Supporting information

Three-Coordinate Organoboron with a B=N Bond: Substituent Effects, Luminescence/Electroluminescence and Reactions with fluoride

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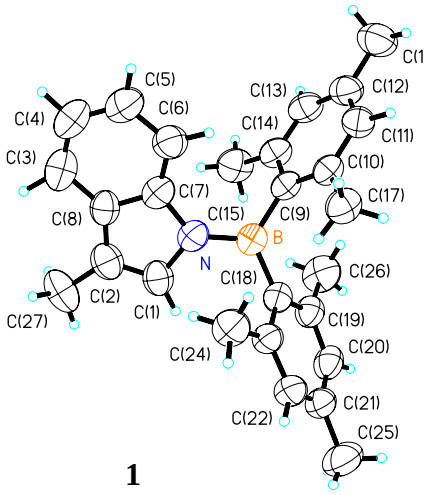
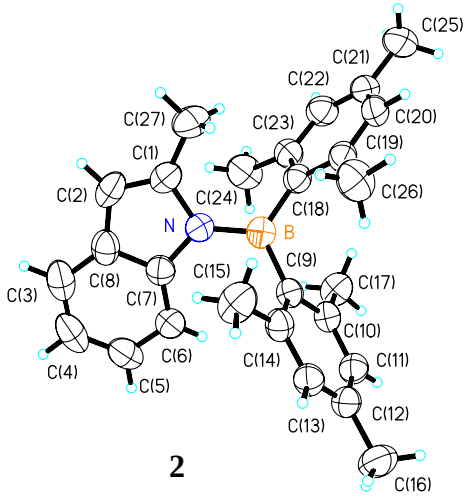
Figure 1S Molecular structures of **1-5** projected down the indolyl plane with labeling schemes with 50% thermal ellipsoids.



1



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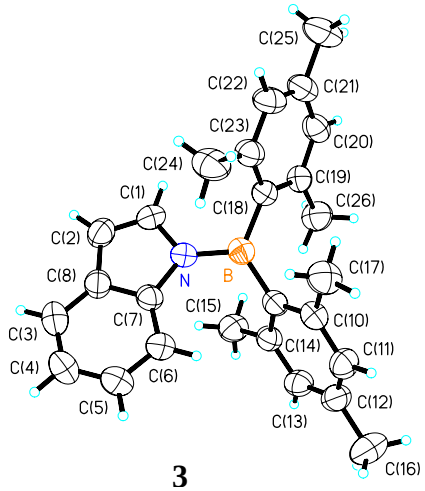

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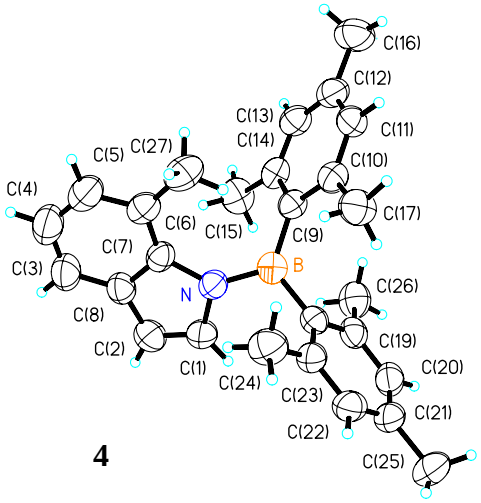
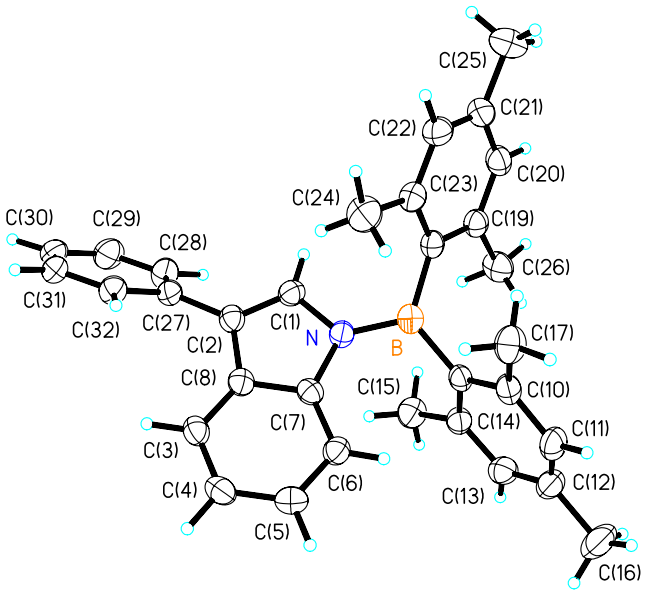


4


C(25)
C(21)
C(22)
C(20)
C(23)
C(24)
C(19)
C(30)
C(29)
C(28)
C(26)
C(31)
C(32)
C(27)
C(1)
N
B
C(17)
C(2)
C(8)
C(15)
C(10)
C(7)
C(14)
C(11)
C(3)
C(6)
C(12)
C(4)
C(13)
C(5)
C(16)

5

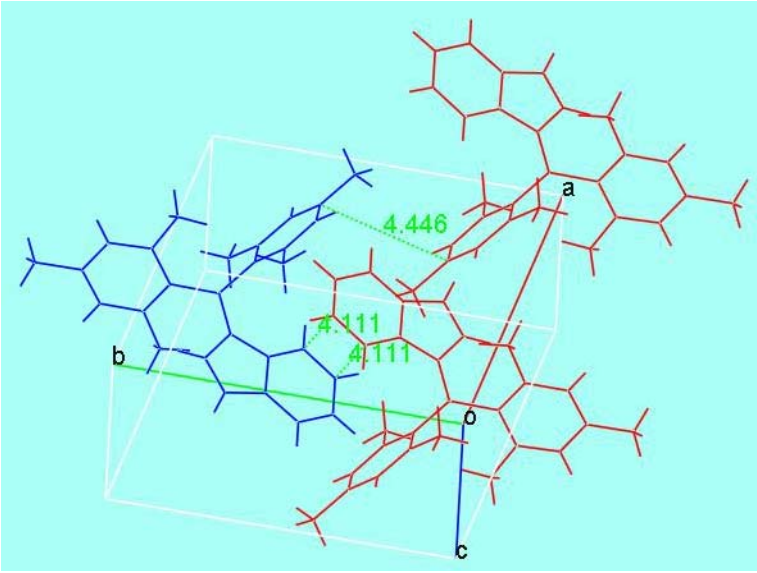


Figure 2S-a Packing diagram of compound **1**

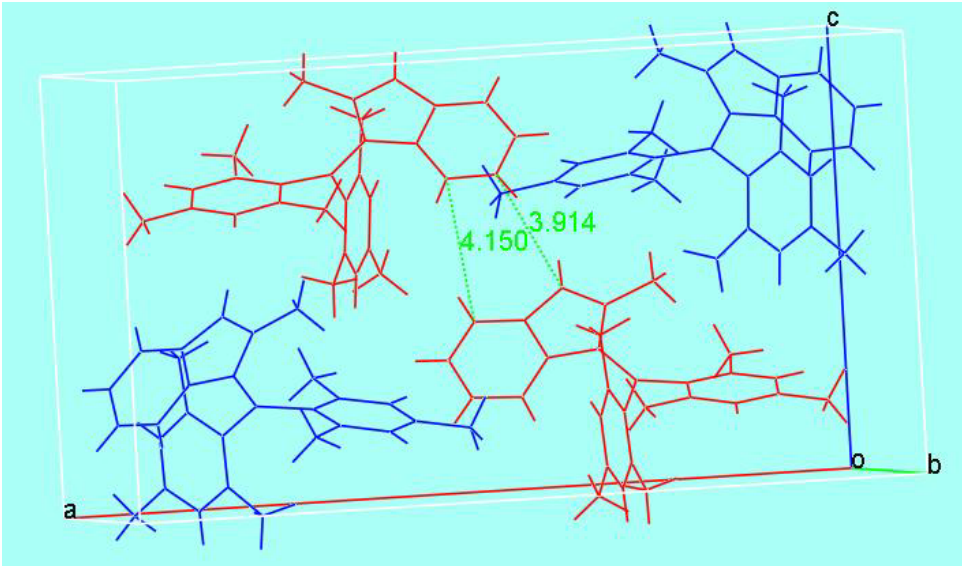


Figure 2S-b Packing diagram of compound **2**

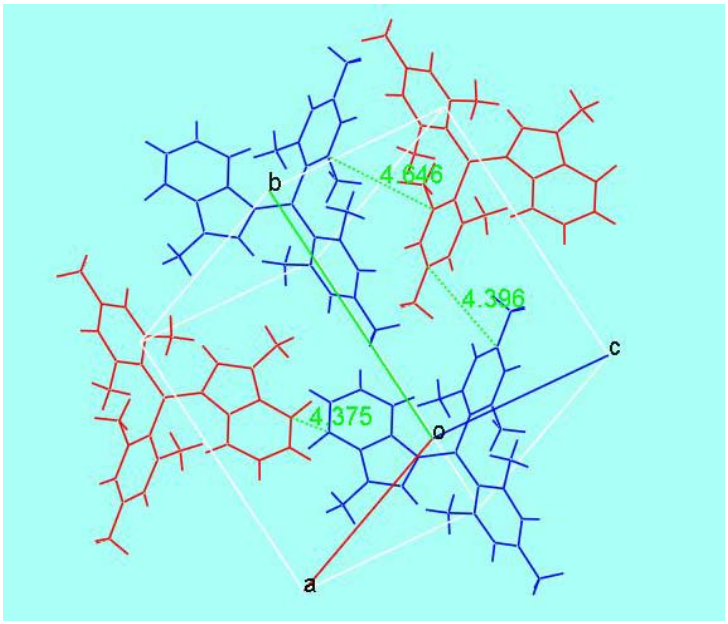


Figure 2S-c Packing diagram of compound **3**

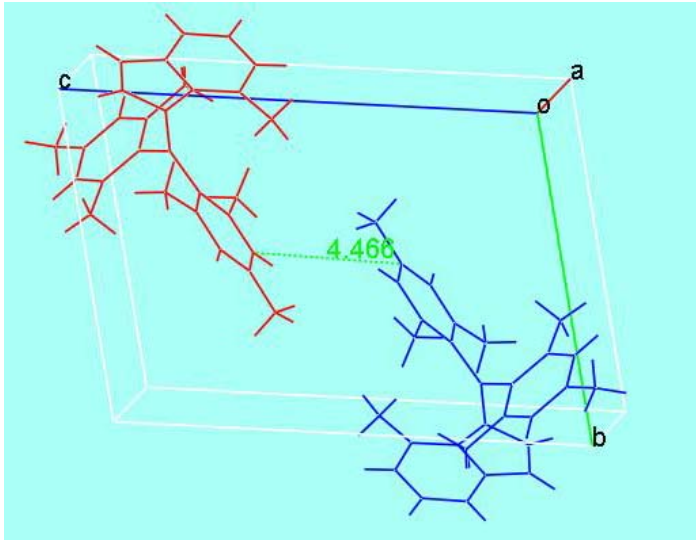


Figure 2S-d Packing diagram of compound **4**

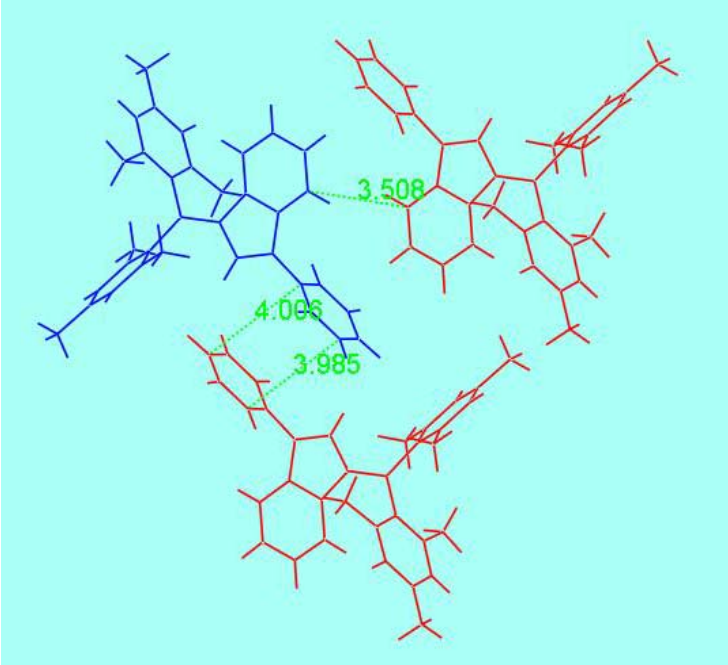


Figure 2S-e Packing diagram of compound **5**

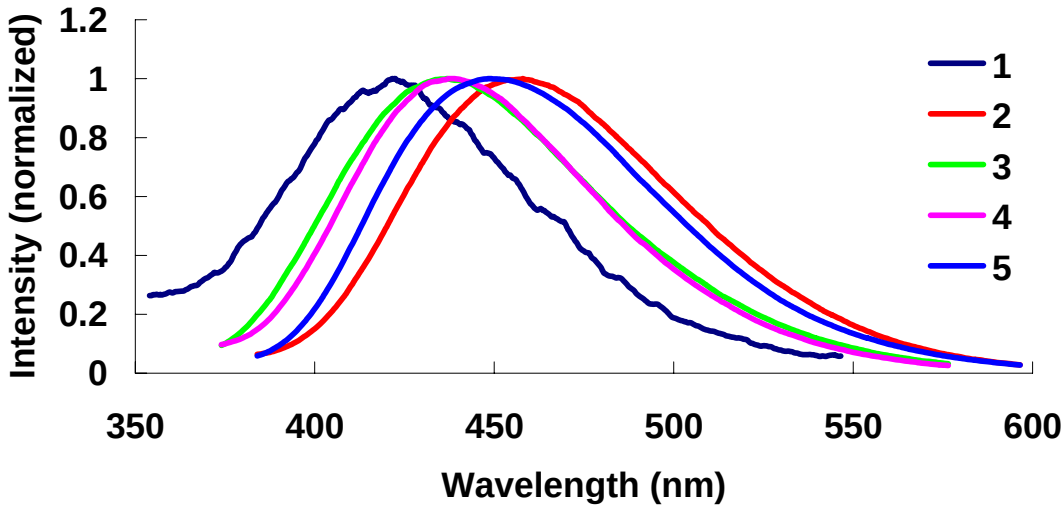
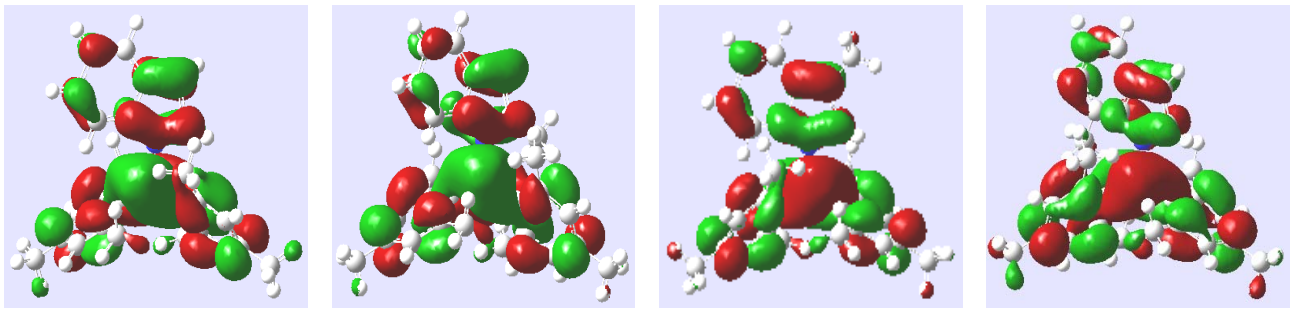
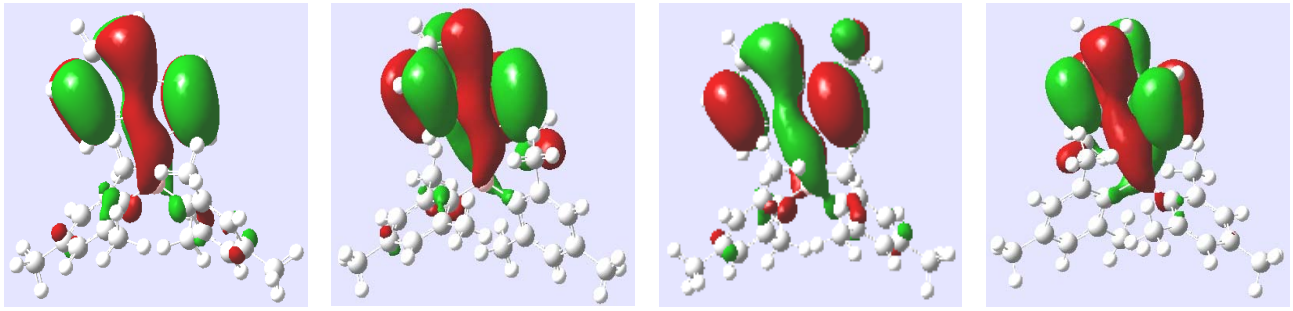


Figure 3s.. The photoluminescent spectra of **1-5** as films at ambient temperature.



