One Well-Placed Methyl Group Increases the Solubility of Phenoxy Boronsubphthalocyanine Two Orders of Magnitude.

Andrew S. Paton,[a] *Alan J. Lough*[b] *and Timothy P. Bender*[a,b,*]

[a] Department of Chemical Engineering and Applied Chemistry, University of Toronto, 200 College Street, Toronto, Ontario, Canada, M5S 3E5

[b] Department of Chemistry, University of Toronto, 80 St. George St., Toronto, Ontario, Canada, M5S 3H6

* To whom correspondences should be addressed. Email: tim.bender@utoronto.ca

ELECTRONIC SUPPORTING INFORMATION.

CONTENTS.

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2a** benzene solvate.

Figure S4. Anisotropic displacement ellipsoid plot of compound **2b** benzene solvate.

Table S17. Crystal data and structure refinement for compound **2b** benzene solvate.

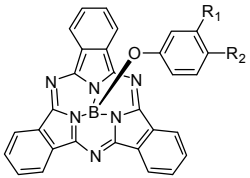
Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for compound **2b** benzene solvate. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S19. Bond lengths [Å] and angles [°] for compound **2b** benzene solvate.

Table S20. Anisotropic displacement parameters ($Å^2$x 10^3) for compound **2b** benzene solvate. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2b** benzene solvate.

Table S1. Solubilities of PhO-**BsubPcs 2a-b** and reference compounds.

	*Acetone*		*Chloroform*		*Chlorobenzene*		*n-Propanol*		*Propyl acetate*		*THF*		*Toluene*	
	MS[a]	SS[b]	MS	SS	MS	SS	MS	SS	MS	SS	MS	SS	MS	SS
R_1=R_2=H[11]	309	1500	597	2920	559	2730	20.9	102	559	2730	796	3890	711	3470
R_1=H, R_2=CH_3[11]	51.3	260	648	3260	554	2780	4.23	21.2	86.4	434	716	3590	635	3190
R_1=CH_3, R_2=H (**2a**)	500	2500	20600	103000	>597	>3000	24.5	123	>597	>3000	>597	>3000	>597	>3000
R_1=R_2=CH_3 (**2b**)	309	1600	17300	90000	>581	>3000	23.3	120	>581	>3000	>581	>3000	>581	>3000

[a] molar solubility in mol/L × 10^{-5}

[b] specific solubility in mg/L

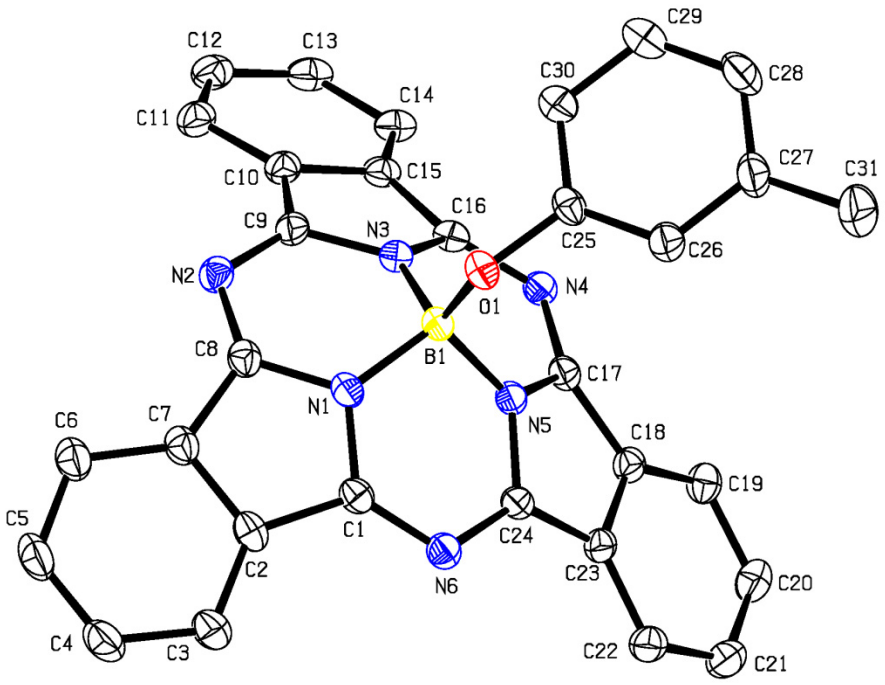


Figure S1. Anisotropic displacement ellipsoid plot of compound **2a**.

Table S2. Crystal data and structure refinement for compound **2a**.

Identification code	**2a**	
Empirical formula	C31 H19 B N6 O	
Formula weight	502.33	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.7992(4) Å	α= 90°.
	b = 13.6438(3) Å	β= 107.4720(14)°.
	c = 14.6775(6) Å	γ = 90°.
Volume	2444.87(14) $Å^3$	
Z	4	
Density (calculated)	1.365 Mg/m^3	

Absorption coefficient	0.086 mm^{-1}
F(000)	1040
Crystal size	0.25 x 0.16 x 0.14 mm^3
Theta range for data collection	2.91 to 27.53°.
Index ranges	-16<=h<=15, -16<=k<=17, -19<=l<=19
Reflections collected	16326
Independent reflections	5569 [R(int) = 0.0690]
Completeness to theta = 27.53°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.004 and 0.869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5569 / 0 / 353
Goodness-of-fit on F^2	1.000
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1290
R indices (all data)	R1 = 0.1528, wR2 = 0.1722
Largest diff. peak and hole	0.257 and -0.237 e.$Å^{-3}$

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

	x	y	z	U(eq)
O(1)	8732(1)	3350(1)	2546(1)	35(1)
N(1)	6876(2)	3274(1)	2606(1)	33(1)
N(2)	6309(2)	4940(1)	2393(1)	35(1)
N(3)	7166(2)	4185(1)	1337(1)	31(1)
N(4)	7111(2)	3350(1)	-106(1)	33(1)
N(5)	7267(2)	2464(1)	1329(1)	30(1)
N(6)	6534(2)	1564(1)	2377(1)	35(1)
C(1)	6476(2)	2406(2)	2836(2)	33(1)
C(2)	5801(2)	2672(2)	3438(2)	38(1)
C(3)	5196(2)	2110(2)	3886(2)	48(1)
C(4)	4554(3)	2590(2)	4353(2)	56(1)
C(5)	4502(2)	3607(2)	4366(2)	54(1)
C(6)	5078(2)	4179(2)	3904(2)	46(1)
C(7)	5748(2)	3711(2)	3448(2)	38(1)
C(8)	6374(2)	4077(2)	2848(2)	35(1)
C(9)	6652(2)	4959(2)	1610(2)	33(1)
C(10)	6323(2)	5610(2)	783(2)	35(1)
C(11)	5778(2)	6508(2)	645(2)	41(1)
C(12)	5524(2)	6914(2)	-254(2)	45(1)
C(13)	5781(2)	6452(2)	-1002(2)	44(1)
C(14)	6286(2)	5542(2)	-884(2)	39(1)
C(15)	6570(2)	5125(2)	20(2)	34(1)
C(16)	7039(2)	4174(2)	379(2)	32(1)
C(17)	7159(2)	2498(2)	374(2)	32(1)
C(18)	6880(2)	1505(2)	23(2)	33(1)
C(19)	6733(2)	1084(2)	-867(2)	38(1)
C(20)	6475(2)	96(2)	-972(2)	44(1)
C(21)	6327(2)	-447(2)	-215(2)	46(1)
C(22)	6416(2)	-31(2)	662(2)	40(1)
C(23)	6710(2)	953(2)	787(2)	32(1)
C(24)	6875(2)	1615(2)	1596(2)	30(1)

C(25)	9548(2)	3371(2)	2108(2)	35(1)
C(26)	10151(2)	2530(2)	2093(2)	43(1)
C(27)	11046(2)	2561(2)	1741(2)	51(1)
C(28)	11302(2)	3435(2)	1387(2)	60(1)
C(29)	10689(2)	4271(2)	1386(2)	59(1)
C(30)	9816(2)	4244(2)	1754(2)	45(1)
C(31)	11739(3)	1669(2)	1765(3)	80(1)
B(1)	7590(2)	3326(2)	1978(2)	32(1)

Table S4. Bond lengths [Å] and angles [°] for compound **2a**.

