9. Appendix B. X-Ray Diffraction Studies

9.1. 2-Phenyl-naphtho[1,8-de][1,3,2]diazaborinane *64*

Table 1. Crystal data and structure refinement for danbph_64.

Identification code	danbph_64	
Empirical formula	C16 H13 B N2	
Formula weight	278.54	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.012 (5) Å	a= 90.000(5)°.
	b = 5.430 (5) Å	b= 117.57(5)°.
	c = 11.745 (5) Å	g = 90.000(5)°.
Volume	702.29 (9) $Å^3$	
Z	2	
Density (calculated)	1.415 Mg/m^3	
Absorption coefficient	0.280 mm^{-1}	
F(000)	288	
Crystal size	0.40 x 0.15 x 0.07 mm^3	
Theta range for data collection	3.61 to 26.05°.	
Index ranges	-5<=h<=5, -12<=k<=11, -16<=l<=16	
Reflections collected	6492	
Independent reflections	2286 [R(int) = 0.0266]	
Completeness to theta = 25.00°	99.8 %	
Max. and min. transmission	0.9807 and 0.8962	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2286 / 1 / 189	
Goodness-of-fit on F^2	0.905	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0945	
R indices (all data)	R1 = 0.0445, wR2 = 0.0977	
Absolute structure parameter	0.05(7)	
Largest diff. peak and hole	0.153 and -0.248 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x10^3) for danbph_64. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	10793(7)	122(3)	9087(6)	45(6)
C(2)	9472(7)	472(3)	8080(1)	41(8)
C(3)	9275(3)	2405(3)	7194(8)	40(6)
C(4)	10377(6)	3948(3)	7336(8)	43(1)
N(5)	11654(4)	3539(3)	8390(9)	49(1)
B(6)	11926(5)	1616(4)	9291(7)	40(3)
C(7)	13375(5)	1227(3)	10455(3)	39(9)
C(8)	14437(9)	2892(3)	10729(3)	47(7)
C(9)	15706(2)	2611(4)	11791(5)	53(1)
C(10)	15947(5)	640(0)	12606(2)	51(1)
C(11)	14918(9)	-1046(4)	12348(8)	56(0)
C(12)	13650(8)	-755(3)	11291(7)	51(7)
C(13)	10168(3)	578(7)	6456(8)	54(3)
C(14)	8862(2)	6115(4)	5419(7)	61(2)
C(15)	7787(2)	4684(4)	5266(3)	58(3)
C(16)	7951(5)	2780(4)	6145(5)	47(5)
C(17)	6869(9)	1231(4)	6032(1)	56(1)
C(18)	7089(1)	-588(4)	6896(4)	58(1)
C(19)	8388(1)	-999(4)	7929(2)	52(2)
H(81)	14293(3)	4288(3)	10166(2)	54(6)
H(91)	16423(1)	3824(4)	11955(6)	60(5)
H(101)	16813(2)	443(4)	13338(6)	59(9)
H(111)	15086(5)	-2397(4)	12902(1)	62(9)
H(121)	12954(2)	-1980(3)	11133(1)	62(8)
H(131)	10918(2)	6844(4)	6551(1)	61(7)
H(141)	8736(2)	7378(4)	4804(8)	71(2)
H(151)	6920(2)	4919(4)	4565(1)	61(6)
H(171)	5981(6)	1487(4)	5315(1)	59(9)
H(181)	6355(4)	-1652(4)	6800(3)	68(4)
H(191)	8546(9)	-2320(4)	8528(8)	60(1)
H(11)	10917(3)	-1139(3)	9595(4)	51(1)
H(51)	12340(4)	4503(3)	8471(3)	52(7)

