Supplementary Material (ESI) for Dalton Transactions

The Synthesis of New Weakly Coordinating Diborate Anions: Anion Stability as a Function of Linker Structure and Steric Bulk.

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Supplementary data for the crystal structure analyses reported

Crystal and structure refinement data for $[Ph_3C][NC\text{-}PBB].0.5(CH_2Cl_2)$,

Compound **1**

Identification code	markh6
Empirical formula	C19 H15, C37 B F27 N, 0.5(C H2 Cl2)
Formula weight	1268.0
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.753(2) Å α = 86.81(3) ° b = 14.636(3) Å β = 76.00(3) ° c = 18.783(4) Å γ = 74.48(3) °
Volume	2506.6(9) $Å^3$
No. of formula units, Z	2
Calculated density	1.680 Mg/m^3
F(000)	1254
Absorption coefficient	0.220 mm^{-1}
Temperature	140(1) K
Wavelength	0.71073 Å
Crystal colour, shape	yellow block
Crystal size	0.15 x 0.15 x 0.10 mm
Crystal mounting	on a glass fibre, in oil, fixed in cold N_2 stream
On the diffractometer:	
Theta range for data collection	1.4 to 23.0 °
Limiting indices	-11<=h<=11, -17<=k<=17, -22<=l<=22
Completeness to theta = 23.0	94.2%
Absorption correction	None
Reflections collected (not including absences)	11153
No. of unique reflections	6572 [R(int) for equivalents = 0.101]
No. of 'observed' reflections ($I > 2\sigma_I$)	3521
Structure determined by:	direct methods, in SHELXS
Refinement:	Full-matrix least-squares on F^2, in SHELXL
Data / restraints / parameters	6572 / 0 / 851

Goodness-of-fit on F^2	0.953
Final R indices ('observed' data)	R1 = 0.087, wR2 = 0.226
Final R indices (all data)	R1 = 0.142, wR2 = 0.257
Reflections weighted: $w = [\sigma^2(Fo^2)+(0.1622P)^2]^{-1}$ where $P=(Fo^2+2Fc^2)/3$	
Extinction coefficient	0.010(2)
Largest diff. peak and hole	0.49 and -0.56 e.Å^{-3}
Location of largest difference peak	near F(96)

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)	S.o.f.
C(1)	1792(7)	2556(4)	-2768(4)	58(2)	
C(11)	1639(7)	2103(4)	-3395(3)	55(2)	
C(12)	2888(8)	1505(4)	-3865(4)	64(2)	
C(13)	2735(8)	1041(5)	-4451(4)	71(2)	
C(14)	1387(9)	1176(6)	-4610(4)	79(2)	
C(15)	160(8)	1778(5)	-4171(4)	71(2)	
C(16)	285(8)	2226(4)	-3565(4)	63(2)	
C(21)	623(7)	2742(5)	-2098(4)	59(2)	
C(22)	-274(7)	2110(5)	-1883(4)	59(2)	
C(23)	-1399(8)	2300(5)	-1250(4)	68(2)	
C(24)	-1649(8)	3088(5)	-837(4)	77(2)	
C(25)	-778(9)	3726(5)	-1033(4)	77(2)	
C(26)	373(8)	3540(5)	-1665(4)	66(2)	
C(31)	3133(8)	2837(4)	-2791(4)	66(2)	
C(32)	3690(8)	2757(4)	-2144(4)	66(2)	
C(33)	4952(9)	2985(5)	-2154(6)	82(2)	
C(34)	5665(9)	3326(6)	-2786(7)	93(3)	
C(35)	5183(10)	3422(5)	-3434(6)	98(3)	
C(36)	3900(9)	3158(4)	-3442(5)	82(2)	
B	4291(9)	2055(5)	2720(5)	67(2)	
C(2)	4998(8)	2321(4)	1924(4)	56(2)	
N	5535(8)	2518(4)	1315(4)	85(2)	
C(41)	5611(7)	1793(4)	3201(3)	52(2)	
C(42)	5318(7)	2087(4)	3936(4)	61(2)	
C(43)	6366(8)	1883(5)	4344(3)	64(2)	
C(44)	7767(8)	1349(5)	4047(4)	63(2)	
C(45)	8086(7)	1029(5)	3326(4)	63(2)	
C(46)	7069(7)	1244(4)	2895(3)	50(2)	
F(42)	3980(4)	2570(3)	4291(2)	76(1)	
F(43)	6014(5)	2204(3)	5041(2)	89(1)	
F(44)	8788(5)	1132(3)	4435(2)	92(1)	
F(45)	9455(4)	486(3)	3029(2)	88(1)	
C(51)	7561(7)	896(4)	2128(3)	49(2)	
C(52)	7315(7)	74(4)	1899(3)	54(2)	
C(53)	7658(7)	-190(5)	1162(4)	60(2)	
C(54)	8287(9)	377(5)	626(4)	73(2)	
C(55)	8629(9)	1158(6)	848(4)	79(2)	
C(56)	8303(8)	1396(5)	1574(4)	64(2)	
F(52)	6697(4)	-491(2)	2404(2)	60(1)	
F(53)	7378(4)	-979(3)	970(2)	76(1)	
F(54)	8535(6)	164(3)	-79(2)	99(2)	
F(55)	9305(6)	1683(3)	325(2)	108(2)	
F(56)	8597(5)	2189(3)	1756(2)	85(1)	
C(61)	3667(7)	1102(4)	2669(4)	56(2)	
C(62)	3666(7)	424(4)	3214(3)	53(2)	
C(63)	3193(7)	-381(4)	3199(3)	55(2)	
C(64)	2690(7)	-541(4)	2608(4)	60(2)	
C(65)	2644(7)	106(4)	2063(3)	55(2)	
C(66)	3118(7)	921(4)	2067(4)	59(2)	
F(62)	4104(4)	529(2)	3838(2)	64(1)	
F(63)	3227(4)	-1011(3)	3766(2)	71(1)	
F(64)	2208(4)	-1325(3)	2588(2)	76(1)	

F(65)	2096(4)	-52(2)	1490(2)	73(1)	
C(71)	2979(8)	1563(5)	1414(4)	65(2)	
C(72)	1960(9)	2411(5)	1425(5)	80(2)	
C(73)	1843(11)	3014(5)	849(7)	92(3)	
C(74)	2854(13)	2748(7)	190(7)	100(3)	
C(75)	3899(10)	1897(6)	122(5)	81(2)	
C(76)	3953(9)	1318(5)	721(4)	67(2)	
F(72)	941(5)	2674(3)	2077(3)	105(2)	
F(73)	803(7)	3837(3)	908(4)	138(2)	
F(74)	2760(8)	3327(3)	-392(3)	140(2)	
F(75)	4885(6)	1673(3)	-524(3)	103(2)	
F(76)	5001(4)	505(3)	653(2)	76(1)	
C(81)	2957(10)	3045(6)	2973(6)	40(4)	0.6
C(82)	1640(12)	2909(5)	3388(6)	51(4)	0.6
C(83)	404(9)	3672(7)	3549(5)	62(4)	0.6
C(84)	485(9)	4571(6)	3295(6)	82(5)	0.6
C(85)	1802(11)	4707(5)	2880(6)	69(4)	0.6
C(86)	3038(9)	3944(7)	2719(5)	63(5)	0.6
F(82)	1412(5)	2026(3)	3749(3)	90(1)	
F(83)	-878(10)	3520(6)	3960(6)	86(2)	0.6
F(84)	-756(8)	5318(5)	3448(6)	97(2)	0.6
F(85)	1798(8)	5609(4)	2681(5)	78(2)	0.6
C(81')	2750(20)	2983(10)	3270(10)	80(10)	0.4
C(82')	1510(30)	2795(10)	3731(11)	75(8)	0.4
C(83')	320(20)	3539(14)	4040(9)	94(9)	0.4
C(84')	376(15)	4471(12)	3889(11)	130(12)	0.4
C(85')	1615(17)	4659(9)	3427(11)	84(7)	0.4
C(86')	2801(15)	3915(12)	3118(9)	66(7)	0.4
F(83')	-893(17)	3362(10)	4507(9)	104(5)	0.4
F(84')	-819(15)	5233(9)	4150(10)	130(5)	0.4
F(85')	1682(16)	5565(9)	3330(11)	128(5)	0.4
C(91)	4272(9)	4239(5)	2392(7)	91(3)	
C(92)	5497(10)	4235(5)	2677(5)	76(2)	
C(93)	6713(9)	4444(5)	2281(5)	70(2)	
C(94)	6766(10)	4694(5)	1558(5)	80(2)	
C(95)	5647(13)	4733(6)	1238(7)	102(3)	
C(96)	4403(13)	4525(5)	1665(7)	106(4)	
F(92)	5412(4)	4010(3)	3402(3)	85(1)	
F(93)	7837(4)	4436(3)	2579(2)	82(1)	
F(94)	7955(6)	4932(3)	1145(3)	105(2)	
F(95)	5692(8)	4977(4)	542(4)	145(3)	
F(96)	3286(7)	4526(3)	1354(4)	153(3)	
Cl(1)	8644(6)	4213(3)	-4499(3)	115(2)	0.5
C(4)	7540(20)	5270(15)	-4750(12)	128(7)	0.5
Cl(2)	6131(7)	5136(5)	-5118(3)	147(2)	0.5