O(1)-C(25)	1.381(3)
O(1)-B(1)	1.450(3)
N(1)-C(8)	1.370(3)
N(1)-C(1)	1.371(3)
N(1)-B(1)	1.482(3)
N(2)-C(8)	1.344(3)
N(2)-C(9)	1.348(3)
N(3)-C(9)	1.366(3)
N(3)-C(16)	1.366(3)
N(3)-B(1)	1.499(3)
N(4)-C(16)	1.349(3)
N(4)-C(17)	1.351(3)
N(5)-C(24)	1.365(3)
N(5)-C(17)	1.367(3)
N(5)-B(1)	1.492(3)
N(6)-C(24)	1.346(3)
N(6)-C(1)	1.346(3)
C(1)-C(2)	1.454(3)
C(2)-C(3)	1.388(3)
C(2)-C(7)	1.419(3)
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.390(4)
C(5)-C(6)	1.382(4)
C(6)-C(7)	1.392(3)
C(7)-C(8)	1.445(3)
C(9)-C(10)	1.460(3)
C(10)-C(11)	1.394(3)
C(10)-C(15)	1.416(3)
C(11)-C(12)	1.378(4)
C(12)-C(13)	1.388(4)
C(13)-C(14)	1.386(3)
C(14)-C(15)	1.389(3)
C(15)-C(16)	1.461(3)
C(17)-C(18)	1.455(3)

C(18)-C(19)	1.387(3)
C(18)-C(23)	1.420(3)
C(19)-C(20)	1.386(3)
C(20)-C(21)	1.394(4)
C(21)-C(22)	1.381(3)
C(22)-C(23)	1.391(3)
C(23)-C(24)	1.455(3)
C(25)-C(30)	1.383(3)
C(25)-C(26)	1.387(3)
C(26)-C(27)	1.391(4)
C(27)-C(28)	1.379(4)
C(27)-C(31)	1.501(4)
C(28)-C(29)	1.385(4)
C(29)-C(30)	1.380(4)

C(25)-O(1)-B(1)	120.29(19)
C(8)-N(1)-C(1)	112.8(2)
C(8)-N(1)-B(1)	123.23(19)
C(1)-N(1)-B(1)	122.72(19)
C(8)-N(2)-C(9)	117.0(2)
C(9)-N(3)-C(16)	113.08(19)
C(9)-N(3)-B(1)	122.4(2)
C(16)-N(3)-B(1)	123.02(19)
C(16)-N(4)-C(17)	116.2(2)
C(24)-N(5)-C(17)	112.96(19)
C(24)-N(5)-B(1)	122.8(2)
C(17)-N(5)-B(1)	123.43(19)
C(24)-N(6)-C(1)	117.62(19)
N(6)-C(1)-N(1)	122.2(2)
N(6)-C(1)-C(2)	130.5(2)
N(1)-C(1)-C(2)	105.56(19)
C(3)-C(2)-C(7)	120.8(2)
C(3)-C(2)-C(1)	131.9(2)
C(7)-C(2)-C(1)	107.1(2)
C(4)-C(3)-C(2)	118.2(2)
C(3)-C(4)-C(5)	121.2(3)

C(6)-C(5)-C(4)	121.4(3)
C(5)-C(6)-C(7)	118.3(2)
C(6)-C(7)-C(2)	120.1(2)
C(6)-C(7)-C(8)	132.0(2)
C(2)-C(7)-C(8)	107.6(2)
N(2)-C(8)-N(1)	122.4(2)
N(2)-C(8)-C(7)	130.0(2)
N(1)-C(8)-C(7)	105.7(2)
N(2)-C(9)-N(3)	122.9(2)
N(2)-C(9)-C(10)	129.4(2)
N(3)-C(9)-C(10)	105.7(2)
C(11)-C(10)-C(15)	121.1(2)
C(11)-C(10)-C(9)	131.5(2)
C(15)-C(10)-C(9)	107.23(19)
C(12)-C(11)-C(10)	117.2(2)
C(11)-C(12)-C(13)	122.1(2)
C(14)-C(13)-C(12)	121.4(3)
C(13)-C(14)-C(15)	117.7(2)
C(14)-C(15)-C(10)	120.6(2)
C(14)-C(15)-C(16)	132.1(2)
C(10)-C(15)-C(16)	107.1(2)
N(4)-C(16)-N(3)	123.2(2)
N(4)-C(16)-C(15)	129.5(2)
N(3)-C(16)-C(15)	105.67(19)
N(4)-C(17)-N(5)	122.6(2)
N(4)-C(17)-C(18)	130.4(2)
N(5)-C(17)-C(18)	105.66(19)
C(19)-C(18)-C(23)	121.0(2)
C(19)-C(18)-C(17)	131.9(2)
C(23)-C(18)-C(17)	107.0(2)
C(20)-C(19)-C(18)	117.9(2)
C(19)-C(20)-C(21)	120.9(2)
C(22)-C(21)-C(20)	122.1(2)
C(21)-C(22)-C(23)	117.6(2)
C(22)-C(23)-C(18)	120.5(2)
C(22)-C(23)-C(24)	132.3(2)

C(18)-C(23)-C(24)	107.23(19)
N(6)-C(24)-N(5)	122.0(2)
N(6)-C(24)-C(23)	131.1(2)
N(5)-C(24)-C(23)	105.5(2)
O(1)-C(25)-C(30)	120.0(2)
O(1)-C(25)-C(26)	119.5(2)
C(30)-C(25)-C(26)	120.3(2)
C(25)-C(26)-C(27)	120.3(2)
C(28)-C(27)-C(26)	118.8(2)
C(28)-C(27)-C(31)	120.3(3)
C(26)-C(27)-C(31)	120.9(3)
C(27)-C(28)-C(29)	120.9(3)
C(30)-C(29)-C(28)	120.2(3)
C(29)-C(30)-C(25)	119.4(2)
O(1)-B(1)-N(1)	110.3(2)
O(1)-B(1)-N(5)	115.11(19)
N(1)-B(1)-N(5)	104.74(19)
O(1)-B(1)-N(3)	117.2(2)
N(1)-B(1)-N(3)	104.61(19)
N(5)-B(1)-N(3)	103.7(2)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2a**. 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)	29(1)	44(1)	33(1)	-1(1)	11(1)	2(1)
N(1)	29(1)	38(1)	34(1)	-1(1)	13(1)	-1(1)
N(2)	34(1)	34(1)	36(1)	-6(1)	9(1)	-1(1)
N(3)	30(1)	30(1)	34(1)	-1(1)	11(1)	-2(1)
N(4)	32(1)	34(1)	33(1)	-1(1)	12(1)	-2(1)
N(5)	30(1)	32(1)	32(1)	1(1)	12(1)	2(1)
N(6)	35(1)	35(1)	37(1)	4(1)	13(1)	4(1)
C(1)	32(2)	39(1)	30(1)	3(1)	10(1)	1(1)
C(2)	36(2)	49(2)	33(2)	1(1)	16(1)	2(1)
C(3)	54(2)	52(2)	46(2)	0(1)	28(2)	-4(1)
C(4)	56(2)	68(2)	58(2)	-8(2)	36(2)	-13(1)
C(5)	45(2)	73(2)	54(2)	-15(2)	29(2)	-3(2)
C(6)	40(2)	56(2)	46(2)	-12(1)	18(1)	-2(1)
C(7)	35(2)	45(2)	34(2)	-7(1)	13(1)	-1(1)
C(8)	28(2)	40(1)	35(2)	-6(1)	8(1)	1(1)
C(9)	29(1)	31(1)	37(2)	-8(1)	9(1)	-4(1)
C(10)	30(1)	31(1)	41(2)	-2(1)	8(1)	-3(1)
C(11)	34(2)	34(1)	52(2)	-2(1)	9(1)	-1(1)
C(12)	31(2)	34(1)	64(2)	4(1)	7(1)	-1(1)
C(13)	35(2)	39(1)	52(2)	8(1)	4(1)	-7(1)
C(14)	36(2)	35(1)	42(2)	4(1)	8(1)	-7(1)
C(15)	27(1)	32(1)	40(2)	2(1)	7(1)	-5(1)
C(16)	30(1)	34(1)	32(2)	1(1)	9(1)	-5(1)
C(17)	29(1)	35(1)	34(2)	2(1)	12(1)	3(1)
C(18)	28(1)	32(1)	38(2)	-2(1)	9(1)	3(1)
C(19)	37(2)	40(1)	37(2)	-2(1)	8(1)	5(1)
C(20)	47(2)	39(2)	44(2)	-8(1)	11(1)	4(1)
C(21)	43(2)	33(1)	57(2)	-4(1)	10(2)	-1(1)
C(22)	34(2)	35(1)	49(2)	4(1)	10(1)	2(1)
C(23)	28(1)	30(1)	39(2)	0(1)	9(1)	3(1)
C(24)	28(1)	31(1)	32(1)	6(1)	10(1)	3(1)

C(25)	25(1)	48(2)	32(1)	-5(1)	8(1)	-1(1)
C(26)	38(2)	43(2)	49(2)	-6(1)	16(1)	0(1)
C(27)	37(2)	57(2)	64(2)	-18(2)	22(2)	1(1)
C(28)	44(2)	73(2)	74(2)	-11(2)	36(2)	-11(2)
C(29)	50(2)	64(2)	74(2)	2(2)	33(2)	-9(2)
C(30)	37(2)	45(2)	56(2)	0(1)	19(1)	-3(1)
C(31)	57(2)	71(2)	122(3)	-19(2)	43(2)	6(2)
B(1)	30(2)	33(2)	34(2)	0(1)	13(1)	1(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **2a**.

	x	y	z	U(eq)
H(3A)	5222	1415	3873	58
H(4A)	4140	2218	4670	68
H(5A)	4062	3917	4700	65
H(6A)	5019	4873	3899	56
H(11A)	5591	6827	1150	49
H(12A)	5161	7530	-367	54
H(13A)	5608	6766	-1607	53
H(14A)	6432	5216	-1404	46
H(19A)	6808	1461	-1388	46
H(20A)	6398	-216	-1567	53
H(21A)	6159	-1125	-307	55
H(22A)	6283	-403	1163	48
H(26A)	9952	1930	2324	51
H(28A)	11908	3463	1140	72
H(29A)	10870	4865	1132	71
H(30A)	9402	4820	1763	54
H(31A)	12511	1833	2066	119
H(31B)	11638	1439	1112	119
H(31C)	11520	1151	2133	119

