Supplementary Information

Variation in crystal packing of phenoxyboronsubphthalocyanines directed by para-substituents on the phenoxy group†

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Figures S1 through S5 are thermal ellipsoid plots and images of unit cells of crystals of compounds **2a** through **2e**, respectively.

Tables S1 through S7 summarize the crystallographic data for crystals of compound **2a**

Tables S8 through S14 summarize the crystallographic data for crystals of compound **2b**

Tables S15 through S21 summarize the crystallographic data for crystals of compound **2c**

Tables S22 through S28 summarize the crystallographic data for crystals of compound **2d**

Tables S29 through S34 summarize the crystallographic data for crystals of compound **2e**.

Figure S6 describes/illustrates the Kauffman column and its use in purification.

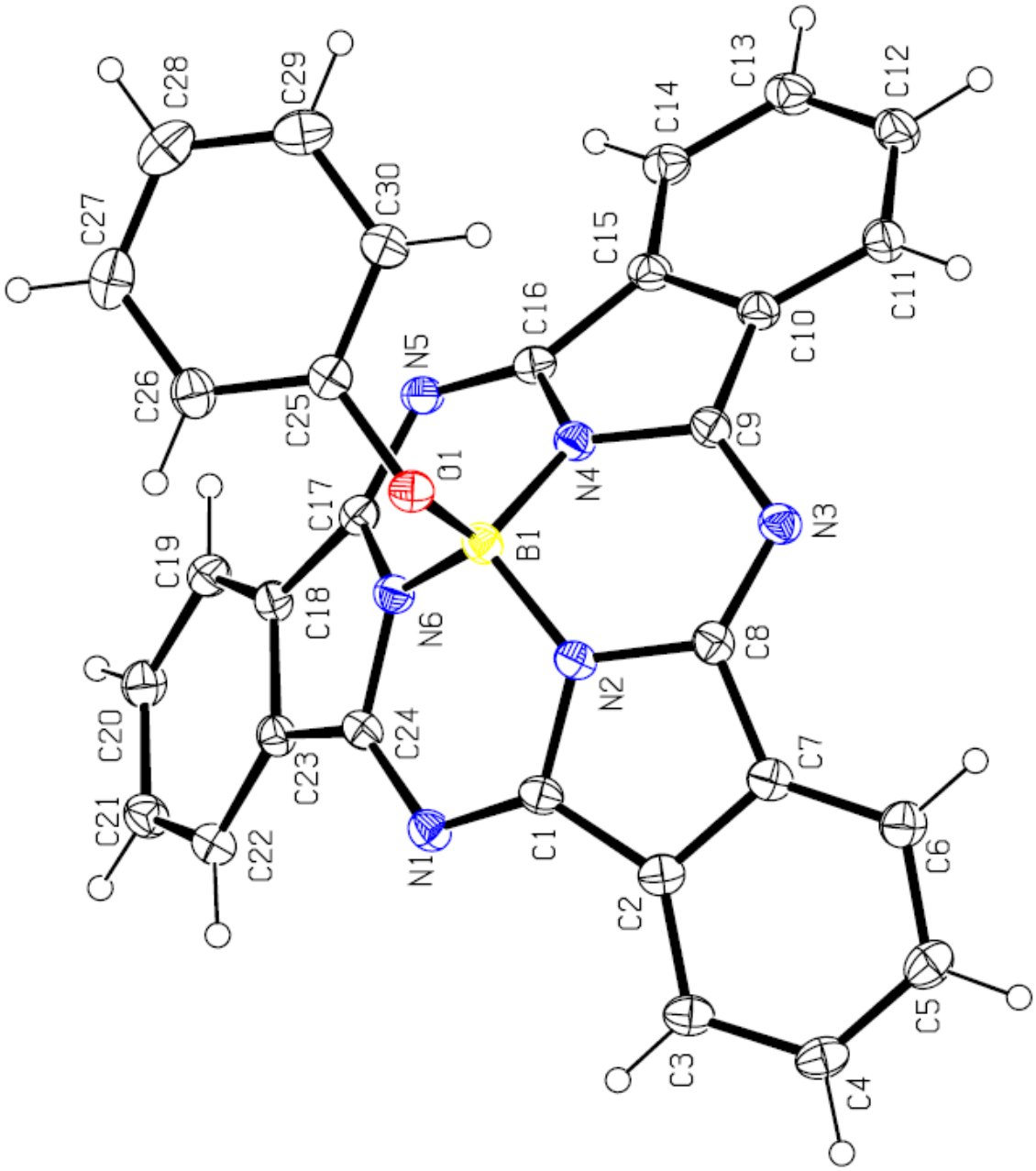


Figure S1A: Thermal ellipsoid plot of compound **2a**, shown with atom numberings.

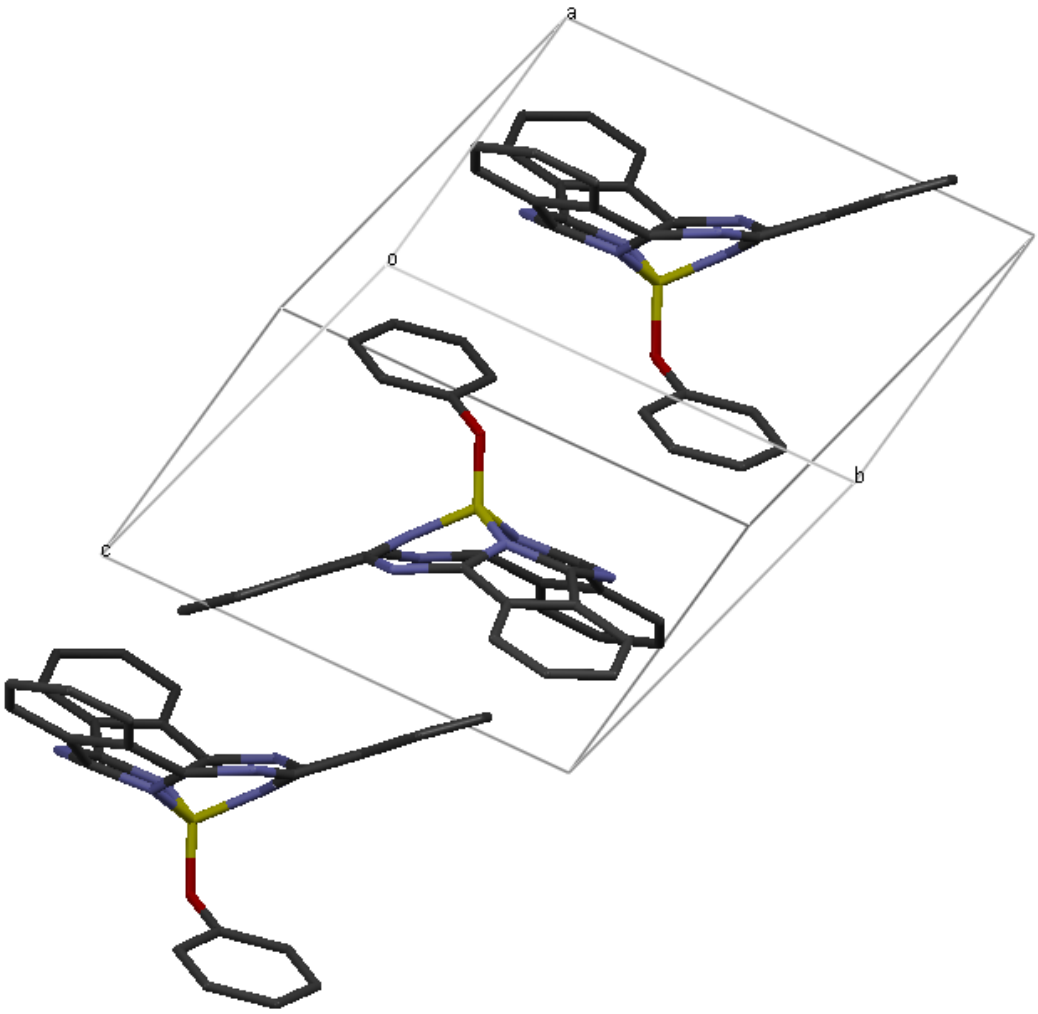


Figure S1B: Image of crystal of compound **2a** showing orientation of crystal axes.

Table S1. Crystal data and structure refinement for compound **2a** (k0970).

Identification code	k0970	
Empirical formula	C30 H17 B N6 O	
Formula weight	488.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.0492(5) Å	α= 85.893(2)°.
	b = 10.7503(4) Å	β= 77.4510(19)°.
	c = 11.8342(5) Å	γ = 66.043(2)°.
Volume	1140.22(9) $Å^3$	
Z	2	
Density (calculated)	1.422 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	504	
Crystal size	0.30 x 0.26 x 0.20 mm^3	
Theta range for data collection	2.57 to 27.46°.	
Index ranges	-12<=h<=13, -13<=k<=13, -15<=l<=15	
Reflections collected	12024	
Independent reflections	5140 [R(int) = 0.0396]	
Completeness to theta = 27.46°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.982 and 0.848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5140 / 0 / 343	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0519, wR2 = 0.1262	
R indices (all data)	R1 = 0.0790, wR2 = 0.1448	
Largest diff. peak and hole	0.277 and -0.257 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2a** (k0970). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6076(1)	5838(1)	3979(1)	29(1)
N(1)	8278(2)	2037(1)	3726(1)	28(1)
N(2)	8624(2)	4110(1)	3636(1)	27(1)
N(3)	9931(2)	5496(1)	2817(1)	29(1)
N(4)	7866(2)	5581(1)	2108(1)	26(1)
N(5)	6681(2)	5018(1)	814(1)	27(1)
N(6)	6975(2)	3866(1)	2601(1)	26(1)
C(1)	8981(2)	2784(2)	3980(1)	27(1)
C(2)	10393(2)	2359(2)	4336(1)	29(1)
C(3)	11299(2)	1147(2)	4776(1)	32(1)
C(4)	12688(2)	1012(2)	4898(2)	36(1)
C(5)	13202(2)	2046(2)	4589(2)	38(1)
C(6)	12315(2)	3255(2)	4146(2)	35(1)
C(7)	10911(2)	3420(2)	4030(1)	29(1)
C(8)	9790(2)	4492(2)	3519(1)	28(1)
C(9)	9002(2)	5976(2)	2080(1)	28(1)
C(10)	9120(2)	6687(2)	992(1)	28(1)
C(11)	9993(2)	7400(2)	512(2)	33(1)
C(12)	9831(2)	7983(2)	-555(2)	37(1)
C(13)	8876(2)	7813(2)	-1171(2)	35(1)
C(14)	8042(2)	7066(2)	-737(2)	31(1)
C(15)	8141(2)	6527(2)	367(1)	28(1)
C(16)	7412(2)	5724(2)	1083(1)	27(1)
C(17)	6561(2)	4038(2)	1557(1)	27(1)
C(18)	6365(2)	2813(2)	1348(1)	27(1)
C(19)	5949(2)	2424(2)	430(2)	31(1)
C(20)	5998(2)	1118(2)	428(2)	34(1)
C(21)	6488(2)	207(2)	1296(2)	33(1)
C(22)	6951(2)	562(2)	2193(2)	31(1)
C(23)	6866(2)	1888(2)	2236(1)	27(1)
C(24)	7348(2)	2562(2)	2994(1)	27(1)

C(25)	4836(2)	6669(2)	3557(1)	29(1)
C(26)	3709(2)	6240(2)	3566(2)	36(1)
C(27)	2468(2)	7070(2)	3131(2)	44(1)
C(28)	2346(2)	8339(2)	2702(2)	46(1)
C(29)	3467(2)	8770(2)	2702(2)	42(1)
C(30)	4711(2)	7942(2)	3129(2)	33(1)
B(1)	7286(2)	4911(2)	3144(2)	27(1)

Table S3. Bond lengths [Å] and angles [°] for compound **2a** (k0970).

O(1)-C(25)	1.379(2)
O(1)-B(1)	1.443(2)
N(1)-C(24)	1.341(2)
N(1)-C(1)	1.349(2)
N(2)-C(8)	1.368(2)
N(2)-C(1)	1.376(2)
N(2)-B(1)	1.489(2)
N(3)-C(9)	1.340(2)
N(3)-C(8)	1.349(2)
N(4)-C(16)	1.364(2)
N(4)-C(9)	1.364(2)
N(4)-B(1)	1.505(2)
N(5)-C(16)	1.344(2)
N(5)-C(17)	1.350(2)
N(6)-C(17)	1.365(2)
N(6)-C(24)	1.371(2)
N(6)-B(1)	1.499(2)
C(1)-C(2)	1.452(2)
C(2)-C(3)	1.394(2)
C(2)-C(7)	1.430(2)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.400(3)
C(5)-C(6)	1.387(3)
C(6)-C(7)	1.385(3)
C(7)-C(8)	1.451(2)
C(9)-C(10)	1.457(2)
C(10)-C(11)	1.395(2)
C(10)-C(15)	1.421(2)
C(11)-C(12)	1.381(3)
C(12)-C(13)	1.397(3)
C(13)-C(14)	1.383(2)
C(14)-C(15)	1.397(2)
C(15)-C(16)	1.462(2)
C(17)-C(18)	1.453(2)

C(18)-C(19)	1.391(2)
C(18)-C(23)	1.421(2)
C(19)-C(20)	1.384(2)
C(20)-C(21)	1.393(3)
C(21)-C(22)	1.380(2)
C(22)-C(23)	1.397(2)
C(23)-C(24)	1.459(2)
C(25)-C(26)	1.383(3)
C(25)-C(30)	1.391(2)
C(26)-C(27)	1.387(3)
C(27)-C(28)	1.388(3)
C(28)-C(29)	1.381(3)
C(29)-C(30)	1.384(3)

C(25)-O(1)-B(1)	115.52(13)
C(24)-N(1)-C(1)	117.72(13)
C(8)-N(2)-C(1)	112.52(14)
C(8)-N(2)-B(1)	122.35(13)
C(1)-N(2)-B(1)	123.22(14)
C(9)-N(3)-C(8)	116.71(14)
C(16)-N(4)-C(9)	114.05(13)
C(16)-N(4)-B(1)	123.25(14)
C(9)-N(4)-B(1)	122.40(14)
C(16)-N(5)-C(17)	116.36(14)
C(17)-N(6)-C(24)	113.15(13)
C(17)-N(6)-B(1)	123.04(13)
C(24)-N(6)-B(1)	122.73(14)
N(1)-C(1)-N(2)	121.98(15)
N(1)-C(1)-C(2)	130.25(15)
N(2)-C(1)-C(2)	105.85(14)
C(3)-C(2)-C(7)	119.85(17)
C(3)-C(2)-C(1)	132.77(16)
C(7)-C(2)-C(1)	107.03(14)
C(4)-C(3)-C(2)	118.18(16)
C(3)-C(4)-C(5)	122.05(17)
C(6)-C(5)-C(4)	120.42(18)

C(7)-C(6)-C(5)	118.55(17)
C(6)-C(7)-C(2)	120.94(16)
C(6)-C(7)-C(8)	131.66(16)
C(2)-C(7)-C(8)	107.11(15)
N(3)-C(8)-N(2)	123.19(16)
N(3)-C(8)-C(7)	128.86(16)
N(2)-C(8)-C(7)	106.16(14)
N(3)-C(9)-N(4)	122.30(14)
N(3)-C(9)-C(10)	131.15(16)
N(4)-C(9)-C(10)	105.06(15)
C(11)-C(10)-C(15)	120.21(16)
C(11)-C(10)-C(9)	132.29(17)
C(15)-C(10)-C(9)	107.47(14)
C(12)-C(11)-C(10)	118.20(18)
C(11)-C(12)-C(13)	121.38(16)
C(14)-C(13)-C(12)	121.60(17)
C(13)-C(14)-C(15)	117.60(17)
C(14)-C(15)-C(10)	120.89(15)
C(14)-C(15)-C(16)	131.99(16)
C(10)-C(15)-C(16)	107.10(14)
N(5)-C(16)-N(4)	122.56(14)
N(5)-C(16)-C(15)	131.24(15)
N(4)-C(16)-C(15)	105.09(14)
N(5)-C(17)-N(6)	122.99(14)
N(5)-C(17)-C(18)	129.48(15)
N(6)-C(17)-C(18)	105.84(13)
C(19)-C(18)-C(23)	121.12(15)
C(19)-C(18)-C(17)	131.41(15)
C(23)-C(18)-C(17)	107.09(14)
C(20)-C(19)-C(18)	117.72(16)
C(19)-C(20)-C(21)	121.39(16)
C(22)-C(21)-C(20)	121.62(15)
C(21)-C(22)-C(23)	118.13(16)
C(22)-C(23)-C(18)	119.95(16)
C(22)-C(23)-C(24)	132.42(16)
C(18)-C(23)-C(24)	107.31(13)