..... LUMO.....

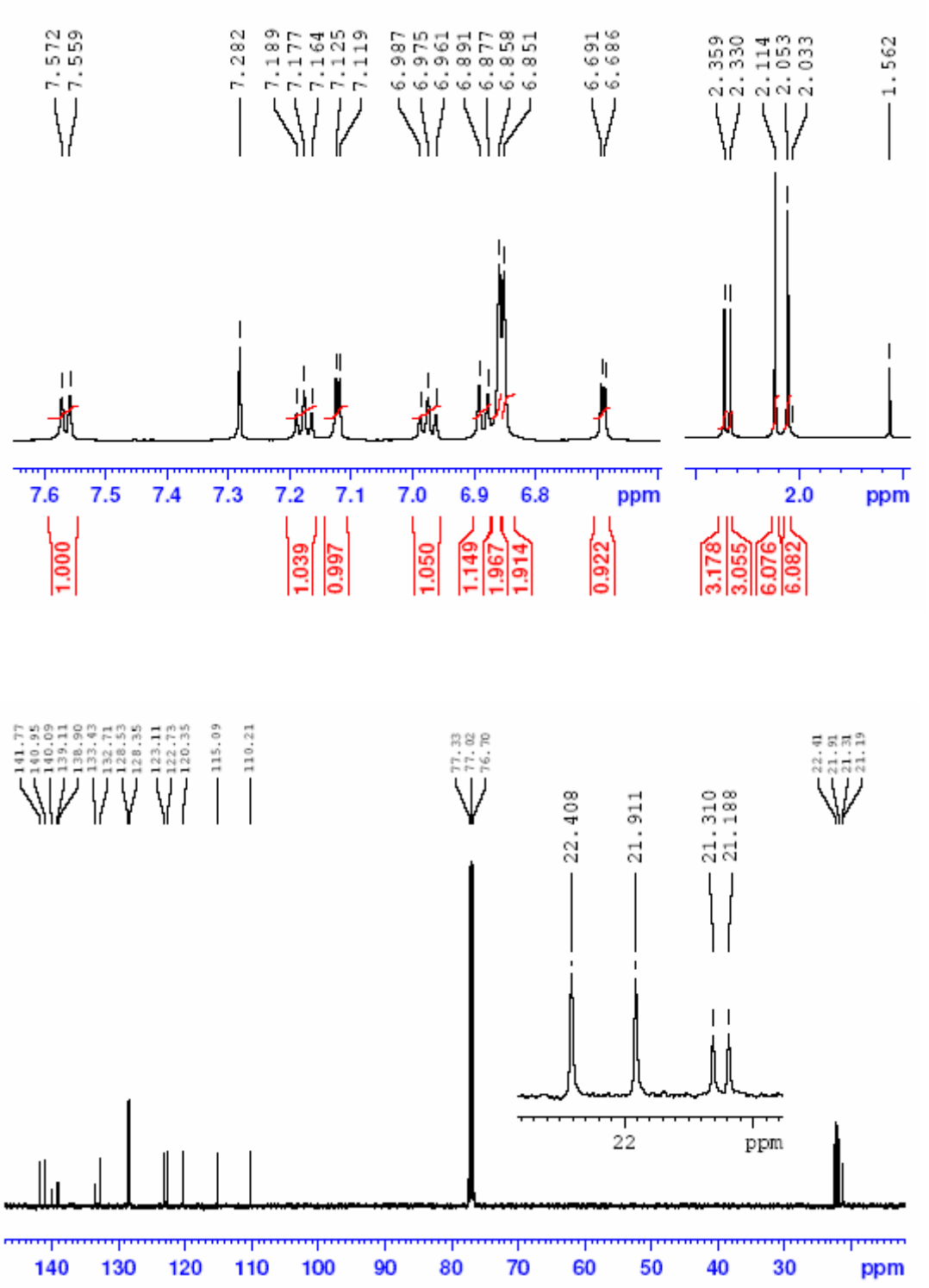


1 2 3 4

..... HOMO.....

Figure 4s. Diagrams showing the HOMO and LUMO levels of compounds **1-4** from optimized structures

Figure 5s. ^{1}H (top) and ^{13}C bottom NMR spectra of **1** at room temperature in $CDCl_3$