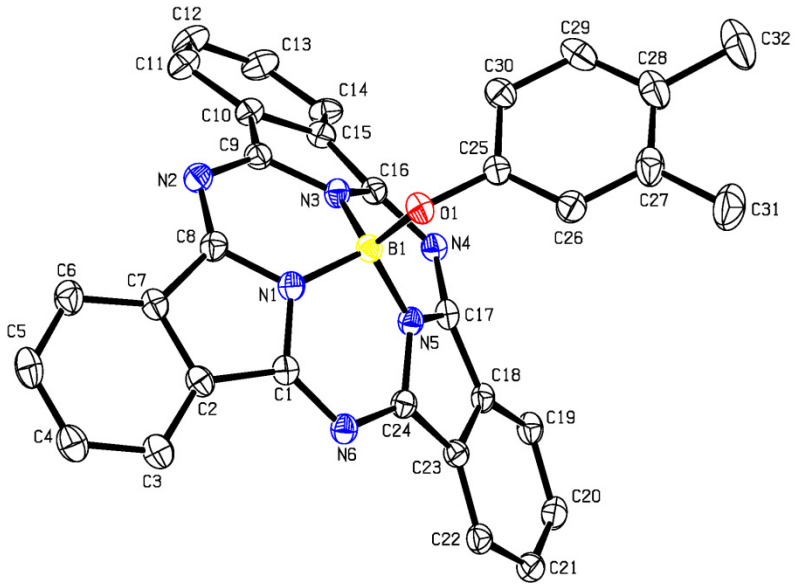


Figure S2. Anisotropic displacement ellipsoid plot of compound **2b**.

Table S7. Crystal data and structure refinement for compound **2b**.

Identification code	**2b**	
Empirical formula	C32 H21 B N6 O	
Formula weight	516.36	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.4280(3) Å	α= 77.850(3)°.
	b = 11.2988(7) Å	β= 80.886(4)°.
	c = 14.0713(9) Å	γ = 77.164(3)°.
Volume	1268.42(12) $Å^3$	
Z	2	
Density (calculated)	1.352 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	536	
Crystal size	0.22 x 0.18 x 0.16 mm^3	

Theta range for data collection	2.60 to 27.42°.
Index ranges	-10<=h<=10, -14<=k<=14, -17<=l<=18
Reflections collected	14664
Independent reflections	5713 [R(int) = 0.0710]
Completeness to theta = 27.42°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.990 and 0.883
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5713 / 0 / 363
Goodness-of-fit on F^2	0.975
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1262
R indices (all data)	R1 = 0.1639, wR2 = 0.1677
Largest diff. peak and hole	0.236 and -0.307 e.$Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5378(2)	5026(2)	2341(1)	35(1)
N(1)	3681(2)	6804(2)	2903(2)	31(1)
N(2)	2503(2)	7924(2)	1469(2)	36(1)
N(3)	2447(2)	5789(2)	2001(2)	30(1)
N(4)	1156(2)	4134(2)	2872(2)	32(1)
N(5)	2985(2)	4886(2)	3612(2)	30(1)
N(6)	3567(2)	6128(2)	4632(2)	33(1)
C(1)	3747(3)	6997(2)	3823(2)	31(1)
C(2)	3649(3)	8310(2)	3730(2)	35(1)
C(3)	3692(3)	9039(2)	4404(2)	42(1)
C(4)	3447(3)	10311(3)	4096(2)	48(1)
C(5)	3131(3)	10845(3)	3145(3)	50(1)
C(6)	3051(3)	10140(2)	2467(2)	45(1)
C(7)	3325(3)	8869(2)	2759(2)	34(1)
C(8)	3245(3)	7881(2)	2265(2)	34(1)
C(9)	2027(3)	6895(2)	1387(2)	32(1)
C(10)	706(3)	6755(2)	891(2)	34(1)
C(11)	-217(3)	7562(3)	205(2)	42(1)
C(12)	-1557(3)	7200(3)	-18(2)	49(1)
C(13)	-1996(3)	6082(3)	433(2)	46(1)
C(14)	-1092(3)	5273(3)	1113(2)	37(1)
C(15)	280(3)	5603(2)	1336(2)	33(1)
C(16)	1352(3)	5031(2)	2086(2)	30(1)
C(17)	1907(3)	4133(2)	3644(2)	30(1)
C(18)	1549(3)	3612(2)	4675(2)	30(1)
C(19)	584(3)	2757(2)	5149(2)	35(1)
C(20)	477(3)	2459(2)	6159(2)	39(1)
C(21)	1271(3)	3016(2)	6690(2)	40(1)
C(22)	2155(3)	3924(2)	6229(2)	35(1)
C(23)	2307(3)	4215(2)	5214(2)	31(1)
C(24)	3111(3)	5104(2)	4518(2)	31(1)

C(25)	5744(3)	3857(2)	2109(2)	32(1)
C(26)	6694(3)	2915(3)	2695(2)	42(1)
C(27)	7215(3)	1747(3)	2444(2)	52(1)
C(28)	6736(3)	1517(3)	1604(3)	52(1)
C(29)	5780(3)	2472(3)	1029(2)	48(1)
C(30)	5289(3)	3641(3)	1271(2)	40(1)
C(31)	8276(4)	748(3)	3085(3)	79(1)
C(32)	7259(4)	260(3)	1308(3)	82(1)
B(1)	3728(3)	5571(3)	2681(2)	30(1)

Table S9. Bond lengths [Å] and angles [°] for compound **2b**.

O(1)-C(25)	1.384(3)
O(1)-B(1)	1.440(3)
N(1)-C(8)	1.367(3)
N(1)-C(1)	1.369(3)
N(1)-B(1)	1.482(3)
N(2)-C(9)	1.343(3)
N(2)-C(8)	1.354(3)
N(3)-C(16)	1.369(3)
N(3)-C(9)	1.371(3)
N(3)-B(1)	1.500(3)
N(4)-C(17)	1.341(3)
N(4)-C(16)	1.350(3)
N(5)-C(17)	1.366(3)
N(5)-C(24)	1.372(3)
N(5)-B(1)	1.495(4)
N(6)-C(24)	1.345(3)
N(6)-C(1)	1.351(3)
C(1)-C(2)	1.446(3)
C(2)-C(3)	1.391(4)
C(2)-C(7)	1.421(4)
C(3)-C(4)	1.389(4)
C(4)-C(5)	1.389(4)
C(5)-C(6)	1.383(4)
C(6)-C(7)	1.386(3)
C(7)-C(8)	1.452(3)
C(9)-C(10)	1.457(3)
C(10)-C(11)	1.386(3)
C(10)-C(15)	1.417(4)
C(11)-C(12)	1.383(4)
C(12)-C(13)	1.390(4)
C(13)-C(14)	1.373(4)
C(14)-C(15)	1.389(3)
C(15)-C(16)	1.450(3)
C(17)-C(18)	1.457(3)

C(18)-C(19)	1.395(4)
C(18)-C(23)	1.419(3)
C(19)-C(20)	1.382(4)
C(20)-C(21)	1.396(4)
C(21)-C(22)	1.391(4)
C(22)-C(23)	1.388(3)
C(23)-C(24)	1.451(3)
C(25)-C(30)	1.380(3)
C(25)-C(26)	1.384(3)
C(26)-C(27)	1.395(4)
C(27)-C(28)	1.398(4)
C(27)-C(31)	1.506(4)
C(28)-C(29)	1.386(4)
C(28)-C(32)	1.516(4)
C(29)-C(30)	1.390(4)

C(25)-O(1)-B(1)	121.03(18)
C(8)-N(1)-C(1)	112.3(2)
C(8)-N(1)-B(1)	123.2(2)
C(1)-N(1)-B(1)	123.2(2)
C(9)-N(2)-C(8)	117.4(2)
C(16)-N(3)-C(9)	112.9(2)
C(16)-N(3)-B(1)	123.2(2)
C(9)-N(3)-B(1)	122.4(2)
C(17)-N(4)-C(16)	116.5(2)
C(17)-N(5)-C(24)	112.8(2)
C(17)-N(5)-B(1)	123.5(2)
C(24)-N(5)-B(1)	123.0(2)
C(24)-N(6)-C(1)	117.0(2)
N(6)-C(1)-N(1)	122.5(2)
N(6)-C(1)-C(2)	129.9(2)
N(1)-C(1)-C(2)	106.0(2)
C(3)-C(2)-C(7)	120.1(2)
C(3)-C(2)-C(1)	132.3(3)
C(7)-C(2)-C(1)	107.5(2)
C(4)-C(3)-C(2)	118.3(3)