N(1)-C(24)-N(6)	122.42(14)
N(1)-C(24)-C(23)	130.36(14)
N(6)-C(24)-C(23)	105.31(14)
O(1)-C(25)-C(26)	119.96(15)
O(1)-C(25)-C(30)	120.17(15)
C(26)-C(25)-C(30)	119.86(17)
C(25)-C(26)-C(27)	119.99(18)
C(26)-C(27)-C(28)	120.10(19)
C(29)-C(28)-C(27)	119.8(2)
C(28)-C(29)-C(30)	120.28(18)
C(29)-C(30)-C(25)	119.94(18)
O(1)-B(1)-N(2)	112.77(14)
O(1)-B(1)-N(6)	116.61(14)
N(2)-B(1)-N(6)	104.68(13)
O(1)-B(1)-N(4)	114.77(14)
N(2)-B(1)-N(4)	103.90(14)
N(6)-B(1)-N(4)	102.68(13)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2a** (k0970). 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}
O(1)	33(1)	29(1)	26(1)	1(1)	-7(1)	-12(1)
N(1)	34(1)	30(1)	24(1)	3(1)	-8(1)	-16(1)
N(2)	31(1)	25(1)	26(1)	3(1)	-7(1)	-13(1)
N(3)	33(1)	26(1)	32(1)	2(1)	-10(1)	-14(1)
N(4)	29(1)	25(1)	27(1)	2(1)	-8(1)	-12(1)
N(5)	29(1)	24(1)	29(1)	3(1)	-9(1)	-10(1)
N(6)	28(1)	25(1)	26(1)	3(1)	-7(1)	-12(1)
C(1)	33(1)	27(1)	22(1)	3(1)	-5(1)	-12(1)
C(2)	34(1)	30(1)	22(1)	-1(1)	-8(1)	-11(1)
C(3)	41(1)	30(1)	25(1)	2(1)	-11(1)	-12(1)
C(4)	41(1)	34(1)	31(1)	2(1)	-16(1)	-9(1)
C(5)	35(1)	41(1)	38(1)	-1(1)	-16(1)	-12(1)
C(6)	39(1)	36(1)	34(1)	0(1)	-14(1)	-16(1)
C(7)	36(1)	30(1)	25(1)	0(1)	-10(1)	-14(1)
C(8)	32(1)	29(1)	26(1)	-2(1)	-8(1)	-14(1)
C(9)	29(1)	24(1)	32(1)	-1(1)	-7(1)	-12(1)
C(10)	28(1)	23(1)	31(1)	1(1)	-4(1)	-8(1)
C(11)	29(1)	30(1)	38(1)	1(1)	-3(1)	-12(1)
C(12)	34(1)	33(1)	40(1)	6(1)	1(1)	-13(1)
C(13)	37(1)	32(1)	30(1)	5(1)	-1(1)	-10(1)
C(14)	31(1)	28(1)	28(1)	0(1)	-4(1)	-7(1)
C(15)	29(1)	22(1)	30(1)	1(1)	-4(1)	-7(1)
C(16)	27(1)	23(1)	27(1)	1(1)	-6(1)	-7(1)
C(17)	25(1)	28(1)	28(1)	1(1)	-7(1)	-9(1)
C(18)	26(1)	27(1)	30(1)	1(1)	-5(1)	-13(1)
C(19)	31(1)	32(1)	32(1)	3(1)	-11(1)	-13(1)
C(20)	36(1)	35(1)	36(1)	-1(1)	-13(1)	-17(1)
C(21)	37(1)	29(1)	36(1)	0(1)	-8(1)	-16(1)
C(22)	34(1)	28(1)	31(1)	3(1)	-6(1)	-14(1)
C(23)	27(1)	29(1)	26(1)	1(1)	-4(1)	-13(1)
C(24)	30(1)	26(1)	26(1)	3(1)	-4(1)	-14(1)

C(25)	30(1)	31(1)	22(1)	-4(1)	-3(1)	-11(1)
C(26)	36(1)	41(1)	33(1)	-1(1)	-4(1)	-19(1)
C(27)	35(1)	63(1)	37(1)	-6(1)	-6(1)	-22(1)
C(28)	37(1)	54(1)	38(1)	-7(1)	-12(1)	-5(1)
C(29)	49(1)	34(1)	35(1)	-1(1)	-11(1)	-8(1)
C(30)	38(1)	30(1)	31(1)	-1(1)	-6(1)	-14(1)
B(1)	31(1)	28(1)	26(1)	1(1)	-7(1)	-15(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2a** (k0970).

	x	y	z	U(eq)
H(3A)	10971	433	4986	38
H(4A)	13313	193	5200	43
H(5A)	14164	1917	4683	46
H(6A)	12663	3955	3927	42
H(11A)	10681	7482	909	39
H(12A)	10380	8510	-876	45
H(13A)	8798	8221	-1906	42
H(14A)	7424	6925	-1173	37
H(19A)	5643	3033	-176	37
H(20A)	5690	838	-177	41
H(21A)	6503	-680	1270	40
H(22A)	7318	-78	2765	37
H(26A)	3784	5378	3871	43
H(27A)	1702	6769	3127	53
H(28A)	1493	8910	2409	56
H(29A)	3384	9639	2408	50
H(30A)	5478	8244	3130	40

Table S6. Selected Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 deg for compound **2a** (k0970).

Cg(I)	->	Cg(J)	Cg-Cg (Å)	Alpha (deg)	Beta (deg)	Gamma (deg)	CgI_Perp (Å)	CgJ_Perp (Å)	Slippage (Å)
Cg(2)	->	Cg(5)	3.6742(10)	2.70(9)	4.95	7.22	-3.6450(7)	-3.6605(7)	
Cg(5)	->	Cg(2)	3.6741(10)	2.70(9)	7.22	4.95	-3.6605(7)	-3.6449(7)	

Table S7. Selected C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) for compound **2a** (k0970).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (deg)	X-H..Cg (deg)	X..Cg (Å)	X-H,Pi (deg)
C(12) -H(12A)	->	Cg(3)	2.77	2.69	13.52	113	3.257(2)	37
C(13) -H(13A)	->	Cg(1)	2.80	-2.74	11.90	119	3.3638(19)	40
C(21) -H(21A)	->	Cg(5)	2.85	2.79	11.31	119	3.4127(19)	39

See lit. [11] for definitions of C-H…π factors
All atoms numbered according to thermal ellipsoid plot in Figure S1. Cg numberings as defined below for ring centroids used in above tables for compound **2a** (k0970):
5-Membered Ring (1) N(2) --> C(1) --> C(2) --> C(7) --> C(8) -->
5-Membered Ring (2) N(4) --> C(9) --> C(10) --> C(15) --> C(16) -->
5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->
6-Membered Ring (5) C(10) --> C(11) --> C(12) --> C(13) --> C(14) --> C(15) -->

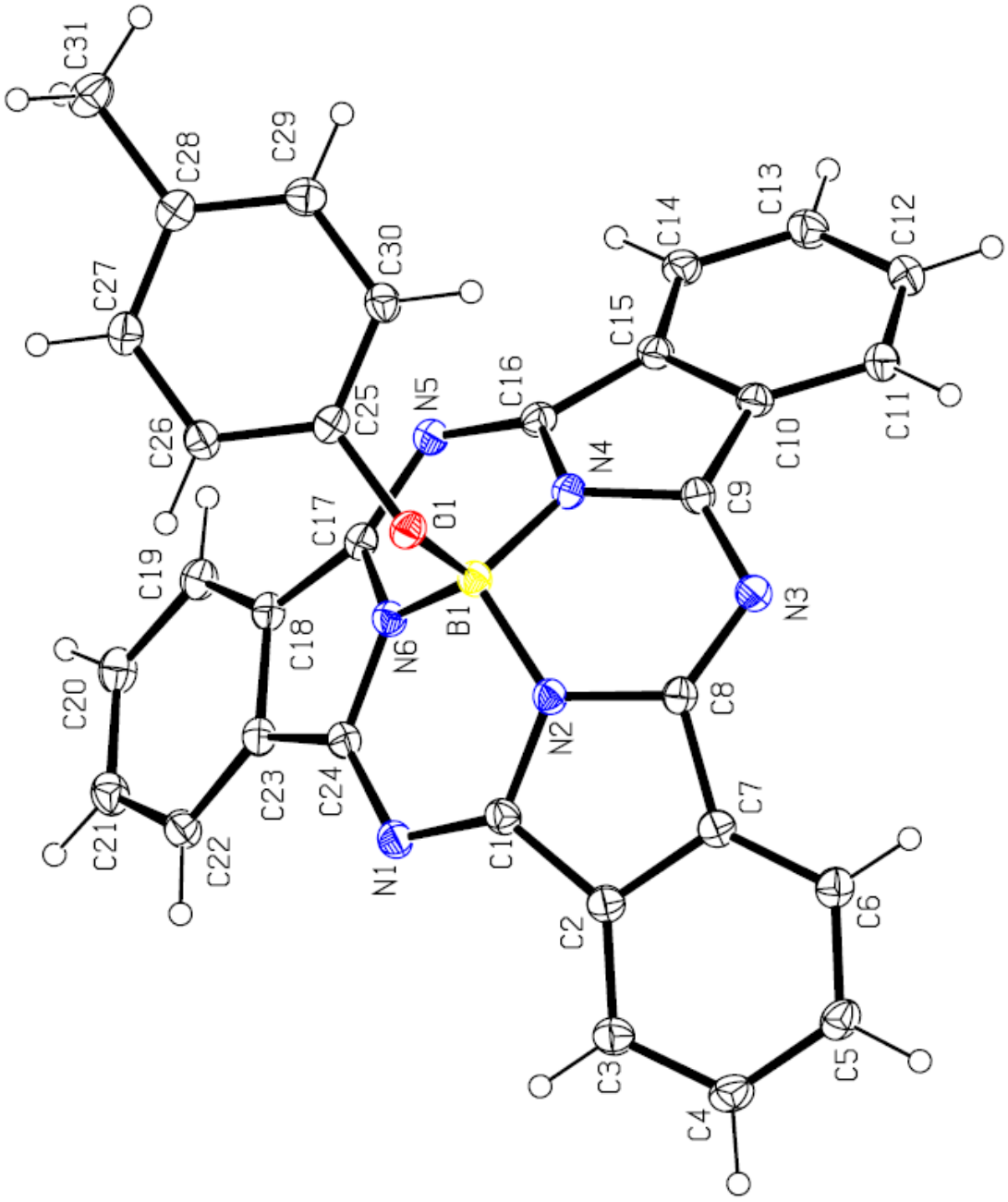


Figure S2A: Thermal ellipsoid plot of compound **2b**, shown with atom numberings.

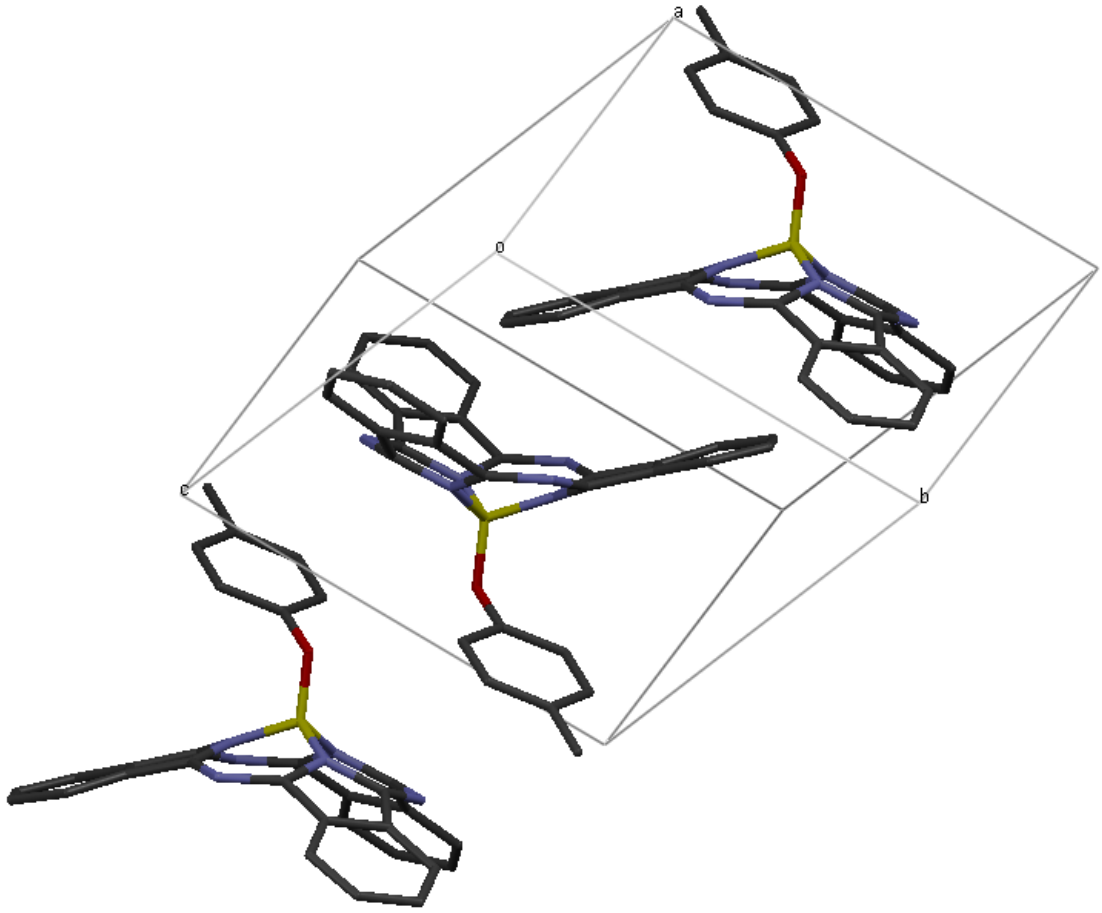


Figure S2B: Image of crystal of compound **2b** showing orientation of crystal axes.

Table S8. Crystal data and structure refinement for compound **2b** (k0971).