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

(a) In the cation

C(1)-C(11)	1.439(8)	C(22)-C(23)	1.393(9)
C(1)-C(21)	1.462(9)	C(23)-C(24)	1.360(9)
C(1)-C(31)	1.463(9)	C(24)-C(25)	1.400(11)
C(11)-C(12)	1.423(9)	C(25)-C(26)	1.405(10)
C(11)-C(16)	1.396(9)	C(31)-C(32)	1.433(9)
C(12)-C(13)	1.382(9)	C(31)-C(36)	1.399(10)
C(13)-C(14)	1.379(10)	C(32)-C(33)	1.355(10)
C(14)-C(15)	1.389(10)	C(33)-C(34)	1.365(12)
C(15)-C(16)	1.390(9)	C(34)-C(35)	1.394(12)
C(21)-C(22)	1.416(9)	C(35)-C(36)	1.409(11)
C(21)-C(26)	1.393(8)		

C(11)-C(1)-C(21)	121.1(6)	C(23)-C(22)-C(21)	119.7(6)
C(11)-C(1)-C(31)	120.3(6)	C(24)-C(23)-C(22)	120.6(7)
C(21)-C(1)-C(31)	118.6(6)	C(23)-C(24)-C(25)	121.1(8)
C(12)-C(11)-C(1)	120.2(6)	C(24)-C(25)-C(26)	119.0(7)
C(16)-C(11)-C(1)	122.2(6)	C(21)-C(26)-C(25)	120.3(7)
C(16)-C(11)-C(12)	117.6(5)	C(32)-C(31)-C(1)	119.6(7)
C(13)-C(12)-C(11)	120.3(6)	C(36)-C(31)-C(1)	120.8(7)
C(14)-C(13)-C(12)	121.0(7)	C(36)-C(31)-C(32)	119.6(7)
C(13)-C(14)-C(15)	119.6(6)	C(33)-C(32)-C(31)	121.0(8)
C(14)-C(15)-C(16)	120.2(6)	C(32)-C(33)-C(34)	118.8(8)
C(15)-C(16)-C(11)	121.2(6)	C(33)-C(34)-C(35)	123.1(8)
C(22)-C(21)-C(1)	120.0(6)	C(34)-C(35)-C(36)	118.9(9)
C(26)-C(21)-C(1)	120.8(7)	C(31)-C(36)-C(35)	118.5(8)
C(26)-C(21)-C(22)	119.3(7)		

(b) In the anion

C(2)-N	1.192(9)	C(56)-F(56)	1.347(7)
B-C(2)	1.564(12)	C(61)-C(62)	1.386(9)
B-C(41)	1.697(9)	C(61)-C(66)	1.427(8)
B-C(61)	1.679(10)	C(62)-F(62)	1.370(6)
B-C(81)	1.670(10)	C(62)-C(63)	1.380(9)
B-C(81')	1.868(16)	C(63)-F(63)	1.370(7)
C(41)-C(42)	1.407(8)	C(63)-C(64)	1.371(9)
C(41)-C(46)	1.429(8)	C(64)-F(64)	1.357(7)
C(42)-F(42)	1.337(7)	C(64)-C(65)	1.356(9)
C(42)-C(43)	1.382(9)	C(65)-F(65)	1.368(6)
C(43)-F(43)	1.348(7)	C(65)-C(66)	1.390(9)
C(43)-C(44)	1.377(9)	C(66)-C(71)	1.514(10)
C(44)-F(44)	1.335(6)	C(71)-C(72)	1.364(9)
C(44)-C(45)	1.391(9)	C(71)-C(76)	1.414(10)
C(45)-F(45)	1.359(7)	C(72)-C(73)	1.365(12)
C(45)-C(46)	1.390(8)	C(72)-F(72)	1.377(9)
C(46)-C(51)	1.478(8)	C(73)-F(73)	1.341(9)
C(51)-C(52)	1.397(8)	C(73)-C(74)	1.383(13)
C(51)-C(56)	1.406(9)	C(74)-F(74)	1.351(9)
C(52)-F(52)	1.360(7)	C(74)-C(75)	1.371(12)
C(52)-C(53)	1.395(8)	C(75)-F(75)	1.348(10)
C(53)-F(53)	1.342(7)	C(75)-C(76)	1.373(11)
C(53)-C(54)	1.399(10)	C(76)-F(76)	1.334(8)
C(54)-F(54)	1.327(8)	C(81)-C(82)	1.3900
C(54)-C(55)	1.385(10)	C(81)-C(86)	1.3900
C(55)-C(56)	1.365(9)	C(82)-C(83)	1.3900
C(55)-F(55)	1.366(9)	C(82)-F(82)	1.471(9)

C(83)-F(83)	1.368(14)	C(85')-F(85')	1.345(17)
C(83)-C(84)	1.3900	C(85')-C(86')	1.3900
C(84)-F(84)	1.379(9)	C(91)-C(86')	1.868(17)
C(84)-C(85)	1.3900	C(91)-C(92)	1.421(10)
C(85)-F(85)	1.350(10)	C(91)-C(96)	1.391(14)
C(85)-C(86)	1.3900	C(92)-C(93)	1.340(11)
C(86)-C(91)	1.380(12)	C(92)-F(92)	1.371(9)
C(81')-C(82')	1.3900	C(93)-F(93)	1.344(7)
C(81')-C(86')	1.3900	C(93)-C(94)	1.380(11)
C(82')-F(82)	1.153(14)	C(94)-F(94)	1.349(10)
C(82')-C(83')	1.3900	C(94)-C(95)	1.355(11)
C(83')-F(83')	1.37(2)	C(95)-F(95)	1.330(11)
C(83')-C(84')	1.3900	C(95)-C(96)	1.382(14)
C(84')-F(84')	1.390(18)	C(96)-F(96)	1.354(9)
C(84')-C(85')	1.3900		