C(5)-C(4)-C(3)	121.0(3)
C(6)-C(5)-C(4)	121.7(3)
C(5)-C(6)-C(7)	117.9(3)
C(6)-C(7)-C(2)	121.0(2)
C(6)-C(7)-C(8)	132.1(3)
C(2)-C(7)-C(8)	106.8(2)
N(2)-C(8)-N(1)	121.9(2)
N(2)-C(8)-C(7)	129.8(2)
N(1)-C(8)-C(7)	106.2(2)
N(2)-C(9)-N(3)	122.5(2)
N(2)-C(9)-C(10)	129.8(2)
N(3)-C(9)-C(10)	105.7(2)
C(11)-C(10)-C(15)	120.5(2)
C(11)-C(10)-C(9)	132.0(2)
C(15)-C(10)-C(9)	107.0(2)
C(12)-C(11)-C(10)	117.5(3)
C(11)-C(12)-C(13)	122.0(3)
C(14)-C(13)-C(12)	121.1(2)
C(13)-C(14)-C(15)	118.1(3)
C(14)-C(15)-C(10)	120.8(2)
C(14)-C(15)-C(16)	131.0(3)
C(10)-C(15)-C(16)	107.7(2)
N(4)-C(16)-N(3)	122.8(2)
N(4)-C(16)-C(15)	129.7(2)
N(3)-C(16)-C(15)	105.7(2)
N(4)-C(17)-N(5)	122.7(2)
N(4)-C(17)-C(18)	130.2(2)
N(5)-C(17)-C(18)	105.8(2)
C(19)-C(18)-C(23)	121.1(2)
C(19)-C(18)-C(17)	131.9(2)
C(23)-C(18)-C(17)	106.9(2)
C(20)-C(19)-C(18)	117.8(3)
C(19)-C(20)-C(21)	121.3(3)
C(22)-C(21)-C(20)	121.4(3)
C(23)-C(22)-C(21)	118.1(3)
C(22)-C(23)-C(18)	120.3(2)

C(22)-C(23)-C(24)	132.2(2)
C(18)-C(23)-C(24)	107.5(2)
N(6)-C(24)-N(5)	122.0(2)
N(6)-C(24)-C(23)	130.9(2)
N(5)-C(24)-C(23)	105.5(2)
C(30)-C(25)-C(26)	119.8(2)
C(30)-C(25)-O(1)	121.3(2)
C(26)-C(25)-O(1)	118.7(2)
C(25)-C(26)-C(27)	120.8(3)
C(26)-C(27)-C(28)	119.6(3)
C(26)-C(27)-C(31)	119.6(3)
C(28)-C(27)-C(31)	120.8(3)
C(29)-C(28)-C(27)	118.7(3)
C(29)-C(28)-C(32)	119.9(3)
C(27)-C(28)-C(32)	121.4(3)
C(28)-C(29)-C(30)	121.6(3)
C(25)-C(30)-C(29)	119.5(3)
O(1)-B(1)-N(1)	110.1(2)
O(1)-B(1)-N(5)	115.6(2)
N(1)-B(1)-N(5)	104.0(2)
O(1)-B(1)-N(3)	117.6(2)
N(1)-B(1)-N(3)	104.6(2)
N(5)-B(1)-N(3)	103.5(2)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2b**. 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)	29(1)	32(1)	44(1)	-11(1)	0(1)	-7(1)
N(1)	30(1)	29(1)	36(1)	-6(1)	-4(1)	-8(1)
N(2)	38(1)	34(1)	35(1)	-4(1)	-1(1)	-10(1)
N(3)	29(1)	26(1)	35(1)	-4(1)	-2(1)	-8(1)
N(4)	34(1)	28(1)	33(1)	-6(1)	-4(1)	-6(1)
N(5)	30(1)	26(1)	34(1)	-5(1)	-7(1)	-7(1)
N(6)	33(1)	30(1)	38(1)	-6(1)	-7(1)	-7(1)
C(1)	25(1)	30(2)	37(2)	-6(1)	-6(1)	-6(1)
C(2)	33(1)	33(2)	43(2)	-12(1)	-3(1)	-10(1)
C(3)	37(2)	40(2)	52(2)	-13(2)	-5(1)	-11(1)
C(4)	48(2)	40(2)	62(2)	-18(2)	-8(2)	-11(1)
C(5)	48(2)	29(2)	74(3)	-12(2)	-5(2)	-10(1)
C(6)	50(2)	33(2)	52(2)	-5(2)	-3(1)	-11(1)
C(7)	29(1)	30(2)	43(2)	-8(1)	2(1)	-9(1)
C(8)	30(1)	32(2)	37(2)	-2(1)	2(1)	-9(1)
C(9)	34(1)	31(2)	31(2)	-6(1)	2(1)	-8(1)
C(10)	37(1)	35(2)	31(2)	-4(1)	-3(1)	-8(1)
C(11)	44(2)	44(2)	34(2)	2(1)	-5(1)	-10(1)
C(12)	49(2)	60(2)	35(2)	5(2)	-14(1)	-12(2)
C(13)	43(2)	60(2)	35(2)	-2(2)	-11(1)	-16(2)
C(14)	40(2)	45(2)	30(2)	-6(1)	0(1)	-16(1)
C(15)	33(1)	35(2)	31(2)	-9(1)	-1(1)	-7(1)
C(16)	30(1)	29(2)	32(2)	-7(1)	-3(1)	-4(1)
C(17)	28(1)	23(1)	39(2)	-6(1)	-5(1)	-3(1)
C(18)	27(1)	24(1)	36(2)	-3(1)	-1(1)	-1(1)
C(19)	30(1)	29(2)	44(2)	-5(1)	-1(1)	-4(1)
C(20)	36(2)	29(2)	44(2)	0(1)	0(1)	-2(1)
C(21)	42(2)	36(2)	36(2)	-4(1)	2(1)	0(1)
C(22)	32(1)	30(2)	39(2)	-6(1)	-3(1)	0(1)
C(23)	27(1)	30(2)	33(2)	-5(1)	-1(1)	1(1)
C(24)	28(1)	30(2)	34(2)	-4(1)	-5(1)	-3(1)

C(25)	27(1)	30(2)	37(2)	-5(1)	4(1)	-8(1)
C(26)	36(1)	41(2)	43(2)	-4(1)	1(1)	-4(1)
C(27)	41(2)	37(2)	65(2)	-1(2)	10(2)	-1(1)
C(28)	46(2)	37(2)	68(2)	-16(2)	18(2)	-13(1)
C(29)	45(2)	52(2)	52(2)	-27(2)	11(1)	-18(2)
C(30)	36(1)	41(2)	43(2)	-12(1)	-1(1)	-8(1)
C(31)	70(2)	55(2)	85(3)	8(2)	6(2)	15(2)
C(32)	78(2)	42(2)	117(3)	-27(2)	37(2)	-17(2)
B(1)	31(2)	28(2)	32(2)	-6(1)	-1(1)	-8(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **2b**.

	x	y	z	U(eq)
H(3A)	3883	8677	5060	50
H(4A)	3497	10822	4543	58
H(5A)	2964	11718	2955	60
H(6A)	2817	10516	1821	54
H(11A)	60	8335	-101	50
H(12A)	-2198	7732	-495	59
H(13A)	-2937	5874	268	55
H(14A)	-1395	4510	1422	45
H(19A)	20	2392	4790	42
H(20A)	-150	1863	6497	47
H(21A)	1207	2770	7382	48
H(22A)	2639	4333	6598	42
H(26A)	6995	3065	3275	50
H(29A)	5453	2324	455	58
H(30A)	4644	4285	862	48
H(31A)	8494	1075	3633	119
H(31B)	9314	462	2701	119
H(31C)	7710	56	3338	119
H(32A)	6881	297	677	122
H(32B)	6778	-350	1806	122
H(32C)	8457	19	1251	122

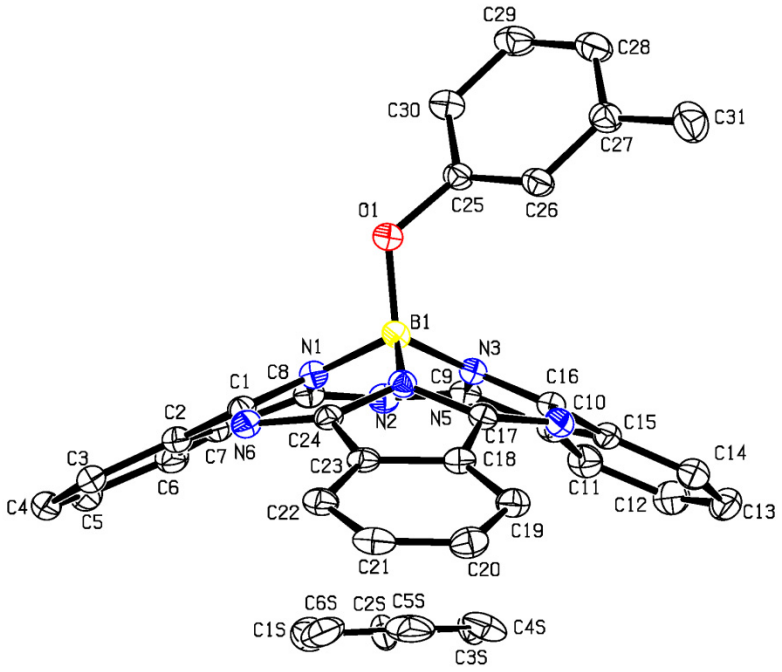


Figure S3. Anisotropic displacement ellipsoid plot of compound **2a** benzene solvate.

Table S12. Crystal data and structure refinement for compound **2a** benzene solvate.