Identification code	k0971	
Empirical formula	C31 H19 B N6 O	
Formula weight	502.33	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.1555(3) Å	α= 86.3530(17)°.
	b = 10.9258(4) Å	β= 78.496(2)°.
	c = 11.7215(4) Å	γ = 66.9870(18)°.
Volume	1172.88(7) $Å^3$	
Z	2	
Density (calculated)	1.422 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	520	
Crystal size	0.34 x 0.30 x 0.20 mm^3	
Theta range for data collection	2.56 to 27.53°.	
Index ranges	-13<=h<=13, -14<=k<=14, -14<=l<=15	
Reflections collected	14448	
Independent reflections	5309 [R(int) = 0.0441]	
Completeness to theta = 27.53°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.983 and 0.804	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5309 / 0 / 353	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0465, wR2 = 0.1138	
R indices (all data)	R1 = 0.0651, wR2 = 0.1264	
Largest diff. peak and hole	0.201 and -0.282 $e.Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2b** (k0971). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8856(1)	4238(1)	991(1)	25(1)
N(1)	5083(1)	4569(1)	2192(1)	26(1)
N(2)	6379(1)	5918(1)	1340(1)	23(1)
N(3)	6741(1)	7954(1)	1236(1)	25(1)
N(4)	8049(1)	6168(1)	2366(1)	23(1)
N(5)	8379(1)	5040(1)	4164(1)	25(1)
N(6)	7160(1)	4484(1)	2878(1)	24(1)
C(1)	5224(2)	5540(1)	1468(1)	25(1)
C(2)	4119(2)	6581(2)	956(1)	26(1)
C(3)	2719(2)	6741(2)	863(1)	31(1)
C(4)	1836(2)	7933(2)	448(1)	34(1)
C(5)	2336(2)	8959(2)	142(1)	31(1)
C(6)	3719(2)	8824(2)	242(1)	28(1)
C(7)	4628(2)	7627(2)	649(1)	25(1)
C(8)	6042(2)	7209(1)	991(1)	24(1)
C(9)	7675(2)	7447(1)	1977(1)	24(1)
C(10)	8141(2)	8128(2)	2746(1)	24(1)
C(11)	8031(2)	9442(2)	2799(1)	28(1)
C(12)	8460(2)	9816(2)	3722(1)	31(1)
C(13)	8953(2)	8927(2)	4601(1)	31(1)
C(14)	9033(2)	7632(2)	4587(1)	28(1)
C(15)	8642(2)	7229(1)	3645(1)	25(1)
C(16)	8472(2)	6009(2)	3424(1)	24(1)
C(17)	7649(2)	4335(1)	3902(1)	24(1)
C(18)	6938(2)	3559(1)	4638(1)	25(1)
C(19)	7070(2)	3030(2)	5743(1)	28(1)
C(20)	6205(2)	2339(2)	6216(1)	31(1)
C(21)	5172(2)	2237(2)	5639(1)	32(1)
C(22)	4984(2)	2808(2)	4562(1)	29(1)
C(23)	5903(2)	3435(1)	4040(1)	25(1)
C(24)	6015(2)	4109(1)	2935(1)	25(1)

C(25)	10099(2)	3436(1)	1404(1)	24(1)
C(26)	10253(2)	2173(2)	1813(1)	27(1)
C(27)	11508(2)	1376(2)	2216(1)	29(1)
C(28)	12625(2)	1813(2)	2219(1)	28(1)
C(29)	12445(2)	3082(2)	1813(1)	29(1)
C(30)	11195(2)	3888(2)	1403(1)	27(1)
C(31)	13996(2)	925(2)	2641(2)	37(1)
B(1)	7712(2)	5141(2)	1830(1)	24(1)

Table S10. Bond lengths [Å] and angles [°] for compound **2b** (k0971).

O(1)-C(25)	1.3858(17)
O(1)-B(1)	1.436(2)
N(1)-C(24)	1.3450(19)
N(1)-C(1)	1.3497(18)
N(2)-C(1)	1.3674(18)
N(2)-C(8)	1.3703(18)
N(2)-B(1)	1.4938(19)
N(3)-C(8)	1.3465(18)
N(3)-C(9)	1.3482(18)
N(4)-C(9)	1.3704(18)
N(4)-C(16)	1.3705(18)
N(4)-B(1)	1.500(2)
N(5)-C(17)	1.3425(18)
N(5)-C(16)	1.3459(18)
N(6)-C(24)	1.3644(18)
N(6)-C(17)	1.3657(18)
N(6)-B(1)	1.505(2)
C(1)-C(2)	1.449(2)
C(2)-C(3)	1.389(2)
C(2)-C(7)	1.427(2)
C(3)-C(4)	1.385(2)
C(4)-C(5)	1.401(2)
C(5)-C(6)	1.382(2)
C(6)-C(7)	1.395(2)
C(7)-C(8)	1.457(2)
C(9)-C(10)	1.456(2)
C(10)-C(11)	1.400(2)
C(10)-C(15)	1.423(2)
C(11)-C(12)	1.382(2)
C(12)-C(13)	1.398(2)
C(13)-C(14)	1.385(2)
C(14)-C(15)	1.395(2)
C(15)-C(16)	1.454(2)
C(17)-C(18)	1.456(2)

C(18)-C(19)	1.395(2)
C(18)-C(23)	1.425(2)
C(19)-C(20)	1.386(2)
C(20)-C(21)	1.399(2)
C(21)-C(22)	1.386(2)
C(22)-C(23)	1.391(2)
C(23)-C(24)	1.455(2)
C(25)-C(30)	1.384(2)
C(25)-C(26)	1.391(2)
C(26)-C(27)	1.387(2)
C(27)-C(28)	1.394(2)
C(28)-C(29)	1.391(2)
C(28)-C(31)	1.510(2)
C(29)-C(30)	1.390(2)

C(25)-O(1)-B(1)	115.61(11)
C(24)-N(1)-C(1)	116.86(12)
C(1)-N(2)-C(8)	112.73(12)
C(1)-N(2)-B(1)	122.47(12)
C(8)-N(2)-B(1)	122.91(12)
C(8)-N(3)-C(9)	117.28(12)
C(9)-N(4)-C(16)	112.83(12)
C(9)-N(4)-B(1)	122.92(12)
C(16)-N(4)-B(1)	122.90(12)
C(17)-N(5)-C(16)	116.63(12)
C(24)-N(6)-C(17)	113.41(12)
C(24)-N(6)-B(1)	122.89(12)
C(17)-N(6)-B(1)	123.35(12)
N(1)-C(1)-N(2)	123.12(13)
N(1)-C(1)-C(2)	128.78(13)
N(2)-C(1)-C(2)	106.10(12)
C(3)-C(2)-C(7)	120.90(14)
C(3)-C(2)-C(1)	131.41(14)
C(7)-C(2)-C(1)	107.23(12)
C(4)-C(3)-C(2)	118.33(15)
C(3)-C(4)-C(5)	120.86(14)

C(6)-C(5)-C(4)	121.65(14)
C(5)-C(6)-C(7)	118.30(14)
C(6)-C(7)-C(2)	119.96(13)
C(6)-C(7)-C(8)	132.69(14)
C(2)-C(7)-C(8)	106.88(12)
N(3)-C(8)-N(2)	122.72(12)
N(3)-C(8)-C(7)	129.34(13)
N(2)-C(8)-C(7)	105.80(12)
N(3)-C(9)-N(4)	122.35(12)
N(3)-C(9)-C(10)	129.74(13)
N(4)-C(9)-C(10)	105.81(12)
C(11)-C(10)-C(15)	120.08(13)
C(11)-C(10)-C(9)	132.39(13)
C(15)-C(10)-C(9)	107.13(12)
C(12)-C(11)-C(10)	118.14(14)
C(11)-C(12)-C(13)	121.46(14)
C(14)-C(13)-C(12)	121.56(14)
C(13)-C(14)-C(15)	117.69(14)
C(14)-C(15)-C(10)	121.03(13)
C(14)-C(15)-C(16)	131.32(13)
C(10)-C(15)-C(16)	107.24(12)
N(5)-C(16)-N(4)	123.04(13)
N(5)-C(16)-C(15)	129.37(13)
N(4)-C(16)-C(15)	105.82(12)
N(5)-C(17)-N(6)	122.20(13)
N(5)-C(17)-C(18)	130.79(13)
N(6)-C(17)-C(18)	105.59(12)
C(19)-C(18)-C(23)	120.74(13)
C(19)-C(18)-C(17)	132.21(14)
C(23)-C(18)-C(17)	106.99(12)
C(20)-C(19)-C(18)	117.83(14)
C(19)-C(20)-C(21)	121.37(14)
C(22)-C(21)-C(20)	121.35(14)
C(21)-C(22)-C(23)	118.15(14)
C(22)-C(23)-C(18)	120.37(14)
C(22)-C(23)-C(24)	132.34(14)

C(18)-C(23)-C(24)	107.22(12)
N(1)-C(24)-N(6)	122.10(13)
N(1)-C(24)-C(23)	130.93(13)
N(6)-C(24)-C(23)	105.60(12)
C(30)-C(25)-O(1)	119.94(13)
C(30)-C(25)-C(26)	119.80(13)
O(1)-C(25)-C(26)	120.25(13)
C(27)-C(26)-C(25)	119.71(14)
C(26)-C(27)-C(28)	121.33(14)
C(29)-C(28)-C(27)	118.03(14)
C(29)-C(28)-C(31)	121.25(14)
C(27)-C(28)-C(31)	120.72(14)
C(30)-C(29)-C(28)	121.18(14)
C(25)-C(30)-C(29)	119.95(14)
O(1)-B(1)-N(2)	112.57(12)
O(1)-B(1)-N(4)	117.09(12)
N(2)-B(1)-N(4)	104.67(12)
O(1)-B(1)-N(6)	114.56(12)
N(2)-B(1)-N(6)	103.83(12)
N(4)-B(1)-N(6)	102.66(12)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2b** (k0971). 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}
O(1)	27(1)	25(1)	23(1)	2(1)	-7(1)	-8(1)
N(1)	30(1)	24(1)	28(1)	2(1)	-9(1)	-12(1)
N(2)	27(1)	22(1)	23(1)	3(1)	-8(1)	-11(1)
N(3)	28(1)	26(1)	22(1)	3(1)	-7(1)	-12(1)
N(4)	24(1)	22(1)	24(1)	4(1)	-7(1)	-9(1)
N(5)	26(1)	24(1)	27(1)	4(1)	-8(1)	-10(1)
N(6)	26(1)	23(1)	24(1)	3(1)	-7(1)	-11(1)
C(1)	28(1)	25(1)	24(1)	0(1)	-8(1)	-12(1)
C(2)	31(1)	28(1)	23(1)	1(1)	-10(1)	-12(1)
C(3)	33(1)	33(1)	33(1)	2(1)	-13(1)	-15(1)
C(4)	31(1)	39(1)	34(1)	1(1)	-15(1)	-12(1)
C(5)	34(1)	31(1)	27(1)	3(1)	-14(1)	-8(1)
C(6)	34(1)	29(1)	22(1)	2(1)	-9(1)	-11(1)
C(7)	30(1)	28(1)	19(1)	1(1)	-7(1)	-12(1)
C(8)	26(1)	24(1)	20(1)	3(1)	-5(1)	-9(1)
C(9)	25(1)	24(1)	23(1)	3(1)	-4(1)	-11(1)
C(10)	23(1)	27(1)	25(1)	2(1)	-5(1)	-11(1)
C(11)	29(1)	25(1)	30(1)	5(1)	-8(1)	-12(1)
C(12)	34(1)	25(1)	36(1)	0(1)	-8(1)	-14(1)
C(13)	35(1)	33(1)	32(1)	0(1)	-12(1)	-16(1)
C(14)	28(1)	31(1)	28(1)	5(1)	-11(1)	-13(1)
C(15)	23(1)	27(1)	26(1)	3(1)	-6(1)	-11(1)
C(16)	24(1)	25(1)	23(1)	2(1)	-7(1)	-9(1)
C(17)	25(1)	21(1)	24(1)	2(1)	-6(1)	-7(1)
C(18)	26(1)	20(1)	26(1)	0(1)	-4(1)	-8(1)
C(19)	30(1)	26(1)	25(1)	1(1)	-5(1)	-9(1)
C(20)	37(1)	29(1)	25(1)	4(1)	-3(1)	-11(1)
C(21)	32(1)	29(1)	33(1)	3(1)	1(1)	-13(1)
C(22)	29(1)	27(1)	32(1)	1(1)	-4(1)	-13(1)
C(23)	27(1)	21(1)	27(1)	1(1)	-4(1)	-8(1)
C(24)	26(1)	21(1)	27(1)	0(1)	-6(1)	-10(1)

C(25)	26(1)	25(1)	19(1)	1(1)	-5(1)	-7(1)
C(26)	32(1)	25(1)	26(1)	1(1)	-7(1)	-13(1)
C(27)	36(1)	24(1)	27(1)	2(1)	-8(1)	-10(1)
C(28)	30(1)	28(1)	24(1)	-2(1)	-6(1)	-7(1)
C(29)	28(1)	33(1)	27(1)	0(1)	-4(1)	-13(1)
C(30)	30(1)	25(1)	27(1)	3(1)	-4(1)	-13(1)
C(31)	35(1)	36(1)	34(1)	0(1)	-13(1)	-6(1)
B(1)	26(1)	23(1)	23(1)	3(1)	-8(1)	-11(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2b** (k0971).

	x	y	z	U(eq)
H(3A)	2375	6050	1078	37
H(4A)	879	8058	370	40
H(5A)	1709	9767	-141	37
H(6A)	4043	9530	38	33
H(11A)	7673	10059	2216	33
H(12A)	8418	10696	3760	37
H(13A)	9239	9217	5223	38
H(14A)	9345	7040	5198	34
H(19A)	7731	3140	6158	34
H(20A)	6316	1926	6949	38
H(21A)	4586	1766	5991	38
H(22A)	4249	2772	4192	35
H(26A)	9503	1859	1818	32
H(27A)	11607	515	2494	35
H(29A)	13188	3404	1817	35
H(30A)	11095	4749	1122	32
H(31A)	14417	71	2219	55
H(31B)	13759	775	3477	55
H(31C)	14700	1352	2501	55

Table S13. Selected Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 deg for compound **2b** (k0971).

Cg(I)	->	Cg(J)	Cg-Cg (Å)	Alpha (deg)	Beta (deg)	Gamma (deg)	CgI_Perp (Å)	CgJ_Perp (Å)	Slippage (Å)
Cg(6)	->	Cg(3)	3.6045(9)	2.08(8)	3.72	1.98	3.6023(6)	3.5970(6)	
Cg(3)	->	Cg(6)	3.6046(9)	2.08(8)	1.98	3.72	3.5970(6)	3.6024(6)	

Table S14. Selected C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) for compound **2b** (k0971).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (deg)	X-H..Cg (deg)	X..Cg (Å)	X-H,Pi (deg)
C(12) -H(12A)	->	Cg(6)	2.94	-2.89	9.86	125	3.5725(17)	45
C(20) -H(20A)	->	Cg(1)	2.75	2.69	11.76	118	3.3001(17)	39
C(21) -H(21A)	->	Cg(2)	2.72	-2.69	8.43	123	3.3339(19)	41

See lit. [11] for definitions of C-H…π factors
All atoms numbered according to thermal ellipsoid plot in Figure S2. Cg numberings as defined below for ring centroids used in above tables for compound **2b** (k0971):
5-Membered Ring (1) N(2) --> C(1) --> C(2) --> C(7) --> C(8) -->
5-Membered Ring (2) N(4) --> C(9) --> C(10) --> C(15) --> C(16) -->
5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->
6-Membered Ring (6) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

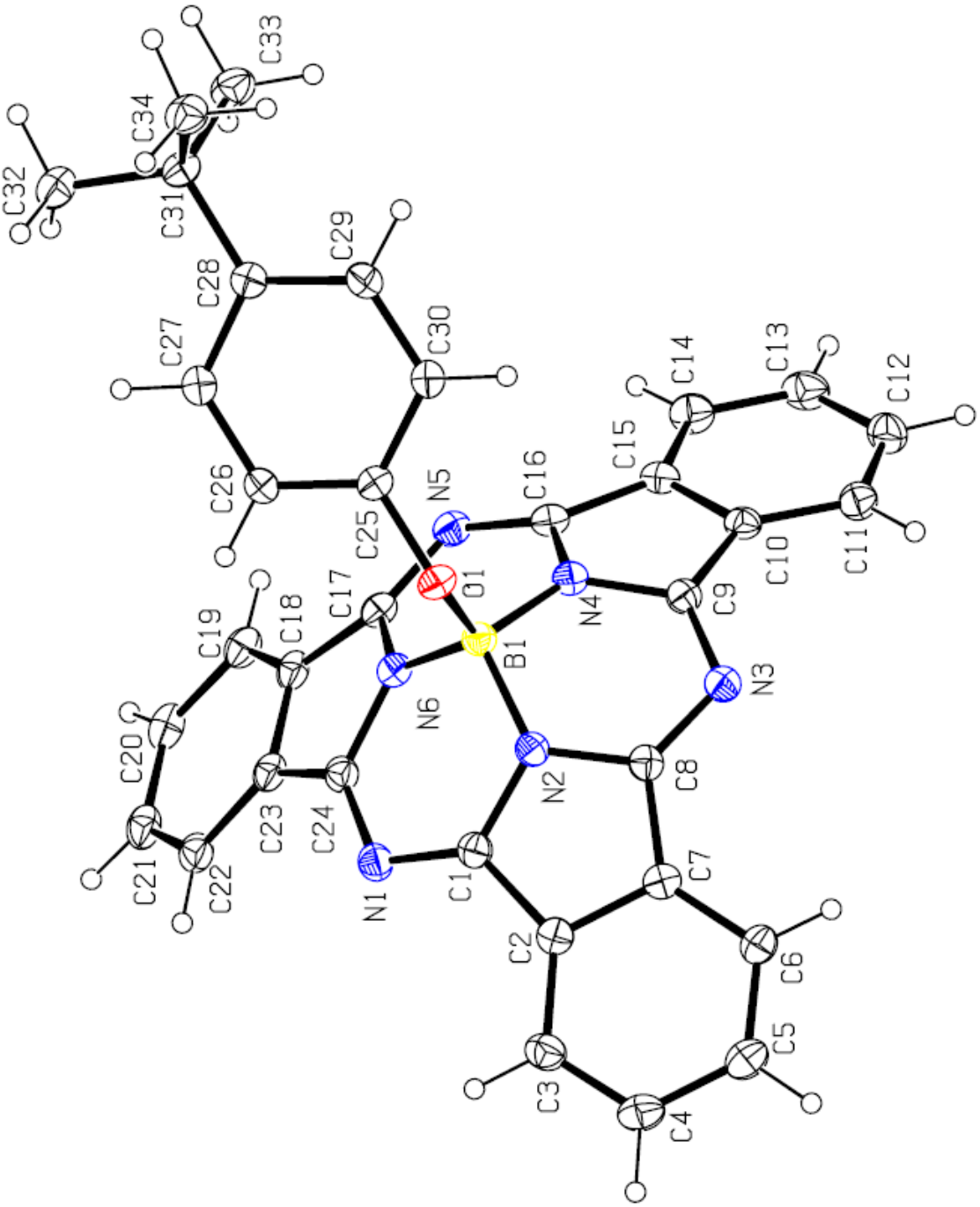


Figure S3A: Thermal ellipsoid plot of compound **2c**, shown with atom numberings.

