(28)-N(10)-C(27)	155.9(4)
N(12)-C(29)-N(11)-C(28)	-152.0(4)
C(36)-C(29)-N(11)-C(28)	13.8(4)
N(12)-C(29)-N(11)-B(2)	14.2(6)
C(36)-C(29)-N(11)-B(2)	-179.9(3)
N(10)-C(28)-N(11)-C(29)	155.1(4)
C(35)-C(28)-N(11)-C(29)	-12.3(4)
N(10)-C(28)-N(11)-B(2)	-11.1(6)
C(35)-C(28)-N(11)-B(2)	-178.5(3)
N(11)-C(29)-N(12)-C(30)	6.1(5)
C(36)-C(29)-N(12)-C(30)	-156.1(4)
N(7)-C(30)-N(12)-C(29)	-8.1(5)
C(31)-C(30)-N(12)-C(29)	156.7(4)
C(26)-N(9)-B(2)-F(14)	-97.4(4)
C(27)-N(9)-B(2)-F(14)	98.9(4)
C(26)-N(9)-B(2)-N(7)	26.9(5)
C(27)-N(9)-B(2)-N(7)	-136.8(3)

C(26)-N(9)-B(2)-N(11)	137.7(3)
C(27)-N(9)-B(2)-N(11)	-26.0(5)
C(30)-N(7)-B(2)-F(14)	-98.7(4)
C(25)-N(7)-B(2)-F(14)	97.5(4)
C(30)-N(7)-B(2)-N(9)	136.9(3)
C(25)-N(7)-B(2)-N(9)	-26.9(5)
C(30)-N(7)-B(2)-N(11)	25.7(5)
C(25)-N(7)-B(2)-N(11)	-138.1(4)
C(29)-N(11)-B(2)-F(14)	96.4(4)
C(28)-N(11)-B(2)-F(14)	-98.7(4)
C(29)-N(11)-B(2)-N(9)	-139.0(3)
C(28)-N(11)-B(2)-N(9)	25.9(5)
C(29)-N(11)-B(2)-N(7)	-27.7(5)
C(28)-N(11)-B(2)-N(7)	137.3(3)
N(16)-C(50)-C(55)-C(61)	18.4(7)
N(17)-C(50)-C(55)-C(61)	-177.3(4)
N(16)-C(50)-C(55)-C(56)	-156.5(4)
N(17)-C(50)-C(55)-C(56)	7.8(4)
C(61)-C(55)-C(56)-C(64)	0.4(6)
C(50)-C(55)-C(56)-C(64)	176.0(4)
C(61)-C(55)-C(56)-C(51)	-175.6(4)
C(50)-C(55)-C(56)-C(51)	-0.1(4)
N(18)-C(51)-C(56)-C(64)	-17.1(8)
N(17)-C(51)-C(56)-C(64)	177.1(4)
N(18)-C(51)-C(56)-C(55)	158.2(4)
N(17)-C(51)-C(56)-C(55)	-7.6(4)
N(18)-C(52)-C(57)-C(65)	10.8(8)
N(13)-C(52)-C(57)-C(65)	176.9(4)
N(18)-C(52)-C(57)-C(58)	-160.5(4)
N(13)-C(52)-C(57)-C(58)	5.7(4)
C(65)-C(57)-C(58)-C(68)	1.9(6)
C(52)-C(57)-C(58)-C(68)	174.6(4)
C(65)-C(57)-C(58)-C(53)	-170.8(4)
C(52)-C(57)-C(58)-C(53)	1.9(4)
N(14)-C(53)-C(58)-C(68)	-17.0(7)
N(13)-C(53)-C(58)-C(68)	179.9(4)