Table 3. Bond lengths [Å] and angles [°] for danbph_64

N(1) - C(2)	1.4001(18)
N(1) - B(6)	1.412(2)
N(1) - H(11)	0.8800
C(2) - C(3)	1.422(2)
C(2) - C(19)	1.377(2)
C(3) - C(4)	1.420(2)
C(3) - C(16)	1.422(2)
C(4) - N(5)	1.3956(19)
C(4) - C(13)	1.378(2)
N(5) - B(6)	1.416(2)
N(5) - H(51)	0.8900
B(6) - C(7)	1.562(2)
C(7) - C(8)	1.393(2)
C(7) - C(12)	1.393(2)
C(8) - C(9)	1.385(2)
C(8) - H(81)	0.9700
C(9) - C(10)	1.377(3)
C(9) - H(91)	0.9800
C(10) - C(11)	1.376(3)
C(10) - H(101)	0.9500
C(11) - C(12)	1.383(2)
C(11) - H(111)	0.9400
C(12) - H(121)	0.9700
C(13) - C(14)	1.401(2)
C(13) - H(131)	0.9700
C(14) - C(15)	1.356(3)
C(14) - H(141)	0.9600
C(15) - C(16)	1.412(3)
C(15) - H(151)	0.9400
C(16) - C(17)	1.413(3)
C(17) - C(18)	1.356(3)
C(17) - H(171)	0.9600
C(18) - C(19)	1.400(2)
C(18) - H(181)	0.9600

C(19) - H(191) 0.9600

C(2) - N(1) - B(6) 123.84(13)
C(2) - N(1) - H(11) 117.0
B(6) - N(1) - H(11) 119.1
N(1) - C(2) - C(3) 117.69(13)
N(1) - C(2) - C(19) 122.02(14)
C(3) - C(2) - C(19) 120.29(14)
C(2) - C(3) - C(4) 121.16(12)
C(2) - C(3) - C(16) 119.17(14)
C(4) - C(3) - C(16) 119.67(14)
C(3) - C(4) - N(5) 117.75(13)
C(3) - C(4) - C(13) 120.18(14)
N(5) - C(4) - C(13) 122.08(15)
C(4) - N(5) - B(6) 123.93(14)
C(4) - N(5) - H(51) 117.3
B(6) - N(5) - H(51) 118.7
N(1) - B(6) - N(5) 115.57(13)
N(1) - B(6) - C(7) 122.37(13)
N(5) - B(6) - C(7) 122.03(14)
B(6) - C(7) - C(8) 121.53(14)
B(6) - C(7) - C(12) 121.48(14)
C(8) - C(7) - C(12) 116.95(14)
C(7) - C(8) - C(9) 121.70(16)
C(7) - C(8) - H(81) 119.6
C(9) - C(8) - H(81) 118.7
C(8) - C(9) - C(10) 120.09(17)
C(8) - C(9) - H(91) 119.3
C(10) - C(9) - H(91) 120.6
C(9) - C(10) - C(11) 119.32(15)
C(9) - C(10) - H(101) 120.5
C(11) - C(10) - H(101) 120.2
C(10) - C(11) - C(12) 120.50(17)
C(10) - C(11) - H(111) 119.3
C(12) - C(11) - H(111) 120.2
C(7) - C(12) - C(11) 121.42(16)
C(7) - C(12) - H(121) 120.1

C(11) - C(12) - H(121) 118.4
C(4) - C(13) - C(14) 119.49(18)
C(4) - C(13) - H(131) 120.4
C(14) - C(13) - H(131) 120.1
C(13) - C(14) - C(15) 121.63(18)
C(13) - C(14) - H(141) 118.6
C(15) - C(14) - H(141) 119.8
C(14) - C(15) - C(16) 120.91(16)
C(14) - C(15) - H(151) 120.7
C(16) - C(15) - H(151) 118.4
C(3) - C(16) - C(15) 118.13(16)
C(3) - C(16) - C(17) 118.52(16)
C(15) - C(16) - C(17) 123.35(16)
C(16) - C(17) - C(18) 120.87(16)
C(16) - C(17) - H(171) 117.9
C(18) - C(17) - H(171) 121.2
C(17) - C(18) - C(19) 121.40(17)
C(17) - C(18) - H(181) 120.3
C(19) - C(18) - H(181) 118.3
C(2) - C(19) - C(18) 119.74(17)
C(2) - C(19) - H(191) 119.0
C(18) - C(19) - H(191) 121.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for danbph_64. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^1	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	46(1)	46(1)	38(8)	8(2)	14(6)	-1(1)
C(2)	42(1)	47(5)	35(8)	-0.5(7)	18(2)	1(3)
C(3)	42(4)	45(2)	35(6)	0.1(6)	19(1)	6(3)
C(4)	45(3)	45(5)	40(1)	5(4)	21(2)	8(4)
N(5)	40(2)	52(9)	50(6)	13(1)	18(1)	1(6)
B(6)	41(5)	41(7)	38(7)	2(9)	19(4)	3(3)
C(7)	41(1)	40(3)	39(1)	3(1)	19(3)	4(1)
C(8)	47(9)	48(1)	44(5)	5(1)	19(1)	1(8)
C(9)	45(1)	58(9)	51(7)	-2(7)	19(1)	-4(7)
C(10)	42(2)	62(6)	43(1)	1(1)	15(1)	7(8)
C(11)	52(6)	58(2)	52(8)	17(9)	20(6)	11(2)
C(12)	45(2)	49(3)	55(5)	12(8)	19(1)	1(5)
C(13)	59(1)	54(1)	54(1)	14(2)	29(7)	10(4)
C(14)	71(6)	60(7)	49(1)	17(9)	26(1)	18(8)
C(15)	56(5)	65(1)	42(1)	5(8)	13(4)	17(9)
C(16)	46(3)	55(8)	37(4)	-2(2)	16(8)	11(1)
C(17)	42(2)	73(2)	45(5)	-7(4)	14(1)	5(5)
C(18)	45(4)	72(9)	54(8)	-7(1)	22(5)	-8(2)
C(19)	49(5)	61(1)	48(8)	1(2)	25(1)	-3(6)