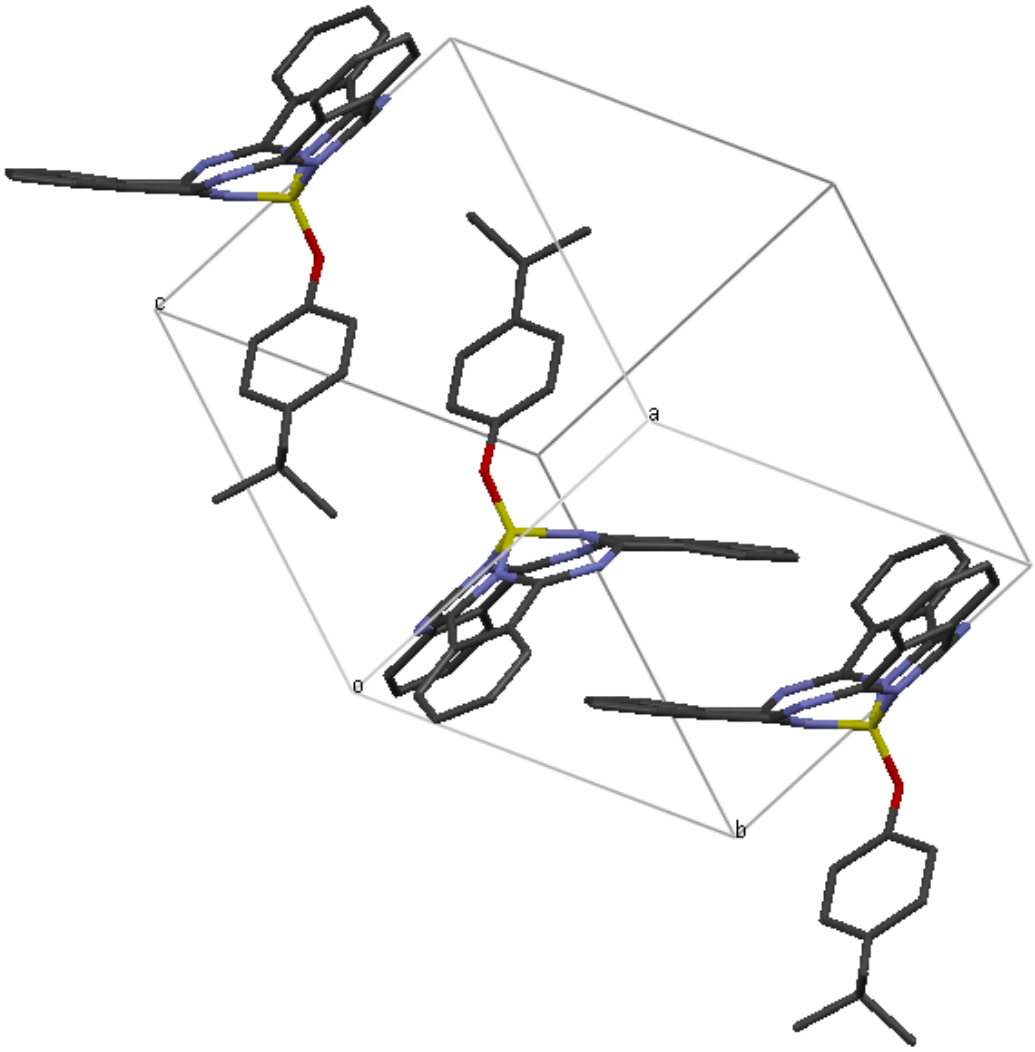


Figure S3B: Image of crystal of compound **2c** showing orientation of crystal axes.

Table S15. Crystal data and structure refinement for compound **2c** (k09107)..

Identification code	k09107	
Empirical formula	C34 H25 B N6 O	
Formula weight	544.41	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.5535(2) Å	α= 79.9663(14)°.
	b = 12.7466(4) Å	β= 78.2792(16)°.
	c = 13.2395(4) Å	γ = 70.9358(17)°.
Volume	1326.76(7) $Å^3$	
Z	2	
Density (calculated)	1.363 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	568	
Crystal size	0.40 x 0.22 x 0.10 mm^3	
Theta range for data collection	2.55 to 27.48°.	
Index ranges	-10<=h<=11, -16<=k<=16, -16<=l<=17	
Reflections collected	15623	
Independent reflections	6009 [R(int) = 0.0566]	
Completeness to theta = 27.48°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.788	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6009 / 0 / 382	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1434	
R indices (all data)	R1 = 0.1178, wR2 = 0.1787	
Largest diff. peak and hole	0.280 and -0.296 $e.Å^{-3}$	

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **2c** (k09107).. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5251(2)	8760(1)	7132(1)	31(1)
N(1)	4300(2)	7894(2)	9944(1)	33(1)
N(2)	6583(2)	8137(1)	8652(1)	27(1)
N(3)	9465(2)	7643(2)	7911(1)	31(1)
N(4)	7563(2)	6969(2)	7311(1)	29(1)
N(5)	6254(2)	5578(2)	7332(1)	33(1)
N(6)	4949(2)	7080(2)	8358(1)	29(1)
C(1)	5633(2)	8279(2)	9614(2)	30(1)
C(2)	6608(3)	8617(2)	10208(2)	31(1)
C(3)	6291(3)	8913(2)	11205(2)	38(1)
C(4)	7540(3)	9106(2)	11581(2)	42(1)
C(5)	9115(3)	9004(2)	10976(2)	42(1)
C(6)	9472(3)	8706(2)	9987(2)	34(1)
C(7)	8204(3)	8525(2)	9587(2)	30(1)
C(8)	8183(2)	8143(2)	8620(2)	28(1)
C(9)	9149(2)	7010(2)	7309(2)	29(1)
C(10)	10278(3)	6070(2)	6775(2)	30(1)
C(11)	12021(3)	5705(2)	6498(2)	37(1)
C(12)	12731(3)	4711(2)	6064(2)	43(1)
C(13)	11765(3)	4068(2)	5932(2)	44(1)
C(14)	10047(3)	4418(2)	6218(2)	41(1)
C(15)	9298(3)	5428(2)	6618(2)	31(1)
C(16)	7560(3)	5988(2)	7029(2)	30(1)
C(17)	5021(3)	6089(2)	8054(2)	30(1)
C(18)	3840(2)	5650(2)	8817(2)	32(1)
C(19)	3375(3)	4690(2)	8890(2)	35(1)
C(20)	2266(3)	4465(2)	9763(2)	38(1)
C(21)	1684(3)	5157(2)	10547(2)	40(1)
C(22)	2179(2)	6097(2)	10502(2)	37(1)
C(23)	3243(2)	6359(2)	9614(2)	32(1)
C(24)	4060(2)	7232(2)	9340(2)	30(1)

C(25)	4502(2)	8621(2)	6350(2)	28(1)
C(26)	2905(2)	8543(2)	6546(2)	32(1)
C(27)	2139(3)	8463(2)	5742(2)	33(1)
C(28)	2948(2)	8475(2)	4717(2)	29(1)
C(29)	4566(3)	8556(2)	4543(2)	35(1)
C(30)	5356(3)	8622(2)	5336(2)	33(1)
C(31)	2105(3)	8436(2)	3812(2)	33(1)
C(32)	330(3)	8350(2)	4171(2)	41(1)
C(33)	3154(3)	7435(2)	3227(2)	44(1)
C(34)	1985(3)	9522(2)	3071(2)	41(1)
B(1)	6018(3)	7794(2)	7803(2)	28(1)

Table S17. Bond lengths [Å] and angles [°] for compound **2c** (k09107)..

O(1)-C(25)	1.387(2)
O(1)-B(1)	1.437(3)
N(1)-C(24)	1.346(3)
N(1)-C(1)	1.349(3)
N(2)-C(8)	1.363(3)
N(2)-C(1)	1.371(3)
N(2)-B(1)	1.490(3)
N(3)-C(9)	1.348(3)
N(3)-C(8)	1.351(3)
N(4)-C(16)	1.367(3)
N(4)-C(9)	1.373(3)
N(4)-B(1)	1.502(3)
N(5)-C(16)	1.345(3)
N(5)-C(17)	1.345(3)
N(6)-C(17)	1.370(3)
N(6)-C(24)	1.377(3)
N(6)-B(1)	1.497(3)
C(1)-C(2)	1.455(3)
C(2)-C(3)	1.385(3)
C(2)-C(7)	1.424(3)
C(3)-C(4)	1.371(3)
C(4)-C(5)	1.399(3)
C(5)-C(6)	1.374(3)
C(6)-C(7)	1.396(3)
C(7)-C(8)	1.451(3)
C(9)-C(10)	1.459(3)
C(10)-C(11)	1.399(3)
C(10)-C(15)	1.412(3)
C(11)-C(12)	1.383(3)
C(12)-C(13)	1.391(4)
C(13)-C(14)	1.381(3)
C(14)-C(15)	1.382(3)
C(15)-C(16)	1.459(3)
C(17)-C(18)	1.453(3)

C(18)-C(19)	1.388(3)
C(18)-C(23)	1.415(3)
C(19)-C(20)	1.390(3)
C(20)-C(21)	1.388(3)
C(21)-C(22)	1.383(3)
C(22)-C(23)	1.396(3)
C(23)-C(24)	1.457(3)
C(25)-C(26)	1.370(3)
C(25)-C(30)	1.391(3)
C(26)-C(27)	1.393(3)
C(27)-C(28)	1.392(3)
C(28)-C(29)	1.390(3)
C(28)-C(31)	1.534(3)
C(29)-C(30)	1.387(3)
C(31)-C(32)	1.529(3)
C(31)-C(33)	1.532(3)
C(31)-C(34)	1.538(3)

C(25)-O(1)-B(1)	118.86(17)
C(24)-N(1)-C(1)	116.79(18)
C(8)-N(2)-C(1)	112.77(18)
C(8)-N(2)-B(1)	123.50(17)
C(1)-N(2)-B(1)	122.73(17)
C(9)-N(3)-C(8)	117.07(18)
C(16)-N(4)-C(9)	112.76(17)
C(16)-N(4)-B(1)	123.23(17)
C(9)-N(4)-B(1)	122.62(19)
C(16)-N(5)-C(17)	116.92(19)
C(17)-N(6)-C(24)	112.39(18)
C(17)-N(6)-B(1)	123.80(18)
C(24)-N(6)-B(1)	122.48(19)
N(1)-C(1)-N(2)	122.5(2)
N(1)-C(1)-C(2)	129.7(2)
N(2)-C(1)-C(2)	105.84(17)
C(3)-C(2)-C(7)	120.2(2)
C(3)-C(2)-C(1)	132.8(2)

C(7)-C(2)-C(1)	106.88(19)
C(4)-C(3)-C(2)	118.9(2)
C(3)-C(4)-C(5)	121.0(2)
C(6)-C(5)-C(4)	121.5(2)
C(5)-C(6)-C(7)	118.2(2)
C(6)-C(7)-C(2)	120.2(2)
C(6)-C(7)-C(8)	132.3(2)
C(2)-C(7)-C(8)	107.24(18)
N(3)-C(8)-N(2)	122.4(2)
N(3)-C(8)-C(7)	130.02(19)
N(2)-C(8)-C(7)	106.03(17)
N(3)-C(9)-N(4)	122.50(19)
N(3)-C(9)-C(10)	130.15(19)
N(4)-C(9)-C(10)	105.52(18)
C(11)-C(10)-C(15)	120.3(2)
C(11)-C(10)-C(9)	132.3(2)
C(15)-C(10)-C(9)	107.21(17)
C(12)-C(11)-C(10)	117.9(2)
C(11)-C(12)-C(13)	121.7(2)
C(14)-C(13)-C(12)	120.6(2)
C(13)-C(14)-C(15)	118.9(2)
C(14)-C(15)-C(10)	120.6(2)
C(14)-C(15)-C(16)	131.8(2)
C(10)-C(15)-C(16)	107.45(19)
N(5)-C(16)-N(4)	122.76(19)
N(5)-C(16)-C(15)	129.7(2)
N(4)-C(16)-C(15)	105.66(18)
N(5)-C(17)-N(6)	122.22(19)
N(5)-C(17)-C(18)	129.9(2)
N(6)-C(17)-C(18)	106.19(18)
C(19)-C(18)-C(23)	121.2(2)
C(19)-C(18)-C(17)	131.4(2)
C(23)-C(18)-C(17)	107.16(19)
C(18)-C(19)-C(20)	117.5(2)
C(21)-C(20)-C(19)	121.3(2)
C(22)-C(21)-C(20)	121.9(2)

C(21)-C(22)-C(23)	117.7(2)
C(22)-C(23)-C(18)	120.4(2)
C(22)-C(23)-C(24)	131.9(2)
C(18)-C(23)-C(24)	107.51(18)
N(1)-C(24)-N(6)	122.62(19)
N(1)-C(24)-C(23)	130.0(2)
N(6)-C(24)-C(23)	105.61(19)
C(26)-C(25)-O(1)	121.24(19)
C(26)-C(25)-C(30)	119.5(2)
O(1)-C(25)-C(30)	119.20(18)
C(25)-C(26)-C(27)	120.5(2)
C(28)-C(27)-C(26)	121.59(19)
C(29)-C(28)-C(27)	116.5(2)
C(29)-C(28)-C(31)	120.89(19)
C(27)-C(28)-C(31)	122.56(18)
C(30)-C(29)-C(28)	122.7(2)
C(29)-C(30)-C(25)	119.25(19)
C(32)-C(31)-C(33)	108.85(19)
C(32)-C(31)-C(28)	112.55(18)
C(33)-C(31)-C(28)	109.88(18)
C(32)-C(31)-C(34)	107.78(18)
C(33)-C(31)-C(34)	109.4(2)
C(28)-C(31)-C(34)	108.38(18)
O(1)-B(1)-N(2)	110.24(19)
O(1)-B(1)-N(6)	117.11(18)
N(2)-B(1)-N(6)	104.18(18)
O(1)-B(1)-N(4)	116.27(18)
N(2)-B(1)-N(4)	104.17(17)
N(6)-B(1)-N(4)	103.45(18)

Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2c** (k09107).. 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}
O(1)	36(1)	31(1)	29(1)	-1(1)	-11(1)	-11(1)
N(1)	29(1)	34(1)	34(1)	-5(1)	-4(1)	-9(1)
N(2)	28(1)	26(1)	28(1)	-3(1)	-3(1)	-9(1)
N(3)	32(1)	29(1)	30(1)	-2(1)	-5(1)	-10(1)
N(4)	32(1)	28(1)	28(1)	-3(1)	-5(1)	-10(1)
N(5)	36(1)	34(1)	31(1)	-5(1)	-8(1)	-13(1)
N(6)	29(1)	29(1)	28(1)	-3(1)	-7(1)	-8(1)
C(1)	29(1)	28(1)	31(1)	-3(1)	-6(1)	-6(1)
C(2)	32(1)	27(1)	34(1)	-4(1)	-6(1)	-8(1)
C(3)	40(1)	39(1)	34(1)	-9(1)	-2(1)	-8(1)
C(4)	53(2)	39(2)	36(1)	-10(1)	-11(1)	-12(1)
C(5)	47(1)	41(2)	44(2)	-8(1)	-14(1)	-17(1)
C(6)	34(1)	32(1)	39(1)	-4(1)	-9(1)	-10(1)
C(7)	35(1)	25(1)	30(1)	-1(1)	-7(1)	-9(1)
C(8)	30(1)	25(1)	30(1)	1(1)	-4(1)	-11(1)
C(9)	31(1)	29(1)	28(1)	-1(1)	-4(1)	-11(1)
C(10)	33(1)	30(1)	23(1)	0(1)	-5(1)	-8(1)
C(11)	35(1)	39(1)	33(1)	2(1)	-8(1)	-10(1)
C(12)	34(1)	46(2)	39(2)	-6(1)	-5(1)	1(1)
C(13)	51(2)	36(2)	40(2)	-13(1)	-8(1)	-1(1)
C(14)	47(1)	34(1)	41(2)	-7(1)	-8(1)	-10(1)
C(15)	37(1)	31(1)	25(1)	-4(1)	-4(1)	-8(1)
C(16)	36(1)	30(1)	25(1)	-2(1)	-7(1)	-10(1)
C(17)	32(1)	29(1)	30(1)	-1(1)	-11(1)	-9(1)
C(18)	26(1)	33(1)	36(1)	3(1)	-12(1)	-9(1)
C(19)	35(1)	32(1)	40(1)	2(1)	-15(1)	-9(1)
C(20)	34(1)	32(1)	51(2)	7(1)	-17(1)	-14(1)
C(21)	32(1)	46(2)	41(2)	13(1)	-13(1)	-17(1)
C(22)	29(1)	45(2)	35(1)	4(1)	-9(1)	-11(1)
C(23)	27(1)	34(1)	35(1)	2(1)	-12(1)	-10(1)
C(24)	27(1)	31(1)	31(1)	-2(1)	-6(1)	-7(1)

C(25)	31(1)	24(1)	29(1)	-1(1)	-8(1)	-8(1)
C(26)	29(1)	37(1)	29(1)	-4(1)	-1(1)	-11(1)
C(27)	29(1)	32(1)	36(1)	-2(1)	-4(1)	-9(1)
C(28)	32(1)	24(1)	30(1)	-1(1)	-6(1)	-7(1)
C(29)	32(1)	43(2)	29(1)	-4(1)	-1(1)	-11(1)
C(30)	28(1)	38(1)	35(1)	-5(1)	-4(1)	-11(1)
C(31)	37(1)	32(1)	33(1)	-4(1)	-10(1)	-12(1)
C(32)	41(1)	44(2)	44(2)	-1(1)	-14(1)	-17(1)
C(33)	48(1)	42(2)	45(2)	-13(1)	-14(1)	-11(1)
C(34)	45(1)	41(2)	37(1)	5(1)	-14(1)	-12(1)
B(1)	29(1)	28(1)	27(1)	-4(1)	-4(1)	-10(1)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2c** (k09107)..

	x	y	z	U(eq)
H(3B)	5226	8980	11622	46
H(4A)	7333	9313	12262	50
H(5B)	9957	9143	11255	50
H(6A)	10551	8624	9587	41
H(11A)	12695	6126	6605	44
H(12A)	13909	4461	5850	51
H(13A)	12292	3383	5643	53
H(14A)	9390	3971	6141	49
H(19A)	3798	4204	8363	43
H(20A)	1900	3826	9823	45
H(21A)	924	4980	11132	48
H(22A)	1808	6548	11056	44
H(26A)	2316	8544	7237	38
H(27A)	1037	8399	5896	39
H(29A)	5154	8566	3852	42
H(30A)	6468	8668	5189	40
H(32A)	-382	9026	4482	61
H(32B)	360	7695	4688	61
H(32C)	-125	8275	3575	61
H(33A)	4288	7490	2982	65
H(33B)	2636	7434	2632	65
H(33C)	3210	6741	3694	65
H(34A)	3093	9633	2880	62
H(34B)	1202	10154	3417	62
H(34C)	1583	9470	2445	62

Table S20. Selected Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 deg for compound **2c** (k09107).

Cg(I)	->	Cg(J)	Cg-Cg (Å)	Alpha (deg)	Beta (deg)	Gamma (deg)	CgI_Perp (Å)	CgJ_Perp (Å)	Slippage (Å)
Cg(3)	->	Cg(6)	3.5482(14)	0.95(12)	9.21	10.13	3.4929(10)	3.5025(10)	
Cg(6)	->	Cg(3)	3.5482(14)	0.95(12)	10.13	9.21	3.5025(10)	3.4929(10)	
Cg(6)	->	Cg(6)	3.8443(14)	0	23.78	23.78	3.5178(10)	3.5178(10)	1.550

Table S21. Selected C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) for compound **2c** (k09107).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (deg)	X-H..Cg (deg)	X..Cg (Å)	X-H,Pi (deg)
C(20) -H(20A)	->	Cg(1)	2.72	-2.72	1.99	136	3.461(3)	46
C(21) -H(21A)	->	Cg(2)	2.71	2.71	3.70	135	3.452(3)	45

See lit. [11] for definitions of C-H…π factors
All atoms numbered according to thermal ellipsoid plot in Figure S3. Cg numberings as defined below for ring centroids used in above tables for compound **2c** (k09107):
5-Membered Ring (1) N(2) --> C(1) --> C(2) --> C(7) --> C(8) -->
5-Membered Ring (2) N(4) --> C(9) --> C(10) --> C(15) --> C(16) -->
5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->
6-Membered Ring (6) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

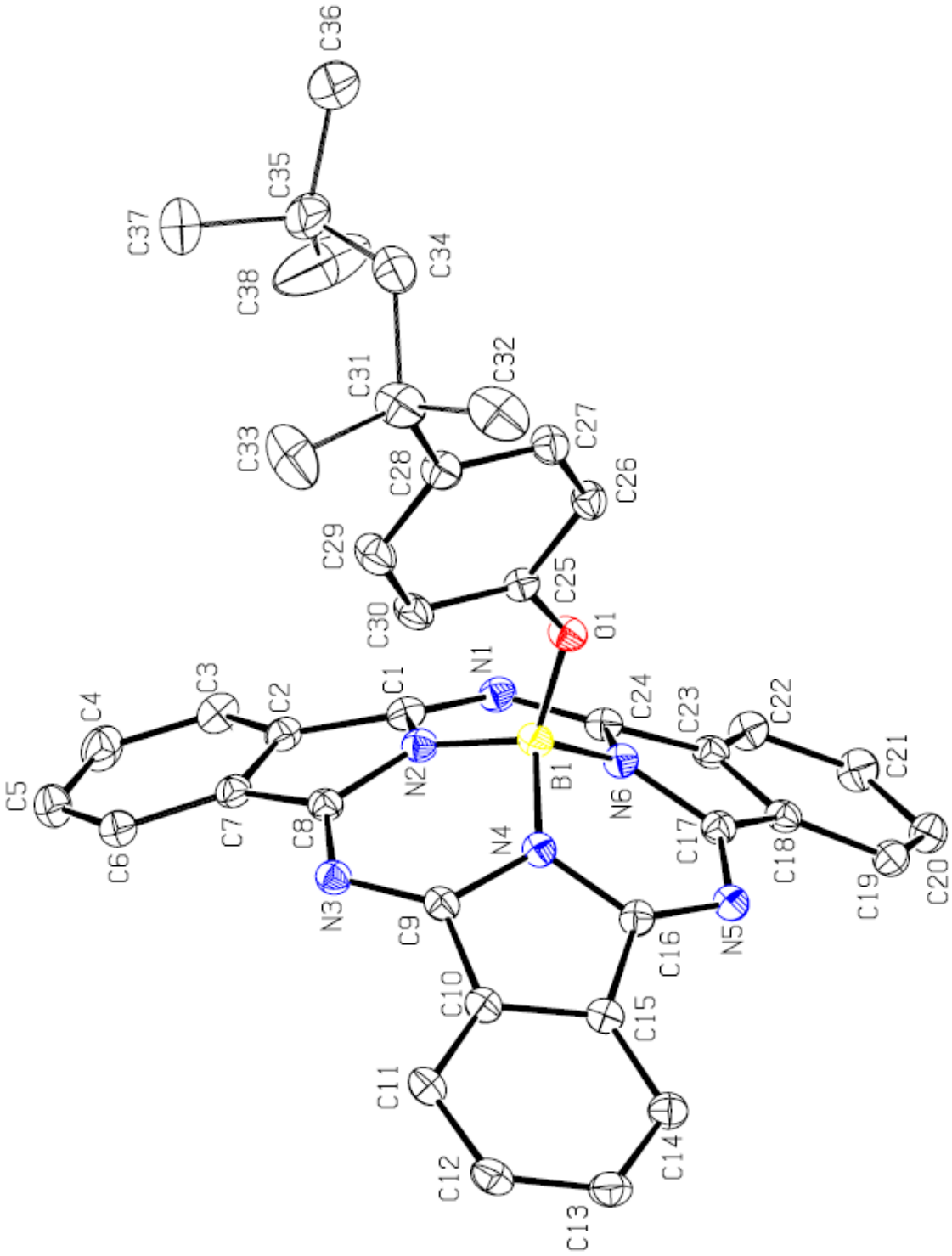


Figure S4A: Thermal ellipsoid plot of compound **2d**, shown with atom numberings.

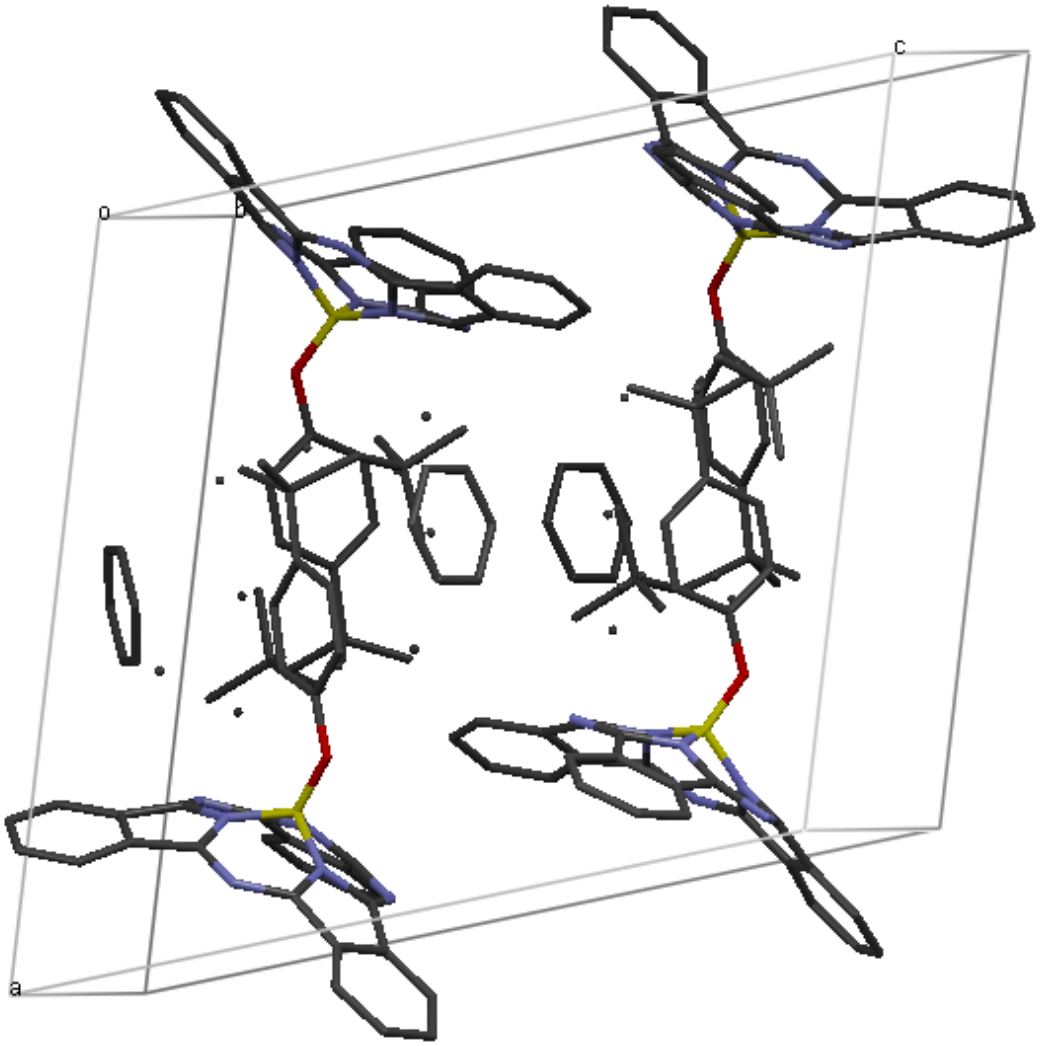


Figure S4B: Image of crystal of compound **2d** showing orientation of crystal axes.

Table S22. Crystal data and structure refinement for compound **2d** (k09104).