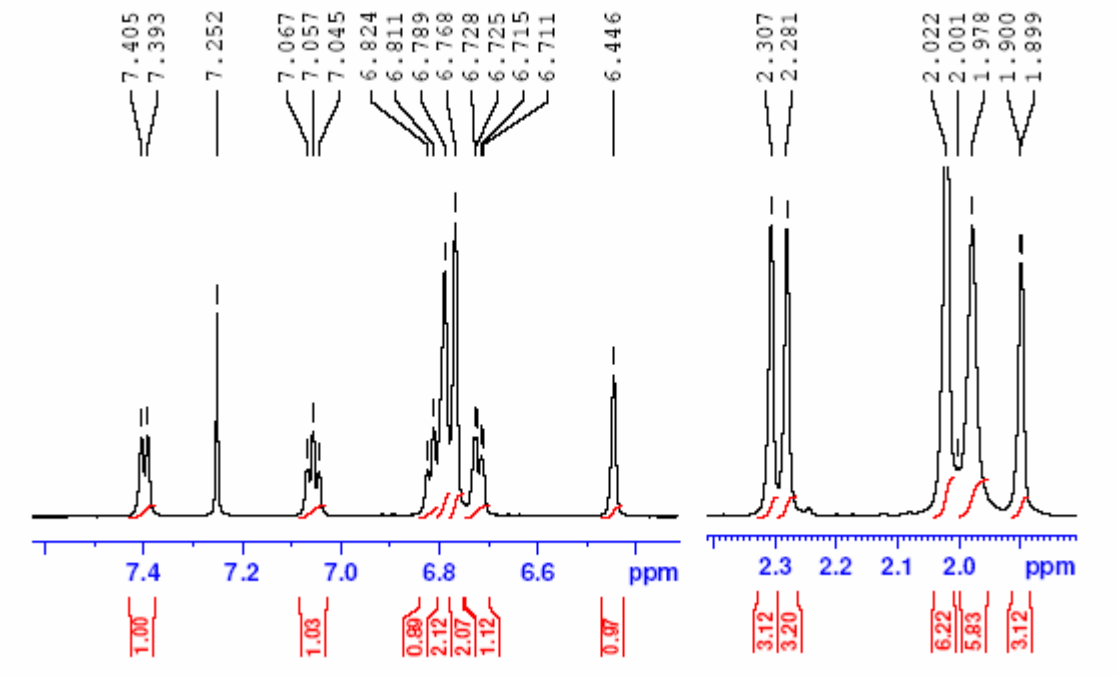


Figure 6S **^{1}H NMR** NMR spectra of **2** at room temperature in $CDCl_3$

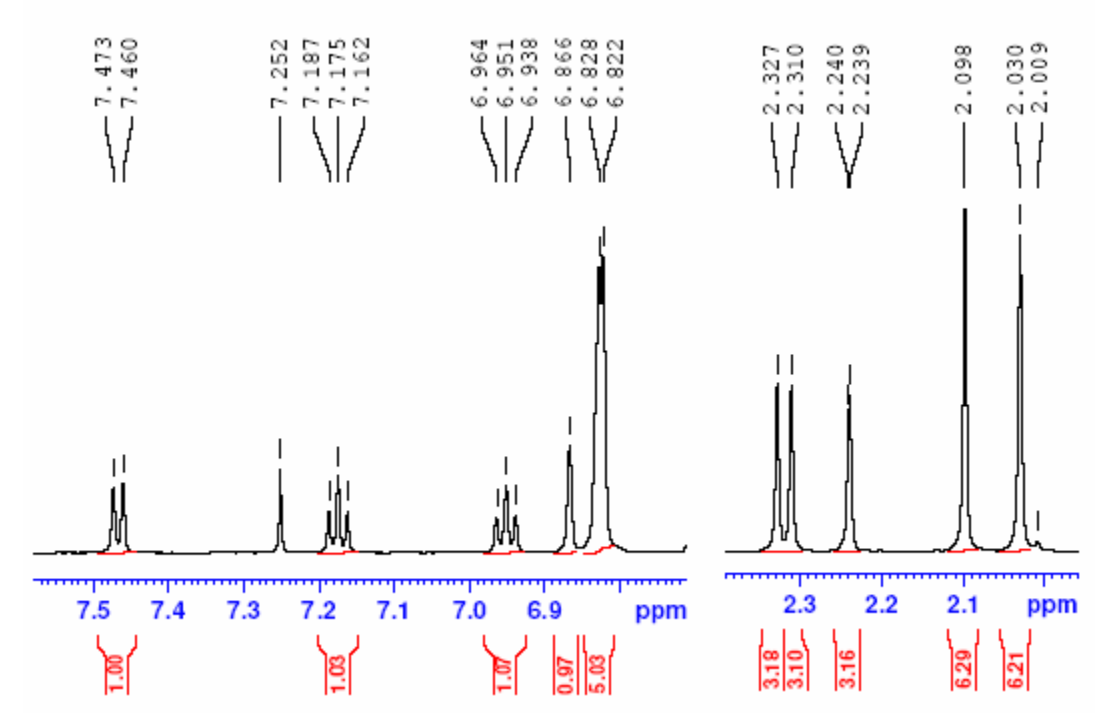


Figure 7S. ^{1}H NMR spectra of **3** at room temperature in $CDCl_3$

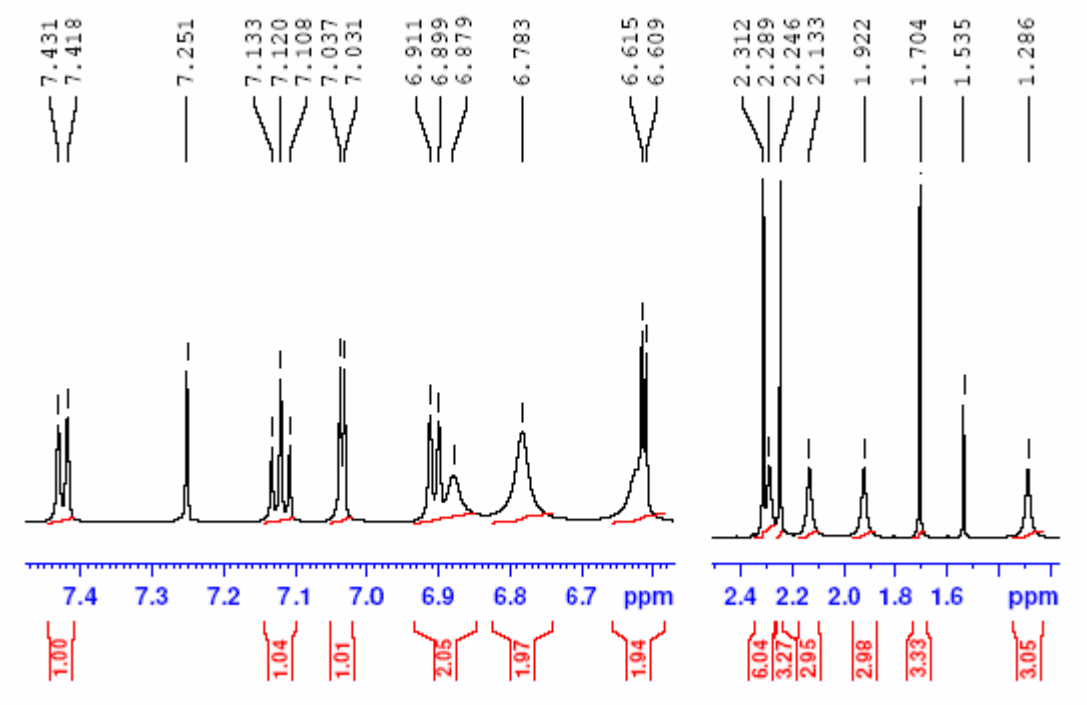


Figure 8S. ^{1}H NMR spectra of **4** at room temperature in $CDCl_3$

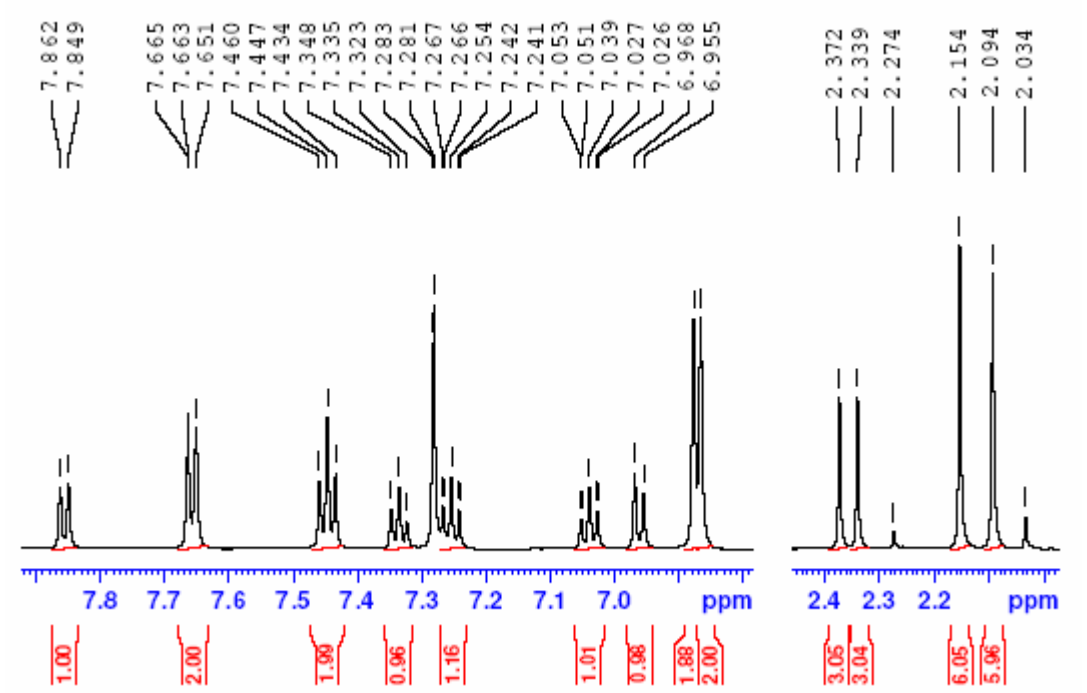


Figure 9S ^{1}H NMR spectra of **5** at room temperature in $CDCl_3$

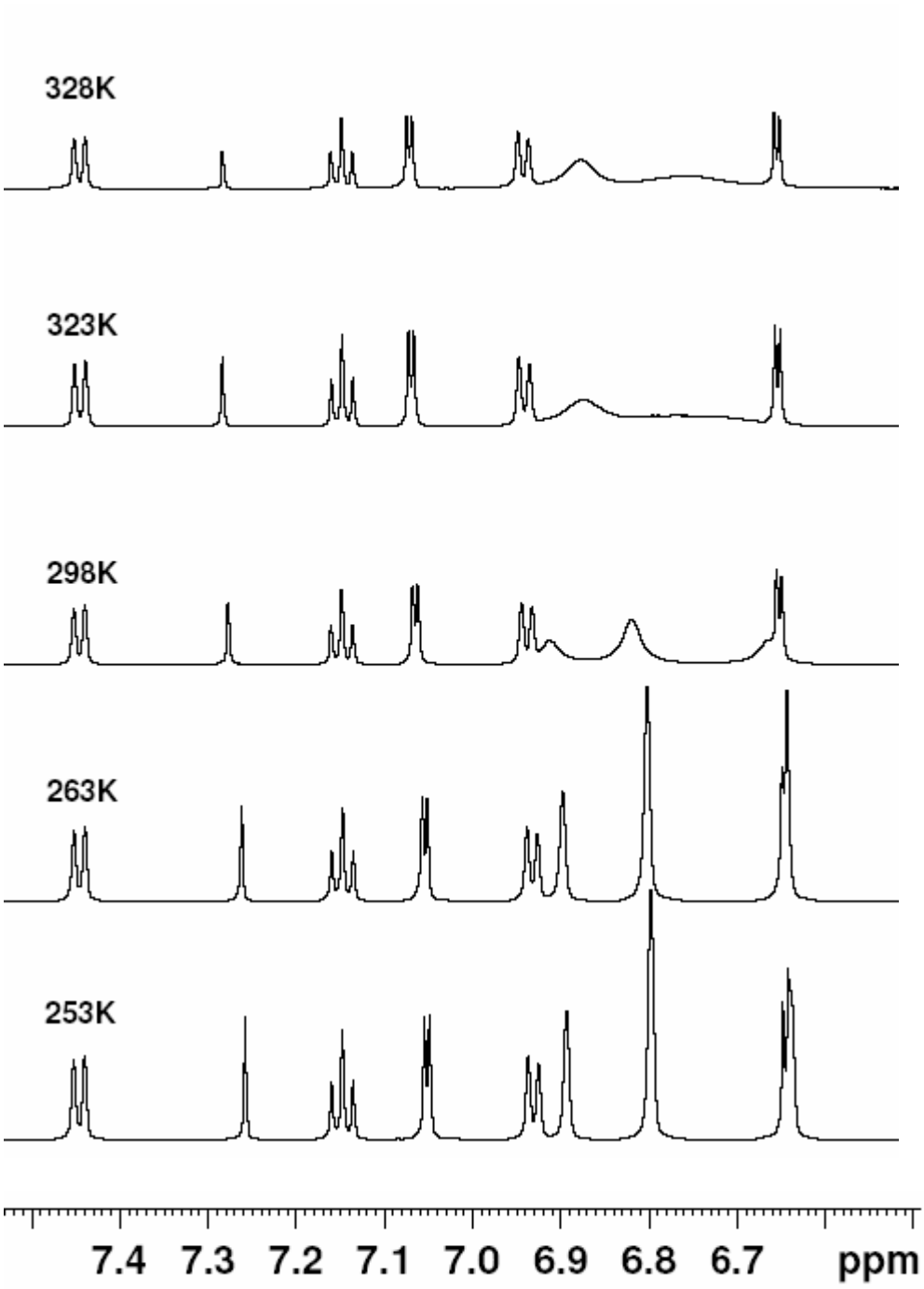


Figure 10s. Variable temperature ^{1}H NMR of **4** in $CDCl_3$ (the aromatic region)

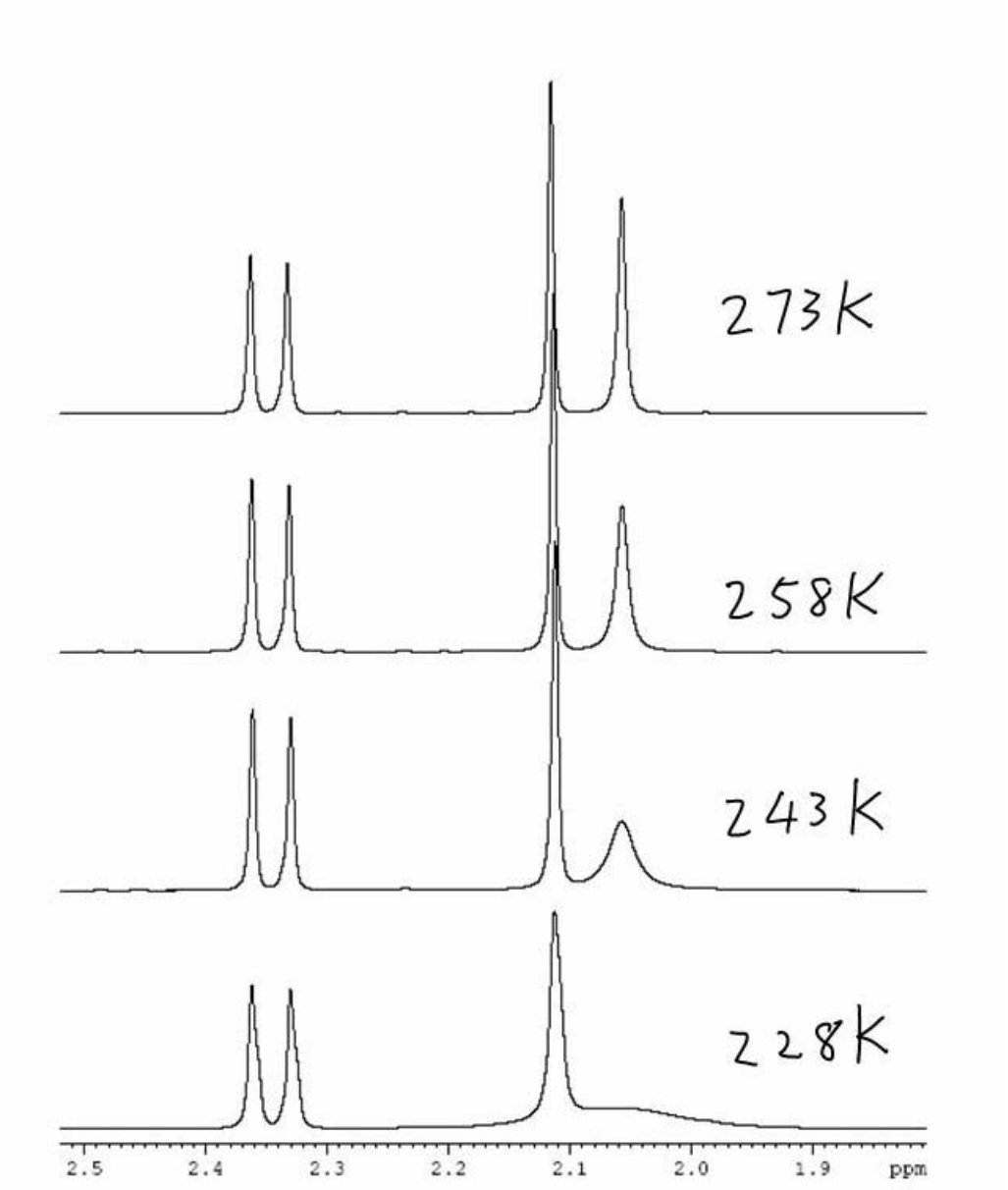
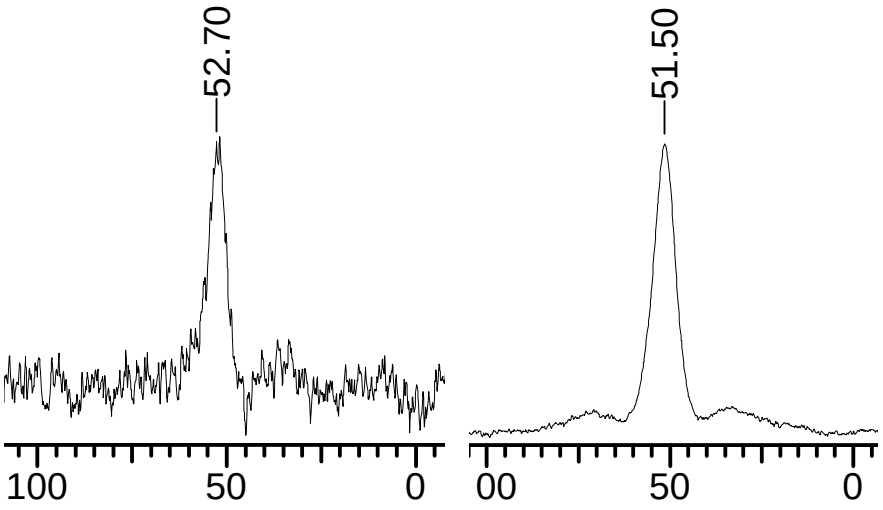


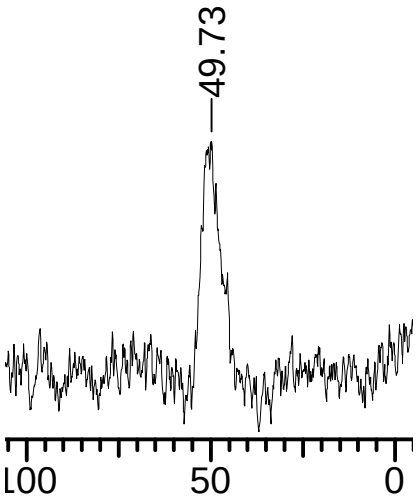
Figure 11s. The variable temperature ^{1}H NMR of **1** in CD_2Cl_2 (the methyl region).