Identification code	**2a** benzene solvate	
Empirical formula	C37 H25 B N6 O	
Formula weight	580.44	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.7554(6) Å	α= 90°.
	b = 13.8025(5) Å	β= 91.924(2)°.
	c = 16.3892(8) Å	γ = 90°.
Volume	2883.8(2) $Å^3$	
Z	4	
Density (calculated)	1.337 Mg/m^3	

Absorption coefficient	0.083 mm^{-1}
F(000)	1208
Crystal size	0.26 x 0.20 x 0.16 mm^3
Theta range for data collection	2.89 to 27.50°.
Index ranges	-16<=h<=16, -15<=k<=17, -21<=l<=21
Reflections collected	19729
Independent reflections	6577 [R(int) = 0.0838]
Completeness to theta = 27.50°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.892
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6577 / 0 / 407
Goodness-of-fit on F^2	0.991
Final R indices [I>2sigma(I)]	R1 = 0.0619, wR2 = 0.1316
R indices (all data)	R1 = 0.1794, wR2 = 0.1788
Largest diff. peak and hole	0.268 and -0.255 e.$Å^{-3}$

Table S13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2a** benzene solvate. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3068(1)	5214(1)	1223(1)	36(1)
C(1)	4427(2)	5760(2)	2923(2)	30(1)
C(2)	4714(2)	6688(2)	3285(2)	32(1)
C(3)	5604(2)	6980(2)	3736(2)	37(1)
C(4)	5633(2)	7915(2)	4036(2)	42(1)
C(5)	4791(2)	8542(2)	3901(2)	45(1)
C(6)	3887(2)	8260(2)	3476(2)	40(1)
C(7)	3850(2)	7320(2)	3160(2)	32(1)
C(8)	3019(2)	6773(2)	2741(2)	32(1)
C(9)	1363(2)	6131(2)	2546(2)	31(1)
C(10)	297(2)	5941(2)	2764(2)	32(1)
C(11)	-497(2)	6542(2)	3027(2)	41(1)
C(12)	-1426(2)	6126(2)	3254(2)	47(1)
C(13)	-1578(2)	5125(2)	3237(2)	44(1)
C(14)	-789(2)	4514(2)	2995(2)	40(1)
C(15)	152(2)	4915(2)	2754(2)	32(1)
C(16)	1141(2)	4494(2)	2533(2)	31(1)
C(17)	2561(2)	3482(2)	2697(2)	32(1)
C(18)	3214(2)	2743(2)	3103(2)	33(1)
C(19)	2975(2)	1832(2)	3410(2)	38(1)
C(20)	3772(2)	1320(2)	3805(2)	43(1)
C(21)	4784(3)	1701(2)	3900(2)	43(1)
C(22)	5020(2)	2617(2)	3621(2)	37(1)
C(23)	4235(2)	3139(2)	3209(1)	31(1)
C(24)	4204(2)	4115(2)	2881(2)	30(1)
C(25)	2351(2)	5010(2)	603(2)	33(1)
C(26)	1800(2)	4136(2)	557(2)	36(1)
C(27)	1113(2)	3947(2)	-99(2)	39(1)
C(28)	978(2)	4637(2)	-702(2)	47(1)
C(29)	1525(2)	5503(2)	-659(2)	48(1)

C(30)	2215(2)	5689(2)	-10(2)	40(1)
C(31)	538(3)	2996(2)	-165(2)	58(1)
N(1)	3468(2)	5901(1)	2544(1)	30(1)
N(2)	1974(2)	6918(2)	2694(1)	34(1)
N(3)	1776(2)	5250(1)	2330(1)	29(1)
N(4)	1513(2)	3590(2)	2668(1)	33(1)
N(5)	3237(2)	4216(1)	2502(1)	28(1)
N(6)	4840(2)	4871(2)	3043(1)	32(1)
B(1)	2882(2)	5130(2)	2085(2)	31(1)
C(1S)	3062(7)	6121(8)	4868(3)	62(2)
C(2S)	1997(9)	6319(2)	4773(3)	50(2)
C(3S)	1288(3)	5568(6)	4633(3)	39(2)
C(4S)	1645(7)	4618(4)	4587(3)	48(2)
C(5S)	2710(9)	4421(5)	4682(4)	65(3)
C(6S)	3419(3)	5172(10)	4822(4)	68(3)
C(1A)	2502(13)	6325(3)	4851(6)	49(3)
C(2A)	1532(9)	5891(11)	4693(6)	45(3)
C(3A)	1465(6)	4893(12)	4591(6)	48(4)
C(4A)	2367(10)	4329(4)	4646(7)	44(3)
C(5A)	3337(7)	4762(7)	4804(6)	46(3)
C(6A)	3404(8)	5760(8)	4906(5)	43(3)

Table S14. Bond lengths [Å] and angles [°] for compound **2a** benzene solvate.

O(1)-C(25)	1.373(3)
O(1)-B(1)	1.446(3)
C(1)-N(6)	1.347(3)
C(1)-N(1)	1.367(3)
C(1)-C(2)	1.454(3)
C(2)-C(3)	1.393(4)
C(2)-C(7)	1.414(4)
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.391(4)
C(5)-C(6)	1.383(4)
C(6)-C(7)	1.398(3)
C(7)-C(8)	1.455(4)
C(8)-N(2)	1.348(3)
C(8)-N(1)	1.376(3)
C(9)-N(2)	1.354(3)
C(9)-N(3)	1.376(3)
C(9)-C(10)	1.442(4)
C(10)-C(11)	1.389(4)
C(10)-C(15)	1.428(3)
C(11)-C(12)	1.379(4)
C(12)-C(13)	1.396(4)
C(13)-C(14)	1.381(4)
C(14)-C(15)	1.391(4)
C(15)-C(16)	1.445(4)
C(16)-N(4)	1.351(3)
C(16)-N(3)	1.370(3)
C(17)-N(4)	1.345(3)
C(17)-N(5)	1.374(3)
C(17)-C(18)	1.464(4)
C(18)-C(19)	1.392(4)
C(18)-C(23)	1.418(4)
C(19)-C(20)	1.382(4)
C(20)-C(21)	1.398(4)
C(21)-C(22)	1.381(4)

C(22)-C(23)	1.390(4)
C(23)-C(24)	1.451(3)
C(24)-N(6)	1.342(3)
C(24)-N(5)	1.369(3)
C(25)-C(30)	1.382(4)
C(25)-C(26)	1.396(4)
C(26)-C(27)	1.388(3)
C(27)-C(28)	1.379(4)
C(27)-C(31)	1.507(4)
C(28)-C(29)	1.384(4)
C(29)-C(30)	1.382(4)
N(1)-B(1)	1.491(3)
N(3)-B(1)	1.489(4)
N(5)-B(1)	1.498(3)
C(1S)-C(2S)	1.3900
C(1S)-C(6S)	1.3900
C(2S)-C(3S)	1.3900
C(3S)-C(4S)	1.3900
C(4S)-C(5S)	1.3900
C(5S)-C(6S)	1.3900
C(1A)-C(2A)	1.3900
C(1A)-C(6A)	1.3900
C(2A)-C(3A)	1.3900
C(3A)-C(4A)	1.3900
C(4A)-C(5A)	1.3900
C(5A)-C(6A)	1.3900

C(25)-O(1)-B(1)	125.4(2)
N(6)-C(1)-N(1)	122.4(2)
N(6)-C(1)-C(2)	130.7(2)
N(1)-C(1)-C(2)	105.6(2)
C(3)-C(2)-C(7)	121.1(2)
C(3)-C(2)-C(1)	131.3(3)
C(7)-C(2)-C(1)	107.4(2)
C(4)-C(3)-C(2)	118.0(3)
C(3)-C(4)-C(5)	120.9(3)

C(6)-C(5)-C(4)	122.1(3)
C(5)-C(6)-C(7)	117.7(3)
C(6)-C(7)-C(2)	120.2(2)
C(6)-C(7)-C(8)	132.2(3)
C(2)-C(7)-C(8)	107.5(2)
N(2)-C(8)-N(1)	122.3(2)
N(2)-C(8)-C(7)	130.8(2)
N(1)-C(8)-C(7)	105.2(2)
N(2)-C(9)-N(3)	122.1(2)
N(2)-C(9)-C(10)	130.1(2)
N(3)-C(9)-C(10)	106.0(2)
C(11)-C(10)-C(15)	120.1(3)
C(11)-C(10)-C(9)	132.2(2)
C(15)-C(10)-C(9)	107.5(2)
C(12)-C(11)-C(10)	118.4(3)
C(11)-C(12)-C(13)	121.9(3)
C(14)-C(13)-C(12)	120.4(3)
C(13)-C(14)-C(15)	118.9(3)
C(14)-C(15)-C(10)	120.2(2)
C(14)-C(15)-C(16)	132.8(3)
C(10)-C(15)-C(16)	106.7(2)
N(4)-C(16)-N(3)	122.5(2)
N(4)-C(16)-C(15)	129.4(2)
N(3)-C(16)-C(15)	106.4(2)
N(4)-C(17)-N(5)	122.8(2)
N(4)-C(17)-C(18)	130.0(2)
N(5)-C(17)-C(18)	105.5(2)
C(19)-C(18)-C(23)	121.0(2)
C(19)-C(18)-C(17)	131.8(3)
C(23)-C(18)-C(17)	107.0(2)
C(20)-C(19)-C(18)	117.7(3)
C(19)-C(20)-C(21)	121.5(3)
C(22)-C(21)-C(20)	121.3(3)
C(21)-C(22)-C(23)	118.2(3)
C(22)-C(23)-C(18)	120.2(2)
C(22)-C(23)-C(24)	132.2(3)