Identification code	k09104	
Empirical formula	C41 H36 B N6 O	
Formula weight	639.57	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 16.4530(4) Å	α= 90°.
	b = 11.9941(2) Å	β= 108.1900(11)°.
	c = 17.5406(4) Å	γ = 90°.
Volume	3288.46(12) $Å^3$	
Z	4	
Density (calculated)	1.292 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	1348	
Crystal size	0.24 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.61 to 27.50°.	
Index ranges	-21<=h<=21, -15<=k<=15, -22<=l<=22	
Reflections collected	21335	
Independent reflections	7488 [R(int) = 0.0473]	
Completeness to theta = 27.50°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.994 and 0.937	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7488 / 26 / 470	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.1309	
R indices (all data)	R1 = 0.1108, wR2 = 0.1595	
Largest diff. peak and hole	0.438 and -0.423 $e.Å^{-3}$	

Table S23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2d** (k09104).. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7667(1)	1765(1)	3426(1)	29(1)
N(1)	9661(1)	3341(1)	4191(1)	29(1)
N(2)	8473(1)	3301(1)	2989(1)	27(1)
N(3)	7841(1)	3385(1)	1572(1)	28(1)
N(4)	8194(1)	1641(1)	2236(1)	25(1)
N(5)	9128(1)	91(1)	2696(1)	28(1)
N(6)	9139(1)	1631(1)	3550(1)	26(1)
C(1)	9081(1)	3864(2)	3578(1)	28(1)
C(2)	9072(1)	5001(2)	3283(1)	29(1)
C(3)	9516(1)	5953(2)	3631(1)	36(1)
C(4)	9389(2)	6911(2)	3166(2)	43(1)
C(5)	8857(2)	6923(2)	2372(2)	41(1)
C(6)	8424(1)	5976(2)	2018(1)	34(1)
C(7)	8523(1)	5013(2)	2478(1)	29(1)
C(8)	8192(1)	3886(2)	2286(1)	26(1)
C(9)	7892(1)	2264(2)	1552(1)	27(1)
C(10)	7874(1)	1520(2)	892(1)	28(1)
C(11)	7557(1)	1646(2)	64(1)	32(1)
C(12)	7670(2)	779(2)	-410(1)	36(1)
C(13)	8113(1)	-183(2)	-71(1)	37(1)
C(14)	8443(1)	-321(2)	749(1)	33(1)
C(15)	8299(1)	523(2)	1237(1)	28(1)
C(16)	8546(1)	651(2)	2106(1)	28(1)
C(17)	9444(1)	623(2)	3402(1)	26(1)
C(18)	10233(1)	450(2)	4063(1)	27(1)
C(19)	10804(1)	-432(2)	4267(1)	31(1)
C(20)	11512(1)	-334(2)	4936(1)	35(1)
C(21)	11672(1)	642(2)	5387(1)	37(1)
C(22)	11133(1)	1551(2)	5181(1)	32(1)
C(23)	10399(1)	1456(2)	4522(1)	28(1)
C(24)	9709(1)	2224(2)	4143(1)	26(1)

C(25)	6799(1)	1901(2)	3153(1)	26(1)
C(26)	6329(1)	1255(2)	3518(1)	31(1)
C(27)	5448(1)	1338(2)	3291(1)	33(1)
C(28)	4998(1)	2078(2)	2698(1)	34(1)
C(29)	5480(1)	2724(2)	2346(1)	41(1)
C(30)	6371(1)	2648(2)	2567(1)	35(1)
C(31)	4024(2)	2161(2)	2475(2)	49(1)
C(32)	3652(2)	968(3)	2298(2)	60(1)
C(33)	3618(2)	2838(5)	1730(3)	72(2)
C(34)	3755(2)	2509(3)	3231(2)	51(1)
C(35)	3988(3)	3657(3)	3645(2)	66(1)
C(36)	3658(3)	3638(4)	4369(3)	77(1)
C(37)	3521(5)	4624(5)	3123(4)	165(4)
C(38)	4954(4)	3890(7)	3942(6)	151(4)
C(31A)	4024(2)	2161(2)	2475(2)	49(1)
C(32A)	3551(8)	1290(9)	2795(8)	61(4)
C(33A)	3708(10)	2220(13)	1557(3)	65(5)
C(34A)	3828(7)	3411(5)	2684(6)	42(3)
C(35A)	4013(7)	3880(8)	3547(6)	66(1)
C(36A)	3394(8)	3324(11)	3930(10)	71(5)
C(37A)	3873(7)	5144(8)	3576(8)	56(4)
C(38A)	4923(6)	3643(11)	4105(8)	28(3)
B(1)	8296(2)	2085(2)	3055(1)	26(1)
C(1S)	5707(3)	-567(4)	4999(3)	91(1)
C(2S)	5792(3)	440(5)	5341(2)	90(1)
C(3S)	5075(4)	1018(3)	5341(2)	93(1)

Table S24. Bond lengths [Å] and angles [°] for compound **2d** (k09104)..

O(1)-C(25)	1.368(2)
O(1)-B(1)	1.436(3)
N(1)-C(24)	1.346(3)
N(1)-C(1)	1.349(3)
N(2)-C(8)	1.368(2)
N(2)-C(1)	1.370(2)
N(2)-B(1)	1.499(3)
N(3)-C(8)	1.346(3)
N(3)-C(9)	1.347(3)
N(4)-C(9)	1.367(2)
N(4)-C(16)	1.371(3)
N(4)-B(1)	1.492(3)
N(5)-C(17)	1.344(3)
N(5)-C(16)	1.350(2)
N(6)-C(24)	1.364(2)
N(6)-C(17)	1.364(2)
N(6)-B(1)	1.491(3)
C(1)-C(2)	1.456(3)
C(2)-C(3)	1.390(3)
C(2)-C(7)	1.418(3)
C(3)-C(4)	1.386(3)
C(4)-C(5)	1.395(3)
C(5)-C(6)	1.381(3)
C(6)-C(7)	1.389(3)
C(7)-C(8)	1.458(3)
C(9)-C(10)	1.455(3)
C(10)-C(11)	1.390(3)
C(10)-C(15)	1.422(3)
C(11)-C(12)	1.380(3)
C(12)-C(13)	1.394(3)
C(13)-C(14)	1.381(3)
C(14)-C(15)	1.392(3)
C(15)-C(16)	1.458(3)
C(17)-C(18)	1.460(3)

C(18)-C(19)	1.385(3)
C(18)-C(23)	1.430(3)
C(19)-C(20)	1.377(3)
C(20)-C(21)	1.390(3)
C(21)-C(22)	1.381(3)
C(22)-C(23)	1.391(3)
C(23)-C(24)	1.451(3)
C(25)-C(30)	1.379(3)
C(25)-C(26)	1.385(3)
C(26)-C(27)	1.382(3)
C(27)-C(28)	1.392(3)
C(28)-C(29)	1.385(3)
C(28)-C(31)	1.530(3)
C(29)-C(30)	1.397(3)
C(31)-C(33)	1.507(3)
C(31)-C(32)	1.550(3)
C(31)-C(34)	1.578(4)
C(34)-C(35)	1.547(5)
C(35)-C(37)	1.528(4)
C(35)-C(36)	1.530(4)
C(35)-C(38)	1.536(4)
C(34A)-C(35A)	1.554(6)
C(35A)-C(36A)	1.537(5)
C(35A)-C(37A)	1.537(5)
C(35A)-C(38A)	1.538(5)
C(1S)-C(2S)	1.337(6)
C(1S)-C(3S)#1	1.352(6)
C(2S)-C(3S)	1.369(6)
C(3S)-C(1S)#1	1.352(6)

C(25)-O(1)-B(1)	129.14(16)
C(24)-N(1)-C(1)	116.99(17)
C(8)-N(2)-C(1)	112.88(16)
C(8)-N(2)-B(1)	123.33(16)
C(1)-N(2)-B(1)	122.34(16)
C(8)-N(3)-C(9)	117.16(17)

C(9)-N(4)-C(16)	112.64(16)
C(9)-N(4)-B(1)	123.37(16)
C(16)-N(4)-B(1)	122.83(16)
C(17)-N(5)-C(16)	116.57(17)
C(24)-N(6)-C(17)	113.69(16)
C(24)-N(6)-B(1)	123.13(16)
C(17)-N(6)-B(1)	122.92(16)
N(1)-C(1)-N(2)	122.68(18)
N(1)-C(1)-C(2)	130.14(18)
N(2)-C(1)-C(2)	105.62(17)
C(3)-C(2)-C(7)	120.8(2)
C(3)-C(2)-C(1)	131.9(2)
C(7)-C(2)-C(1)	107.24(17)
C(4)-C(3)-C(2)	117.5(2)
C(3)-C(4)-C(5)	121.8(2)
C(6)-C(5)-C(4)	121.0(2)
C(5)-C(6)-C(7)	118.1(2)
C(6)-C(7)-C(2)	120.66(19)
C(6)-C(7)-C(8)	132.0(2)
C(2)-C(7)-C(8)	107.24(17)
N(3)-C(8)-N(2)	122.42(18)
N(3)-C(8)-C(7)	130.60(18)
N(2)-C(8)-C(7)	105.65(17)
N(3)-C(9)-N(4)	122.12(18)
N(3)-C(9)-C(10)	130.21(18)
N(4)-C(9)-C(10)	105.90(17)
C(11)-C(10)-C(15)	120.66(19)
C(11)-C(10)-C(9)	132.32(19)
C(15)-C(10)-C(9)	106.99(17)
C(12)-C(11)-C(10)	118.1(2)
C(11)-C(12)-C(13)	121.2(2)
C(14)-C(13)-C(12)	121.7(2)
C(13)-C(14)-C(15)	117.8(2)
C(14)-C(15)-C(10)	120.35(19)
C(14)-C(15)-C(16)	132.38(19)
C(10)-C(15)-C(16)	107.18(17)

N(5)-C(16)-N(4)	122.67(18)
N(5)-C(16)-C(15)	130.45(18)
N(4)-C(16)-C(15)	105.68(16)
N(5)-C(17)-N(6)	122.44(17)
N(5)-C(17)-C(18)	130.97(18)
N(6)-C(17)-C(18)	105.27(16)
C(19)-C(18)-C(23)	120.31(18)
C(19)-C(18)-C(17)	132.58(19)
C(23)-C(18)-C(17)	107.05(17)
C(20)-C(19)-C(18)	118.7(2)
C(19)-C(20)-C(21)	121.1(2)
C(22)-C(21)-C(20)	121.6(2)
C(21)-C(22)-C(23)	118.2(2)
C(22)-C(23)-C(18)	120.05(19)
C(22)-C(23)-C(24)	132.85(19)
C(18)-C(23)-C(24)	107.06(17)
N(1)-C(24)-N(6)	121.80(17)
N(1)-C(24)-C(23)	131.01(18)
N(6)-C(24)-C(23)	105.73(17)
O(1)-C(25)-C(30)	124.95(18)
O(1)-C(25)-C(26)	116.36(17)
C(30)-C(25)-C(26)	118.66(19)
C(27)-C(26)-C(25)	120.88(19)
C(26)-C(27)-C(28)	121.8(2)
C(29)-C(28)-C(27)	116.4(2)
C(29)-C(28)-C(31)	123.37(19)
C(27)-C(28)-C(31)	120.21(19)
C(28)-C(29)-C(30)	122.5(2)
C(25)-C(30)-C(29)	119.7(2)
C(33)-C(31)-C(28)	113.7(2)
C(33)-C(31)-C(32)	106.4(3)
C(28)-C(31)-C(32)	107.9(2)
C(33)-C(31)-C(34)	115.0(3)
C(28)-C(31)-C(34)	110.4(2)
C(32)-C(31)-C(34)	102.5(2)
C(35)-C(34)-C(31)	122.4(3)

C(37)-C(35)-C(36)	105.4(3)
C(37)-C(35)-C(38)	109.8(5)
C(36)-C(35)-C(38)	108.6(5)
C(37)-C(35)-C(34)	113.0(4)
C(36)-C(35)-C(34)	106.0(3)
C(38)-C(35)-C(34)	113.5(4)
C(36A)-C(35A)-C(37A)	106.7(6)
C(36A)-C(35A)-C(38A)	106.8(6)
C(37A)-C(35A)-C(38A)	106.7(6)
C(36A)-C(35A)-C(34A)	108.3(11)
C(37A)-C(35A)-C(34A)	113.8(9)
C(38A)-C(35A)-C(34A)	114.1(10)
O(1)-B(1)-N(6)	108.04(16)
O(1)-B(1)-N(4)	117.43(17)
N(6)-B(1)-N(4)	103.58(16)
O(1)-B(1)-N(2)	118.73(18)
N(6)-B(1)-N(2)	103.45(16)
N(4)-B(1)-N(2)	103.80(16)
C(2S)-C(1S)-C(3S)#1	120.7(4)
C(1S)-C(2S)-C(3S)	119.3(4)
C(1S)#1-C(3S)-C(2S)	120.0(4)

Symmetry transformations used to generate equivalent atoms:

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

Table S25. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2d** (k09104). 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}
O(1)	20(1)	39(1)	28(1)	4(1)	7(1)	0(1)
N(1)	24(1)	32(1)	29(1)	-1(1)	8(1)	2(1)
N(2)	23(1)	30(1)	27(1)	0(1)	8(1)	1(1)
N(3)	26(1)	31(1)	28(1)	1(1)	9(1)	0(1)
N(4)	22(1)	27(1)	26(1)	1(1)	6(1)	0(1)
N(5)	25(1)	31(1)	28(1)	2(1)	7(1)	0(1)
N(6)	22(1)	28(1)	26(1)	0(1)	6(1)	0(1)
C(1)	24(1)	32(1)	29(1)	-5(1)	9(1)	-2(1)
C(2)	28(1)	29(1)	33(1)	-3(1)	12(1)	1(1)
C(3)	31(1)	36(1)	40(1)	-7(1)	9(1)	0(1)
C(4)	48(2)	29(1)	56(2)	-9(1)	19(1)	-6(1)
C(5)	48(1)	31(1)	49(2)	5(1)	20(1)	-1(1)
C(6)	36(1)	33(1)	38(1)	2(1)	16(1)	3(1)
C(7)	26(1)	29(1)	34(1)	-1(1)	14(1)	2(1)
C(8)	22(1)	31(1)	27(1)	2(1)	9(1)	2(1)
C(9)	21(1)	32(1)	27(1)	3(1)	7(1)	-2(1)
C(10)	24(1)	31(1)	29(1)	0(1)	8(1)	-4(1)
C(11)	34(1)	35(1)	27(1)	4(1)	8(1)	-3(1)
C(12)	43(1)	42(1)	26(1)	0(1)	12(1)	-7(1)
C(13)	43(1)	40(1)	34(1)	-5(1)	18(1)	-2(1)
C(14)	30(1)	35(1)	34(1)	-1(1)	11(1)	-2(1)
C(15)	25(1)	32(1)	26(1)	-1(1)	7(1)	-3(1)
C(16)	24(1)	28(1)	30(1)	0(1)	8(1)	0(1)
C(17)	24(1)	28(1)	28(1)	1(1)	9(1)	-1(1)
C(18)	23(1)	32(1)	26(1)	3(1)	9(1)	-1(1)
C(19)	26(1)	33(1)	33(1)	3(1)	10(1)	3(1)
C(20)	29(1)	38(1)	36(1)	5(1)	8(1)	6(1)
C(21)	27(1)	45(1)	32(1)	1(1)	0(1)	4(1)
C(22)	26(1)	37(1)	31(1)	-3(1)	5(1)	0(1)
C(23)	23(1)	35(1)	27(1)	2(1)	10(1)	1(1)
C(24)	22(1)	33(1)	24(1)	-2(1)	6(1)	-1(1)

C(25)	22(1)	29(1)	26(1)	-2(1)	6(1)	0(1)
C(26)	28(1)	32(1)	33(1)	5(1)	8(1)	2(1)
C(27)	26(1)	35(1)	40(1)	5(1)	12(1)	-2(1)
C(28)	25(1)	43(1)	34(1)	3(1)	7(1)	2(1)
C(29)	29(1)	55(2)	38(1)	19(1)	10(1)	10(1)
C(30)	27(1)	45(1)	36(1)	12(1)	14(1)	3(1)
C(31)	25(1)	73(2)	47(2)	12(1)	9(1)	5(1)
C(32)	25(2)	91(3)	59(2)	9(2)	5(2)	-19(2)
C(33)	22(2)	104(4)	83(3)	52(3)	4(2)	12(2)
C(34)	29(2)	61(2)	69(2)	26(2)	24(2)	12(2)
C(35)	68(2)	51(2)	98(3)	15(2)	56(2)	16(2)
C(36)	89(3)	68(3)	93(4)	16(3)	57(3)	23(3)
C(37)	305(10)	90(4)	172(7)	83(5)	177(8)	112(6)
C(38)	140(6)	116(6)	252(10)	-104(6)	143(7)	-57(5)
C(31A)	25(1)	73(2)	47(2)	12(1)	9(1)	5(1)
C(35A)	68(2)	51(2)	98(3)	15(2)	56(2)	16(2)
B(1)	24(1)	30(1)	24(1)	1(1)	6(1)	-1(1)
C(1S)	108(4)	104(3)	73(3)	37(2)	47(3)	15(3)
C(2S)	95(3)	116(4)	46(2)	21(2)	3(2)	-45(3)
C(3S)	169(5)	67(2)	47(2)	0(2)	42(3)	-22(3)

Table S26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2d** (k09104).

	x	y	z	U(eq)
H(3A)	9891	5947	4166	43
H(4A)	9672	7578	3396	52
H(5A)	8793	7592	2069	50
H(6A)	8067	5983	1475	41
H(11A)	7272	2310	-169	39
H(12A)	7442	837	-977	44
H(13A)	8190	-758	-414	45
H(14A)	8757	-970	974	39
H(19A)	10708	-1092	3951	37
H(20A)	11897	-943	5093	42
H(21A)	12164	684	5847	44
H(22A)	11259	2223	5482	39
H(26A)	6616	747	3930	38
H(27A)	5141	878	3547	40
H(29A)	5195	3238	1939	49
H(30A)	6681	3109	2315	42
H(32A)	3784	665	1832	90
H(32B)	3030	994	2186	90
H(32C)	3906	491	2765	90
H(33A)	3822	2570	1294	108
H(33B)	3773	3625	1837	108
H(33C)	2994	2760	1573	108
H(34A)	3125	2441	3074	61
H(34B)	3993	1937	3648	61
H(36A)	3038	3514	4187	115
H(36B)	3785	4352	4652	115
H(36C)	3940	3035	4733	115
H(37A)	2907	4463	2924	248
H(37B)	3740	4720	2668	248
H(37C)	3617	5310	3443	248

H(38A)	5174	3908	3483	226
H(38B)	5245	3300	4314	226
H(38C)	5060	4611	4219	226
H(32D)	3707	546	2657	92
H(32E)	2933	1400	2556	92
H(32F)	3706	1359	3380	92
H(33D)	3794	1496	1335	97
H(33E)	4031	2793	1376	97
H(33F)	3098	2409	1373	97
H(34C)	4136	3902	2413	50
H(34D)	3210	3533	2410	50
H(36D)	2803	3465	3597	106
H(36E)	3485	3633	4468	106
H(36F)	3499	2518	3971	106
H(37D)	3297	5333	3229	83
H(37E)	4297	5536	3388	83
H(37F)	3936	5369	4128	83
H(38D)	5036	2840	4115	42
H(38E)	4976	3901	4648	42
H(38F)	5338	4038	3906	42
H(1S)	6203	-971	4994	109
H(2S)	6344	750	5582	108
H(3S)	5128	1737	5579	111

Table S27. Selected Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 deg for compound **2d** (k09104).