N(14)-C(53)-C(58)-C(57)	154.4(4)
N(13)-C(53)-C(58)-C(57)	-8.7(4)
N(14)-C(54)-C(59)-C(69)	16.1(7)
N(15)-C(54)-C(59)-C(69)	-179.5(4)
N(14)-C(54)-C(59)-C(60)	-158.0(4)
N(15)-C(54)-C(59)-C(60)	6.4(4)
C(69)-C(59)-C(60)-C(72)	0.8(6)
C(54)-C(59)-C(60)-C(72)	175.8(4)
C(69)-C(59)-C(60)-C(49)	-175.0(4)
C(54)-C(59)-C(60)-C(49)	0.0(4)
N(16)-C(49)-C(60)-C(72)	-17.4(8)
N(15)-C(49)-C(60)-C(72)	178.6(4)
N(16)-C(49)-C(60)-C(59)	157.7(4)
N(15)-C(49)-C(60)-C(59)	-6.3(4)
C(56)-C(55)-C(61)-F(36)	179.7(4)
C(50)-C(55)-C(61)-F(36)	5.4(7)
C(56)-C(55)-C(61)-C(62)	-0.9(6)
C(50)-C(55)-C(61)-C(62)	-175.2(4)
F(36)-C(61)-C(62)-F(37)	-1.0(6)
C(55)-C(61)-C(62)-F(37)	179.6(4)
F(36)-C(61)-C(62)-C(63)	179.2(4)
C(55)-C(61)-C(62)-C(63)	-0.2(6)
F(37)-C(62)-C(63)-F(38)	1.3(6)
C(61)-C(62)-C(63)-F(38)	-178.9(4)
F(37)-C(62)-C(63)-C(64)	-178.0(4)
C(61)-C(62)-C(63)-C(64)	1.8(7)
F(38)-C(63)-C(64)-F(39)	-1.0(6)
C(62)-C(63)-C(64)-F(39)	178.3(4)
F(38)-C(63)-C(64)-C(56)	178.5(4)
C(62)-C(63)-C(64)-C(56)	-2.2(7)
C(55)-C(56)-C(64)-F(39)	-179.4(4)
C(51)-C(56)-C(64)-F(39)	-4.6(7)
C(55)-C(56)-C(64)-C(63)	1.1(6)
C(51)-C(56)-C(64)-C(63)	176.0(4)
C(58)-C(57)-C(65)-F(28)	175.7(4)
C(52)-C(57)-C(65)-F(28)	5.2(7)

C(58)-C(57)-C(65)-C(66)	-1.7(6)
C(52)-C(57)-C(65)-C(66)	-172.2(4)
F(28)-C(65)-C(66)-F(29)	0.3(6)
C(57)-C(65)-C(66)-F(29)	177.8(4)
F(28)-C(65)-C(66)-C(67)	-176.7(4)
C(57)-C(65)-C(66)-C(67)	0.8(6)
F(29)-C(66)-C(67)-F(30)	-1.5(6)
C(65)-C(66)-C(67)-F(30)	175.6(4)
F(29)-C(66)-C(67)-C(68)	-177.0(3)
C(65)-C(66)-C(67)-C(68)	0.1(6)
F(30)-C(67)-C(68)-F(31)	2.5(6)
C(66)-C(67)-C(68)-F(31)	178.0(4)
F(30)-C(67)-C(68)-C(58)	-175.4(4)
C(66)-C(67)-C(68)-C(58)	0.0(6)
C(57)-C(58)-C(68)-F(31)	-178.9(4)
C(53)-C(58)-C(68)-F(31)	-8.4(7)
C(57)-C(58)-C(68)-C(67)	-1.0(6)
C(53)-C(58)-C(68)-C(67)	169.5(4)
C(60)-C(59)-C(69)-F(32)	179.7(3)
C(54)-C(59)-C(69)-F(32)	6.2(7)
C(60)-C(59)-C(69)-C(70)	-1.0(6)
C(54)-C(59)-C(69)-C(70)	-174.6(4)
F(32)-C(69)-C(70)-F(33)	0.1(6)
C(59)-C(69)-C(70)-F(33)	-179.2(4)
F(32)-C(69)-C(70)-C(71)	179.6(4)
C(59)-C(69)-C(70)-C(71)	0.3(7)
F(33)-C(70)-C(71)-F(34)	0.2(7)
C(69)-C(70)-C(71)-F(34)	-179.2(4)
F(33)-C(70)-C(71)-C(72)	-179.9(4)
C(69)-C(70)-C(71)-C(72)	0.7(7)
F(34)-C(71)-C(72)-F(35)	-1.4(6)
C(70)-C(71)-C(72)-F(35)	178.7(4)
F(34)-C(71)-C(72)-C(60)	179.0(4)
C(70)-C(71)-C(72)-C(60)	-0.9(7)
C(59)-C(60)-C(72)-F(35)	-179.5(4)
C(49)-C(60)-C(72)-F(35)	-4.8(7)