9.2. 2-(4-Chlorophenyl)-naphtho[1,8-de][1,3,2]diazaborinane *65*

Table 1. Crystal data and structure refinement for danbphcl_65.

Identification code	danbphcl_65	
Empirical formula	C16 H12 B Cl N2	
Formula weight	278.54	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 4.716(5) Å	a= 90.000(5)°.
	b = 10.281(5) Å	b= 96.554(5)°.
	c = 13.571(5) Å	g = 90.000(5)°.
Volume	653.7(8) $Å^3$	
Z	2	
Density (calculated)	1.415 Mg/m^3	
Absorption coefficient	0.280 mm^{-1}	
F(000)	288	
Crystal size	0.40 x 0.15 x 0.07 mm^3	
Theta range for data collection	3.61 to 26.05°.	
Index ranges	-5<=h<=5, -12<=k<=11, -16<=l<=16	
Reflections collected	4902	
Independent reflections	2286 [R(int) = 0.0266]	
Completeness to theta = 25.00°	99.8 %	
Max. and min. transmission	0.9807 and 0.8962	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2286 / 1 / 189	
Goodness-of-fit on F^2	0.997	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0945	
R indices (all data)	R1 = 0.0445, wR2 = 0.0977	
Absolute structure parameter	0.05(7)	
Largest diff. peak and hole	0.153 and -0.248 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x10^3) for danbphcl_65. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl	-10368(1)	4127(1)	4250(1)	55(1)
N(2)	-1196(4)	9013(2)	3043(1)	40(1)
N(1)	-1813(4)	7869(2)	1503(2)	39(1)
C(9)	1391(4)	9690(2)	1708(2)	35(1)
C(005)	105(4)	8681(2)	1103(2)	36(1)
C(5)	3366(5)	10540(2)	1326(2)	39(1)
C(10)	-4634(5)	7024(2)	2924(2)	36(1)
C(1)	738(5)	9863(2)	2695(2)	36(1)
C(6)	4036(5)	10340(2)	348(2)	45(1)
C(7)	2761(5)	9356(3)	-213(2)	49(1)
C(8)	804(5)	8527(2)	147(2)	46(1)
C(14)	-6900(5)	6218(3)	4322(2)	47(1)
C(13)	-8199(4)	5247(2)	3739(2)	39(1)
C(2)	2031(5)	10847(2)	3277(2)	46(1)
C(11)	-6037(5)	6040(2)	2365(2)	44(1)
C(4)	4629(5)	11536(2)	1945(2)	48(1)
C(12)	-7810(5)	5155(2)	2754(2)	45(1)
C(15)	-5137(5)	7092(3)	3915(2)	49(1)
B	-2545(5)	7993(3)	2482(2)	35(1)
C(3)	3950(6)	11682(2)	2886(2)	50(1)