Cg(I) ->	Cg(J)	Cg-Cg (Å)	Alpha (deg)	Beta (deg)	Gamma (deg)	CgI_Perp (Å)	CgJ_Perp (Å)	Slippage (Å)
Cg(3) ->	Cg(6)	3.6910(12)	1.58(11)	16.58	17.84	-3.5135(9)	-3.5375(9)	
Cg(6) ->	Cg(3)	3.6912(12)	1.58(11)	17.84	16.58	-3.5376(9)	-3.5135(9)	
Cg(6) ->	Cg(6)	3.8131(13)	0	22.15	22.15	-3.5318(9)	-3.5317(9)	1.438

Table S28. Selected C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) for compound **2d** (k09104).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (deg)	X-H..Cg (deg)	X..Cg (Å)	X-H,Pi (deg)
C(27) -H(27A)	->	Cg(8)	2.83	-2.81	7.37	148	3.672(3)	53
C(37A)-H(37D)	->	Cg(2)	2.77	-2.74	8.42	137	3.553(12)	56
C(37A)-H(37E)	->	Cg(7)	2.83	-2.81	6.96	131	3.552(12)	42

See lit. [11] for definitions of C-H…π factors
All atoms numbered according to thermal ellipsoid plot in Figure S4. Cg numberings as defined below for ring centroids used in above tables for compound **2d** (k09104):
5-Membered Ring (2) N(4) --> C(9) --> C(10) --> C(15) --> C(16) -->
5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->
6-Membered Ring (6) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->
6-Membered Ring (7) C(25) --> C(26) --> C(27) --> C(28) --> C(29) --> C(30) -->
6-Membered Ring (8) C(1S) --> C(2S) --> C(3S) --> C(1S)a --> C(2S)a --> C(3S)a -->

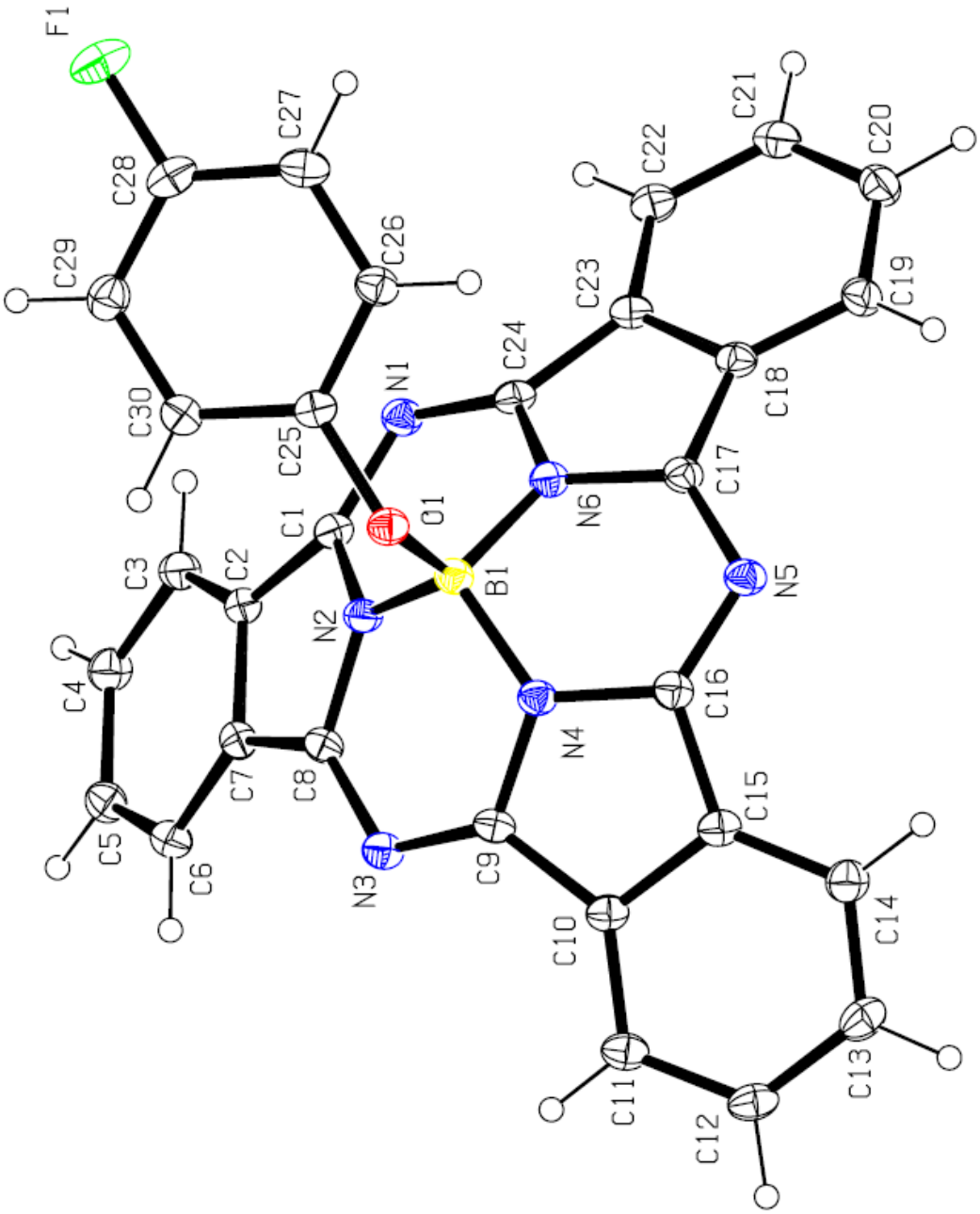


Figure S5A: Thermal ellipsoid plot of compound **2e**, shown with atom numberings.

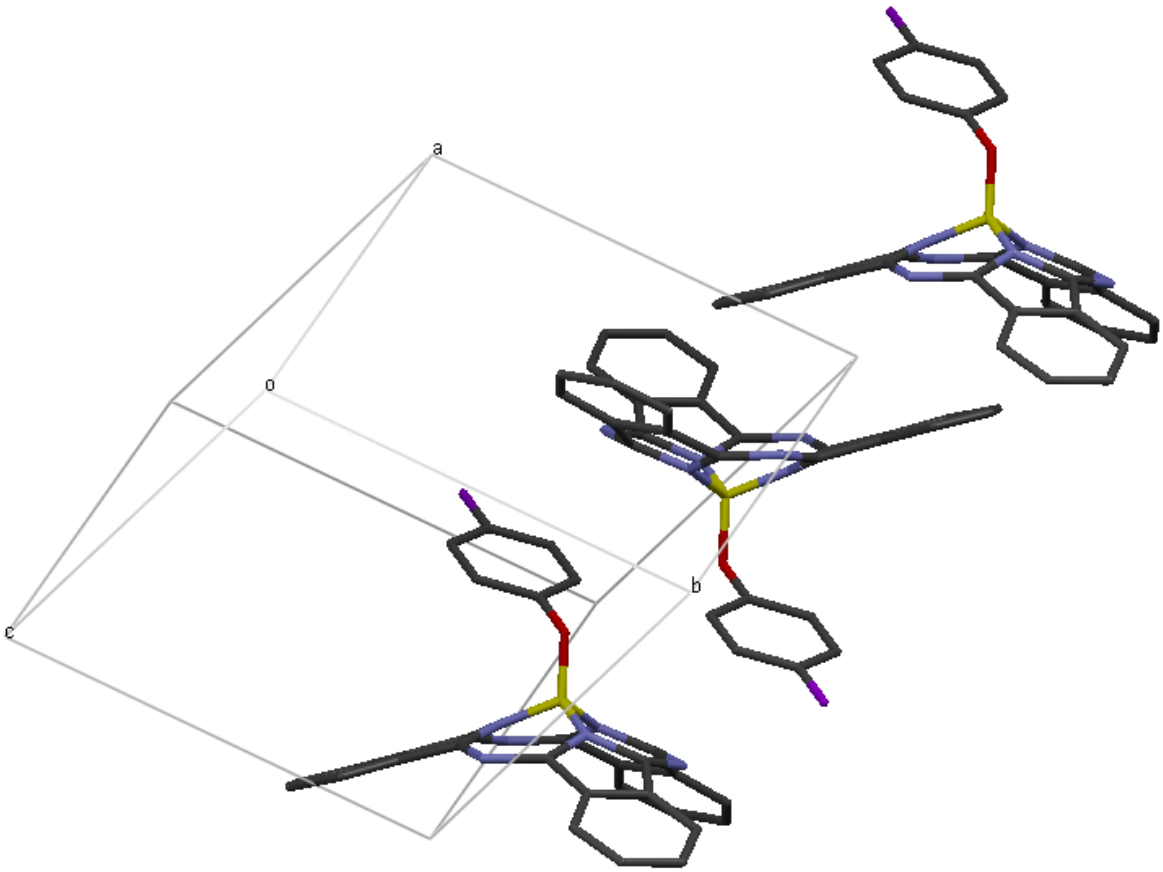


Figure S5B: Image of crystal of compound **2e** showing orientation of crystal axes.

Table S29. Crystal data and structure refinement for compound **2e** (k08356).

Identification code	k08356	
Empirical formula	C30 H16 B F N6 O	
Formula weight	506.30	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.0420(3) Å	α= 85.8210(18)°.
	b = 10.7558(4) Å	β= 77.1560(19)°.
	c = 11.7366(4) Å	γ = 66.5820(19)°.
Volume	1133.97(7) $Å^3$	
Z	2	
Density (calculated)	1.483 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	520	
Crystal size	0.30 x 0.22 x 0.16 mm^3	
Theta range for data collection	2.57 to 27.54°.	
Index ranges	-12<=h<=12, -13<=k<=13, -14<=l<=15	
Reflections collected	10460	
Independent reflections	5099 [R(int) = 0.0511]	
Completeness to theta = 27.54°	99.4 %	
Max. and min. transmission	0.990 and 0.753	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5099 / 0 / 352	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1262	
R indices (all data)	R1 = 0.1005, wR2 = 0.1536	
Largest diff. peak and hole	0.311 and -0.301 $e.Å^{-3}$	

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2e** (k08356). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	1224(2)	4055(2)	2294(1)	51(1)
O(1)	6107(2)	808(2)	4005(1)	26(1)
N(1)	6699(2)	2(2)	818(2)	26(1)
N(2)	6992(2)	-1150(2)	2615(1)	24(1)
N(3)	8279(2)	-2971(2)	3752(1)	26(1)
N(4)	8643(2)	-901(2)	3651(1)	24(1)
N(5)	9955(2)	486(2)	2816(2)	27(1)
N(6)	7891(2)	562(2)	2111(1)	24(1)
C(1)	6577(2)	-973(2)	1562(2)	24(1)
C(2)	6365(2)	-2193(2)	1359(2)	24(1)
C(3)	5934(2)	-2579(2)	435(2)	29(1)
C(4)	5982(2)	-3877(2)	434(2)	32(1)
C(5)	6491(2)	-4799(2)	1292(2)	30(1)
C(6)	6960(2)	-4445(2)	2196(2)	27(1)
C(7)	6868(2)	-3123(2)	2248(2)	24(1)
C(8)	7355(2)	-2446(2)	3008(2)	24(1)
C(9)	8982(2)	-2219(2)	3999(2)	24(1)
C(10)	10397(2)	-2645(2)	4344(2)	25(1)
C(11)	11293(2)	-3850(2)	4780(2)	29(1)
C(12)	12688(2)	-3986(2)	4881(2)	32(1)
C(13)	13209(2)	-2966(2)	4554(2)	34(1)
C(14)	12338(2)	-1761(2)	4117(2)	32(1)
C(15)	10924(2)	-1590(2)	4024(2)	25(1)
C(16)	9813(2)	-520(2)	3522(2)	25(1)
C(17)	9024(2)	970(2)	2075(2)	25(1)
C(18)	9138(2)	1690(2)	982(2)	25(1)
C(19)	9981(2)	2437(2)	507(2)	29(1)
C(20)	9804(2)	3034(2)	-558(2)	33(1)
C(21)	8855(2)	2850(2)	-1183(2)	32(1)
C(22)	8043(2)	2076(2)	-742(2)	29(1)
C(23)	8150(2)	1525(2)	357(2)	26(1)

C(24)	7437(2)	712(2)	1079(2)	24(1)
C(25)	4872(2)	1633(2)	3578(2)	24(1)
C(26)	4753(2)	2899(2)	3154(2)	28(1)
C(27)	3518(2)	3723(2)	2720(2)	33(1)
C(28)	2438(2)	3248(2)	2720(2)	34(1)
C(29)	2529(2)	1996(3)	3129(2)	33(1)
C(30)	3760(2)	1184(2)	3572(2)	29(1)
B(1)	7316(3)	-107(3)	3154(2)	24(1)

Table S31. Bond lengths [Å] and angles [°] for compound **2e** (k08356).