Figure 12s. ^{11}B NMR for 1-5

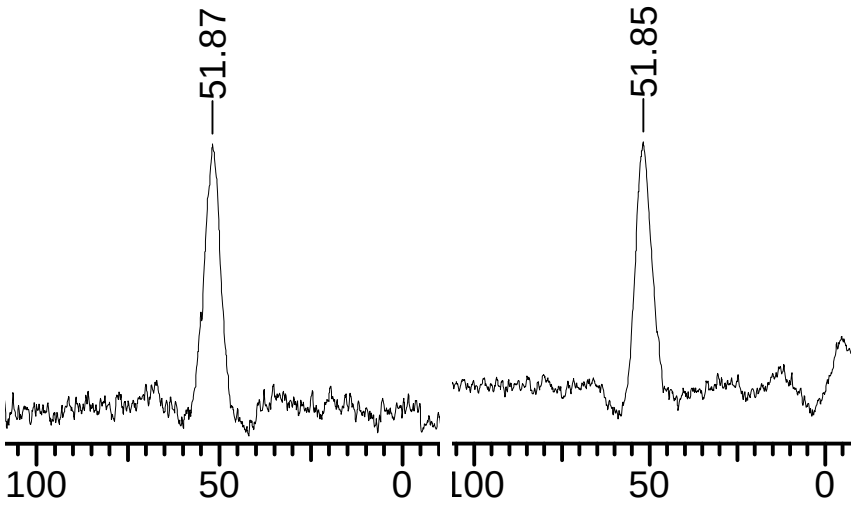


Compound 1

Compound 2

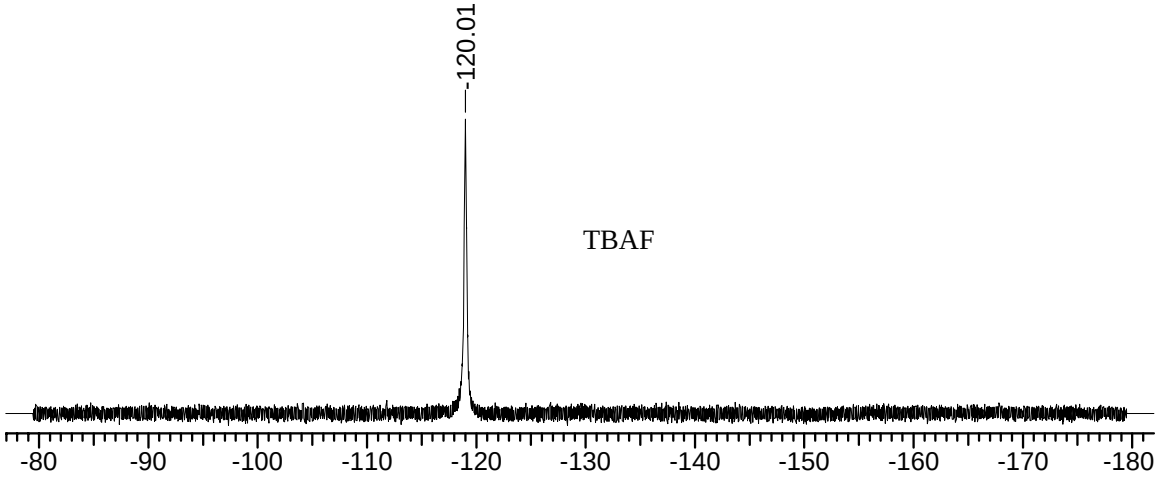


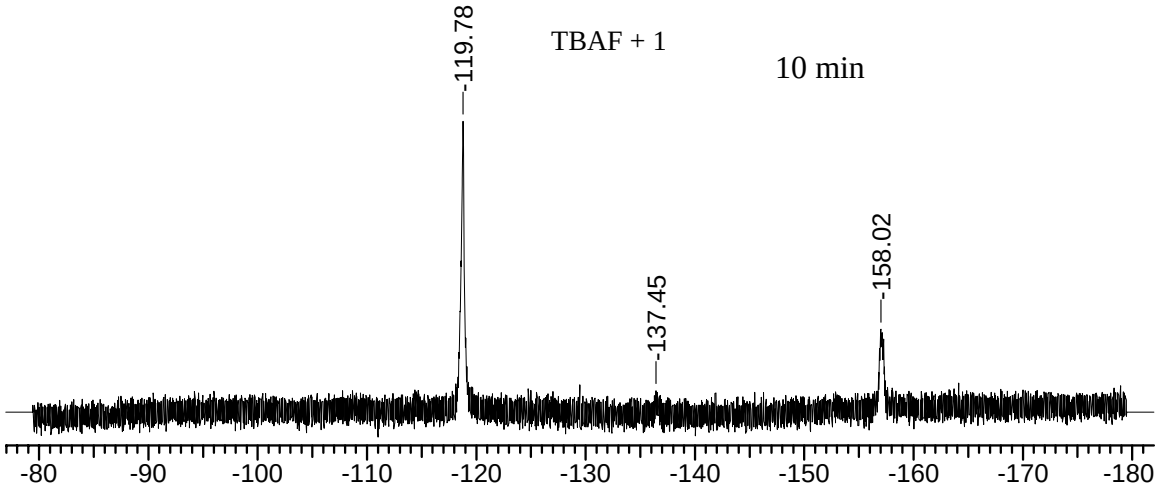
Compound 3

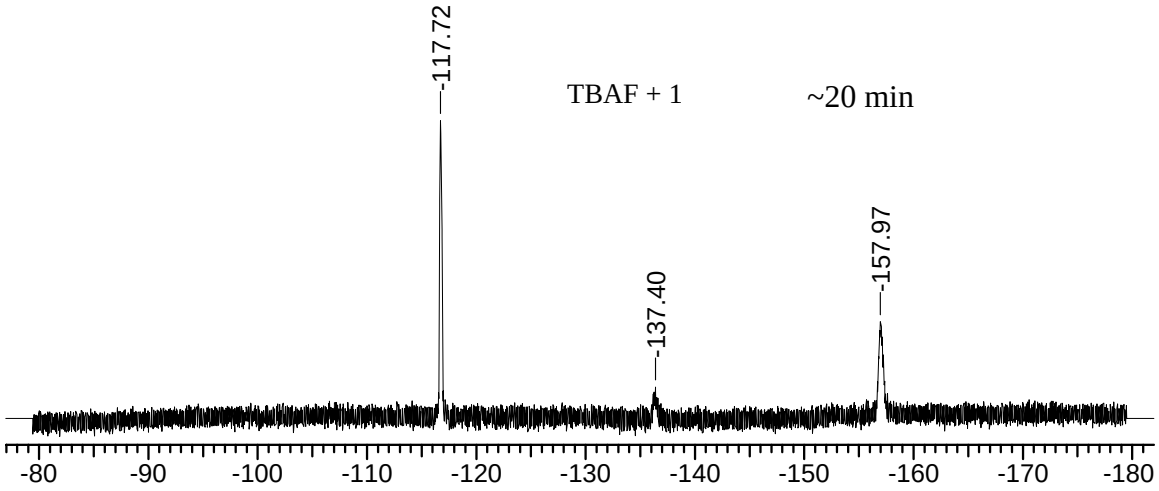


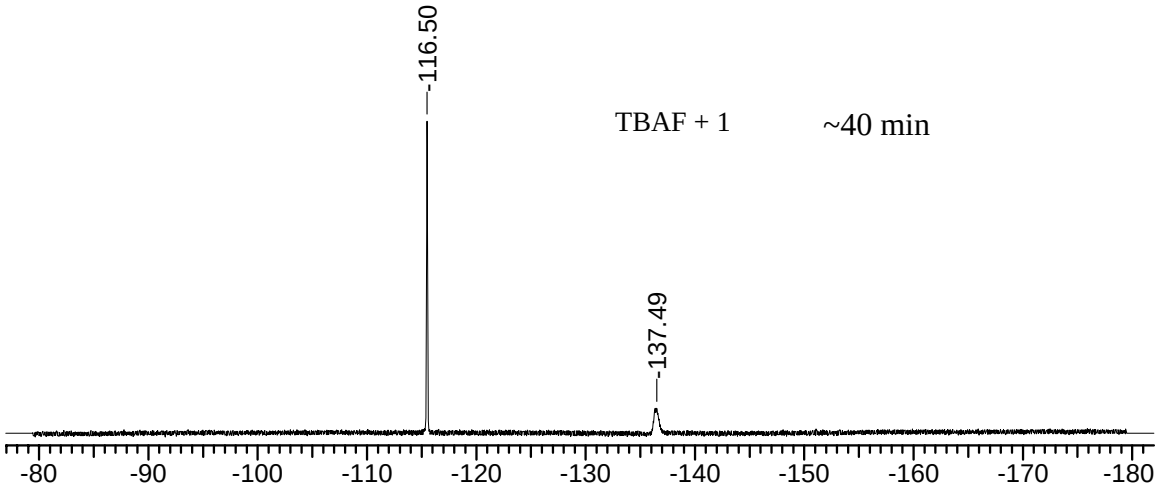
Compound 4 **Compound 5**

Figure 13s. ^{19}F NMR of TBAF before and after the addition of **1** in CD_2Cl_2.




-119.78
TBAF + 1
10 min
-137.45
-158.02
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180


-117.72
TBAF + 1
~20 min
-137.40
-157.97
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180


-116.50
TBAF + 1
~40 min
-137.49
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180

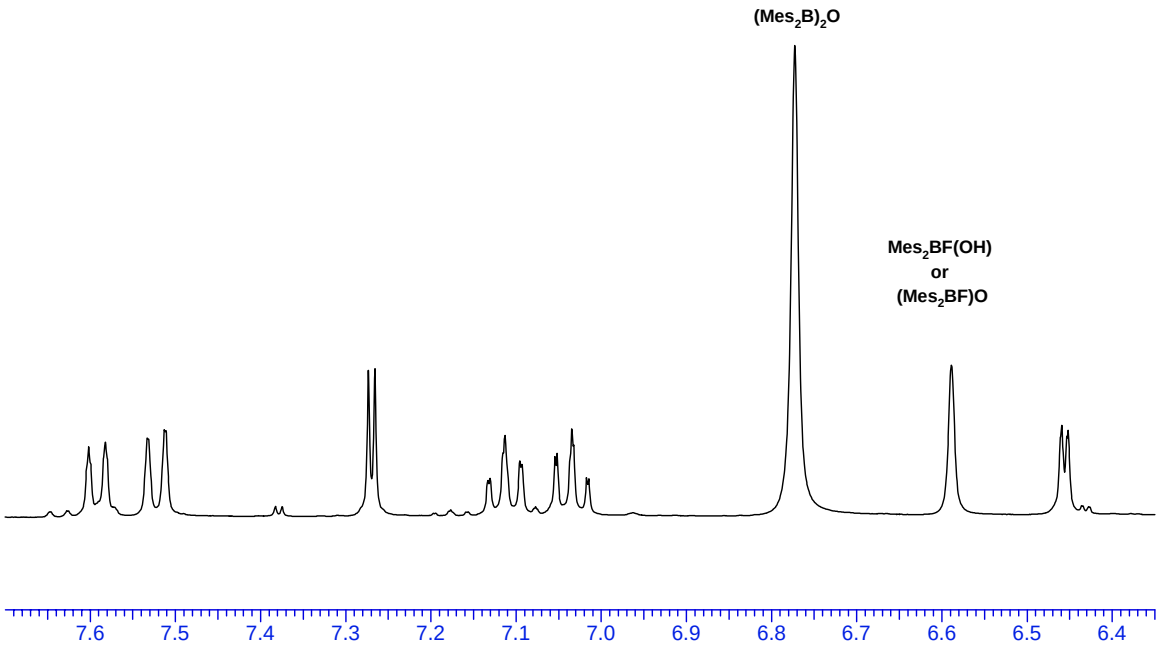


Figure 14S ^{1}H NMR spectra of **1** and **TBAF** (1:1) at room temperature in $CDCl_3$

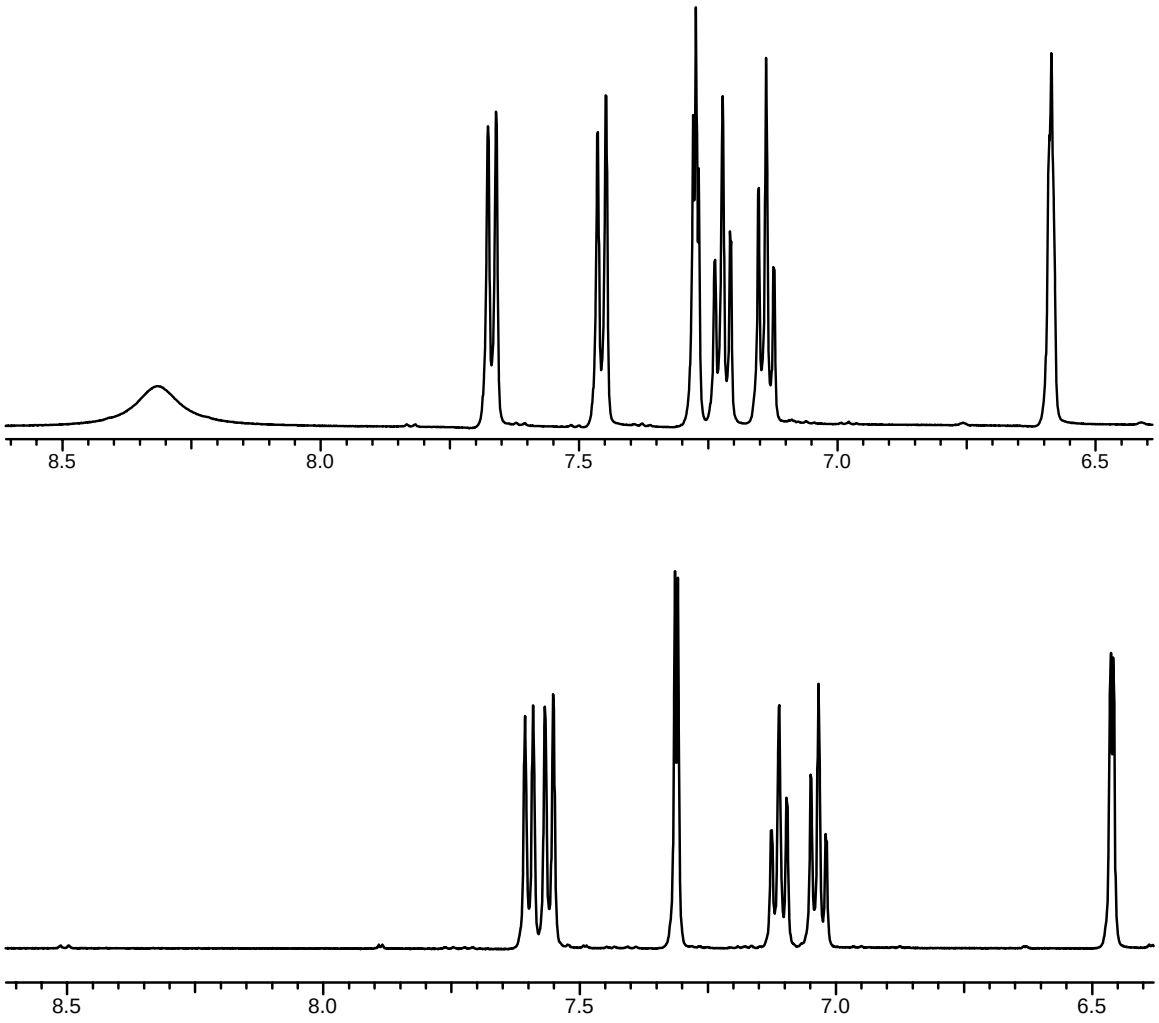


Figure 15s. ^{1}H-NMR (CD_2Cl_2, in 500MHz) for **indole** (top) and **Indole + TBAF** (1:1)

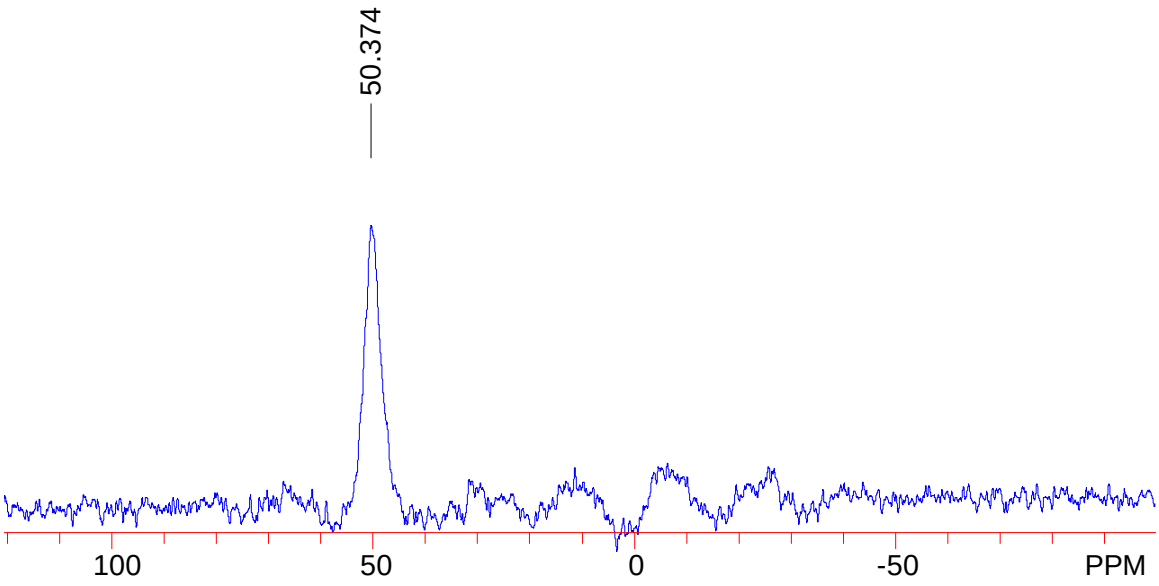


Figure.16S. ^{11}B-NMR spectra of **$(Mes_2B)_2O$** in the presence of **Indole** at room temperature in $CDCl_3$

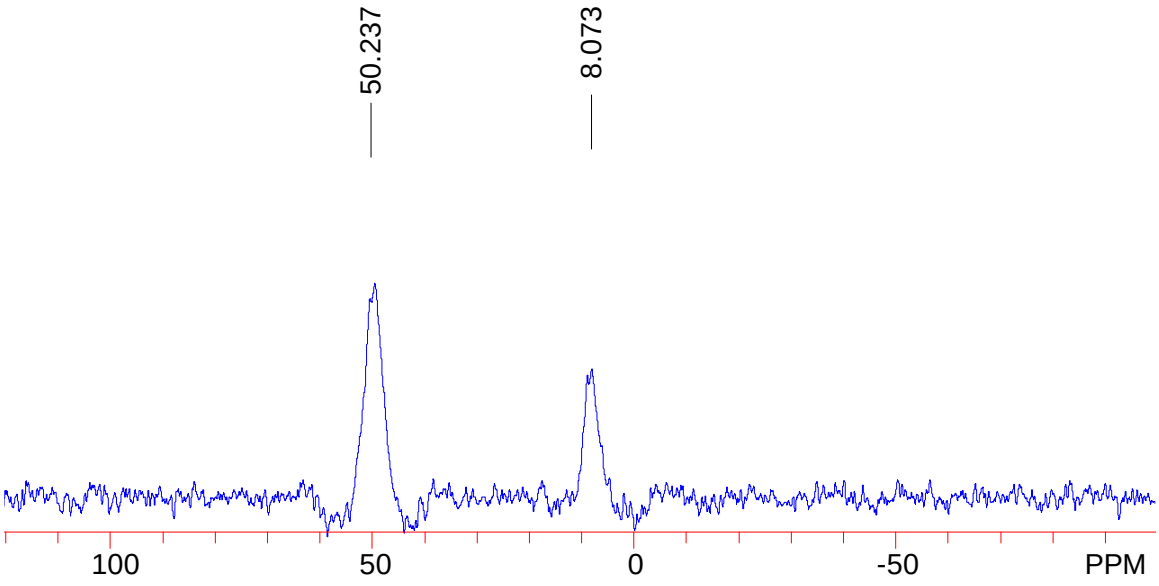


Figure 17s. ^{11}B-NMR spectra of **$(Mes_2B)_2O$** and **TBAF** (1:1) at RT in $CDCl_3$