C(59)-C(60)-C(72)-C(71)	0.2(6)
C(49)-C(60)-C(72)-C(71)	174.8(4)
N(18)-C(52)-N(13)-C(53)	155.2(4)
C(57)-C(52)-N(13)-C(53)	-11.9(4)
N(18)-C(52)-N(13)-B(3)	-9.4(6)
C(57)-C(52)-N(13)-B(3)	-176.5(3)
N(14)-C(53)-N(13)-C(52)	-151.1(4)
C(58)-C(53)-N(13)-C(52)	13.1(4)
N(14)-C(53)-N(13)-B(3)	13.6(6)
C(58)-C(53)-N(13)-B(3)	177.8(3)
N(13)-C(53)-N(14)-C(54)	7.4(5)
C(58)-C(53)-N(14)-C(54)	-153.0(4)
N(15)-C(54)-N(14)-C(53)	-9.1(5)
C(59)-C(54)-N(14)-C(53)	153.0(4)
N(16)-C(49)-N(15)-C(54)	-154.4(4)
C(60)-C(49)-N(15)-C(54)	11.0(4)
N(16)-C(49)-N(15)-B(3)	10.1(6)
C(60)-C(49)-N(15)-B(3)	175.5(3)
N(14)-C(54)-N(15)-C(49)	154.7(4)
C(59)-C(54)-N(15)-C(49)	-11.0(4)
N(14)-C(54)-N(15)-B(3)	-9.9(5)
C(59)-C(54)-N(15)-B(3)	-175.6(3)
N(15)-C(49)-N(16)-C(50)	8.7(6)
C(60)-C(49)-N(16)-C(50)	-152.9(4)
N(17)-C(50)-N(16)-C(49)	-7.2(5)
C(55)-C(50)-N(16)-C(49)	154.7(4)
N(16)-C(50)-N(17)-C(51)	152.3(4)
C(55)-C(50)-N(17)-C(51)	-13.4(4)
N(16)-C(50)-N(17)-B(3)	-13.3(6)
C(55)-C(50)-N(17)-B(3)	-179.0(3)
N(18)-C(51)-N(17)-C(50)	-153.7(4)
C(56)-C(51)-N(17)-C(50)	13.4(4)
N(18)-C(51)-N(17)-B(3)	12.1(6)
C(56)-C(51)-N(17)-B(3)	179.1(3)
N(13)-C(52)-N(18)-C(51)	-9.0(6)
C(57)-C(52)-N(18)-C(51)	154.8(4)

N(17)-C(51)-N(18)-C(52)	7.6(6)
C(56)-C(51)-N(18)-C(52)	-156.0(4)
C(52)-N(13)-B(3)-F(27)	-100.8(4)
C(53)-N(13)-B(3)-F(27)	96.0(4)
C(52)-N(13)-B(3)-N(17)	24.8(5)
C(53)-N(13)-B(3)-N(17)	-138.4(4)
C(52)-N(13)-B(3)-N(15)	135.2(4)
C(53)-N(13)-B(3)-N(15)	-28.0(5)
C(50)-N(17)-B(3)-F(27)	-96.5(4)
C(51)-N(17)-B(3)-F(27)	99.2(4)
C(50)-N(17)-B(3)-N(13)	138.2(4)
C(51)-N(17)-B(3)-N(13)	-26.0(5)
C(50)-N(17)-B(3)-N(15)	27.3(5)
C(51)-N(17)-B(3)-N(15)	-136.9(3)
C(49)-N(15)-B(3)-F(27)	98.9(4)
C(54)-N(15)-B(3)-F(27)	-98.2(4)
C(49)-N(15)-B(3)-N(13)	-136.7(4)
C(54)-N(15)-B(3)-N(13)	26.3(5)
C(49)-N(15)-B(3)-N(17)	-25.8(5)
C(54)-N(15)-B(3)-N(17)	137.2(3)

Symmetry transformations used to generate equivalent atoms:

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