F(1)-C(28)	1.363(2)
O(1)-C(25)	1.383(2)
O(1)-B(1)	1.447(3)
N(1)-C(1)	1.341(3)
N(1)-C(24)	1.345(3)
N(2)-C(8)	1.366(3)
N(2)-C(1)	1.367(2)
N(2)-B(1)	1.500(3)
N(3)-C(8)	1.347(3)
N(3)-C(9)	1.347(3)
N(4)-C(16)	1.366(3)
N(4)-C(9)	1.373(3)
N(4)-B(1)	1.488(3)
N(5)-C(17)	1.345(3)
N(5)-C(16)	1.347(3)
N(6)-C(24)	1.364(2)
N(6)-C(17)	1.364(3)
N(6)-B(1)	1.496(3)
C(1)-C(2)	1.453(3)
C(2)-C(3)	1.397(3)
C(2)-C(7)	1.423(3)
C(3)-C(4)	1.378(3)
C(4)-C(5)	1.393(3)
C(5)-C(6)	1.385(3)
C(6)-C(7)	1.393(3)
C(7)-C(8)	1.462(3)
C(9)-C(10)	1.451(3)
C(10)-C(11)	1.390(3)
C(10)-C(15)	1.426(3)
C(11)-C(12)	1.381(3)
C(12)-C(13)	1.389(3)
C(13)-C(14)	1.382(3)
C(14)-C(15)	1.386(3)
C(15)-C(16)	1.446(3)

C(17)-C(18)	1.456(3)
C(18)-C(19)	1.392(3)
C(18)-C(23)	1.426(3)
C(19)-C(20)	1.378(3)
C(20)-C(21)	1.403(3)
C(21)-C(22)	1.384(3)
C(22)-C(23)	1.388(3)
C(23)-C(24)	1.455(3)
C(25)-C(30)	1.383(3)
C(25)-C(26)	1.384(3)
C(26)-C(27)	1.388(3)
C(27)-C(28)	1.370(3)
C(28)-C(29)	1.371(3)
C(29)-C(30)	1.388(3)

C(25)-O(1)-B(1)	115.24(15)
C(1)-N(1)-C(24)	116.67(17)
C(8)-N(2)-C(1)	113.31(17)
C(8)-N(2)-B(1)	122.95(17)
C(1)-N(2)-B(1)	122.62(18)
C(8)-N(3)-C(9)	117.16(18)
C(16)-N(4)-C(9)	112.80(17)
C(16)-N(4)-B(1)	122.11(18)
C(9)-N(4)-B(1)	123.09(17)
C(17)-N(5)-C(16)	117.04(17)
C(24)-N(6)-C(17)	113.60(17)
C(24)-N(6)-B(1)	123.70(17)
C(17)-N(6)-B(1)	122.44(16)
N(1)-C(1)-N(2)	123.19(18)
N(1)-C(1)-C(2)	129.73(18)
N(2)-C(1)-C(2)	105.50(17)
C(3)-C(2)-C(7)	120.8(2)
C(3)-C(2)-C(1)	131.4(2)
C(7)-C(2)-C(1)	107.41(17)
C(4)-C(3)-C(2)	117.6(2)
C(3)-C(4)-C(5)	121.8(2)

C(6)-C(5)-C(4)	121.3(2)
C(5)-C(6)-C(7)	118.2(2)
C(6)-C(7)-C(2)	120.14(18)
C(6)-C(7)-C(8)	132.58(19)
C(2)-C(7)-C(8)	106.90(18)
N(3)-C(8)-N(2)	122.51(18)
N(3)-C(8)-C(7)	130.17(19)
N(2)-C(8)-C(7)	105.55(17)
N(3)-C(9)-N(4)	122.56(18)
N(3)-C(9)-C(10)	129.67(19)
N(4)-C(9)-C(10)	105.72(17)
C(11)-C(10)-C(15)	119.98(19)
C(11)-C(10)-C(9)	132.8(2)
C(15)-C(10)-C(9)	106.85(18)
C(12)-C(11)-C(10)	118.1(2)
C(11)-C(12)-C(13)	122.0(2)
C(14)-C(13)-C(12)	120.9(2)
C(13)-C(14)-C(15)	118.3(2)
C(14)-C(15)-C(10)	120.8(2)
C(14)-C(15)-C(16)	131.4(2)
C(10)-C(15)-C(16)	107.51(17)
N(5)-C(16)-N(4)	123.14(18)
N(5)-C(16)-C(15)	129.20(19)
N(4)-C(16)-C(15)	105.87(18)
N(5)-C(17)-N(6)	121.72(19)
N(5)-C(17)-C(18)	131.42(19)
N(6)-C(17)-C(18)	105.33(16)
C(19)-C(18)-C(23)	120.3(2)
C(19)-C(18)-C(17)	132.45(19)
C(23)-C(18)-C(17)	107.28(18)
C(20)-C(19)-C(18)	118.3(2)
C(19)-C(20)-C(21)	121.4(2)
C(22)-C(21)-C(20)	121.1(2)
C(21)-C(22)-C(23)	118.2(2)
C(22)-C(23)-C(18)	120.7(2)
C(22)-C(23)-C(24)	132.4(2)

C(18)-C(23)-C(24)	106.97(17)
N(1)-C(24)-N(6)	121.96(19)
N(1)-C(24)-C(23)	131.48(18)
N(6)-C(24)-C(23)	105.58(17)
C(30)-C(25)-O(1)	119.71(19)
C(30)-C(25)-C(26)	120.18(19)
O(1)-C(25)-C(26)	120.11(18)
C(25)-C(26)-C(27)	120.1(2)
C(28)-C(27)-C(26)	118.4(2)
F(1)-C(28)-C(27)	118.5(2)
F(1)-C(28)-C(29)	118.7(2)
C(27)-C(28)-C(29)	122.7(2)
C(28)-C(29)-C(30)	118.5(2)
C(25)-C(30)-C(29)	120.0(2)
O(1)-B(1)-N(4)	112.56(17)
O(1)-B(1)-N(6)	114.95(18)
N(4)-B(1)-N(6)	104.39(17)
O(1)-B(1)-N(2)	116.16(17)
N(4)-B(1)-N(2)	104.65(17)
N(6)-B(1)-N(2)	102.79(16)

Symmetry transformations used to generate equivalent atoms:

Table S32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2e** (k08356). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	42(1)	48(1)	58(1)	7(1)	-27(1)	-3(1)
O(1)	28(1)	26(1)	24(1)	2(1)	-8(1)	-10(1)
N(1)	28(1)	22(1)	29(1)	1(1)	-8(1)	-9(1)
N(2)	26(1)	20(1)	26(1)	3(1)	-8(1)	-8(1)
N(3)	31(1)	23(1)	25(1)	1(1)	-9(1)	-11(1)
N(4)	27(1)	23(1)	23(1)	2(1)	-8(1)	-10(1)
N(5)	31(1)	22(1)	29(1)	1(1)	-10(1)	-10(1)
N(6)	26(1)	22(1)	25(1)	1(1)	-8(1)	-9(1)
C(1)	24(1)	23(1)	25(1)	1(1)	-8(1)	-7(1)
C(2)	24(1)	24(1)	26(1)	3(1)	-7(1)	-10(1)
C(3)	31(1)	26(1)	33(1)	3(1)	-12(1)	-11(1)
C(4)	35(1)	32(1)	32(1)	-1(1)	-12(1)	-14(1)
C(5)	32(1)	26(1)	34(1)	0(1)	-7(1)	-13(1)
C(6)	31(1)	23(1)	27(1)	1(1)	-5(1)	-10(1)
C(7)	24(1)	24(1)	25(1)	0(1)	-4(1)	-11(1)
C(8)	27(1)	23(1)	21(1)	2(1)	-4(1)	-10(1)
C(9)	30(1)	20(1)	20(1)	1(1)	-6(1)	-8(1)
C(10)	30(1)	25(1)	19(1)	0(1)	-9(1)	-9(1)
C(11)	37(1)	27(1)	22(1)	2(1)	-10(1)	-11(1)
C(12)	38(1)	29(1)	28(1)	2(1)	-16(1)	-7(1)
C(13)	31(1)	37(1)	37(1)	-1(1)	-16(1)	-9(1)
C(14)	34(1)	31(1)	34(1)	0(1)	-12(1)	-14(1)
C(15)	30(1)	23(1)	22(1)	-2(1)	-10(1)	-8(1)
C(16)	30(1)	23(1)	25(1)	-2(1)	-8(1)	-11(1)
C(17)	28(1)	19(1)	28(1)	0(1)	-8(1)	-9(1)
C(18)	26(1)	20(1)	27(1)	0(1)	-5(1)	-5(1)
C(19)	28(1)	23(1)	34(1)	1(1)	-5(1)	-10(1)
C(20)	30(1)	27(1)	36(1)	3(1)	1(1)	-11(1)
C(21)	32(1)	26(1)	27(1)	4(1)	-2(1)	-5(1)
C(22)	30(1)	26(1)	26(1)	-2(1)	-6(1)	-6(1)
C(23)	27(1)	19(1)	27(1)	1(1)	-7(1)	-5(1)

C(24)	27(1)	19(1)	26(1)	0(1)	-10(1)	-5(1)
C(25)	26(1)	24(1)	19(1)	-2(1)	-5(1)	-6(1)
C(26)	34(1)	25(1)	27(1)	0(1)	-8(1)	-12(1)
C(27)	41(1)	25(1)	30(1)	0(1)	-9(1)	-8(1)
C(28)	30(1)	35(1)	29(1)	-2(1)	-11(1)	-3(1)
C(29)	31(1)	38(2)	31(1)	0(1)	-8(1)	-14(1)
C(30)	31(1)	28(1)	27(1)	2(1)	-6(1)	-13(1)
B(1)	27(1)	23(1)	23(1)	2(1)	-7(1)	-11(1)

Table S33. Selected Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 deg for compound **2e** (k08356).

Cg(I)	->	Cg(J)	Cg-Cg (Å)	Alpha (deg)	Beta (deg)	Gamma (deg)	CgI_Perp (Å)	CgJ_Perp (Å)	Slippage (Å)
Cg(3)	->	Cg(6)	3.6942(12)	3.49(11)	5.67	8.93	-3.6495(9)	-3.6761(8)	
Cg(6)	->	Cg(3)	3.6941(12)	3.49(11)	8.93	5.67	-3.6761(8)	-3.6494(9)	

Table S34. Selected C-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 30.0 Deg) for compound **2e** (k08356).

X-H(I)	->	Cg(J)	H..Cg (Å)	H-Perp (Å)	Gamma (deg)	X-H..Cg (deg)	X..Cg (Å)	X-H,Pi (deg)
C(5) -H(5A)	->	Cg(6)	2.82	2.78	9.90	120	3.403(2)	39
C(20)-H(20A)	->	Cg(1)	2.81	2.72	14.63	110	3.267(2)	35
C(21)-H(21A)	->	Cg(2)	2.81	-2.73	13.07	117	3.345(2)	40

See lit. [11] for definitions of C-H…π factors
All atoms numbered according to thermal ellipsoid plot in Figure S5. Cg numberings as defined below for ring centroids used in above tables for compound **2e** (k08356):
5-Membered Ring (1) N(2) --> C(1) --> C(2) --> C(7) --> C(8) -->
5-Membered Ring (2) N(4) --> C(9) --> C(10) --> C(15) --> C(16) -->
5-Membered Ring (3) N(6) --> C(17) --> C(18) --> C(23) --> C(24) -->
6-Membered Ring (6) C(18) --> C(19) --> C(20) --> C(21) --> C(22) --> C(23) -->

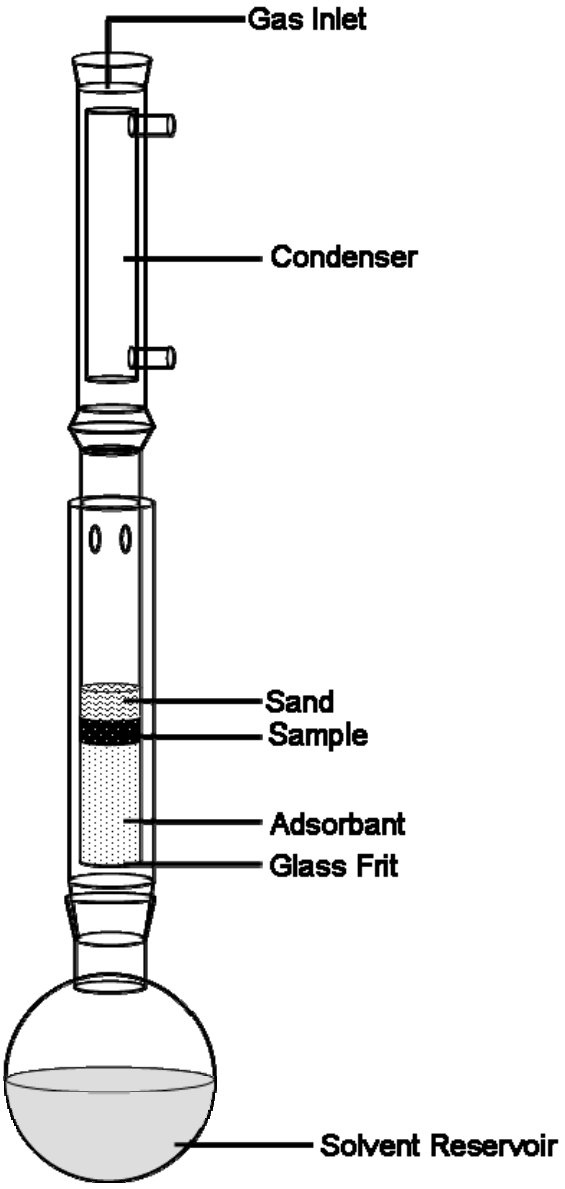
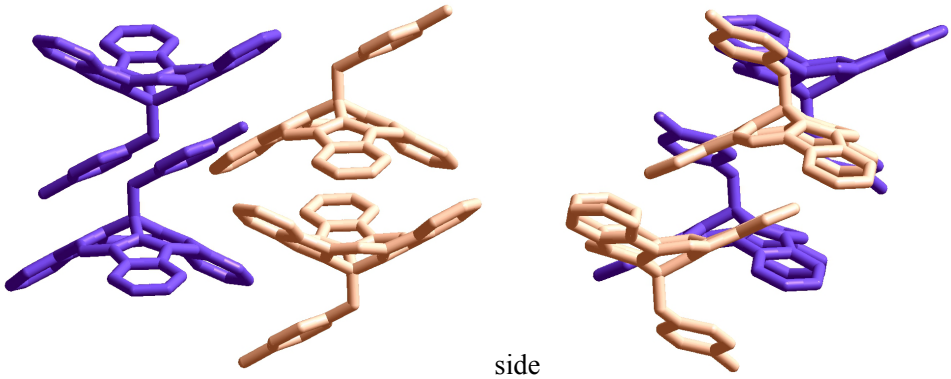
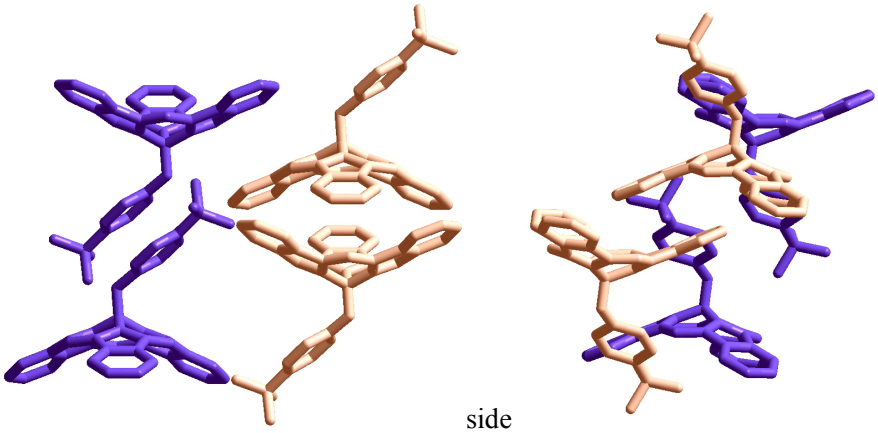


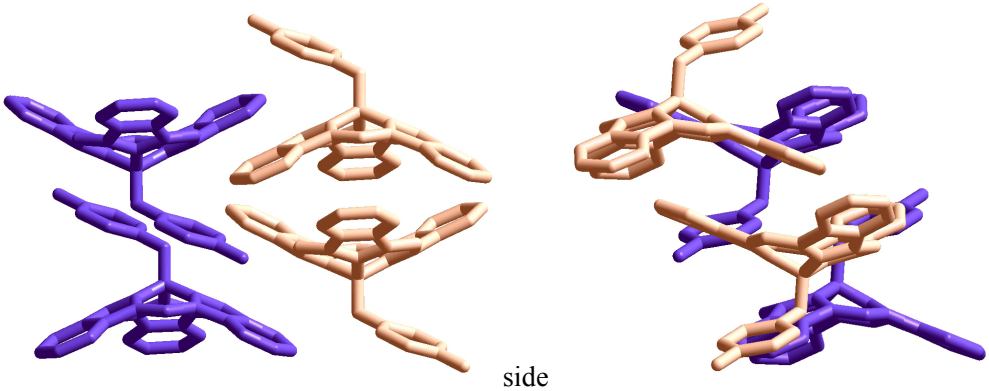
Figure S6: Kauffman column set up used for purification of derivatized subphthalocyanine. The column consists of two concentric cylinders mounted above a solvent reservoir and below a condenser and gas inlet. The sample is loaded onto the adsorbant by dissolving in solvent and pipetting onto the sand with the condenser removed. The solvent in the reservoir is heated under stirring and holes in the top of the small cylinder allow the vapours to rise and liquefy in the condenser. The solvent liquid then drips into the inner cylinder, eluting through the adsorbant and bringing the **BsubPc** product with it. The excess phenol from the reaction is remains on the adsorbant, and the product is collected in the solvent reservoir.



(**2b**) front side



(**2c**) front side



(**2e**) front side

Figure S7. Depictions of the single crystal arrangement of compounds **2b**, **2c** and **2e**.