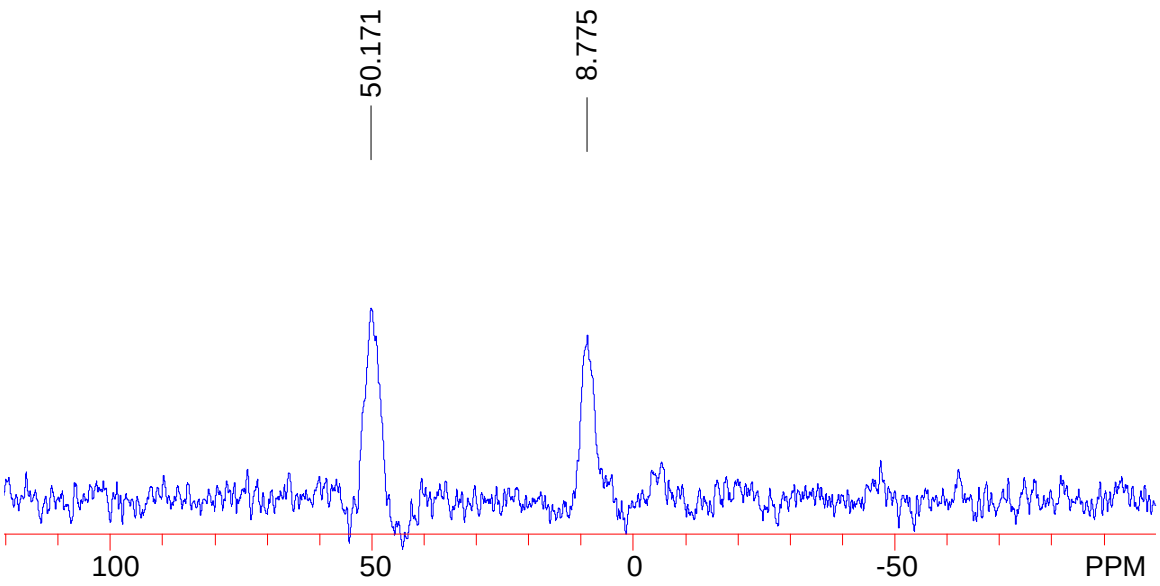


Figure 18S ^{11}B-NMR spectra of the mixture of **1** and **TBAF** (1:1) at RT in $CDCl_3$

Figure 19s The CV diagrams for compounds **1-5**

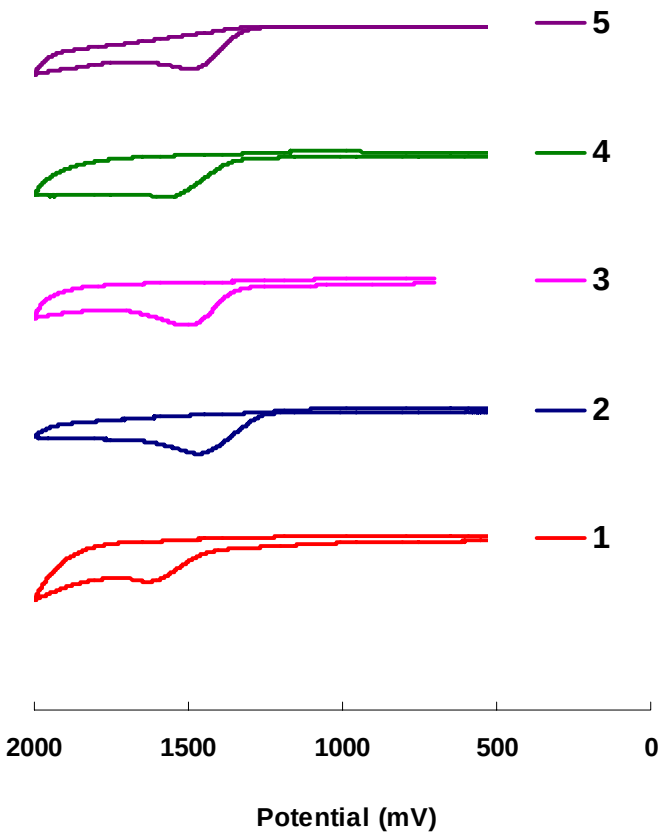


Figure 20s. The structure of $\{B(mesityl)_2\}_2O$ (BOB) isolated from the mixture of TBAF + 1

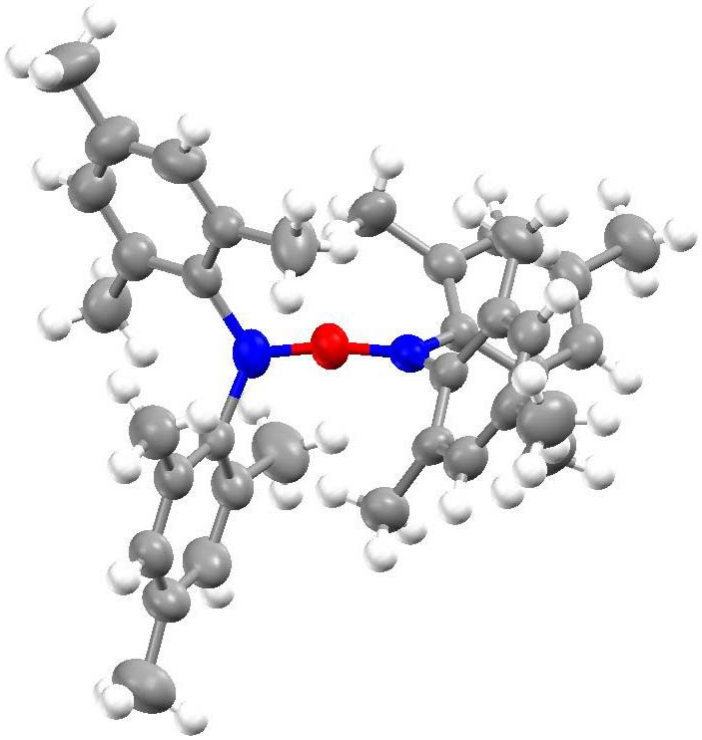


Table 1. Crystal data and structure refinement for 1.

Identification code	1	
Empirical formula	C26 H28 B N	
Formula weight	365.30	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2148(10) Å	α= 105.341(2)°.
	b = 11.6163(13) Å	β= 94.143(2)°.
	c = 12.2308(14) Å	γ = 106.575(2)°.
Volume	1064.9(2) $Å^3$	
Z	2	
Density (calculated)	1.139 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	392	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Theta range for data collection	1.92 to 28.22°.	
Index ranges	-10<=h<=9, -15<=k<=13, -16<=l<=15	
Reflections collected	7481	
Independent reflections	4761 [R(int) = 0.0164]	
Completeness to theta = 28.22°	90.7 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.820	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4761 / 0 / 259	
Goodness-of-fit on F^2	0.917	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1406	
R indices (all data)	R1 = 0.0955, wR2 = 0.1558	
Largest diff. peak and hole	0.279 and -0.144 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	3503(2)	1677(1)	1962(1)	48(1)
B	2236(3)	982(2)	2507(2)	47(1)
C(1)	4112(2)	1146(2)	973(2)	55(1)
C(2)	5189(2)	2018(2)	623(2)	60(1)
C(3)	6392(3)	4440(2)	1549(2)	73(1)
C(4)	6356(3)	5401(2)	2478(2)	78(1)
C(5)	5325(3)	5154(2)	3297(2)	68(1)
C(6)	4297(2)	3957(2)	3193(2)	56(1)
C(7)	4331(2)	2988(2)	2248(2)	47(1)
C(8)	5379(2)	3221(2)	1428(2)	54(1)
C(9)	1101(2)	1665(1)	3231(2)	44(1)
C(10)	1041(2)	1726(2)	4392(2)	50(1)
C(11)	23(2)	2350(2)	5000(2)	57(1)
C(12)	-976(2)	2910(2)	4502(2)	57(1)
C(13)	-928(2)	2837(2)	3363(2)	54(1)
C(14)	70(2)	2233(2)	2713(2)	48(1)
C(15)	-7(3)	2189(2)	1469(2)	62(1)
C(16)	-2070(3)	3586(2)	5185(2)	86(1)
C(17)	2127(3)	1170(2)	5013(2)	66(1)
C(18)	2067(2)	-461(2)	2279(2)	47(1)
C(19)	492(2)	-1415(2)	1797(2)	48(1)
C(20)	411(3)	-2673(2)	1548(2)	56(1)
C(21)	1829(3)	-3031(2)	1790(2)	59(1)
C(22)	3360(3)	-2087(2)	2308(2)	61(1)
C(23)	3511(2)	-817(2)	2551(2)	55(1)
C(24)	5241(3)	133(2)	3131(2)	77(1)
C(25)	1693(3)	-4409(2)	1520(2)	86(1)
C(26)	-1147(2)	-1140(2)	1512(2)	66(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

N-C(1)	1.400(2)	C(7)-N-B	129.39(15)
N-C(7)	1.414(2)	N-B-C(9)	119.17(14)
N-B	1.444(2)	N-B-C(18)	115.99(15)
B-C(9)	1.566(3)	C(9)-B-C(18)	124.81(15)
B-C(18)	1.587(2)	C(2)-C(1)-N	111.87(16)
C(1)-C(2)	1.329(2)	C(1)-C(2)-C(8)	107.34(17)
C(2)-C(8)	1.439(2)	C(4)-C(3)-C(8)	119.37(19)
C(3)-C(4)	1.375(3)	C(3)-C(4)-C(5)	120.52(19)
C(3)-C(8)	1.386(3)	C(6)-C(5)-C(4)	121.3(2)
C(4)-C(5)	1.393(3)	C(5)-C(6)-C(7)	117.92(18)
C(5)-C(6)	1.373(2)	C(6)-C(7)-C(8)	121.32(16)
C(6)-C(7)	1.392(2)	C(6)-C(7)-N	130.12(16)
C(7)-C(8)	1.399(2)	C(8)-C(7)-N	108.44(15)
C(9)-C(10)	1.408(2)	C(3)-C(8)-C(7)	119.53(18)
C(9)-C(14)	1.420(2)	C(3)-C(8)-C(2)	133.58(18)
C(10)-C(11)	1.388(2)	C(7)-C(8)-C(2)	106.79(16)
C(10)-C(17)	1.511(2)	C(10)-C(9)-C(14)	117.90(15)
C(11)-C(12)	1.382(2)	C(10)-C(9)-B	122.16(15)
C(12)-C(13)	1.377(3)	C(14)-C(9)-B	119.94(15)
C(12)-C(16)	1.512(3)	C(11)-C(10)-C(9)	120.01(16)
C(13)-C(14)	1.386(2)	C(11)-C(10)-C(17)	118.72(16)
C(14)-C(15)	1.506(2)	C(9)-C(10)-C(17)	121.22(16)
C(18)-C(19)	1.406(2)	C(12)-C(11)-C(10)	122.32(17)
C(18)-C(23)	1.409(2)	C(13)-C(12)-C(11)	117.49(17)
C(19)-C(20)	1.392(2)	C(13)-C(12)-C(16)	121.28(19)
C(19)-C(26)	1.508(2)	C(11)-C(12)-C(16)	121.22(19)
C(20)-C(21)	1.382(3)	C(12)-C(13)-C(14)	122.82(17)
C(21)-C(22)	1.384(3)	C(13)-C(14)-C(9)	119.44(16)
C(21)-C(25)	1.516(2)	C(13)-C(14)-C(15)	118.20(15)
C(22)-C(23)	1.392(2)	C(9)-C(14)-C(15)	122.35(15)
C(23)-C(24)	1.512(3)	C(19)-C(18)-C(23)	118.18(14)
		C(19)-C(18)-B	121.45(15)
C(1)-N-C(7)	105.52(14)	C(23)-C(18)-B	120.37(16)
C(1)-N-B	125.04(14)	C(20)-C(19)-C(18)	119.95(17)

C(20)-C(19)-C(26)	117.42(16)	C(22)-C(21)-C(25)	121.50(19)
C(18)-C(19)-C(26)	122.63(15)	C(21)-C(22)-C(23)	122.23(18)
C(21)-C(20)-C(19)	122.21(18)	C(22)-C(23)-C(18)	119.79(17)
C(20)-C(21)-C(22)	117.56(16)	C(22)-C(23)-C(24)	117.65(17)
C(20)-C(21)-C(25)	120.92(19)	C(18)-C(23)-C(24)	122.54(15)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. 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}
N	50(1)	41(1)	54(1)	14(1)	13(1)	18(1)
B	44(1)	48(1)	50(1)	18(1)	2(1)	15(1)
C(1)	57(1)	52(1)	57(1)	10(1)	15(1)	25(1)
C(2)	58(1)	66(1)	61(1)	20(1)	20(1)	23(1)
C(3)	69(2)	67(1)	86(2)	35(1)	29(1)	12(1)
C(4)	77(2)	52(1)	98(2)	24(1)	22(1)	7(1)
C(5)	72(2)	48(1)	79(2)	13(1)	14(1)	14(1)
C(6)	58(1)	48(1)	61(1)	14(1)	12(1)	17(1)
C(7)	46(1)	45(1)	55(1)	18(1)	8(1)	16(1)
C(8)	49(1)	55(1)	60(1)	22(1)	13(1)	16(1)
C(9)	44(1)	40(1)	49(1)	15(1)	8(1)	13(1)
C(10)	50(1)	45(1)	53(1)	17(1)	5(1)	11(1)
C(11)	64(1)	60(1)	46(1)	14(1)	13(1)	18(1)
C(12)	55(1)	54(1)	61(1)	10(1)	13(1)	20(1)
C(13)	51(1)	52(1)	64(1)	18(1)	7(1)	21(1)
C(14)	48(1)	44(1)	53(1)	16(1)	8(1)	15(1)
C(15)	69(1)	69(1)	60(1)	28(1)	9(1)	33(1)
C(16)	94(2)	96(2)	78(2)	13(1)	28(1)	51(2)
C(17)	76(2)	71(1)	57(1)	25(1)	7(1)	29(1)
C(18)	47(1)	44(1)	51(1)	17(1)	10(1)	16(1)
C(19)	49(1)	48(1)	49(1)	16(1)	11(1)	14(1)
C(20)	61(1)	47(1)	53(1)	15(1)	6(1)	9(1)
C(21)	81(2)	44(1)	52(1)	16(1)	12(1)	20(1)
C(22)	70(1)	57(1)	66(1)	23(1)	9(1)	32(1)
C(23)	53(1)	49(1)	65(1)	20(1)	8(1)	18(1)

C(24)	55(1)	63(1)	112(2)	28(1)	-3(1)	20(1)
C(25)	126(2)	50(1)	81(2)	17(1)	3(1)	34(1)
C(26)	50(1)	64(1)	78(2)	15(1)	3(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	3801	286	606	66
H(2A)	5720	1878	-24	72
H(3A)	7090	4607	1007	88
H(4A)	7026	6222	2559	93
H(5A)	5334	5814	3927	82
H(6A)	3599	3798	3737	67
H(11A)	12	2391	5769	69
H(13A)	-1593	3208	3014	65
H(15A)	-901	2507	1256	92
H(15B)	-246	1335	1001	92
H(15C)	1077	2696	1355	92
H(16A)	-2915	3690	4668	129
H(16B)	-1352	4396	5667	129
H(16C)	-2637	3100	5652	129
H(17A)	1818	1209	5761	99
H(17B)	3321	1638	5090	99
H(17C)	1933	308	4583	99
H(20A)	-633	-3293	1208	67
H(22A)	4320	-2308	2501	73
H(24A)	5075	853	3653	115
H(24B)	5877	389	2561	115
H(24C)	5869	-241	3547	115
H(25A)	841	-4889	852	128
H(25B)	1367	-4702	2161	128
H(25C)	2786	-4509	1376	128
H(26A)	-1022	-718	931	100
H(26B)	-1382	-611	2189	100
H(26C)	-2082	-1915	1234	100

Table 1. Crystal data and structure refinement for 2.