C(18)-C(23)-C(24)	107.4(2)
N(6)-C(24)-N(5)	122.7(2)
N(6)-C(24)-C(23)	129.8(2)
N(5)-C(24)-C(23)	106.0(2)
O(1)-C(25)-C(30)	117.6(2)
O(1)-C(25)-C(26)	122.6(2)
C(30)-C(25)-C(26)	119.7(2)
C(27)-C(26)-C(25)	120.5(2)
C(28)-C(27)-C(26)	119.1(3)
C(28)-C(27)-C(31)	120.1(3)
C(26)-C(27)-C(31)	120.8(3)
C(27)-C(28)-C(29)	120.6(3)
C(30)-C(29)-C(28)	120.4(3)
C(25)-C(30)-C(29)	119.7(3)
C(1)-N(1)-C(8)	113.0(2)
C(1)-N(1)-B(1)	123.6(2)
C(8)-N(1)-B(1)	122.5(2)
C(8)-N(2)-C(9)	117.0(2)
C(16)-N(3)-C(9)	112.1(2)
C(16)-N(3)-B(1)	123.6(2)
C(9)-N(3)-B(1)	122.9(2)
C(17)-N(4)-C(16)	116.8(2)
C(24)-N(5)-C(17)	112.5(2)
C(24)-N(5)-B(1)	123.2(2)
C(17)-N(5)-B(1)	122.9(2)
C(24)-N(6)-C(1)	116.6(2)
O(1)-B(1)-N(3)	116.3(2)
O(1)-B(1)-N(1)	109.9(2)
N(3)-B(1)-N(1)	104.3(2)
O(1)-B(1)-N(5)	117.2(2)
N(3)-B(1)-N(5)	104.3(2)
N(1)-B(1)-N(5)	103.4(2)
C(2S)-C(1S)-C(6S)	120.0
C(1S)-C(2S)-C(3S)	120.0
C(4S)-C(3S)-C(2S)	120.0
C(5S)-C(4S)-C(3S)	120.0

C(4S)-C(5S)-C(6S)	120.0
C(5S)-C(6S)-C(1S)	120.0
C(2A)-C(1A)-C(6A)	120.0
C(1A)-C(2A)-C(3A)	120.0
C(4A)-C(3A)-C(2A)	120.0
C(3A)-C(4A)-C(5A)	120.0
C(6A)-C(5A)-C(4A)	120.0
C(5A)-C(6A)-C(1A)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2a** benzene solvate. 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)	47(1)	27(1)	-1(1)	1(1)	-5(1)
C(1)	26(2)	40(2)	24(1)	0(1)	5(1)	1(1)
C(2)	35(2)	37(2)	25(1)	-1(1)	4(1)	-4(1)
C(3)	34(2)	50(2)	28(2)	0(1)	5(1)	-8(1)
C(4)	45(2)	50(2)	29(2)	-6(1)	4(1)	-16(2)
C(5)	52(2)	43(2)	40(2)	-13(1)	10(2)	-13(2)
C(6)	44(2)	41(2)	34(2)	-4(1)	7(1)	-2(1)
C(7)	41(2)	32(2)	23(1)	1(1)	6(1)	-6(1)
C(8)	37(2)	34(2)	26(2)	4(1)	2(1)	0(1)
C(9)	37(2)	34(2)	23(1)	3(1)	-1(1)	3(1)
C(10)	30(2)	39(2)	27(2)	3(1)	-2(1)	6(1)
C(11)	39(2)	42(2)	41(2)	5(1)	-4(1)	8(1)
C(12)	36(2)	63(2)	42(2)	5(2)	2(2)	10(2)
C(13)	34(2)	59(2)	40(2)	7(2)	4(1)	-1(2)
C(14)	39(2)	45(2)	35(2)	5(1)	-2(1)	-1(2)
C(15)	28(2)	44(2)	26(2)	3(1)	-1(1)	0(1)
C(16)	33(2)	35(2)	24(1)	0(1)	0(1)	-2(1)
C(17)	35(2)	36(2)	24(1)	-6(1)	2(1)	-4(1)
C(18)	37(2)	35(2)	26(2)	-1(1)	4(1)	3(1)
C(19)	45(2)	39(2)	31(2)	-1(1)	2(1)	0(1)
C(20)	55(2)	37(2)	38(2)	3(1)	8(2)	5(2)
C(21)	57(2)	45(2)	27(2)	1(1)	2(1)	20(2)
C(22)	42(2)	42(2)	27(2)	-3(1)	4(1)	8(1)
C(23)	34(2)	35(2)	23(1)	-3(1)	6(1)	7(1)
C(24)	28(2)	39(2)	24(1)	-1(1)	5(1)	2(1)
C(25)	28(2)	44(2)	26(2)	0(1)	-1(1)	4(1)
C(26)	37(2)	43(2)	28(2)	0(1)	-3(1)	3(1)
C(27)	36(2)	47(2)	33(2)	-7(1)	3(1)	4(1)
C(28)	45(2)	64(2)	30(2)	-3(2)	-3(1)	6(2)
C(29)	52(2)	60(2)	33(2)	9(2)	-2(2)	13(2)

C(30)	46(2)	40(2)	33(2)	1(1)	0(1)	3(1)
C(31)	55(2)	58(2)	60(2)	-12(2)	-4(2)	-7(2)
N(1)	31(1)	31(1)	28(1)	1(1)	1(1)	-1(1)
N(2)	36(2)	34(1)	32(1)	4(1)	0(1)	0(1)
N(3)	29(1)	33(1)	24(1)	-1(1)	0(1)	-2(1)
N(4)	32(2)	37(1)	29(1)	-3(1)	-1(1)	-2(1)
N(5)	28(1)	30(1)	27(1)	-2(1)	1(1)	2(1)
N(6)	31(1)	38(1)	29(1)	-1(1)	4(1)	0(1)
B(1)	30(2)	35(2)	26(2)	-2(1)	-2(1)	-2(1)
C(1S)	48(5)	93(5)	44(4)	24(3)	-9(3)	-3(5)
C(2S)	43(5)	60(4)	45(3)	7(3)	-12(3)	-23(3)
C(3S)	47(3)	34(4)	35(3)	10(2)	-13(3)	-19(3)
C(4S)	79(6)	37(3)	27(3)	0(3)	-15(3)	7(4)
C(5S)	66(7)	103(6)	27(3)	-8(3)	13(4)	22(5)
C(6S)	45(5)	120(10)	40(4)	28(5)	13(3)	7(4)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **2a** benzene solvate.

	x	y	z	U(eq)
H(3A)	6175	6548	3834	44
H(4A)	6236	8133	4339	50
H(5A)	4838	9184	4108	54
H(6A)	3310	8691	3402	47
H(11A)	-403	7225	3049	49
H(12A)	-1977	6532	3426	57
H(13A)	-2230	4861	3394	53
H(14A)	-888	3832	2992	48
H(19A)	2287	1571	3349	46
H(20A)	3629	695	4017	52
H(21A)	5319	1323	4161	52
H(22A)	5702	2883	3708	45
H(26A)	1896	3668	977	43
H(28A)	506	4517	-1151	56
H(29A)	1425	5972	-1079	58
H(30A)	2595	6281	14	48
H(31A)	90	2992	-662	87
H(31B)	105	2911	313	87
H(31C)	1047	2465	-188	87
H(1SA)	3547	6635	4964	74
H(2SA)	1753	6968	4804	60
H(3SA)	560	5703	4568	47
H(4SA)	1160	4105	4491	58
H(5SA)	2954	3772	4651	78
H(6SA)	4147	5037	4887	82
H(1AA)	2548	7007	4920	59
H(2AA)	916	6277	4655	54
H(3AA)	803	4597	4483	58
H(4AA)	2322	3647	4576	53
H(5AA)	3953	4377	4841	56

H(6AA)	4066	6057	5014	51

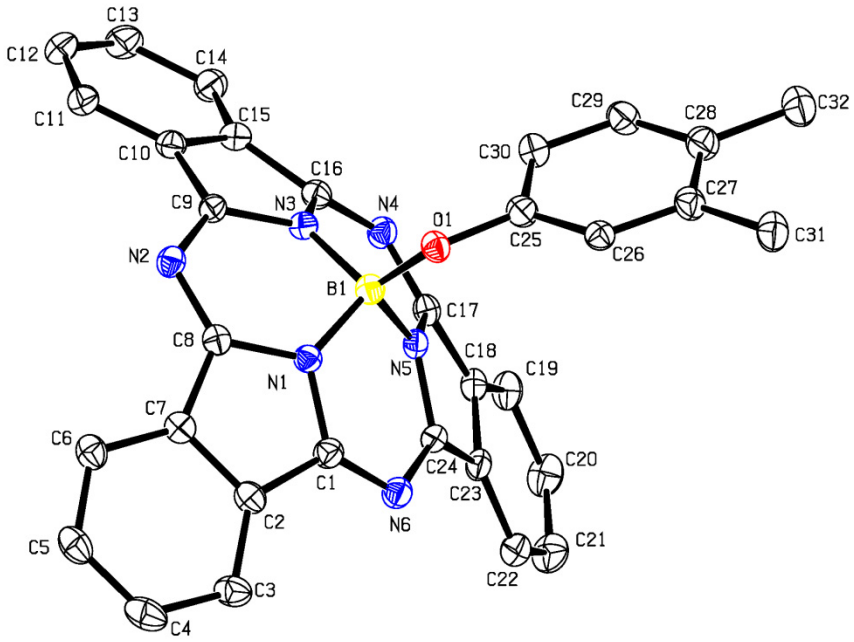


Figure S4. Anisotropic displacement ellipsoid plot of compound **2b** benzene solvate.