Table 3. Bond lengths [Å] and angles [°] for danbphcl_65

Cl-C(13)	1.736(2)
N(2)-C(1)	1.384(3)
N(2)-B	1.405(3)
N(2)-H(200)	0.78(2)
N(1)-C(005)	1.386(3)
N(1)-B	1.416(3)
N(1)-H(100)	0.82(3)
C(9)-C(005)	1.416(3)
C(9)-C(5)	1.418(3)
C(9)-C(1)	1.419(3)
C(005)-C(8)	1.384(3)
C(5)-C(4)	1.411(3)
C(5)-C(6)	1.414(3)
C(10)-C(11)	1.387(3)
C(10)-C(15)	1.393(3)
C(10)-B	1.567(3)
C(1)-C(2)	1.382(3)
C(6)-C(7)	1.364(4)
C(6)-H(6)	0.9300
C(7)-C(8)	1.385(3)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(14)-C(13)	1.373(3)
C(14)-C(15)	1.382(3)
C(14)-H(14)	0.9300
C(13)-C(12)	1.373(3)
C(2)-C(3)	1.395(3)
C(2)-H(2)	0.9300
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.9300
C(4)-C(3)	1.361(3)
C(4)-H(4)	0.9300
C(12)-H(12)	0.9300
C(15)-H(15)	0.9300
C(3)-H(3)	0.9300

C(1)-N(2)-B	124.20(18)
C(1)-N(2)-H(200)	113(2)
B-N(2)-H(200)	123(2)
C(005)-N(1)-B	123.6(2)
C(005)-N(1)-H(100)	114.6(17)
B-N(1)-H(100)	121.7(17)
C(005)-C(9)-C(5)	119.67(19)
C(005)-C(9)-C(1)	120.99(19)
C(5)-C(9)-C(1)	119.3(2)
C(8)-C(005)-N(1)	122.3(2)
C(8)-C(005)-C(9)	119.74(19)
N(1)-C(005)-C(9)	117.99(19)
C(4)-C(5)-C(6)	122.6(2)
C(4)-C(5)-C(9)	118.7(2)
C(6)-C(5)-C(9)	118.7(2)
C(11)-C(10)-C(15)	116.2(2)
C(11)-C(10)-B	122.39(18)
C(15)-C(10)-B	121.4(2)
C(2)-C(1)-N(2)	122.2(2)
C(2)-C(1)-C(9)	120.1(2)
N(2)-C(1)-C(9)	117.69(19)
C(7)-C(6)-C(5)	120.1(2)
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	121.9(2)
C(6)-C(7)-H(7)	119.1
C(8)-C(7)-H(7)	119.1
C(005)-C(8)-C(7)	120.0(2)
C(005)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(13)-C(14)-C(15)	119.4(2)
C(13)-C(14)-H(14)	120.3
C(15)-C(14)-H(14)	120.3
C(12)-C(13)-C(14)	120.7(2)
C(12)-C(13)-Cl	119.54(18)
C(14)-C(13)-Cl	119.78(18)

C(1)-C(2)-C(3)	119.8(2)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(12)-C(11)-C(10)	122.9(2)
C(12)-C(11)-H(11)	118.5
C(10)-C(11)-H(11)	118.5
C(3)-C(4)-C(5)	120.7(2)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(13)-C(12)-C(11)	118.8(2)
C(13)-C(12)-H(12)	120.6
C(11)-C(12)-H(12)	120.6
C(14)-C(15)-C(10)	122.0(2)
C(14)-C(15)-H(15)	119.0
C(10)-C(15)-H(15)	119.0
N(2)-B-N(1)	115.57(19)
N(2)-B-C(10)	122.17(18)
N(1)-B-C(10)	122.2(2)
C(4)-C(3)-C(2)	121.4(2)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for danbphcl_65. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl	57(1)	52(1)	56(1)	7(1)	13(1)	-13(1)
N(2)	44(1)	45(1)	32(1)	-2(1)	11(1)	-4(1)
N(1)	43(1)	41(1)	34(1)	-3(1)	6(1)	-6(1)
C(9)	34(1)	34(1)	36(1)	3(1)	2(1)	7(1)
C(005)	34(1)	39(1)	35(1)	3(1)	5(1)	3(1)
C(5)	36(1)	36(1)	44(1)	9(1)	2(1)	4(1)
C(10)	35(1)	37(1)	35(1)	4(1)	5(1)	4(1)
C(1)	35(1)	34(1)	40(1)	2(1)	5(1)	3(1)
C(6)	49(1)	47(1)	40(1)	12(1)	11(1)	1(1)
C(7)	55(1)	58(2)	36(1)	6(1)	12(1)	4(1)
C(8)	53(1)	52(1)	34(1)	-6(1)	9(1)	-3(1)
C(14)	56(1)	54(2)	33(1)	-3(1)	11(1)	-10(1)
C(13)	35(1)	38(1)	44(1)	6(1)	5(1)	2(1)
C(2)	52(1)	45(1)	42(1)	-5(1)	7(1)	-2(1)
C(11)	52(1)	47(2)	34(1)	-1(1)	9(1)	-4(1)
C(4)	51(1)	39(1)	55(2)	9(1)	7(1)	-2(1)
C(12)	52(1)	44(1)	40(1)	-4(1)	2(1)	-7(1)
C(15)	55(2)	51(2)	40(1)	-9(1)	7(1)	-14(1)
B	32(1)	36(1)	36(1)	5(1)	4(1)	3(1)
C(3)	55(2)	42(2)	51(2)	-5(1)	1(1)	-9(1)