Identification code	2	
Empirical formula	C27 H30 B N	
Formula weight	379.33	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 22.3981(18) Å	α= 90°.
	b = 8.1607(7) Å	β= 90°.
	c = 12.2170(10) Å	γ = 90°.
Volume	2233.1(3) $Å^3$	
Z	4	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	816	
Crystal size	0.40 x 0.30 x 0.20 mm^3	
Theta range for data collection	1.82 to 28.25°.	
Index ranges	-27<=h<=28, -10<=k<=10, -14<=l<=15	
Reflections collected	14894	
Independent reflections	5067 [R(int) = 0.0275]	
Completeness to theta = 28.25°	96.4 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.810	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5067 / 1 / 281	
Goodness-of-fit on F^2	0.900	
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0795	
R indices (all data)	R1 = 0.0686, wR2 = 0.0868	
Absolute structure parameter	Cannot be reliably determined	
Largest diff. peak and hole	0.119 and -0.116 $e.Å^{-3}$	

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

	x	y	z	U(eq)
B	8295(1)	8388(2)	2561(2)	46(1)
N	8653(1)	9374(2)	1821(1)	48(1)
C(1)	8459(1)	10205(2)	861(2)	56(1)
C(2)	8914(1)	11053(2)	434(2)	63(1)
C(3)	10009(1)	11488(2)	1075(2)	73(1)
C(4)	10397(1)	11088(3)	1900(3)	80(1)
C(5)	10223(1)	10086(2)	2756(2)	70(1)
C(6)	9653(1)	9421(2)	2796(2)	60(1)
C(7)	9264(1)	9788(2)	1956(2)	50(1)
C(8)	9433(1)	10846(2)	1105(2)	57(1)
C(9)	8604(1)	6955(2)	3212(1)	44(1)
C(10)	8559(1)	6845(2)	4370(1)	46(1)
C(11)	8814(1)	5526(2)	4915(2)	52(1)
C(12)	9115(1)	4283(2)	4367(2)	53(1)
C(13)	9152(1)	4393(2)	3244(2)	53(1)
C(14)	8912(1)	5699(2)	2655(2)	50(1)
C(15)	8982(1)	5674(2)	1425(2)	74(1)
C(16)	9380(1)	2853(2)	4981(2)	77(1)
C(17)	8267(1)	8160(2)	5041(2)	61(1)
C(18)	7613(1)	8797(2)	2696(2)	47(1)
C(19)	7166(1)	7614(2)	2519(1)	52(1)
C(20)	6571(1)	8000(3)	2704(2)	61(1)
C(21)	6395(1)	9514(2)	3094(2)	63(1)
C(22)	6832(1)	10664(2)	3271(2)	62(1)
C(23)	7434(1)	10351(2)	3063(2)	54(1)
C(24)	7880(1)	11718(2)	3266(2)	74(1)
C(25)	5741(1)	9880(3)	3303(2)	90(1)
C(26)	7318(1)	5938(2)	2063(2)	77(1)
C(27)	7855(1)	9975(3)	383(2)	80(1)

Table 3. Bond lengths [Å] and angles [°] for 2.

B-N	1.452(2)	N-B-C(9)	118.90(14)
B-C(18)	1.572(3)	C(18)-B-C(9)	122.12(15)
B-C(9)	1.575(3)	C(7)-N-C(1)	106.08(14)
N-C(7)	1.420(2)	C(7)-N-B	126.32(14)
N-C(1)	1.423(2)	C(1)-N-B	127.49(14)
C(1)-C(2)	1.338(3)	C(2)-C(1)-N	109.63(17)
C(1)-C(27)	1.487(3)	C(2)-C(1)-C(27)	127.27(19)
C(2)-C(8)	1.431(3)	N-C(1)-C(27)	122.80(16)
C(3)-C(4)	1.370(3)	C(1)-C(2)-C(8)	109.45(18)
C(3)-C(8)	1.393(3)	C(4)-C(3)-C(8)	118.6(2)
C(4)-C(5)	1.383(3)	C(3)-C(4)-C(5)	121.19(18)
C(5)-C(6)	1.386(2)	C(4)-C(5)-C(6)	121.2(2)
C(6)-C(7)	1.379(3)	C(7)-C(6)-C(5)	118.0(2)
C(7)-C(8)	1.403(2)	C(6)-C(7)-C(8)	121.04(17)
C(9)-C(14)	1.411(2)	C(6)-C(7)-N	130.11(17)
C(9)-C(10)	1.421(2)	C(8)-C(7)-N	108.60(16)
C(10)-C(11)	1.389(2)	C(3)-C(8)-C(7)	119.94(19)
C(10)-C(17)	1.501(2)	C(3)-C(8)-C(2)	133.80(19)
C(11)-C(12)	1.390(2)	C(7)-C(8)-C(2)	106.23(16)
C(12)-C(13)	1.378(3)	C(14)-C(9)-C(10)	117.97(15)
C(12)-C(16)	1.508(2)	C(14)-C(9)-B	120.74(16)
C(13)-C(14)	1.393(2)	C(10)-C(9)-B	121.23(14)
C(14)-C(15)	1.511(3)	C(11)-C(10)-C(9)	119.81(15)
C(18)-C(23)	1.404(2)	C(11)-C(10)-C(17)	118.12(16)
C(18)-C(19)	1.408(2)	C(9)-C(10)-C(17)	122.00(15)
C(19)-C(20)	1.387(2)	C(10)-C(11)-C(12)	122.28(17)
C(19)-C(26)	1.516(3)	C(13)-C(12)-C(11)	117.46(16)
C(20)-C(21)	1.382(3)	C(13)-C(12)-C(16)	121.50(17)
C(21)-C(22)	1.374(2)	C(11)-C(12)-C(16)	121.03(18)
C(21)-C(25)	1.516(3)	C(12)-C(13)-C(14)	122.77(16)
C(22)-C(23)	1.396(2)	C(13)-C(14)-C(9)	119.69(16)
C(23)-C(24)	1.517(2)	C(13)-C(14)-C(15)	117.64(16)
		C(9)-C(14)-C(15)	122.65(16)
N-B-C(18)	118.98(15)	C(23)-C(18)-C(19)	117.70(14)

C(23)-C(18)-B	120.18(13)	C(22)-C(21)-C(25)	121.82(19)
C(19)-C(18)-B	122.02(14)	C(20)-C(21)-C(25)	120.66(18)
C(20)-C(19)-C(18)	120.21(16)	C(21)-C(22)-C(23)	122.34(17)
C(20)-C(19)-C(26)	118.77(16)	C(22)-C(23)-C(18)	119.97(15)
C(18)-C(19)-C(26)	120.93(15)	C(22)-C(23)-C(24)	118.09(15)
C(21)-C(20)-C(19)	122.21(17)	C(18)-C(23)-C(24)	121.92(14)
C(22)-C(21)-C(20)	117.52(16)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2. 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}
B	54(1)	41(1)	43(1)	-10(1)	-1(1)	-5(1)
N	49(1)	49(1)	47(1)	3(1)	0(1)	2(1)
C(1)	66(1)	53(1)	48(1)	3(1)	0(1)	7(1)
C(2)	86(2)	57(1)	47(1)	12(1)	10(1)	6(1)
C(3)	69(1)	70(1)	81(2)	0(1)	28(1)	-7(1)
C(4)	52(1)	79(1)	110(2)	-17(1)	22(1)	-10(1)
C(5)	50(1)	72(1)	89(2)	-6(1)	-2(1)	1(1)
C(6)	53(1)	57(1)	69(2)	6(1)	2(1)	0(1)
C(7)	51(1)	45(1)	53(1)	-2(1)	8(1)	5(1)
C(8)	62(1)	52(1)	58(1)	-2(1)	17(1)	1(1)
C(9)	43(1)	44(1)	44(1)	-3(1)	2(1)	-4(1)
C(10)	47(1)	46(1)	47(1)	-3(1)	4(1)	-5(1)
C(11)	55(1)	56(1)	46(1)	3(1)	-2(1)	-5(1)
C(12)	51(1)	48(1)	59(1)	5(1)	-2(1)	-4(1)
C(13)	51(1)	45(1)	62(1)	-4(1)	9(1)	4(1)
C(14)	50(1)	50(1)	51(1)	-1(1)	9(1)	-1(1)
C(15)	100(2)	68(1)	54(1)	-6(1)	15(1)	14(1)
C(16)	85(1)	64(1)	83(2)	11(1)	-4(1)	18(1)
C(17)	76(1)	57(1)	49(1)	-7(1)	4(1)	5(1)
C(18)	51(1)	47(1)	45(1)	1(1)	-1(1)	-3(1)
C(19)	54(1)	55(1)	46(1)	6(1)	-2(1)	-7(1)
C(20)	51(1)	74(1)	59(1)	15(1)	-5(1)	-17(1)

C(21)	48(1)	80(1)	59(1)	20(1)	0(1)	4(1)
C(22)	61(1)	63(1)	63(1)	4(1)	6(1)	13(1)
C(23)	51(1)	52(1)	58(1)	3(1)	1(1)	1(1)
C(24)	73(1)	48(1)	102(2)	-14(1)	4(1)	1(1)
C(25)	52(1)	119(2)	99(2)	29(2)	5(1)	15(1)
C(26)	81(1)	62(1)	87(2)	-17(1)	-7(1)	-18(1)
C(27)	80(2)	99(2)	61(1)	12(1)	-14(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2.

	x	y	z	U(eq)
H(3A)	10128	12173	507	88
H(4A)	10784	11498	1885	96
H(5A)	10492	9854	3313	84
H(11A)	8783	5473	5674	63
H(13A)	9344	3560	2862	63
H(15A)	9164	4662	1205	111
H(15B)	9229	6574	1201	111
H(15C)	8596	5772	1088	111
H(16A)	9645	2259	4508	116
H(16B)	9065	2140	5222	116
H(16C)	9597	3249	5605	116
H(17A)	8248	7817	5792	91
H(17B)	7871	8355	4772	91
H(17C)	8497	9151	4989	91
H(22A)	6723	11688	3540	74
H(24A)	7686	12598	3649	112
H(24B)	8030	12112	2579	112
H(24C)	8204	11309	3700	112
H(25A)	5707	10863	3731	135
H(25B)	5563	8983	3694	135
H(25C)	5539	10027	2617	135
H(26A)	6983	5219	2152	115

H(26B)	7656	5500	2449	115
H(26C)	7413	6034	1299	115
H(27A)	7844	10442	-338	120
H(27B)	7564	10508	837	120
H(27C)	7766	8826	340	120
H(20)	6275(7)	7254(19)	2580(15)	55(5)
H(6)	9576(8)	8790(20)	3343(16)	60(6)
H(2)	8877(8)	11630(20)	-218(17)	68(6)

Table 1. Crystal data and structure refinement for 3.

Identification code	3	
Empirical formula	C27 H30 B N	
Formula weight	379.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.635(4) Å	α= 99.281(9)°.
	b = 11.606(6) Å	β= 98.716(9)°.
	c = 12.262(7) Å	γ = 107.487(9)°.
Volume	1130.3(10) $Å^3$	
Z	2	
Density (calculated)	1.115 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	408	
Crystal size	0.40 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.72 to 25.00°.	
Index ranges	-9<=h<=10, -12<=k<=13, -14<=l<=14	
Reflections collected	6724	
Independent reflections	3961 [R(int) = 0.0326]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.628	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3961 / 0 / 301	
Goodness-of-fit on F^2	0.983	
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1590	
R indices (all data)	R1 = 0.0843, wR2 = 0.1761	
Largest diff. peak and hole	0.305 and -0.141 e.$Å^{-3}$	

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

	x	y	z	U(eq)
B	2845(3)	8751(2)	2312(2)	55(1)
N	1574(2)	8010(2)	2789(1)	62(1)
C(1)	1014(3)	8503(3)	3760(2)	68(1)
C(2)	43(3)	7588(3)	4137(2)	76(1)
C(3)	-1065(3)	5207(3)	3331(3)	93(1)
C(4)	-1023(4)	4313(3)	2463(3)	97(1)
C(5)	-119(3)	4614(2)	1674(2)	91(1)
C(6)	830(3)	5837(2)	1716(2)	72(1)
C(7)	809(2)	6724(2)	2573(2)	65(1)
C(8)	-147(2)	6454(2)	3389(2)	64(1)
C(9)	3941(2)	8118(2)	1689(2)	54(1)
C(10)	4044(2)	8150(2)	569(2)	57(1)
C(11)	5045(3)	7598(2)	55(2)	66(1)
C(12)	5994(3)	7023(2)	632(2)	68(1)
C(13)	5898(3)	7007(2)	1740(2)	68(1)
C(14)	4892(2)	7537(2)	2281(2)	63(1)
C(15)	4897(3)	7464(2)	3499(2)	82(1)
C(16)	7066(3)	6415(3)	69(2)	94(1)
C(17)	3038(3)	8747(2)	-120(2)	71(1)
C(18)	3103(2)	10177(2)	2515(2)	56(1)
C(19)	4652(2)	11066(2)	3054(2)	62(1)
C(20)	4813(3)	12314(2)	3268(2)	70(1)
C(21)	3535(3)	12734(2)	2944(2)	71(1)
C(22)	2033(3)	11865(2)	2384(2)	68(1)
C(23)	1781(2)	10607(2)	2178(2)	58(1)
C(24)	71(3)	9737(2)	1585(2)	77(1)
C(25)	3768(4)	14102(2)	3204(3)	102(1)
C(26)	6159(3)	10719(2)	3438(2)	90(1)
C(27)	-715(3)	7720(3)	5149(2)	96(1)