N-C(2)-B	179.6(7)	C(66)-C(61)-B	123.3(6)
C(2)-B-C(41)	107.8(6)	C(62)-C(61)-C(66)	115.0(6)
C(2)-B-C(61)	108.3(5)	F(62)-C(62)-C(63)	114.2(5)
C(2)-B-C(81)	100.4(6)	F(62)-C(62)-C(61)	121.2(5)
C(2)-B-C(81')	117.1(7)	C(63)-C(62)-C(61)	124.5(5)
C(61)-B-C(41)	110.2(5)	F(63)-C(63)-C(64)	120.6(6)
C(81)-B-C(41)	116.0(6)	F(63)-C(63)-C(62)	120.4(5)
C(41)-B-C(81')	105.8(8)	C(64)-C(63)-C(62)	119.0(6)
C(81)-B-C(61)	113.3(7)	F(64)-C(64)-C(65)	121.2(5)
C(61)-B-C(81')	107.5(9)	F(64)-C(64)-C(63)	119.7(6)
C(42)-C(41)-B	121.6(6)	C(65)-C(64)-C(63)	119.1(6)
C(46)-C(41)-B	122.4(5)	C(64)-C(65)-F(65)	118.1(5)
C(42)-C(41)-C(46)	116.0(5)	C(64)-C(65)-C(66)	122.8(5)
F(42)-C(42)-C(43)	115.4(6)	F(65)-C(65)-C(66)	119.1(6)
F(42)-C(42)-C(41)	121.5(5)	C(65)-C(66)-C(61)	119.6(6)
C(43)-C(42)-C(41)	123.1(6)	C(65)-C(66)-C(71)	115.4(5)
F(43)-C(43)-C(44)	119.5(6)	C(61)-C(66)-C(71)	125.0(6)
F(43)-C(43)-C(42)	119.8(6)	C(72)-C(71)-C(76)	113.8(7)
C(44)-C(43)-C(42)	120.6(6)	C(72)-C(71)-C(66)	125.3(8)
F(44)-C(44)-C(43)	121.6(6)	C(76)-C(71)-C(66)	120.9(6)
F(44)-C(44)-C(45)	120.6(6)	C(73)-C(72)-C(71)	126.2(9)
C(43)-C(44)-C(45)	117.8(5)	C(73)-C(72)-F(72)	117.1(7)
F(45)-C(45)-C(46)	118.5(6)	C(71)-C(72)-F(72)	116.7(8)
F(45)-C(45)-C(44)	118.6(5)	F(73)-C(73)-C(72)	122.3(10)
C(46)-C(45)-C(44)	122.9(6)	F(73)-C(73)-C(74)	120.4(9)
C(45)-C(46)-C(41)	119.6(5)	C(72)-C(73)-C(74)	117.3(8)
C(45)-C(46)-C(51)	117.7(5)	F(74)-C(74)-C(75)	120.7(11)
C(41)-C(46)-C(51)	122.7(5)	F(74)-C(74)-C(73)	118.7(10)
C(52)-C(51)-C(56)	115.6(5)	C(75)-C(74)-C(73)	120.6(8)
C(52)-C(51)-C(46)	123.4(6)	F(75)-C(75)-C(74)	118.8(8)
C(56)-C(51)-C(46)	120.9(5)	F(75)-C(75)-C(76)	121.8(8)
F(52)-C(52)-C(53)	117.8(5)	C(74)-C(75)-C(76)	119.3(9)
F(52)-C(52)-C(51)	119.8(5)	F(76)-C(76)-C(75)	118.7(8)
C(53)-C(52)-C(51)	122.4(6)	F(76)-C(76)-C(71)	118.5(6)
F(53)-C(53)-C(52)	120.1(6)	C(75)-C(76)-C(71)	122.7(7)
F(53)-C(53)-C(54)	120.5(6)	C(82)-C(81)-B	115.2(7)
C(52)-C(53)-C(54)	119.4(6)	C(86)-C(81)-B	124.2(7)
F(54)-C(54)-C(55)	121.3(7)	C(82)-C(81)-C(86)	120.0
F(54)-C(54)-C(53)	120.0(6)	C(83)-C(82)-C(81)	120.0
C(55)-C(54)-C(53)	118.8(6)	C(83)-C(82)-F(82)	113.5(7)
C(56)-C(55)-F(55)	120.7(7)	C(81)-C(82)-F(82)	126.3(7)
C(56)-C(55)-C(54)	120.8(7)	F(83)-C(83)-C(84)	121.2(7)
F(55)-C(55)-C(54)	118.5(6)	F(83)-C(83)-C(82)	118.8(7)
F(56)-C(56)-C(55)	118.2(7)	C(84)-C(83)-C(82)	120.0
F(56)-C(56)-C(51)	118.9(5)	F(84)-C(84)-C(83)	119.4(8)
C(55)-C(56)-C(51)	122.6(6)	F(84)-C(84)-C(85)	120.6(8)
C(62)-C(61)-B	121.7(5)	C(83)-C(84)-C(85)	120.0

F(85)-C(85)-C(84)	116.1(8)	C(85')-C(86')-C(91)	116.2(10)
F(85)-C(85)-C(86)	123.9(7)	C(81')-C(86')-C(91)	123.0(10)
C(84)-C(85)-C(86)	120.0	C(86)-C(91)-C(96)	116.6(9)
C(91)-C(86)-C(85)	111.3(7)	C(86)-C(91)-C(92)	129.0(10)
C(91)-C(86)-C(81)	128.1(7)	C(96)-C(91)-C(92)	114.3(9)
C(85)-C(86)-C(81)	120.0	C(96)-C(91)-C(86')	134.9(9)
C(82')-C(81')-B	123.8(12)	C(92)-C(91)-C(86')	110.7(9)
C(86')-C(81')-B	115.7(11)	C(93)-C(92)-F(92)	118.7(7)
C(82')-C(81')-C(86')	120.0	C(93)-C(92)-C(91)	123.8(9)
F(82)-C(82')-C(81')	117.5(16)	F(92)-C(92)-C(91)	117.5(9)
F(82)-C(82')-C(83')	121.4(17)	C(92)-C(93)-F(93)	121.4(8)
C(81')-C(82')-C(83')	120.0	C(92)-C(93)-C(94)	118.0(7)
F(83')-C(83')-C(84')	119.5(15)	F(93)-C(93)-C(94)	120.5(8)
F(83')-C(83')-C(82')	120.5(15)	F(94)-C(94)-C(95)	117.4(9)
C(84')-C(83')-C(82')	120.0	F(94)-C(94)-C(93)	119.9(7)
F(84')-C(84')-C(83')	121.7(13)	C(95)-C(94)-C(93)	122.7(10)
F(84')-C(84')-C(85')	118.2(13)	F(95)-C(95)-C(94)	122.9(12)
C(83')-C(84')-C(85')	120.0	F(95)-C(95)-C(96)	119.3(9)
F(85')-C(85')-C(84')	118.8(13)	C(94)-C(95)-C(96)	117.8(10)
F(85')-C(85')-C(86')	121.0(13)	F(96)-C(96)-C(95)	119.2(11)
C(84')-C(85')-C(86')	120.0	F(96)-C(96)-C(91)	117.3(12)
C(85')-C(86')-C(81')	120.0	C(95)-C(96)-C(91)	123.3(8)

(c) In the disordered solvent molecule

Cl(1)-C(4)	1.746(19)	Cl(2)-C(4)-Cl(1)	114.7(13)
C(4)-Cl(2)	1.74(2)		

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3) for the expression:

$$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$$

E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	60(4)	47(4)	72(5)	14(3)	-27(4)	-17(3)
C(11)	58(4)	49(4)	58(4)	0(3)	-20(4)	-9(3)
C(12)	62(5)	66(4)	64(4)	7(4)	-21(4)	-16(4)
C(13)	78(5)	82(5)	48(4)	-9(4)	-13(4)	-14(4)
C(14)	84(6)	97(6)	61(5)	-5(4)	-29(5)	-20(5)
C(15)	71(5)	92(5)	60(4)	9(4)	-28(4)	-28(4)
C(16)	63(5)	57(4)	68(4)	-1(3)	-22(4)	-8(3)
C(21)	52(4)	63(4)	67(5)	-1(4)	-25(4)	-13(3)
C(22)	57(4)	70(4)	61(4)	0(3)	-25(4)	-24(4)
C(23)	77(5)	75(5)	64(5)	0(4)	-26(4)	-29(4)
C(24)	68(5)	79(5)	79(5)	-18(4)	-21(4)	-5(4)
C(25)	84(6)	65(5)	85(6)	-14(4)	-33(5)	-7(4)
C(26)	70(5)	53(4)	75(5)	-18(4)	-21(4)	-10(3)
C(31)	59(5)	51(4)	90(6)	-2(4)	-18(4)	-18(3)
C(32)	67(5)	47(4)	86(5)	-15(3)	-21(4)	-13(3)
C(33)	69(6)	62(5)	120(7)	-18(5)	-22(5)	-23(4)
C(34)	62(6)	65(5)	156(10)	-43(6)	-28(7)	-12(4)
C(35)	75(6)	63(5)	146(9)	-1(5)	7(6)	-34(4)
C(36)	87(6)	46(4)	117(7)	2(4)	-24(5)	-24(4)
B	60(5)	46(4)	108(7)	-10(4)	-49(5)	-8(4)
C(2)	74(5)	44(4)	61(5)	10(3)	-39(4)	-18(3)
N	108(5)	63(4)	107(6)	2(4)	-61(5)	-30(4)
C(41)	69(5)	47(3)	45(4)	4(3)	-24(3)	-17(3)
C(42)	59(5)	53(4)	70(5)	-11(3)	-21(4)	-7(3)
C(43)	74(5)	78(5)	46(4)	-13(3)	-17(4)	-26(4)
C(44)	66(5)	92(5)	48(4)	2(4)	-33(4)	-29(4)
C(45)	48(4)	71(4)	71(5)	6(4)	-24(4)	-9(3)
C(46)	53(4)	45(3)	55(4)	3(3)	-23(3)	-10(3)
F(42)	73(3)	70(2)	78(3)	-15(2)	-11(2)	-9(2)
F(43)	116(4)	110(3)	54(2)	-16(2)	-23(2)	-49(3)
F(44)	83(3)	142(4)	71(3)	10(2)	-44(2)	-43(3)
F(45)	54(3)	121(3)	79(3)	-6(2)	-26(2)	5(2)
C(51)	55(4)	52(4)	45(4)	-1(3)	-20(3)	-14(3)
C(52)	51(4)	60(4)	47(4)	-1(3)	-11(3)	-10(3)
C(53)	73(5)	61(4)	52(4)	-9(4)	-22(4)	-20(4)
C(54)	91(6)	85(5)	49(5)	-3(4)	-21(4)	-27(4)
C(55)	102(6)	89(5)	51(5)	13(4)	-11(4)	-42(5)
C(56)	83(5)	59(4)	55(4)	-6(3)	-22(4)	-20(4)
F(52)	64(2)	55(2)	60(2)	3(2)	-12(2)	-15(2)
F(53)	85(3)	75(2)	72(3)	-20(2)	-20(2)	-24(2)
F(54)	133(4)	124(3)	45(2)	-13(2)	-15(2)	-46(3)
F(55)	153(5)	116(4)	64(3)	14(3)	-10(3)	-69(3)
F(56)	118(4)	76(3)	75(3)	-2(2)	-22(3)	-49(2)
C(61)	53(4)	56(4)	63(4)	-5(3)	-26(3)	-7(3)
C(62)	53(4)	69(4)	47(4)	2(3)	-26(3)	-18(3)
C(63)	53(4)	58(4)	56(4)	-1(3)	-17(3)	-13(3)
C(64)	57(4)	56(4)	77(5)	0(4)	-25(4)	-20(3)
C(65)	58(4)	59(4)	58(4)	-7(3)	-27(3)	-17(3)
C(66)	55(4)	50(4)	76(5)	-10(3)	-33(4)	-2(3)
F(62)	77(3)	63(2)	63(2)	0(2)	-30(2)	-24(2)
F(63)	76(3)	73(2)	74(3)	13(2)	-30(2)	-30(2)
F(64)	79(3)	71(2)	95(3)	-1(2)	-39(2)	-31(2)