Table S17. Crystal data and structure refinement for compound **2b** benzene solvate.

Identification code	**2b** benzene solvate	
Empirical formula	C38 H27 B N6 O	
Formula weight	594.47	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.3006(4) Å	α= 90°.
	b = 13.8287(7) Å	β= 90.754(2)°.
	c = 17.4739(7) Å	γ = 90°.
Volume	2972.1(2) $Å^3$	
Z	4	
Density (calculated)	1.329 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	

F(000)	1240
Crystal size	0.18 x 0.18 x 0.10 mm^3
Theta range for data collection	2.76 to 25.00°.
Index ranges	-14<=h<=14, -16<=k<=16, -15<=l<=20
Reflections collected	15799
Independent reflections	5201 [R(int) = 0.0766]
Completeness to theta = 25.00°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.994 and 0.880
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5201 / 12 / 449
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0735, wR2 = 0.1759
R indices (all data)	R1 = 0.1557, wR2 = 0.2322
Largest diff. peak and hole	0.551 and -0.281 e.$Å^{-3}$

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2b** benzene solvate. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8028(2)	4982(2)	3673(1)	31(1)
N(1)	8358(2)	5858(2)	2497(2)	27(1)
N(2)	9866(2)	5032(2)	1967(2)	30(1)
N(3)	8311(2)	4166(2)	2398(2)	27(1)
N(4)	6609(2)	3397(2)	2149(2)	33(1)
N(5)	6692(2)	5022(2)	2588(2)	27(1)
N(6)	6675(2)	6725(2)	2395(2)	34(1)
C(1)	7775(3)	6686(3)	2355(2)	32(1)
C(2)	8523(3)	7347(3)	1989(2)	33(1)
C(3)	8384(3)	8286(3)	1721(2)	41(1)
C(4)	9211(3)	8693(3)	1309(2)	49(1)
C(5)	10162(3)	8170(3)	1147(2)	42(1)
C(6)	10303(3)	7235(3)	1404(2)	37(1)
C(7)	9487(3)	6823(3)	1840(2)	32(1)
C(8)	9341(3)	5852(3)	2136(2)	29(1)
C(9)	9319(3)	4200(3)	2060(2)	29(1)
C(10)	9453(3)	3274(3)	1678(2)	31(1)
C(11)	10317(3)	2884(3)	1271(2)	36(1)
C(12)	10165(3)	2002(3)	924(2)	43(1)
C(13)	9163(3)	1520(3)	954(2)	46(1)
C(14)	8304(3)	1896(3)	1351(2)	39(1)
C(15)	8446(3)	2776(3)	1724(2)	32(1)
C(16)	7708(3)	3395(2)	2143(2)	31(1)
C(17)	6122(3)	4231(3)	2333(2)	29(1)
C(18)	5035(3)	4587(3)	2148(2)	32(1)
C(19)	4088(3)	4121(3)	1895(2)	39(1)
C(20)	3189(3)	4686(3)	1736(2)	47(1)
C(21)	3214(3)	5687(3)	1816(2)	49(1)
C(22)	4144(3)	6163(3)	2047(2)	39(1)
C(23)	5059(3)	5609(3)	2226(2)	31(1)

C(24)	6156(3)	5876(3)	2454(2)	29(1)
C(25)	7335(3)	4520(3)	4166(2)	35(1)
C(26)	7000(3)	5014(2)	4806(2)	30(1)
C(27)	6302(3)	4612(3)	5337(2)	38(1)
C(28)	5928(3)	3659(3)	5221(2)	41(1)
C(29)	6285(3)	3162(3)	4581(2)	41(1)
C(30)	6985(3)	3573(3)	4060(2)	38(1)
C(31)	5954(3)	5175(3)	6024(2)	46(1)
C(32)	5161(3)	3180(3)	5773(2)	50(1)
B(1)	7859(3)	4988(3)	2846(2)	30(1)
C(1S)	7830(20)	4520(20)	232(11)	86(7)
C(2S)	6720(20)	4571(14)	371(12)	86(7)
C(3S)	6230(10)	5461(13)	472(10)	68(5)
C(4S)	6840(14)	6301(8)	434(9)	57(4)
C(5S)	7944(16)	6250(18)	295(13)	59(5)
C(6S)	8438(15)	5360(30)	193(13)	80(8)
C(7S)	7330(20)	4286(15)	332(11)	95(8)
C(8S)	6458(15)	4830(30)	462(13)	119(11)
C(9S)	6550(20)	5800(30)	464(11)	116(11)
C(10S)	7510(30)	6214(18)	337(11)	96(9)
C(11S)	8385(18)	5665(19)	206(13)	76(7)
C(12S)	8296(13)	4701(16)	204(11)	73(6)

Table S19. Bond lengths [Å] and angles [°] for compound **2b** benzene solvate.

O(1)-C(25)	1.377(4)
O(1)-B(1)	1.458(5)
N(1)-C(8)	1.371(4)
N(1)-C(1)	1.372(4)
N(1)-B(1)	1.485(5)
N(2)-C(8)	1.339(4)
N(2)-C(9)	1.344(4)
N(3)-C(16)	1.370(4)
N(3)-C(9)	1.381(4)
N(3)-B(1)	1.492(5)
N(4)-C(17)	1.341(4)
N(4)-C(16)	1.351(4)
N(5)-C(24)	1.370(4)
N(5)-C(17)	1.372(4)
N(5)-B(1)	1.499(5)
N(6)-C(24)	1.341(4)
N(6)-C(1)	1.357(4)
C(1)-C(2)	1.451(5)
C(2)-C(3)	1.391(5)
C(2)-C(7)	1.416(5)
C(3)-C(4)	1.374(5)
C(4)-C(5)	1.407(5)
C(5)-C(6)	1.379(5)
C(6)-C(7)	1.390(5)
C(7)-C(8)	1.451(5)
C(9)-C(10)	1.455(5)
C(10)-C(11)	1.395(5)
C(10)-C(15)	1.420(5)
C(11)-C(12)	1.374(5)
C(12)-C(13)	1.403(5)
C(13)-C(14)	1.373(5)
C(14)-C(15)	1.390(5)
C(15)-C(16)	1.454(5)
C(17)-C(18)	1.457(5)

C(18)-C(19)	1.399(5)
C(18)-C(23)	1.420(5)
C(19)-C(20)	1.380(5)
C(20)-C(21)	1.392(6)
C(21)-C(22)	1.376(5)
C(22)-C(23)	1.393(5)
C(23)-C(24)	1.450(5)
C(25)-C(26)	1.378(5)
C(25)-C(30)	1.390(5)
C(26)-C(27)	1.389(5)
C(27)-C(28)	1.409(5)
C(27)-C(31)	1.498(5)
C(28)-C(29)	1.388(5)
C(28)-C(32)	1.512(5)
C(29)-C(30)	1.384(5)
C(1S)-C(2S)	1.385(11)
C(1S)-C(6S)	1.385(11)
C(2S)-C(3S)	1.385(11)
C(3S)-C(4S)	1.385(11)
C(4S)-C(5S)	1.385(11)
C(5S)-C(6S)	1.385(11)
C(7S)-C(8S)	1.338(12)
C(7S)-C(12S)	1.338(12)
C(8S)-C(9S)	1.338(12)
C(9S)-C(10S)	1.338(12)
C(10S)-C(11S)	1.338(12)
C(11S)-C(12S)	1.338(12)

C(25)-O(1)-B(1)	122.8(3)
C(8)-N(1)-C(1)	112.6(3)
C(8)-N(1)-B(1)	123.7(3)
C(1)-N(1)-B(1)	122.2(3)
C(8)-N(2)-C(9)	117.1(3)
C(16)-N(3)-C(9)	111.9(3)
C(16)-N(3)-B(1)	124.0(3)
C(9)-N(3)-B(1)	122.8(3)

C(17)-N(4)-C(16)	117.0(3)
C(24)-N(5)-C(17)	112.9(3)
C(24)-N(5)-B(1)	122.3(3)
C(17)-N(5)-B(1)	123.8(3)
C(24)-N(6)-C(1)	116.4(3)
N(6)-C(1)-N(1)	122.9(3)
N(6)-C(1)-C(2)	129.5(3)
N(1)-C(1)-C(2)	105.8(3)
C(3)-C(2)-C(7)	121.0(3)
C(3)-C(2)-C(1)	131.4(3)
C(7)-C(2)-C(1)	107.3(3)
C(4)-C(3)-C(2)	118.1(4)
C(3)-C(4)-C(5)	121.2(4)
C(6)-C(5)-C(4)	121.2(4)
C(5)-C(6)-C(7)	118.3(4)
C(6)-C(7)-C(2)	120.3(3)
C(6)-C(7)-C(8)	131.9(3)
C(2)-C(7)-C(8)	107.5(3)
N(2)-C(8)-N(1)	122.5(3)
N(2)-C(8)-C(7)	130.0(3)
N(1)-C(8)-C(7)	105.8(3)
N(2)-C(9)-N(3)	122.3(3)
N(2)-C(9)-C(10)	129.7(3)
N(3)-C(9)-C(10)	105.9(3)
C(11)-C(10)-C(15)	120.9(3)
C(11)-C(10)-C(9)	131.7(3)
C(15)-C(10)-C(9)	107.2(3)
C(12)-C(11)-C(10)	117.8(3)
C(11)-C(12)-C(13)	121.3(4)
C(14)-C(13)-C(12)	121.4(4)
C(13)-C(14)-C(15)	118.4(4)
C(14)-C(15)-C(10)	120.1(3)
C(14)-C(15)-C(16)	132.6(3)
C(10)-C(15)-C(16)	107.1(3)
N(4)-C(16)-N(3)	122.3(3)
N(4)-C(16)-C(15)	129.5(3)