9.3. 2-(4-Methylphenyl)-naphtho[1,8-de][1,3,2]diazaborinane *67*

Table 1. Crystal data and structure refinement for danbtol_67

Identification code	danbtol_67	
Empirical formula	C17 H15 B N2	
Formula weight	258.12	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.7838(18) Å	a= 90°.
	b = 10.1485(10) Å	b= 112.991(16)°.
	c = 13.5349(17) Å	g = 90°.
Volume	1363.6(3) $Å^3$	
Z	4	
Density (calculated)	1.257 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	544	
Crystal size	0.40 x 0.25 x 0.10 mm^3	
Theta range for data collection	2.88 to 28.75°.	
Index ranges	-8<=h<=13, -13<=k<=11, -17<=l<=18	
Reflections collected	6057	
Independent reflections	2855 [R(int) = 0.0397]	
Completeness to theta = 25.00°	92.9 %	
Max. and min. transmission	0.9927 and 0.9712	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2855 / 0 / 190	
Goodness-of-fit on F^2	0.903	
Final R indices [I>2sigma(I)]	R1 = 0.0575, wR2 = 0.1510	
R indices (all data)	R1 = 0.0918, wR2 = 0.1688	
Largest diff. peak and hole	0.194 and -0.317 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for danbtol_67. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6948(2)	2784(1)	685(1)	46(1)
N(2)	7114(2)	790(2)	1665(1)	46(1)
C(10)	9125(2)	1990(2)	1865(1)	39(1)
C(11)	4700(2)	1661(2)	478(1)	43(1)
C(1)	8335(2)	2976(2)	1149(1)	40(1)
C(9)	8514(2)	871(2)	2120(1)	41(1)
C(14)	1852(2)	1713(2)	-255(2)	54(1)
C(15)	2522(2)	2414(2)	-780(2)	54(1)
C(5)	10550(2)	2138(2)	2348(1)	46(1)
C(2)	8952(2)	4065(2)	941(1)	50(1)
C(16)	3907(2)	2391(2)	-417(2)	51(1)
C(8)	9310(2)	-71(2)	2815(2)	53(1)
C(12)	4013(2)	948(2)	986(2)	57(1)
C(13)	2634(2)	981(2)	629(2)	63(1)
C(6)	11317(2)	1142(2)	3048(2)	57(1)
C(3)	10347(2)	4197(2)	1411(2)	57(1)
C(4)	11137(2)	3267(2)	2095(2)	56(1)
C(7)	10704(2)	72(2)	3265(2)	59(1)
C(17)	342(2)	1743(2)	-650(2)	74(1)
B(1)	6270(2)	1721(2)	934(2)	42(1)

Table 3. Bond lengths [Å] and angles [°] for danbtol_67.