F(65)	84(3)	69(2)	84(3)	0(2)	-46(2)	-29(2)
C(71)	64(5)	58(4)	91(6)	3(4)	-47(5)	-20(4)
C(72)	56(5)	65(5)	121(7)	-19(5)	-42(5)	4(4)
C(73)	110(7)	50(5)	133(8)	16(6)	-84(7)	-3(5)
C(74)	131(9)	78(6)	131(9)	48(6)	-97(8)	-46(6)
C(75)	110(7)	84(6)	81(6)	14(5)	-59(6)	-47(5)
C(76)	84(5)	60(4)	75(5)	3(4)	-51(5)	-20(4)
F(72)	80(3)	80(3)	162(5)	-17(3)	-69(4)	7(2)
F(73)	149(5)	73(3)	200(6)	27(3)	-102(5)	4(3)
F(74)	216(6)	99(3)	156(5)	62(4)	-124(5)	-69(4)
F(75)	153(5)	112(3)	76(3)	20(3)	-55(3)	-65(3)
F(76)	93(3)	76(3)	66(2)	-1(2)	-38(2)	-13(2)
C(81)	32(7)	43(9)	49(9)	-17(6)	-16(6)	-6(6)
C(82)	62(11)	32(7)	67(11)	-13(6)	-17(9)	-20(7)
C(83)	36(7)	56(9)	97(11)	-11(8)	-15(7)	-13(6)
C(84)	58(10)	51(8)	130(13)	-28(9)	-22(10)	4(7)
C(85)	64(9)	70(10)	91(10)	3(8)	-36(9)	-30(7)
C(86)	74(11)	36(7)	78(11)	-9(7)	-40(9)	12(8)
F(82)	78(3)	71(3)	119(4)	-14(3)	-24(3)	-14(2)
F(83)	59(5)	61(5)	132(8)	-6(5)	-10(6)	-18(4)
F(84)	55(5)	62(5)	155(8)	-8(5)	-13(5)	8(3)
F(85)	69(5)	39(4)	129(6)	-5(4)	-37(5)	-7(3)
C(81')	120(30)	59(16)	80(20)	24(13)	-33(17)	-50(16)
C(82')	58(15)	78(18)	80(20)	-5(14)	-6(13)	-10(14)
C(83')	130(30)	72(15)	110(20)	19(16)	-50(20)	-64(18)
C(84')	49(15)	130(30)	190(30)	-80(20)	23(18)	-21(15)
C(85')	58(14)	42(12)	140(20)	-9(14)	-1(15)	-14(10)
C(86')	37(11)	58(14)	110(20)	-12(13)	-13(12)	-25(10)
F(83')	90(10)	88(9)	110(11)	24(9)	21(10)	-27(7)
F(84')	83(9)	82(9)	180(15)	3(10)	27(11)	0(7)
F(85')	97(10)	69(9)	189(16)	0(10)	19(12)	-21(7)
C(91)	62(5)	40(4)	188(10)	-3(5)	-65(6)	-12(4)
C(92)	88(6)	49(4)	100(6)	3(4)	-43(5)	-15(4)
C(93)	70(5)	56(4)	102(6)	0(4)	-44(5)	-25(4)
C(94)	94(7)	51(4)	109(7)	9(4)	-47(6)	-20(4)
C(95)	128(9)	70(5)	145(9)	18(5)	-91(8)	-41(6)
C(96)	125(9)	50(4)	174(11)	13(6)	-117(9)	-7(5)
F(92)	78(3)	66(2)	119(4)	-11(2)	-25(3)	-29(2)
F(93)	76(3)	80(3)	108(3)	6(2)	-45(3)	-30(2)
F(94)	122(4)	81(3)	128(4)	10(3)	-53(4)	-35(3)
F(95)	229(7)	102(4)	158(5)	36(4)	-137(5)	-60(4)
F(96)	162(5)	77(3)	278(8)	23(4)	-171(6)	-27(3)
Cl(1)	142(4)	106(3)	99(3)	4(3)	-45(3)	-22(3)
C(4)	123(17)	127(15)	127(17)	31(13)	-42(14)	-15(13)
Cl(2)	143(5)	162(5)	123(4)	25(4)	-42(4)	-12(4)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) of the parent carbon atom.

	x	y	z	U(eq)
H(12)	3811	1427	-3779	76
H(13)	3554	631	-4742	85
H(14)	1300	865	-5009	95
H(15)	-748	1883	-4282	86
H(16)	-549	2614	-3268	76
H(22)	-112	1571	-2164	71
H(23)	-1986	1883	-1108	82
H(24)	-2410	3206	-418	92
H(25)	-960	4264	-748	93
H(26)	970	3952	-1796	79
H(32)	3177	2546	-1712	79
H(33)	5326	2911	-1737	98
H(34)	6512	3503	-2785	112
H(35)	5701	3657	-3854	117
H(36)	3570	3196	-3871	98
H(4A)	7118	5680	-4321	154
H(4B)	8154	5586	-5107	154

Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(21)-C(1)-C(11)-C(16)	32.0(9)
C(31)-C(1)-C(11)-C(16)	-148.2(6)
C(21)-C(1)-C(11)-C(12)	-147.9(6)
C(31)-C(1)-C(11)-C(12)	32.0(8)
C(11)-C(1)-C(21)-C(26)	-146.7(6)
C(31)-C(1)-C(21)-C(26)	33.4(8)
C(11)-C(1)-C(21)-C(22)	33.0(8)
C(31)-C(1)-C(21)-C(22)	-146.9(6)
C(11)-C(1)-C(31)-C(36)	34.6(8)
C(21)-C(1)-C(31)-C(36)	-145.6(6)
C(11)-C(1)-C(31)-C(32)	-143.7(6)
C(21)-C(1)-C(31)-C(32)	36.2(8)
C(81)-B-C(2)-N	-124(100)
C(61)-B-C(2)-N	-5(100)
C(41)-B-C(2)-N	114(100)
C(81')-B-C(2)-N	-127(100)
C(2)-B-C(41)-C(42)	139.8(6)
C(81)-B-C(41)-C(42)	28.3(10)
C(61)-B-C(41)-C(42)	-102.2(7)
C(81')-B-C(41)-C(42)	13.7(10)
C(2)-B-C(41)-C(46)	-41.9(7)
C(81)-B-C(41)-C(46)	-153.4(7)
C(61)-B-C(41)-C(46)	76.1(8)
C(81')-B-C(41)-C(46)	-168.0(8)
C(45)-C(46)-C(51)-C(52)	98.2(7)
C(41)-C(46)-C(51)-C(52)	-82.5(7)
C(45)-C(46)-C(51)-C(56)	-82.6(7)
C(41)-C(46)-C(51)-C(56)	96.7(7)
C(2)-B-C(61)-C(62)	147.1(6)
C(81)-B-C(61)-C(62)	-102.5(8)
C(41)-B-C(61)-C(62)	29.3(9)
C(81')-B-C(61)-C(62)	-85.5(9)
C(2)-B-C(61)-C(66)	-32.2(8)
C(81)-B-C(61)-C(66)	78.2(9)
C(41)-B-C(61)-C(66)	-149.9(6)
C(81')-B-C(61)-C(66)	95.2(9)
C(65)-C(66)-C(71)-C(72)	106.2(7)
C(61)-C(66)-C(71)-C(72)	-73.0(9)
C(65)-C(66)-C(71)-C(76)	-74.6(8)
C(61)-C(66)-C(71)-C(76)	106.3(8)
C(2)-B-C(81)-C(82)	141.1(5)
C(61)-B-C(81)-C(82)	25.9(8)
C(41)-B-C(81)-C(82)	-103.1(7)
C(2)-B-C(81)-C(86)	-30.4(8)
C(61)-B-C(81)-C(86)	-145.6(6)
C(41)-B-C(81)-C(86)	85.4(9)
C(85)-C(86)-C(91)-C(96)	-73.9(9)
C(81)-C(86)-C(91)-C(96)	115.2(8)
C(85)-C(86)-C(91)-C(92)	110.8(8)
C(81)-C(86)-C(91)-C(92)	-60.1(12)
C(2)-B-C(81')-C(82')	140.4(9)
C(61)-B-C(81')-C(82')	18.4(12)
C(41)-B-C(81')-C(82')	-99.4(10)
C(2)-B-C(81')-C(86')	-31.0(14)
C(61)-B-C(81')-C(86')	-153.0(9)
C(41)-B-C(81')-C(86')	89.2(11)
C(96)-C(91)-C(86')-C(85')	-73.1(14)