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

B-N	1.442(3)	N-B-C(18)	116.66(18)
B-C(9)	1.573(3)	C(9)-B-C(18)	124.25(18)
B-C(18)	1.574(3)	C(7)-N-B	130.45(18)
N-C(7)	1.401(3)	C(7)-N-C(1)	105.49(18)
N-C(1)	1.449(3)	B-N-C(1)	123.47(19)
C(1)-C(2)	1.336(3)	C(2)-C(1)-N	110.7(2)
C(2)-C(8)	1.426(3)	C(1)-C(2)-C(8)	107.2(2)
C(2)-C(27)	1.496(3)	C(1)-C(2)-C(27)	126.7(3)
C(3)-C(4)	1.374(4)	C(8)-C(2)-C(27)	126.1(2)
C(3)-C(8)	1.410(3)	C(4)-C(3)-C(8)	118.6(3)
C(4)-C(5)	1.357(4)	C(5)-C(4)-C(3)	121.2(3)
C(5)-C(6)	1.398(4)	C(4)-C(5)-C(6)	121.8(3)
C(6)-C(7)	1.354(3)	C(7)-C(6)-C(5)	117.5(3)
C(7)-C(8)	1.405(3)	C(6)-C(7)-N	129.4(2)
C(9)-C(10)	1.395(3)	C(6)-C(7)-C(8)	122.4(2)
C(9)-C(14)	1.403(3)	N-C(7)-C(8)	108.04(19)
C(10)-C(11)	1.386(3)	C(7)-C(8)-C(3)	118.4(2)
C(10)-C(17)	1.509(3)	C(7)-C(8)-C(2)	108.5(2)
C(11)-C(12)	1.387(3)	C(3)-C(8)-C(2)	133.1(2)
C(12)-C(13)	1.375(3)	C(10)-C(9)-C(14)	118.46(19)
C(12)-C(16)	1.503(3)	C(10)-C(9)-B	122.04(17)
C(13)-C(14)	1.392(3)	C(14)-C(9)-B	119.47(18)
C(14)-C(15)	1.508(3)	C(11)-C(10)-C(9)	120.3(2)
C(18)-C(19)	1.405(3)	C(11)-C(10)-C(17)	118.51(19)
C(18)-C(23)	1.410(3)	C(9)-C(10)-C(17)	121.12(18)
C(19)-C(20)	1.390(3)	C(10)-C(11)-C(12)	121.7(2)
C(19)-C(26)	1.506(3)	C(13)-C(12)-C(11)	117.6(2)
C(20)-C(21)	1.366(3)	C(13)-C(12)-C(16)	120.8(2)
C(21)-C(22)	1.376(3)	C(11)-C(12)-C(16)	121.6(2)
C(21)-C(25)	1.512(3)	C(12)-C(13)-C(14)	122.4(2)
C(22)-C(23)	1.384(3)	C(13)-C(14)-C(9)	119.5(2)
C(23)-C(24)	1.507(3)	C(13)-C(14)-C(15)	117.5(2)
		C(9)-C(14)-C(15)	123.01(19)
N-B-C(9)	119.00(19)	C(19)-C(18)-C(23)	117.62(19)

C(19)-C(18)-B	121.20(18)	C(20)-C(21)-C(25)	121.0(2)
C(23)-C(18)-B	121.18(17)	C(22)-C(21)-C(25)	121.6(2)
C(20)-C(19)-C(18)	119.6(2)	C(21)-C(22)-C(23)	122.3(2)
C(20)-C(19)-C(26)	118.0(2)	C(22)-C(23)-C(18)	120.1(2)
C(18)-C(19)-C(26)	122.4(2)	C(22)-C(23)-C(24)	117.78(19)
C(21)-C(20)-C(19)	122.9(2)	C(18)-C(23)-C(24)	122.16(19)
C(20)-C(21)-C(22)	117.4(2)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. 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}
B	53(1)	58(2)	51(1)	14(1)	2(1)	15(1)
N	66(1)	57(1)	63(1)	17(1)	12(1)	19(1)
C(1)	63(1)	79(2)	63(1)	22(1)	15(1)	23(1)
C(2)	64(1)	95(2)	69(2)	21(1)	14(1)	26(1)
C(3)	81(2)	87(2)	107(2)	34(2)	27(2)	10(2)
C(4)	96(2)	63(2)	117(2)	17(2)	26(2)	3(2)
C(5)	97(2)	63(2)	103(2)	11(2)	18(2)	17(2)
C(6)	74(1)	69(2)	74(2)	15(1)	15(1)	23(1)
C(7)	61(1)	59(1)	71(1)	17(1)	6(1)	18(1)
C(8)	52(1)	70(2)	66(1)	20(1)	12(1)	14(1)
C(9)	54(1)	46(1)	58(1)	11(1)	5(1)	12(1)
C(10)	56(1)	47(1)	61(1)	10(1)	8(1)	11(1)
C(11)	71(1)	59(1)	62(1)	7(1)	17(1)	15(1)
C(12)	61(1)	58(1)	80(2)	6(1)	13(1)	18(1)
C(13)	63(1)	57(1)	80(2)	16(1)	3(1)	22(1)
C(14)	63(1)	55(1)	67(1)	13(1)	7(1)	18(1)
C(15)	97(2)	87(2)	70(2)	28(1)	7(1)	42(2)
C(16)	85(2)	92(2)	107(2)	3(2)	25(2)	39(2)
C(17)	82(1)	68(2)	62(1)	18(1)	9(1)	26(1)
C(18)	60(1)	54(1)	52(1)	13(1)	13(1)	16(1)
C(19)	60(1)	56(1)	60(1)	11(1)	10(1)	10(1)
C(20)	72(2)	57(2)	67(2)	9(1)	14(1)	5(1)

C(21)	92(2)	54(1)	70(1)	14(1)	31(1)	20(1)
C(22)	80(2)	62(2)	71(2)	22(1)	24(1)	31(1)
C(23)	63(1)	55(1)	58(1)	15(1)	15(1)	20(1)
C(24)	64(1)	76(2)	90(2)	21(1)	5(1)	25(1)
C(25)	135(2)	57(2)	112(2)	14(2)	32(2)	28(2)
C(26)	65(1)	82(2)	102(2)	9(2)	-7(1)	12(1)
C(27)	80(2)	138(3)	79(2)	23(2)	34(1)	42(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3.

	x	y	z	U(eq)
H(1)	1390(30)	9390(20)	4090(19)	82(7)
H(3)	-1720(40)	5100(30)	3980(30)	141(12)
H(4)	-1740(40)	3440(30)	2430(20)	117(9)
H(5A)	-131	3989	1090	109
H(6)	1420(30)	6050(20)	1120(19)	72(6)
H(11)	5080(20)	7602(19)	-730(20)	71(6)
H(13)	6510(30)	6655(19)	2161(17)	63(6)
H(15A)	5742	7137	3771	123
H(15B)	3832	6932	3553	123
H(15C)	5120	8277	3947	123
H(16A)	7674	6951	-353	141
H(16B)	6378	5646	-433	141
H(16C)	7831	6260	634	141
H(17A)	3297	9596	255	106
H(17B)	1876	8314	-197	106
H(17C)	3301	8712	-855	106
H(20)	5900(30)	12880(20)	3664(19)	78(7)
H(22)	1130(30)	12170(20)	2172(19)	80(7)
H(24A)	-530	10180	1200	115
H(24B)	-512	9401	2131	115
H(24C)	165	9075	1047	115
H(25A)	2717	14212	3237	153

H(25B)	4209	14470	2621	153
H(25C)	4526	14492	3918	153
H(26A)	7108	11456	3726	135
H(26B)	6358	10213	2810	135
H(26C)	5972	10266	4023	135
H(27A)	-404	8581	5501	144
H(27B)	-325	7290	5678	144
H(27C)	-1903	7373	4918	144

Table 1. Crystal data and structure refinement for 4.

Identification code	4	
Empirical formula	C27 H30 B N	
Formula weight	379.33	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4989(11) Å	α= 100.384(2)°.
	b = 10.0999(14) Å	β= 106.956(2)°.
	c = 14.424(2) Å	γ = 103.731(2)°.
Volume	1108.2(3) $Å^3$	
Z	2	
Density (calculated)	1.137 Mg/m^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	408	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.15 to 28.28°.	
Index ranges	-9<=h<=11, -13<=k<=13, -17<=l<=18	
Reflections collected	7919	
Independent reflections	5020 [R(int) = 0.0228]	
Completeness to theta = 28.28°	91.0 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.820	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5020 / 0 / 269	
Goodness-of-fit on F^2	0.832	
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1197	
R indices (all data)	R1 = 0.1386, wR2 = 0.1419	
Largest diff. peak and hole	0.144 and -0.159 e.$Å^{-3}$	

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

	x	y	z	U(eq)
N	681(2)	9574(2)	2234(1)	52(1)
B	-579(3)	8222(3)	2083(2)	48(1)
C(1)	649(3)	10120(2)	1389(2)	64(1)
C(2)	2093(3)	11148(2)	1586(2)	71(1)
C(3)	4716(3)	12389(3)	3213(2)	77(1)
C(4)	5337(3)	12437(3)	4206(2)	84(1)
C(5)	4396(3)	11514(3)	4598(2)	74(1)
C(6)	2826(3)	10493(2)	4031(2)	57(1)
C(7)	2249(2)	10419(2)	3005(2)	51(1)
C(8)	3147(3)	11388(2)	2610(2)	58(1)
C(9)	-105(2)	7062(2)	2607(1)	48(1)
C(10)	-1164(2)	6322(2)	3052(2)	53(1)
C(11)	-745(3)	5259(2)	3468(2)	58(1)
C(12)	691(3)	4853(2)	3445(2)	61(1)
C(13)	1711(3)	5565(2)	2989(2)	60(1)
C(14)	1365(2)	6646(2)	2581(2)	53(1)
C(15)	2586(3)	7312(2)	2099(2)	72(1)
C(16)	1084(3)	3671(3)	3878(2)	87(1)
C(17)	-2768(3)	6670(3)	3136(2)	73(1)
C(18)	-2406(2)	7983(2)	1284(2)	48(1)
C(19)	-3079(3)	6936(2)	363(2)	54(1)
C(20)	-4703(3)	6776(2)	-320(2)	66(1)
C(21)	-5686(3)	7632(3)	-127(2)	62(1)
C(22)	-4996(3)	8667(2)	764(2)	62(1)
C(23)	-3401(2)	8858(2)	1474(2)	54(1)
C(24)	-2804(3)	9993(2)	2446(2)	75(1)
C(25)	-7459(3)	7431(3)	-868(2)	95(1)
C(26)	-2031(3)	6021(2)	72(2)	73(1)
C(27)	1827(3)	9614(3)	4531(2)	75(1)

Table 3. Bond lengths [Å] and angles [°] for 4.

N-C(7)	1.412(2)	C(7)-N-B	134.71(18)
N-C(1)	1.422(2)	C(1)-N-B	118.48(18)
N-B	1.457(3)	N-B-C(9)	122.73(18)
B-C(9)	1.572(3)	N-B-C(18)	113.85(18)
B-C(18)	1.574(3)	C(9)-B-C(18)	123.23(18)
C(1)-C(2)	1.323(3)	C(2)-C(1)-N	111.1(2)
C(2)-C(8)	1.428(3)	C(1)-C(2)-C(8)	108.1(2)
C(3)-C(4)	1.362(3)	C(4)-C(3)-C(8)	118.4(2)
C(3)-C(8)	1.386(3)	C(3)-C(4)-C(5)	120.2(2)
C(4)-C(5)	1.389(3)	C(6)-C(5)-C(4)	123.8(2)
C(5)-C(6)	1.385(3)	C(5)-C(6)-C(7)	115.1(2)
C(6)-C(7)	1.398(3)	C(5)-C(6)-C(27)	120.2(2)
C(6)-C(27)	1.504(3)	C(7)-C(6)-C(27)	124.57(19)
C(7)-C(8)	1.402(3)	C(6)-C(7)-C(8)	121.5(2)
C(9)-C(10)	1.405(3)	C(6)-C(7)-N	129.77(19)
C(9)-C(14)	1.417(2)	C(8)-C(7)-N	108.28(19)
C(10)-C(11)	1.390(3)	C(3)-C(8)-C(7)	120.9(2)
C(10)-C(17)	1.517(3)	C(3)-C(8)-C(2)	131.9(2)
C(11)-C(12)	1.383(3)	C(7)-C(8)-C(2)	107.09(19)
C(12)-C(13)	1.381(3)	C(10)-C(9)-C(14)	116.97(19)
C(12)-C(16)	1.504(3)	C(10)-C(9)-B	122.27(17)
C(13)-C(14)	1.381(3)	C(14)-C(9)-B	120.61(17)
C(14)-C(15)	1.508(3)	C(11)-C(10)-C(9)	120.71(18)
C(18)-C(19)	1.404(3)	C(11)-C(10)-C(17)	116.97(19)
C(18)-C(23)	1.405(3)	C(9)-C(10)-C(17)	122.28(19)
C(19)-C(20)	1.395(3)	C(12)-C(11)-C(10)	122.3(2)
C(19)-C(26)	1.513(3)	C(13)-C(12)-C(11)	116.8(2)
C(20)-C(21)	1.385(3)	C(13)-C(12)-C(16)	122.2(2)
C(21)-C(22)	1.369(3)	C(11)-C(12)-C(16)	121.0(2)
C(21)-C(25)	1.513(3)	C(14)-C(13)-C(12)	123.04(19)
C(22)-C(23)	1.385(3)	C(13)-C(14)-C(9)	120.17(19)
C(23)-C(24)	1.506(3)	C(13)-C(14)-C(15)	116.97(18)
		C(9)-C(14)-C(15)	122.8(2)
C(7)-N-C(1)	105.32(16)	C(19)-C(18)-C(23)	117.98(19)

C(19)-C(18)-B	122.28(18)	C(22)-C(21)-C(25)	121.2(2)
C(23)-C(18)-B	119.72(19)	C(20)-C(21)-C(25)	121.5(2)
C(20)-C(19)-C(18)	119.8(2)	C(21)-C(22)-C(23)	122.9(2)
C(20)-C(19)-C(26)	119.0(2)	C(22)-C(23)-C(18)	119.9(2)
C(18)-C(19)-C(26)	121.06(19)	C(22)-C(23)-C(24)	118.2(2)
C(21)-C(20)-C(19)	122.0(2)	C(18)-C(23)-C(24)	121.92(19)
C(22)-C(21)-C(20)	117.4(2)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. 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}
N	49(1)	55(1)	48(1)	14(1)	13(1)	13(1)
B	51(1)	54(2)	45(2)	10(1)	25(1)	18(1)
C(1)	64(1)	70(2)	53(2)	27(1)	13(1)	13(1)
C(2)	69(2)	70(2)	77(2)	35(2)	27(2)	13(1)
C(3)	57(2)	66(2)	95(2)	15(2)	19(2)	8(1)
C(4)	59(2)	74(2)	95(2)	6(2)	8(2)	11(1)
C(5)	66(2)	76(2)	65(2)	6(2)	9(1)	24(1)
C(6)	53(1)	63(2)	54(2)	10(1)	14(1)	26(1)
C(7)	42(1)	52(1)	55(2)	8(1)	11(1)	17(1)
C(8)	49(1)	54(1)	71(2)	18(1)	21(1)	14(1)
C(9)	44(1)	54(1)	45(1)	12(1)	16(1)	15(1)
C(10)	49(1)	57(1)	51(1)	12(1)	15(1)	16(1)
C(11)	60(1)	57(1)	56(2)	18(1)	20(1)	13(1)
C(12)	64(1)	56(2)	53(2)	9(1)	9(1)	23(1)
C(13)	53(1)	65(2)	62(2)	12(1)	17(1)	26(1)
C(14)	47(1)	56(1)	51(1)	7(1)	15(1)	14(1)
C(15)	64(1)	77(2)	87(2)	21(2)	41(1)	29(1)
C(16)	105(2)	76(2)	85(2)	29(2)	22(2)	44(2)
C(17)	65(1)	88(2)	89(2)	40(2)	43(1)	30(1)
C(18)	49(1)	48(1)	50(1)	18(1)	20(1)	14(1)
C(19)	55(1)	52(1)	54(2)	18(1)	23(1)	8(1)
C(20)	64(1)	65(2)	53(2)	18(1)	13(1)	1(1)