N(1)-C(1)	1.391(2)
N(1)-B(1)	1.417(2)
N(1)-H(100)	0.92(2)
N(2)-C(9)	1.392(2)
N(2)-B(1)	1.413(3)
N(2)-H(200)	0.86(2)
C(10)-C(9)	1.420(2)
C(10)-C(1)	1.422(2)
C(10)-C(5)	1.424(2)
C(11)-C(16)	1.392(2)
C(11)-C(12)	1.394(3)
C(11)-B(1)	1.560(3)
C(1)-C(2)	1.375(2)
C(9)-C(8)	1.381(2)
C(14)-C(13)	1.380(3)
C(14)-C(15)	1.391(3)
C(14)-C(17)	1.503(3)
C(15)-C(16)	1.378(2)
C(15)-H(15)	0.9300
C(5)-C(6)	1.412(3)
C(5)-C(4)	1.414(3)
C(2)-C(3)	1.392(3)
C(2)-H(2)	0.9300
C(16)-H(16)	0.9300
C(8)-C(7)	1.391(3)
C(8)-H(8)	0.9300
C(12)-C(13)	1.373(3)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(6)-C(7)	1.361(3)
C(6)-H(6)	0.9300
C(3)-C(4)	1.363(3)
C(3)-H(3)	0.9300
C(4)-H(4)	0.9300
C(7)-H(7)	0.9300

C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600

C(1)-N(1)-B(1)	124.25(16)
C(1)-N(1)-H(100)	117.3(12)
B(1)-N(1)-H(100)	118.4(12)
C(9)-N(2)-B(1)	124.13(16)
C(9)-N(2)-H(200)	113.6(14)
B(1)-N(2)-H(200)	121.5(14)
C(9)-C(10)-C(1)	121.11(16)
C(9)-C(10)-C(5)	119.53(16)
C(1)-C(10)-C(5)	119.35(16)
C(16)-C(11)-C(12)	116.15(18)
C(16)-C(11)-B(1)	121.79(16)
C(12)-C(11)-B(1)	121.90(17)
C(2)-C(1)-N(1)	122.75(16)
C(2)-C(1)-C(10)	119.74(17)
N(1)-C(1)-C(10)	117.51(15)
C(8)-C(9)-N(2)	122.58(17)
C(8)-C(9)-C(10)	119.68(17)
N(2)-C(9)-C(10)	117.73(16)
C(13)-C(14)-C(15)	117.03(18)
C(13)-C(14)-C(17)	122.01(19)
C(15)-C(14)-C(17)	120.96(19)
C(16)-C(15)-C(14)	121.03(18)
C(16)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(6)-C(5)-C(4)	122.86(19)
C(6)-C(5)-C(10)	118.46(17)
C(4)-C(5)-C(10)	118.67(17)
C(1)-C(2)-C(3)	120.46(18)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(15)-C(16)-C(11)	122.14(17)
C(15)-C(16)-H(16)	118.9
C(11)-C(16)-H(16)	118.9

C(9)-C(8)-C(7)	120.26(18)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(13)-C(12)-C(11)	121.65(19)
C(13)-C(12)-H(12)	119.2
C(11)-C(12)-H(12)	119.2
C(12)-C(13)-C(14)	121.99(19)
C(12)-C(13)-H(13)	119.0
C(14)-C(13)-H(13)	119.0
C(7)-C(6)-C(5)	120.62(18)
C(7)-C(6)-H(6)	119.7
C(5)-C(6)-H(6)	119.7
C(4)-C(3)-C(2)	121.42(18)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	120.34(18)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(6)-C(7)-C(8)	121.43(18)
C(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(2)-B(1)-N(1)	115.12(18)
N(2)-B(1)-C(11)	123.64(17)
N(1)-B(1)-C(11)	121.12(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for danbtol_67. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	39(1)	48(1)	48(1)	7(1)	14(1)	2(1)
N(2)	45(1)	43(1)	45(1)	2(1)	14(1)	-5(1)
C(10)	41(1)	44(1)	34(1)	-5(1)	15(1)	2(1)
C(11)	40(1)	47(1)	41(1)	-2(1)	15(1)	-2(1)
C(1)	39(1)	46(1)	37(1)	-4(1)	16(1)	-1(1)
C(9)	43(1)	43(1)	36(1)	-5(1)	14(1)	2(1)
C(14)	42(1)	65(1)	57(1)	-16(1)	20(1)	-3(1)
C(15)	46(1)	59(1)	50(1)	0(1)	12(1)	2(1)
C(5)	41(1)	57(1)	38(1)	-9(1)	12(1)	2(1)
C(2)	51(1)	49(1)	49(1)	3(1)	17(1)	-5(1)
C(16)	48(1)	54(1)	50(1)	3(1)	18(1)	-3(1)
C(8)	59(1)	48(1)	43(1)	4(1)	13(1)	4(1)
C(12)	47(1)	71(1)	52(1)	12(1)	19(1)	-1(1)
C(13)	50(2)	85(2)	58(1)	6(1)	26(1)	-7(1)
C(6)	40(1)	73(1)	48(1)	-7(1)	7(1)	7(1)
C(3)	54(1)	60(1)	57(1)	-4(1)	21(1)	-18(1)
C(4)	39(1)	71(1)	57(1)	-11(1)	16(1)	-11(1)
C(7)	58(2)	61(1)	45(1)	3(1)	7(1)	16(1)
C(17)	45(2)	100(2)	76(2)	-16(1)	23(1)	-1(1)
B(1)	43(1)	46(1)	39(1)	-4(1)	19(1)	-1(1)