C(92)-C(91)-C(86')-C(85')	102.8(10)
C(96)-C(91)-C(86')-C(81')	96.9(13)
C(92)-C(91)-C(86')-C(81')	-87.2(10)

Table 1. Crystal data and structure refinement of $C_{36}H_2BF_{26}N \cdot CH_2Cl_2$, Compound **3**

Identification code	03src0530	
Empirical formula	$C_{37}H_4BCl_2F_{26}N$	
Formula weight	1038.12	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 10.9769(3) Å	α = 87.181(2)°
	b = 14.3059(6) Å	β = 83.930(3)°
	c = 22.4108(10) Å	γ = 85.923(2)°
Volume	3487.6(2) Å^3	
Z	4	
Density (calculated)	1.977 Mg / m^3	
Absorption coefficient	0.361 mm^{-1}	
F(000)	2024	
Crystal	Slab; Colourless	
Crystal size	0.24 × 0.16 × 0.06 mm^3	
θ range for data collection	2.96 – 27.45°	
Index ranges	$-14 \le h \le 14$, $-18 \le k \le 18$, $-28 \le l \le 29$	
Reflections collected	49270	
Independent reflections	15151 [R_{int} = 0.0752]	
Completeness to θ = 27.45°	95.0 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9787 and 0.9183	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15151 / 0 / 1208	
Goodness-of-fit on F^2	0.948	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0558, *wR2* = 0.1208	
R indices (all data)	*R1* = 0.1444, *wR2* = 0.1510	
Extinction coefficient	0.0002(2)	
Largest diff. peak and hole	0.674 and –0.490 e Å^{-3}	

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). Cell determination: DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) Data collection: Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). Data reduction and cell refinement: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. 276: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). Absorption correction: *SORTAV* (R. H. Blessing, Acta Cryst. A51 (1995) 33–37; R. H. Blessing, J. Appl. Cryst. 30 (1997) 421–426). Structure solution: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A46 467–473). Structure refinement: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). Graphics: Cameron - A Molecular Graphics Package. (D. M. Watkin, L. Pearce and C. K. Prout, Chemical Crystallography Laboratory, University of Oxford, 1993).

Special details:

All hydrogen atoms were fixed.

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	2637(3)	7976(2)	1579(2)	20(1)	1
C2	3574(3)	8151(2)	1907(2)	22(1)	1
C3	4018(3)	9028(3)	1922(2)	25(1)	1
C4	3455(3)	9779(2)	1630(2)	26(1)	1
C5	2511(3)	9632(2)	1298(2)	24(1)	1
C6	2130(3)	8750(2)	1244(2)	23(1)	1
C7	1204(3)	8573(2)	834(2)	20(1)	1
C8	1128(3)	9004(2)	270(2)	24(1)	1
C9	317(3)	8762(2)	−111(2)	23(1)	1
C10	−472(3)	8074(2)	53(2)	24(1)	1
C11	−398(3)	7605(2)	600(2)	24(1)	1
C12	419(3)	7851(2)	985(2)	21(1)	1
C13	2337(3)	6254(2)	1112(2)	20(1)	1
C14	1665(3)	5463(2)	1124(2)	22(1)	1
C15	1883(3)	4741(3)	735(2)	26(1)	1
C16	2818(3)	4800(3)	281(2)	27(1)	1
C17	3454(3)	5595(2)	220(2)	24(1)	1
C18	3246(3)	6314(2)	614(2)	21(1)	1
C19	3935(3)	7163(2)	410(2)	24(1)	1
C20	4967(3)	7427(3)	646(2)	29(1)	1
C21	5604(3)	8181(3)	408(2)	32(1)	1
C22	5223(4)	8684(3)	−82(2)	34(1)	1
C23	4213(3)	8434(3)	−336(2)	31(1)	1
C24	3606(3)	7689(3)	−92(2)	26(1)	1
C25	1907(3)	6578(2)	2348(2)	22(1)	1
C26	1419(3)	7197(3)	2788(2)	25(1)	1
C27	1303(3)	7005(3)	3394(2)	26(1)	1
C28	1692(3)	6129(3)	3607(2)	27(1)	1
C29	2166(3)	5492(3)	3199(2)	27(1)	1
C30	2295(3)	5689(2)	2583(2)	22(1)	1
C31	2849(3)	4877(2)	2227(2)	22(1)	1
C32	2229(3)	4066(3)	2214(2)	27(1)	1
C33	2721(4)	3286(3)	1926(2)	32(1)	1
C34	3916(4)	3281(3)	1656(2)	31(1)	1
C35	4567(3)	4055(3)	1672(2)	28(1)	1
C36	4036(3)	4843(3)	1948(2)	25(1)	1
B1	1969(3)	6995(3)	1643(2)	22(1)	1
F1	4117(2)	7467(1)	2242(1)	27(1)	1
F2	4939(2)	9159(1)	2255(1)	32(1)	1
F3	3830(2)	10644(1)	1674(1)	34(1)	1
F4	1950(2)	10402(1)	1050(1)	29(1)	1
F5	1919(2)	9651(1)	54(1)	29(1)	1
F6	324(2)	9195(1)	−658(1)	31(1)	1
F7	−1273(2)	7843(1)	−311(1)	31(1)	1
F8	−1114(2)	6895(1)	760(1)	30(1)	1
F9	702(2)	5369(1)	1554(1)	26(1)	1
F10	1216(2)	3990(1)	807(1)	36(1)	1
F11	3063(2)	4108(2)	−107(1)	37(1)	1
F12	4302(2)	5672(1)	−261(1)	33(1)	1
F13	2649(2)	7436(2)	−364(1)	33(1)	1
F14	3852(2)	8923(2)	−820(1)	45(1)	1
F15	5846(2)	9410(2)	−312(1)	47(1)	1
F16	6591(2)	8417(2)	653(1)	47(1)	1
F17	5387(2)	6933(2)	1117(1)	34(1)	1