N(3)-C(16)-C(15)	106.4(3)
N(4)-C(17)-N(5)	122.4(3)
N(4)-C(17)-C(18)	130.5(3)
N(5)-C(17)-C(18)	105.4(3)
C(19)-C(18)-C(23)	120.3(3)
C(19)-C(18)-C(17)	132.2(4)
C(23)-C(18)-C(17)	107.4(3)
C(20)-C(19)-C(18)	117.7(4)
C(19)-C(20)-C(21)	121.8(4)
C(22)-C(21)-C(20)	121.5(4)
C(21)-C(22)-C(23)	118.0(4)
C(22)-C(23)-C(18)	120.7(3)
C(22)-C(23)-C(24)	131.9(3)
C(18)-C(23)-C(24)	107.3(3)
N(6)-C(24)-N(5)	122.6(3)
N(6)-C(24)-C(23)	130.1(3)
N(5)-C(24)-C(23)	105.8(3)
O(1)-C(25)-C(26)	118.1(3)
O(1)-C(25)-C(30)	123.2(3)
C(26)-C(25)-C(30)	118.7(3)
C(25)-C(26)-C(27)	122.5(3)
C(26)-C(27)-C(28)	118.8(3)
C(26)-C(27)-C(31)	120.8(4)
C(28)-C(27)-C(31)	120.3(3)
C(29)-C(28)-C(27)	118.2(3)
C(29)-C(28)-C(32)	120.2(4)
C(27)-C(28)-C(32)	121.5(4)
C(30)-C(29)-C(28)	122.1(4)
C(29)-C(30)-C(25)	119.6(4)
O(1)-B(1)-N(1)	110.9(3)
O(1)-B(1)-N(3)	117.7(3)
N(1)-B(1)-N(3)	104.1(3)
O(1)-B(1)-N(5)	115.0(3)
N(1)-B(1)-N(5)	104.5(3)
N(3)-B(1)-N(5)	103.2(3)
C(2S)-C(1S)-C(6S)	120.0

C(1S)-C(2S)-C(3S)	120.0
C(4S)-C(3S)-C(2S)	120.0
C(3S)-C(4S)-C(5S)	120.0
C(4S)-C(5S)-C(6S)	120.0
C(5S)-C(6S)-C(1S)	120.0
C(8S)-C(7S)-C(12S)	120.0
C(7S)-C(8S)-C(9S)	120.0
C(8S)-C(9S)-C(10S)	120.0
C(9S)-C(10S)-C(11S)	120.0
C(12S)-C(11S)-C(10S)	120.0
C(11S)-C(12S)-C(7S)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **2b** benzene solvate. 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)	28(1)	36(2)	29(2)	3(1)	1(1)	-3(1)
N(1)	27(2)	26(2)	28(2)	1(1)	0(1)	0(1)
N(2)	25(2)	35(2)	31(2)	-2(1)	0(1)	0(2)
N(3)	26(2)	26(2)	29(2)	0(1)	-1(1)	-1(1)
N(4)	30(2)	33(2)	36(2)	0(2)	4(1)	-2(2)
N(5)	25(2)	29(2)	27(2)	-1(1)	5(1)	-1(1)
N(6)	31(2)	31(2)	39(2)	0(2)	4(1)	0(2)
C(1)	30(2)	33(2)	34(2)	0(2)	1(2)	1(2)
C(2)	34(2)	31(2)	35(2)	1(2)	0(2)	-8(2)
C(3)	39(2)	32(2)	51(3)	7(2)	-4(2)	-4(2)
C(4)	55(3)	32(2)	60(3)	13(2)	-5(2)	-15(2)
C(5)	40(2)	47(3)	40(3)	9(2)	0(2)	-15(2)
C(6)	30(2)	43(3)	37(2)	3(2)	0(2)	-7(2)
C(7)	31(2)	32(2)	32(2)	-1(2)	-3(2)	-4(2)
C(8)	28(2)	33(2)	27(2)	0(2)	-1(2)	-2(2)
C(9)	24(2)	33(2)	29(2)	3(2)	1(2)	2(2)
C(10)	34(2)	30(2)	30(2)	2(2)	-1(2)	3(2)
C(11)	33(2)	39(2)	35(2)	3(2)	1(2)	6(2)
C(12)	46(3)	38(3)	45(3)	-2(2)	8(2)	13(2)
C(13)	61(3)	28(2)	48(3)	-8(2)	4(2)	4(2)
C(14)	37(2)	36(2)	43(3)	0(2)	3(2)	1(2)
C(15)	33(2)	29(2)	33(2)	2(2)	-2(2)	2(2)
C(16)	32(2)	27(2)	33(2)	1(2)	2(2)	-2(2)
C(17)	27(2)	31(2)	30(2)	1(2)	3(2)	-6(2)
C(18)	29(2)	39(2)	28(2)	-1(2)	5(2)	-1(2)
C(19)	33(2)	47(3)	36(2)	-6(2)	3(2)	-7(2)
C(20)	27(2)	65(3)	49(3)	-9(2)	-5(2)	-5(2)
C(21)	31(2)	67(3)	48(3)	0(2)	-5(2)	5(2)
C(22)	33(2)	44(2)	41(2)	4(2)	5(2)	5(2)
C(23)	24(2)	39(2)	29(2)	-1(2)	4(2)	2(2)

C(24)	26(2)	30(2)	32(2)	3(2)	5(2)	4(2)
C(25)	32(2)	38(2)	35(2)	4(2)	0(2)	-1(2)
C(26)	30(2)	32(2)	29(2)	0(2)	-2(2)	0(2)
C(27)	34(2)	49(3)	30(2)	5(2)	-1(2)	2(2)
C(28)	35(2)	46(3)	42(3)	6(2)	1(2)	0(2)
C(29)	44(2)	39(2)	40(3)	6(2)	3(2)	-2(2)
C(30)	40(2)	41(3)	33(2)	2(2)	5(2)	0(2)
C(31)	35(2)	67(3)	36(2)	2(2)	2(2)	1(2)
C(32)	46(3)	59(3)	45(3)	5(2)	6(2)	-5(2)
B(1)	26(2)	33(3)	30(2)	0(2)	-1(2)	-1(2)
C(1S)	130(20)	81(12)	45(10)	13(10)	-12(14)	22(15)
C(2S)	130(20)	100(12)	24(9)	-3(10)	-17(12)	-69(12)
C(3S)	56(8)	99(12)	47(11)	-26(9)	6(7)	-30(8)
C(4S)	66(12)	55(7)	50(10)	2(6)	1(8)	-3(7)
C(5S)	49(9)	82(11)	47(9)	23(8)	-7(7)	-15(8)
C(6S)	47(10)	130(20)	60(13)	22(14)	12(9)	4(11)
C(7S)	108(17)	106(12)	70(13)	47(10)	-37(12)	-53(10)
C(8S)	71(8)	230(30)	56(15)	70(20)	5(9)	-42(14)
C(9S)	111(15)	210(30)	32(11)	20(20)	15(14)	40(20)
C(10S)	140(30)	101(13)	44(12)	-13(9)	-25(18)	12(11)
C(11S)	75(12)	86(13)	66(13)	23(10)	-42(10)	-26(11)
C(12S)	66(8)	90(12)	64(11)	17(10)	-25(8)	-13(9)

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **2b** benzene solvate.

	x	y	z	U(eq)
H(3A)	7737	8636	1819	49
H(4A)	9140	9339	1131	59
H(5A)	10717	8467	856	51
H(6A)	10941	6881	1286	44
H(11A)	10990	3218	1235	43
H(12A)	10750	1712	659	52
H(13A)	9077	920	695	55
H(14A)	7629	1563	1370	47
H(19A)	4064	3438	1834	46
H(20A)	2535	4384	1567	56
H(21A)	2574	6051	1710	59
H(22A)	4163	6848	2083	47
H(26A)	7256	5655	4886	36
H(29A)	6040	2518	4499	49
H(30A)	7225	3210	3633	45
H(31A)	6192	5848	5974	69
H(31B)	6283	4891	6486	69
H(31C)	5161	5154	6062	69
H(32A)	4913	2562	5560	75
H(32B)	4533	3602	5856	75
H(32C)	5540	3066	6262	75
H(1S)	8166	3910	162	103
H(2S)	6304	3995	397	104
H(3S)	5472	5496	568	81
H(4S)	6502	6911	504	68
H(5S)	8363	6826	268	71
H(6S)	9195	5325	98	96
H(7S)	7269	3601	330	114
H(8S)	5774	4540	553	143
H(9S)	5927	6189	557	139

H(10S)	7574	6899	338	116
H(11S)	9069	5960	116	91
H(12S)	8916	4311	112	88