9.4. 2-[4-(Methylsulfanyl)phenyl]-naphtho[1,8-de][1,3,2]diazaborinane *68*

Table 1. Crystal data and structure refinement for danbphs_68.

Identification code	danbphs_68	
Empirical formula	C17 H15 B N2 S	
Formula weight	290.18	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.7594(6) Å	a= 90°.
	b = 9.0545(3) Å	b= 113.411(5)°.
	c = 12.7830(5) Å	g = 90°.
Volume	1461.46(10) $Å^3$	
Z	4	
Density (calculated)	1.319 Mg/m^3	
Absorption coefficient	0.214 mm^{-1}	
F(000)	608	
Crystal size	0.40 x 0.40 x 0.30 mm^3	
Theta range for data collection	2.84 to 32.07°.	
Index ranges	-19<=h<=20, -12<=k<=12, -16<=l<=18	
Reflections collected	14782	
Independent reflections	4709 [R(int) = 0.0334]	
Completeness to theta = 25.00°	99.9 %	
Max. and min. transmission	0.9385 and 0.9192	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4709 / 0 / 199	
Goodness-of-fit on F^2	0.981	
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1347	
R indices (all data)	R1 = 0.0868, wR2 = 0.1491	
Largest diff. peak and hole	0.415 and -0.485 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for danbphs_68. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(17)	-568(1)	1664(2)	3451(2)	67(1)
S(1)	663(1)	748(1)	4165(1)	70(1)
C(10)	3636(1)	-734(1)	-856(1)	37(1)
C(5)	4167(1)	-889(1)	-1604(1)	39(1)
N(2)	3425(1)	-1414(1)	865(1)	44(1)
C(9)	3951(1)	-1623(2)	140(1)	38(1)
B	2626(1)	-340(2)	681(1)	41(1)
N(1)	2335(1)	488(2)	-335(1)	46(1)
C(1)	2815(1)	327(2)	-1106(1)	40(1)
C(11)	2102(1)	-77(2)	1545(1)	42(1)
C(8)	4765(1)	-2624(2)	370(1)	44(1)
C(14)	1140(1)	426(2)	3101(1)	44(1)
C(6)	4999(1)	-1924(2)	-1326(1)	45(1)
C(4)	3842(1)	9(2)	-2589(1)	49(1)
C(7)	5281(1)	-2761(2)	-369(1)	46(1)
C(2)	2529(1)	1168(2)	-2076(1)	51(1)
C(12)	2577(1)	-528(2)	2684(1)	49(1)
C(15)	640(1)	868(2)	1974(1)	45(1)
C(13)	2117(1)	-280(2)	3444(1)	51(1)
C(16)	1120(1)	626(2)	1221(1)	45(1)
C(3)	3043(1)	991(2)	-2816(1)	53(1)

Table 3. Bond lengths [Å] and angles [°] for danbphs_68.