F18	968(2)	8077(1)	2621(1)	30(1)	1
F19	805(2)	7648(2)	3776(1)	37(1)	1
F20	1595(2)	5919(2)	4199(1)	37(1)	1
F21	2545(2)	4634(2)	3416(1)	34(1)	1
F22	1079(2)	4038(1)	2495(1)	34(1)	1
F23	2065(2)	2535(2)	1915(1)	48(1)	1
F24	4421(2)	2515(2)	1380(1)	49(1)	1
F25	5739(2)	4032(2)	1432(1)	39(1)	1
F26	4708(2)	5586(1)	1949(1)	31(1)	1
N1	514(2)	7349(2)	1554(1)	21(1)	1
C41	7423(3)	2219(2)	3318(2)	23(1)	1
C42	6511(3)	2055(3)	2969(2)	26(1)	1
C43	6041(3)	1185(3)	2947(2)	33(1)	1
C44	6552(4)	428(3)	3260(2)	34(1)	1
C45	7472(3)	564(3)	3608(2)	29(1)	1
C46	7893(3)	1443(2)	3663(2)	22(1)	1
C47	8829(3)	1599(2)	4071(2)	22(1)	1
C48	8928(3)	1146(2)	4625(2)	24(1)	1
C49	9829(3)	1324(2)	4981(2)	24(1)	1
C50	10636(3)	2000(3)	4812(2)	25(1)	1
C51	10520(3)	2500(2)	4276(2)	26(1)	1
C52	9652(3)	2304(2)	3910(2)	22(1)	1
C53	7713(3)	3871(2)	3861(2)	22(1)	1
C54	8423(3)	4618(3)	3911(2)	23(1)	1
C55	8218(3)	5273(3)	4345(2)	27(1)	1
C56	7258(3)	5177(3)	4781(2)	29(1)	1
C57	6577(3)	4415(3)	4779(2)	27(1)	1
C58	6765(3)	3758(2)	4336(2)	23(1)	1
C59	5986(3)	2937(3)	4455(2)	26(1)	1
C60	6180(3)	2322(3)	4948(2)	27(1)	1
C61	5460(4)	1592(3)	5107(2)	36(1)	1
C62	4500(4)	1447(3)	4791(2)	38(1)	1
C63	4271(3)	2038(3)	4299(2)	37(1)	1
C64	5000(3)	2783(3)	4150(2)	30(1)	1
C65	8153(3)	3708(2)	2603(2)	22(1)	1
C66	8622(3)	3130(3)	2137(2)	24(1)	1
C67	8764(3)	3397(3)	1536(2)	26(1)	1
C68	8425(3)	4308(3)	1370(2)	29(1)	1
C69	7961(3)	4902(3)	1809(2)	28(1)	1
C70	7817(3)	4640(3)	2413(2)	23(1)	1
C71	7322(3)	5404(3)	2809(2)	25(1)	1
C72	8006(3)	6171(3)	2875(2)	28(1)	1
C73	7578(4)	6918(3)	3206(2)	31(1)	1
C74	6376(4)	6961(3)	3464(2)	37(1)	1
C75	5643(3)	6243(3)	3390(2)	31(1)	1
C76	6121(3)	5480(3)	3071(2)	28(1)	1
B41	8079(3)	3206(3)	3286(2)	22(1)	1
F41	6004(2)	2749(1)	2626(1)	32(1)	1
F42	5152(2)	1071(2)	2601(1)	47(1)	1
F43	6166(2)	–429(2)	3215(1)	49(1)	1
F44	8011(2)	–206(1)	3867(1)	35(1)	1
F45	8114(2)	535(1)	4854(1)	29(1)	1
F46	9893(2)	845(1)	5509(1)	30(1)	1
F47	11492(2)	2178(2)	5158(1)	34(1)	1
F48	11266(2)	3190(1)	4103(1)	33(1)	1
F49	9407(2)	4752(1)	3499(1)	27(1)	1
F50	8936(2)	5994(2)	4341(1)	40(1)	1
F51	7023(2)	5797(2)	5215(1)	41(1)	1
F52	5693(2)	4300(2)	5236(1)	37(1)	1
F53	7092(2)	2462(2)	5283(1)	37(1)	1

F54	5663(2)	1024(2)	5586(1)	46(1)	1
F55	3782(2)	741(2)	4942(1)	54(1)	1
F56	3353(2)	1896(2)	3979(1)	49(1)	1
F57	4723(2)	3361(2)	3691(1)	36(1)	1
F58	9013(2)	2219(1)	2261(1)	31(1)	1
F59	9228(2)	2785(2)	1128(1)	34(1)	1
F60	8552(2)	4594(2)	789(1)	40(1)	1
F61	7648(2)	5796(2)	1631(1)	36(1)	1
F62	9164(2)	6172(1)	2599(1)	33(1)	1
F63	8295(2)	7619(2)	3277(1)	46(1)	1
F64	5929(2)	7701(2)	3781(1)	56(1)	1
F65	4464(2)	6308(2)	3614(1)	47(1)	1
F66	5388(2)	4790(2)	3011(1)	34(1)	1
N41	9536(2)	2829(2)	3352(1)	22(1)	1
C81	7786(4)	9394(3)	1722(2)	52(1)	1
Cl81	9052(1)	9773(1)	2037(1)	60(1)	1
Cl82	7608(1)	8184(1)	1899(1)	48(1)	1
C83	1329(4)	36(3)	3360(2)	54(1)	1
Cl83	2772(1)	–556(1)	3362(1)	65(1)	1
Cl84	1273(1)	877(1)	2766(1)	60(1)	1

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

C1–C2	1.371(5)	C26–F18	1.370(4)
C1–C6	1.420(5)	C27–F19	1.335(4)
C1–B1	1.623(5)	C27–C28	1.374(5)
C2–F1	1.347(4)	C28–F20	1.342(4)
C2–C3	1.381(5)	C28–C29	1.360(5)
C3–F2	1.347(4)	C29–F21	1.352(4)
C3–C4	1.374(5)	C29–C30	1.389(5)
C4–F3	1.343(4)	C30–C31	1.497(5)
C4–C5	1.372(5)	C31–C36	1.383(5)
C5–F4	1.348(4)	C31–C32	1.389(5)
C5–C6	1.372(5)	C32–F22	1.352(4)
C6–C7	1.483(5)	C32–C33	1.365(5)
C7–C8	1.385(5)	C33–F23	1.337(4)
C7–C12	1.397(5)	C33–C34	1.386(5)
C8–F5	1.351(4)	C34–F24	1.341(4)
C8–C9	1.369(5)	C34–C35	1.364(5)
C9–F6	1.347(4)	C35–F25	1.339(4)
C9–C10	1.368(5)	C35–C36	1.375(5)
C10–F7	1.330(4)	C36–F26	1.337(4)
C10–C11	1.376(5)	B1–N1	1.670(5)
C11–F8	1.339(4)	N1–H1A	0.9200
C11–C12	1.382(5)	N1–H1B	0.9200
C12–N1	1.443(4)	C41–C42	1.373(5)
C13–C14	1.391(5)	C41–C46	1.421(5)
C13–C18	1.420(5)	C41–B41	1.625(5)
C13–B1	1.632(5)	C42–F41	1.349(4)
C14–F9	1.363(4)	C42–C43	1.386(5)
C14–C15	1.376(5)	C43–F42	1.333(4)
C15–F10	1.337(4)	C43–C44	1.379(5)
C15–C16	1.370(5)	C44–F43	1.337(4)
C16–F11	1.344(4)	C44–C45	1.369(5)
C16–C17	1.370(5)	C45–F44	1.349(4)
C17–F12	1.353(4)	C45–C46	1.385(5)
C17–C18	1.378(5)	C46–C47	1.480(5)
C18–C19	1.503(5)	C47–C48	1.384(5)
C19–C20	1.382(5)	C47–C52	1.409(5)
C19–C24	1.388(5)	C48–F45	1.340(4)
C20–F17	1.346(4)	C48–C49	1.380(5)
C20–C21	1.382(5)	C49–F46	1.343(4)
C21–F16	1.335(4)	C49–C50	1.371(5)
C21–C22	1.368(6)	C50–F47	1.326(4)
C22–F15	1.336(4)	C50–C51	1.379(5)
C22–C23	1.376(6)	C51–F48	1.344(4)
C23–F14	1.341(4)	C51–C52	1.373(5)
C23–C24	1.359(5)	C52–N41	1.441(4)
C24–F13	1.349(4)	C53–C54	1.382(5)
C25–C26	1.396(5)	C53–C58	1.421(5)
C25–C30	1.407(5)	C53–B41	1.638(6)
C25–B1	1.659(5)	C54–F49	1.363(4)
C26–C27	1.367(5)	C54–C55	1.373(5)

C55–F50	1.342(4)	C69–F61	1.352(4)
C55–C56	1.369(5)	C69–C70	1.383(5)
C56–F51	1.342(4)	C70–C71	1.479(5)
C56–C57	1.366(5)	C71–C76	1.385(5)
C57–F52	1.347(4)	C71–C72	1.395(5)
C57–C58	1.389(5)	C72–F62	1.354(4)
C58–C59	1.499(5)	C72–C73	1.359(5)
C59–C64	1.376(5)	C73–F63	1.343(4)
C59–C60	1.403(5)	C73–C74	1.381(5)
C60–F53	1.344(4)	C74–F64	1.340(4)
C60–C61	1.365(6)	C74–C75	1.375(6)
C61–F54	1.342(4)	C75–F65	1.336(4)
C61–C62	1.364(6)	C75–C76	1.377(5)
C62–F55	1.333(4)	C76–F66	1.337(4)
C62–C63	1.389(6)	B41–N41	1.670(5)
C63–F56	1.329(5)	N41–H41A	0.9200
C63–C64	1.385(6)	N41–H41B	0.9200
C64–F57	1.336(4)	C81–Cl81	1.754(5)
C65–C66	1.396(5)	C81–Cl82	1.776(5)
C65–C70	1.414(5)	C81–H81A	0.9900
C65–B41	1.655(5)	C81–H81B	0.9900
C66–F58	1.367(4)	C83–Cl83	1.742(5)
C66–C67	1.377(5)	C83–Cl84	1.753(5)
C67–F59	1.335(4)	C83–H83A	0.9900
C67–C68	1.374(5)	C83–H83B	0.9900
C68–F60	1.341(4)		
C68–C69	1.365(5)		