C(21)	52(1)	71(2)	60(2)	32(1)	12(1)	11(1)
C(22)	56(1)	70(2)	68(2)	31(2)	22(1)	23(1)
C(23)	51(1)	56(1)	53(2)	18(1)	16(1)	13(1)
C(24)	82(2)	75(2)	71(2)	15(2)	25(1)	36(1)
C(25)	66(2)	112(2)	88(2)	44(2)	-3(2)	18(2)
C(26)	78(2)	68(2)	65(2)	5(1)	24(1)	17(1)
C(27)	75(2)	99(2)	49(2)	15(1)	19(1)	29(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4.

	x	y	z	U(eq)
H(1A)	-267	9797	778	77
H(2A)	2373	11631	1136	86
H(3A)	5328	13013	2945	92
H(4A)	6395	13089	4622	101
H(5A)	4845	11586	5282	89
H(11A)	-1454	4803	3774	70
H(13A)	2675	5303	2954	72
H(15A)	3254	6704	1969	107
H(15B)	3347	8210	2543	107
H(15C)	1934	7448	1476	107
H(16A)	292	3374	4212	130
H(16B)	2246	3996	4351	130
H(16C)	964	2888	3345	130
H(17A)	-3376	5986	3395	110
H(17B)	-3506	6647	2483	110
H(17C)	-2435	7596	3582	110
H(20A)	-5138	6072	-924	79
H(22A)	-5625	9268	899	74
H(24A)	-3767	10283	2521	112
H(24B)	-1934	10791	2437	112
H(24C)	-2330	9630	2999	112
H(25A)	-7790	8267	-715	143

H(25B)	-8283	6636	-820	143
H(25C)	-7428	7263	-1538	143
H(26A)	-2782	5208	-469	110
H(26B)	-1475	5720	641	110
H(26C)	-1172	6557	-139	110
H(27A)	648	9616	4305	113
H(27B)	2332	10005	5247	113
H(27C)	1864	8661	4360	113

Table 1. Crystal data and structure refinement for 5.

Identification code	5	
Empirical formula	C32 H32 B N	
Formula weight	441.40	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.4353(10) Å	α= 90°.
	b = 18.5158(15) Å	β= 92.2680(10)°.
	c = 11.9490(10) Å	γ = 90°.
Volume	2528.0(4) $Å^3$	
Z	4	
Density (calculated)	1.160 Mg/m^3	
Absorption coefficient	0.066 mm^{-1}	
F(000)	944	
Crystal size	0.30 x 0.20 x 0.12 mm^3	
Theta range for data collection	1.78 to 28.25°.	
Index ranges	-13<=h<=14, -24<=k<=24, -15<=l<=14	
Reflections collected	17595	
Independent reflections	5892 [R(int) = 0.0336]	
Completeness to theta = 28.25°	94.1 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000 and 0.879	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5892 / 0 / 369	
Goodness-of-fit on F^2	0.905	
Final R indices [I>2sigma(I)]	R1 = 0.0496, wR2 = 0.1110	
R indices (all data)	R1 = 0.0945, wR2 = 0.1230	
Largest diff. peak and hole	0.277 and -0.200 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	2621(1)	955(1)	8156(1)	30(1)
B	3045(2)	1236(1)	9225(2)	30(1)
C(1)	3317(2)	633(1)	7350(1)	33(1)
C(2)	2686(2)	456(1)	6408(1)	32(1)
C(3)	486(2)	702(1)	5890(2)	35(1)
C(4)	-530(2)	982(1)	6292(2)	38(1)
C(5)	-554(2)	1249(1)	7380(2)	37(1)
C(6)	441(2)	1258(1)	8083(2)	32(1)
C(7)	1471(1)	980(1)	7672(1)	29(1)
C(8)	1498(1)	693(1)	6583(1)	30(1)
C(9)	2146(1)	1306(1)	10179(1)	29(1)
C(10)	1844(2)	1990(1)	10601(1)	34(1)
C(11)	1042(2)	2043(1)	11437(2)	41(1)
C(12)	530(2)	1438(1)	11897(2)	42(1)
C(13)	827(2)	766(1)	11485(2)	39(1)
C(14)	1607(1)	689(1)	10626(1)	33(1)
C(15)	1858(2)	-64(1)	10203(2)	42(1)
C(16)	-346(2)	1503(1)	12812(2)	63(1)
C(17)	2325(2)	2668(1)	10087(2)	44(1)
C(18)	4372(1)	1477(1)	9366(1)	31(1)
C(19)	5081(2)	1254(1)	10302(1)	33(1)
C(20)	6208(2)	1517(1)	10459(2)	39(1)
C(21)	6692(2)	2009(1)	9737(2)	42(1)
C(22)	5996(2)	2232(1)	8827(2)	42(1)
C(23)	4859(2)	1980(1)	8625(1)	35(1)
C(24)	4175(2)	2295(1)	7626(2)	48(1)
C(25)	7916(2)	2297(1)	9954(2)	63(1)
C(26)	4643(2)	725(1)	11148(2)	44(1)
C(27)	3086(1)	64(1)	5416(1)	33(1)
C(28)	3711(2)	-578(1)	5532(2)	42(1)
C(29)	4027(2)	-968(1)	4600(2)	48(1)

C(30)	3718(2)	-726(1)	3537(2)	45(1)
C(31)	3117(2)	-83(1)	3409(2)	42(1)
C(32)	2806(2)	311(1)	4333(2)	37(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

N-C(1)	1.406(2)	C(21)-C(25)	1.511(3)
N-C(7)	1.416(2)	C(22)-C(23)	1.393(2)
N-B	1.444(2)	C(23)-C(24)	1.518(2)
B-C(9)	1.570(2)	C(27)-C(28)	1.390(2)
B-C(18)	1.584(2)	C(27)-C(32)	1.397(2)
C(1)-C(2)	1.353(2)	C(28)-C(29)	1.389(2)
C(2)-C(8)	1.451(2)	C(29)-C(30)	1.380(3)
C(2)-C(27)	1.479(2)	C(30)-C(31)	1.380(3)
C(3)-C(4)	1.376(2)	C(31)-C(32)	1.382(2)
C(3)-C(8)	1.396(2)		
C(4)-C(5)	1.393(3)	C(1)-N-C(7)	106.02(13)
C(5)-C(6)	1.386(2)	C(1)-N-B	125.40(14)
C(6)-C(7)	1.393(2)	C(7)-N-B	128.48(14)
C(7)-C(8)	1.408(2)	N-B-C(9)	117.76(15)
C(9)-C(10)	1.411(2)	N-B-C(18)	118.79(15)
C(9)-C(14)	1.412(2)	C(9)-B-C(18)	123.43(15)
C(10)-C(11)	1.386(2)	C(2)-C(1)-N	112.02(15)
C(10)-C(17)	1.512(2)	C(1)-C(2)-C(8)	106.20(14)
C(11)-C(12)	1.388(3)	C(1)-C(2)-C(27)	127.92(15)
C(12)-C(13)	1.384(2)	C(8)-C(2)-C(27)	125.80(15)
C(12)-C(16)	1.517(2)	C(4)-C(3)-C(8)	119.22(17)
C(13)-C(14)	1.393(2)	C(3)-C(4)-C(5)	120.54(18)
C(14)-C(15)	1.515(2)	C(6)-C(5)-C(4)	121.57(17)
C(18)-C(23)	1.416(2)	C(5)-C(6)-C(7)	117.88(17)
C(18)-C(19)	1.416(2)	C(6)-C(7)-C(8)	120.97(16)
C(19)-C(20)	1.384(2)	C(6)-C(7)-N	130.81(15)
C(19)-C(26)	1.507(2)	C(8)-C(7)-N	108.14(14)
C(20)-C(21)	1.384(3)	C(3)-C(8)-C(7)	119.78(16)
C(21)-C(22)	1.384(3)	C(3)-C(8)-C(2)	132.61(16)

C(7)-C(8)-C(2)	107.56(14)	C(20)-C(19)-C(26)	118.03(16)
C(10)-C(9)-C(14)	118.30(15)	C(18)-C(19)-C(26)	121.58(15)
C(10)-C(9)-B	120.66(14)	C(19)-C(20)-C(21)	122.70(18)
C(14)-C(9)-B	121.03(14)	C(22)-C(21)-C(20)	117.00(17)
C(11)-C(10)-C(9)	119.96(16)	C(22)-C(21)-C(25)	121.91(18)
C(11)-C(10)-C(17)	119.73(15)	C(20)-C(21)-C(25)	121.07(18)
C(9)-C(10)-C(17)	120.16(15)	C(21)-C(22)-C(23)	122.66(17)
C(10)-C(11)-C(12)	121.97(17)	C(22)-C(23)-C(18)	119.98(17)
C(13)-C(12)-C(11)	118.08(17)	C(22)-C(23)-C(24)	117.13(16)
C(13)-C(12)-C(16)	120.48(18)	C(18)-C(23)-C(24)	122.82(16)
C(11)-C(12)-C(16)	121.43(17)	C(28)-C(27)-C(32)	118.06(16)
C(12)-C(13)-C(14)	121.85(17)	C(28)-C(27)-C(2)	120.88(15)
C(13)-C(14)-C(9)	119.80(16)	C(32)-C(27)-C(2)	121.00(15)
C(13)-C(14)-C(15)	118.40(15)	C(29)-C(28)-C(27)	120.92(19)
C(9)-C(14)-C(15)	121.80(15)	C(30)-C(29)-C(28)	120.27(19)
C(23)-C(18)-C(19)	117.28(15)	C(29)-C(30)-C(31)	119.38(18)
C(23)-C(18)-B	121.20(15)	C(30)-C(31)-C(32)	120.67(19)
C(19)-C(18)-B	121.22(14)	C(31)-C(32)-C(27)	120.67(18)
C(20)-C(19)-C(18)	120.38(16)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5. 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}
N	31(1)	32(1)	28(1)	-2(1)	1(1)	1(1)
B	40(1)	22(1)	30(1)	3(1)	-1(1)	3(1)
C(1)	31(1)	35(1)	32(1)	0(1)	4(1)	2(1)
C(2)	36(1)	31(1)	28(1)	1(1)	1(1)	-2(1)
C(3)	39(1)	36(1)	30(1)	0(1)	-2(1)	-9(1)
C(4)	32(1)	41(1)	40(1)	4(1)	-7(1)	-7(1)
C(5)	32(1)	37(1)	43(1)	4(1)	4(1)	-1(1)
C(6)	33(1)	34(1)	31(1)	1(1)	3(1)	-1(1)
C(7)	31(1)	26(1)	31(1)	3(1)	-1(1)	-3(1)
C(8)	35(1)	26(1)	30(1)	1(1)	1(1)	-5(1)

C(9)	29(1)	32(1)	26(1)	-3(1)	-4(1)	2(1)
C(10)	37(1)	34(1)	31(1)	-6(1)	-5(1)	3(1)
C(11)	44(1)	42(1)	38(1)	-12(1)	1(1)	10(1)
C(12)	37(1)	57(1)	33(1)	-3(1)	4(1)	8(1)
C(13)	36(1)	45(1)	37(1)	5(1)	2(1)	-1(1)
C(14)	33(1)	37(1)	29(1)	-2(1)	-1(1)	0(1)
C(15)	51(1)	34(1)	42(1)	0(1)	5(1)	-5(1)
C(16)	60(1)	82(2)	49(1)	-3(1)	22(1)	12(1)
C(17)	55(1)	32(1)	47(1)	-6(1)	3(1)	5(1)
C(18)	34(1)	30(1)	28(1)	-5(1)	2(1)	2(1)
C(19)	35(1)	31(1)	32(1)	-5(1)	1(1)	4(1)
C(20)	35(1)	44(1)	37(1)	-7(1)	-5(1)	6(1)
C(21)	36(1)	46(1)	44(1)	-12(1)	4(1)	-5(1)
C(22)	43(1)	40(1)	42(1)	-2(1)	10(1)	-8(1)
C(23)	40(1)	34(1)	31(1)	-2(1)	3(1)	1(1)
C(24)	54(1)	48(1)	41(1)	12(1)	1(1)	-6(1)
C(25)	41(1)	79(2)	69(2)	-7(1)	1(1)	-16(1)
C(26)	44(1)	48(1)	38(1)	9(1)	-6(1)	2(1)
C(27)	33(1)	35(1)	30(1)	-3(1)	3(1)	-6(1)
C(28)	45(1)	44(1)	36(1)	-1(1)	1(1)	4(1)
C(29)	46(1)	48(1)	51(1)	-11(1)	9(1)	6(1)
C(30)	36(1)	59(1)	41(1)	-16(1)	12(1)	-9(1)
C(31)	39(1)	60(1)	29(1)	-1(1)	5(1)	-11(1)
C(32)	38(1)	40(1)	35(1)	0(1)	4(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5.

	x	y	z	U(eq)
H(1)	4123(15)	559(9)	7515(14)	39(5)
H(3)	510(14)	518(8)	5122(15)	37(5)
H(4)	-1250(16)	1000(9)	5832(15)	48(5)
H(5)	-1277(14)	1448(8)	7685(13)	33(4)
H(6)	399(14)	1453(8)	8837(14)	34(4)

H(11)	837(14)	2500(9)	11687(14)	41(5)
H(13)	474(14)	340(9)	11778(14)	37(5)
H(15A)	1809	-410	10820	63
H(15B)	2646	-78	9909	63
H(15C)	1282	-191	9606	63
H(16A)	-966	1843	12575	95
H(16B)	52	1681	13499	95
H(16C)	-691	1029	12953	95
H(17A)	2097	3089	10526	67
H(17B)	2009	2718	9316	67
H(17C)	3180	2638	10084	67
H(20)	6679(15)	1350(8)	11073(14)	37(5)
H(22)	6330(14)	2574(8)	8324(14)	38(5)
H(24A)	4515	2762	7427	72
H(24B)	3357	2364	7817	72
H(24C)	4213	1964	6989	72
H(25A)	8470	1894	10007	95
H(25B)	7949	2570	10658	95
H(25C)	8123	2616	9337	95
H(26A)	5270	619	11706	66
H(26B)	4401	278	10767	66
H(26C)	3974	934	11520	66
H(28)	3924(16)	-759(9)	6320(16)	52(5)
H(29)	4501(16)	-1413(10)	4715(16)	62(6)
H(30)	3915(15)	-1024(9)	2851(16)	50(5)
H(31)	2915(14)	91(9)	2654(15)	44(5)
H(32)	2386(14)	772(9)	4225(14)	38(5)