C(17)-S(1)	1.7790(18)
S(1)-C(14)	1.7533(15)
C(10)-C(1)	1.4190(19)
C(10)-C(9)	1.4211(18)
C(10)-C(5)	1.4230(18)
C(5)-C(6)	1.411(2)
C(5)-C(4)	1.414(2)
N(2)-C(9)	1.3963(17)
N(2)-B	1.416(2)
C(9)-C(8)	1.3776(19)
B-N(1)	1.413(2)
B-C(11)	1.559(2)
N(1)-C(1)	1.3946(18)
C(1)-C(2)	1.373(2)
C(11)-C(16)	1.398(2)
C(11)-C(12)	1.400(2)
C(8)-C(7)	1.3948(19)
C(14)-C(15)	1.386(2)
C(14)-C(13)	1.393(2)
C(6)-C(7)	1.358(2)
C(4)-C(3)	1.353(2)
C(2)-C(3)	1.397(2)
C(12)-C(13)	1.372(2)
C(15)-C(16)	1.385(2)

C(14)-S(1)-C(17)	104.67(8)
C(1)-C(10)-C(9)	121.18(12)
C(1)-C(10)-C(5)	119.38(12)
C(9)-C(10)-C(5)	119.42(12)
C(6)-C(5)-C(4)	122.98(13)
C(6)-C(5)-C(10)	118.54(12)
C(4)-C(5)-C(10)	118.48(13)
C(9)-N(2)-B	123.79(12)
C(8)-C(9)-N(2)	122.61(12)
C(8)-C(9)-C(10)	119.77(12)

N(2)-C(9)-C(10)	117.60(12)
N(1)-B-N(2)	115.76(13)
N(1)-B-C(11)	121.89(13)
N(2)-B-C(11)	122.35(13)
C(1)-N(1)-B	123.61(13)
C(2)-C(1)-N(1)	122.26(13)
C(2)-C(1)-C(10)	119.74(13)
N(1)-C(1)-C(10)	117.99(12)
C(16)-C(11)-C(12)	115.99(13)
C(16)-C(11)-B	121.59(13)
C(12)-C(11)-B	122.42(13)
C(9)-C(8)-C(7)	120.22(13)
C(15)-C(14)-C(13)	118.59(13)
C(15)-C(14)-S(1)	125.00(11)
C(13)-C(14)-S(1)	116.36(12)
C(7)-C(6)-C(5)	120.69(13)
C(3)-C(4)-C(5)	120.75(14)
C(6)-C(7)-C(8)	121.36(14)
C(1)-C(2)-C(3)	120.45(14)
C(13)-C(12)-C(11)	122.17(14)
C(16)-C(15)-C(14)	119.97(13)
C(12)-C(13)-C(14)	120.76(14)
C(15)-C(16)-C(11)	122.50(14)
C(4)-C(3)-C(2)	121.17(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for danbphs_68. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(17)	62(1)	65(1)	85(1)	0(1)	39(1)	10(1)
S(1)	69(1)	94(1)	59(1)	10(1)	37(1)	24(1)
C(10)	41(1)	33(1)	33(1)	-4(1)	12(1)	-6(1)
C(5)	47(1)	36(1)	36(1)	-7(1)	16(1)	-7(1)
N(2)	53(1)	44(1)	41(1)	9(1)	24(1)	6(1)
C(9)	43(1)	35(1)	37(1)	-2(1)	16(1)	-3(1)
B	41(1)	42(1)	41(1)	-1(1)	17(1)	-4(1)
N(1)	45(1)	49(1)	47(1)	6(1)	21(1)	10(1)
C(1)	42(1)	38(1)	38(1)	-1(1)	13(1)	-2(1)
C(11)	41(1)	42(1)	44(1)	0(1)	18(1)	-2(1)
C(8)	53(1)	39(1)	40(1)	4(1)	18(1)	5(1)
C(14)	45(1)	42(1)	50(1)	-1(1)	22(1)	-1(1)
C(6)	52(1)	44(1)	42(1)	-7(1)	23(1)	-3(1)
C(4)	66(1)	45(1)	38(1)	-1(1)	25(1)	-2(1)
C(7)	49(1)	41(1)	48(1)	-4(1)	18(1)	6(1)
C(2)	56(1)	48(1)	46(1)	9(1)	17(1)	10(1)
C(12)	44(1)	54(1)	48(1)	6(1)	20(1)	11(1)
C(15)	37(1)	49(1)	49(1)	1(1)	15(1)	3(1)
C(13)	50(1)	58(1)	45(1)	7(1)	20(1)	9(1)
C(16)	41(1)	50(1)	41(1)	1(1)	13(1)	-2(1)
C(3)	68(1)	50(1)	39(1)	10(1)	17(1)	4(1)