C2–C1–C6	116.6(3)	F6–C9–C10	120.0(3)
C2–C1–B1	122.8(3)	F6–C9–C8	119.1(3)
C6–C1–B1	119.8(3)	C10–C9–C8	120.9(3)
F1–C2–C1	121.4(3)	F7–C10–C9	121.3(3)
F1–C2–C3	115.7(3)	F7–C10–C11	120.3(3)
C1–C2–C3	122.9(3)	C9–C10–C11	118.4(3)
F2–C3–C4	120.1(3)	F8–C11–C10	119.9(3)
F2–C3–C2	120.3(3)	F8–C11–C12	119.5(3)
C4–C3–C2	119.5(3)	C10–C11–C12	120.6(3)
F3–C4–C5	120.9(3)	C11–C12–C7	121.8(3)
F3–C4–C3	119.9(3)	C11–C12–N1	120.7(3)
C5–C4–C3	119.2(3)	C7–C12–N1	117.5(3)
F4–C5–C6	122.1(3)	C14–C13–C18	113.8(3)
F4–C5–C4	116.4(3)	C14–C13–B1	117.6(3)
C6–C5–C4	121.5(3)	C18–C13–B1	128.6(3)
C5–C6–C1	120.0(3)	F9–C14–C15	115.3(3)
C5–C6–C7	121.6(3)	F9–C14–C13	119.0(3)
C1–C6–C7	118.3(3)	C15–C14–C13	125.8(3)
C8–C7–C12	115.7(3)	F10–C15–C16	120.8(3)
C8–C7–C6	124.9(3)	F10–C15–C14	120.7(3)
C12–C7–C6	119.0(3)	C16–C15–C14	118.5(3)
F5–C8–C9	116.4(3)	F11–C16–C15	120.3(3)
F5–C8–C7	120.8(3)	F11–C16–C17	121.4(3)
C9–C8–C7	122.6(3)	C15–C16–C17	118.3(3)

F12–C17–C16	117.2(3)	F24–C34–C33	119.6(4)
F12–C17–C18	119.6(3)	C35–C34–C33	119.7(3)
C16–C17–C18	123.2(3)	F25–C35–C34	119.4(3)
C17–C18–C13	120.2(3)	F25–C35–C36	120.3(3)
C17–C18–C19	113.4(3)	C34–C35–C36	120.2(3)
C13–C18–C19	126.0(3)	F26–C36–C35	118.0(3)
C20–C19–C24	115.5(3)	F26–C36–C31	119.9(3)
C20–C19–C18	125.4(3)	C35–C36–C31	122.0(3)
C24–C19–C18	118.8(3)	C1–B1–C13	117.2(3)
F17–C20–C19	119.7(3)	C1–B1–C25	109.9(3)
F17–C20–C21	118.1(3)	C13–B1–C25	117.8(3)
C19–C20–C21	122.2(4)	C1–B1–N1	102.2(3)
F16–C21–C22	120.1(3)	C13–B1–N1	103.5(3)
F16–C21–C20	120.2(4)	C25–B1–N1	103.8(3)
C22–C21–C20	119.7(4)	C12–N1–B1	111.3(2)
F15–C22–C21	119.5(4)	C12–N1–H1A	109.4
F15–C22–C23	120.6(4)	B1–N1–H1A	109.4
C21–C22–C23	119.9(3)	C12–N1–H1B	109.4
F14–C23–C24	121.4(4)	B1–N1–H1B	109.4
F14–C23–C22	119.7(3)	H1A–N1–H1B	108.0
C24–C23–C22	118.9(4)	C42–C41–C46	116.9(3)
F13–C24–C23	117.7(3)	C42–C41–B41	122.9(3)
F13–C24–C19	118.5(3)	C46–C41–B41	119.7(3)
C23–C24–C19	123.7(4)	F41–C42–C41	121.3(3)
C26–C25–C30	113.5(3)	F41–C42–C43	115.6(3)
C26–C25–B1	116.4(3)	C41–C42–C43	123.1(3)
C30–C25–B1	130.1(3)	F42–C43–C44	120.4(3)
C27–C26–F18	114.3(3)	F42–C43–C42	120.3(3)
C27–C26–C25	126.0(3)	C44–C43–C42	119.2(3)
F18–C26–C25	119.6(3)	F43–C44–C45	120.7(3)
F19–C27–C26	121.0(3)	F43–C44–C43	120.2(3)
F19–C27–C28	120.2(3)	C45–C44–C43	119.1(4)
C26–C27–C28	118.8(3)	F44–C45–C44	117.0(3)
F20–C28–C29	121.8(3)	F44–C45–C46	120.8(3)
F20–C28–C27	120.3(3)	C44–C45–C46	122.1(3)
C29–C28–C27	117.9(3)	C45–C46–C41	119.3(3)
F21–C29–C28	117.1(3)	C45–C46–C47	122.0(3)
F21–C29–C30	119.5(3)	C41–C46–C47	118.7(3)
C28–C29–C30	123.4(3)	C48–C47–C52	115.8(3)
C29–C30–C25	120.4(3)	C48–C47–C46	125.3(3)
C29–C30–C31	113.4(3)	C52–C47–C46	118.7(3)
C25–C30–C31	126.2(3)	F45–C48–C49	116.5(3)
C36–C31–C32	115.9(3)	F45–C48–C47	121.2(3)
C36–C31–C30	122.9(3)	C49–C48–C47	122.3(3)
C32–C31–C30	120.8(3)	F46–C49–C50	119.7(3)
F22–C32–C33	117.6(3)	F46–C49–C48	119.4(3)
F22–C32–C31	119.2(3)	C50–C49–C48	120.9(3)
C33–C32–C31	123.2(3)	F47–C50–C49	120.8(3)
F23–C33–C32	120.5(3)	F47–C50–C51	121.0(3)
F23–C33–C34	120.7(3)	C49–C50–C51	118.2(3)
C32–C33–C34	118.8(4)	F48–C51–C52	118.8(3)
F24–C34–C35	120.7(3)	F48–C51–C50	120.1(3)

C52–C51–C50	121.1(3)	F60–C68–C67	120.1(3)
C51–C52–C47	121.6(3)	C69–C68–C67	118.3(3)
C51–C52–N41	120.8(3)	F61–C69–C68	116.9(3)
C47–C52–N41	117.6(3)	F61–C69–C70	119.5(3)
C54–C53–C58	114.7(3)	C68–C69–C70	123.7(3)
C54–C53–B41	117.6(3)	C69–C70–C65	119.8(3)
C58–C53–B41	127.7(3)	C69–C70–C71	114.3(3)
F49–C54–C55	115.1(3)	C65–C70–C71	125.9(3)
F49–C54–C53	119.3(3)	C76–C71–C72	115.2(3)
C55–C54–C53	125.6(3)	C76–C71–C70	123.4(3)
F50–C55–C56	120.5(3)	C72–C71–C70	120.9(3)
F50–C55–C54	121.0(3)	F62–C72–C73	117.9(3)
C56–C55–C54	118.5(3)	F62–C72–C71	118.4(3)
F51–C56–C57	120.7(3)	C73–C72–C71	123.6(3)
F51–C56–C55	120.7(3)	F63–C73–C72	121.2(3)
C57–C56–C55	118.5(3)	F63–C73–C74	119.8(4)
F52–C57–C56	117.5(3)	C72–C73–C74	119.0(4)
F52–C57–C58	119.2(3)	F64–C74–C75	120.3(4)
C56–C57–C58	123.2(3)	F64–C74–C73	120.0(4)
C57–C58–C53	119.2(3)	C75–C74–C73	119.7(4)
C57–C58–C59	113.9(3)	F65–C75–C74	119.6(4)
C53–C58–C59	126.7(3)	F65–C75–C76	120.7(4)
C64–C59–C60	116.2(3)	C74–C75–C76	119.7(3)
C64–C59–C58	124.8(3)	F66–C76–C75	118.3(3)
C60–C59–C58	118.8(3)	F66–C76–C71	119.1(3)
F53–C60–C61	118.6(3)	C75–C76–C71	122.6(4)
F53–C60–C59	119.2(3)	C41–B41–C53	115.8(3)
C61–C60–C59	122.3(4)	C41–B41–C65	111.9(3)
F54–C61–C62	119.1(4)	C53–B41–C65	118.3(3)
F54–C61–C60	120.6(4)	C41–B41–N41	101.2(3)
C62–C61–C60	120.3(4)	C53–B41–N41	103.9(3)
F55–C62–C61	121.1(4)	C65–B41–N41	102.9(3)
F55–C62–C63	119.3(4)	C52–N41–B41	111.4(3)
C61–C62–C63	119.6(4)	C52–N41–H41A	109.3
F56–C63–C64	120.4(4)	B41–N41–H41A	109.3
F56–C63–C62	120.3(4)	C52–N41–H41B	109.3
C64–C63–C62	119.2(4)	B41–N41–H41B	109.3
F57–C64–C59	119.9(3)	H41A–N41–H41B	108.0
F57–C64–C63	117.7(4)	Cl81–C81–Cl82	111.0(2)
C59–C64–C63	122.4(4)	Cl81–C81–H81A	109.4
C66–C65–C70	114.2(3)	Cl82–C81–H81A	109.4
C66–C65–B41	115.6(3)	Cl81–C81–H81B	109.4
C70–C65–B41	130.2(3)	Cl82–C81–H81B	109.4
F58–C66–C67	114.2(3)	H81A–C81–H81B	108.0
F58–C66–C65	120.2(3)	Cl83–C83–Cl84	112.1(2)
C67–C66–C65	125.6(3)	Cl83–C83–H83A	109.2
F59–C67–C68	121.0(3)	Cl84–C83–H83A	109.2
F59–C67–C66	120.6(3)	Cl83–C83–H83B	109.2
C68–C67–C66	118.4(3)	Cl84–C83–H83B	109.2
F60–C68–C69	121.7(3)	H83A–C83–H83B	107.9

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	20(2)	22(2)	19(2)	−5(2)	1(1)	1(1)
C2	22(2)	23(2)	20(2)	−2(2)	−2(2)	−1(2)
C3	20(2)	30(2)	26(2)	−4(2)	−6(2)	−5(2)
C4	29(2)	18(2)	31(2)	−4(2)	0(2)	−10(2)
C5	25(2)	22(2)	23(2)	3(2)	−1(2)	2(2)
C6	21(2)	24(2)	23(2)	−2(2)	−1(2)	−1(2)
C7	19(2)	16(2)	24(2)	−3(2)	−2(2)	1(1)
C8	23(2)	18(2)	29(2)	2(2)	1(2)	−2(2)
C9	26(2)	24(2)	20(2)	2(2)	−9(2)	5(2)
C10	23(2)	22(2)	28(2)	−5(2)	−8(2)	2(2)
C11	21(2)	18(2)	34(2)	−3(2)	−1(2)	−4(2)
C12	21(2)	20(2)	22(2)	0(2)	−1(2)	0(2)
C13	18(2)	21(2)	21(2)	5(2)	−7(1)	−1(1)
C14	22(2)	23(2)	21(2)	−1(2)	−2(2)	−3(2)
C15	27(2)	22(2)	29(2)	1(2)	−7(2)	−5(2)
C16	32(2)	23(2)	27(2)	−6(2)	−7(2)	3(2)
C17	27(2)	21(2)	23(2)	1(2)	−3(2)	3(2)
C18	21(2)	21(2)	21(2)	3(2)	−1(2)	−1(1)
C19	26(2)	24(2)	22(2)	−4(2)	4(2)	2(2)
C20	29(2)	30(2)	26(2)	−3(2)	−1(2)	0(2)
C21	24(2)	38(3)	35(2)	−5(2)	3(2)	−10(2)
C22	40(2)	26(2)	33(2)	5(2)	13(2)	−8(2)
C23	37(2)	30(2)	24(2)	6(2)	3(2)	4(2)
C24	25(2)	25(2)	29(2)	0(2)	−1(2)	0(2)
C25	19(2)	27(2)	22(2)	0(2)	−3(2)	−5(2)
C26	23(2)	28(2)	25(2)	2(2)	−3(2)	−2(2)
C27	27(2)	28(2)	24(2)	−9(2)	−2(2)	−1(2)
C28	28(2)	36(2)	15(2)	−1(2)	−3(2)	−4(2)
C29	26(2)	28(2)	28(2)	6(2)	−4(2)	−3(2)
C30	19(2)	23(2)	23(2)	0(2)	−2(2)	0(1)
C31	24(2)	22(2)	20(2)	2(2)	−3(2)	−2(2)
C32	24(2)	29(2)	26(2)	7(2)	3(2)	−1(2)
C33	43(2)	18(2)	36(2)	1(2)	−1(2)	−5(2)
C34	41(2)	19(2)	29(2)	1(2)	1(2)	7(2)
C35	26(2)	36(3)	22(2)	2(2)	4(2)	−1(2)
C36	27(2)	26(2)	21(2)	5(2)	−6(2)	−3(2)
B1	19(2)	25(2)	22(2)	1(2)	−2(2)	1(2)
F1	28(1)	24(1)	30(1)	4(1)	−10(1)	−1(1)
F2	31(1)	30(1)	37(1)	−6(1)	−14(1)	−6(1)
F3	40(1)	24(1)	40(1)	−1(1)	−12(1)	−10(1)
F4	33(1)	20(1)	36(1)	2(1)	−10(1)	−2(1)
F5	29(1)	27(1)	30(1)	5(1)	−3(1)	−9(1)
F6	38(1)	28(1)	27(1)	4(1)	−11(1)	0(1)
F7	33(1)	34(1)	30(1)	−4(1)	−14(1)	−2(1)
F8	30(1)	28(1)	35(1)	1(1)	−7(1)	−11(1)
F9	24(1)	26(1)	27(1)	0(1)	3(1)	−5(1)
F10	37(1)	27(1)	45(1)	−9(1)	−2(1)	−10(1)
F11	46(1)	30(1)	35(1)	−13(1)	1(1)	0(1)
F12	40(1)	31(1)	25(1)	−1(1)	9(1)	3(1)
F13	34(1)	38(1)	29(1)	1(1)	−7(1)	0(1)
F14	54(2)	39(2)	37(1)	14(1)	4(1)	6(1)
F15	55(2)	30(1)	52(2)	2(1)	14(1)	−14(1)

F16	38(1)	51(2)	54(2)	−8(1)	−2(1)	−21(1)
F17	31(1)	40(1)	31(1)	3(1)	−9(1)	−4(1)
F18	40(1)	24(1)	26(1)	−5(1)	−2(1)	4(1)
F19	43(1)	40(1)	27(1)	−10(1)	1(1)	3(1)
F20	43(1)	49(2)	17(1)	2(1)	−1(1)	2(1)
F21	42(1)	31(1)	27(1)	10(1)	−1(1)	5(1)
F22	30(1)	29(1)	43(1)	3(1)	6(1)	−9(1)
F23	57(2)	28(1)	59(2)	−3(1)	3(1)	−16(1)
F24	64(2)	28(1)	52(2)	−9(1)	9(1)	10(1)
F25	27(1)	50(2)	36(1)	1(1)	6(1)	5(1)
F26	28(1)	33(1)	33(1)	0(1)	−1(1)	−7(1)
N1	24(2)	20(2)	18(2)	1(1)	−1(1)	−4(1)
C41	25(2)	22(2)	22(2)	−4(2)	1(2)	−1(2)
C42	30(2)	28(2)	22(2)	5(2)	−5(2)	−5(2)
C43	36(2)	34(3)	31(2)	−2(2)	−15(2)	−9(2)
C44	47(2)	22(2)	36(2)	−4(2)	−15(2)	−14(2)
C45	35(2)	21(2)	31(2)	5(2)	−7(2)	−3(2)
C46	24(2)	22(2)	20(2)	−5(2)	−1(2)	−2(2)
C47	23(2)	20(2)	22(2)	−2(2)	−2(2)	−2(1)
C48	28(2)	18(2)	24(2)	2(2)	2(2)	−2(2)
C49	34(2)	21(2)	18(2)	−3(2)	−3(2)	5(2)
C50	23(2)	24(2)	29(2)	−3(2)	−12(2)	0(2)
C51	22(2)	20(2)	35(2)	−1(2)	−1(2)	0(2)
C52	21(2)	26(2)	18(2)	0(2)	−1(2)	2(2)
C53	19(2)	24(2)	23(2)	2(2)	−6(2)	1(2)
C54	23(2)	25(2)	20(2)	2(2)	−1(2)	−2(2)
C55	29(2)	21(2)	33(2)	−7(2)	−7(2)	−3(2)
C56	38(2)	25(2)	23(2)	−5(2)	−6(2)	7(2)
C57	27(2)	29(2)	23(2)	5(2)	2(2)	5(2)
C58	26(2)	23(2)	19(2)	2(2)	−2(2)	1(2)
C59	24(2)	23(2)	29(2)	4(2)	7(2)	1(2)
C60	23(2)	28(2)	27(2)	3(2)	4(2)	4(2)
C61	38(2)	32(3)	33(2)	2(2)	10(2)	6(2)
C62	36(2)	20(2)	55(3)	−4(2)	16(2)	−5(2)
C63	21(2)	36(3)	53(3)	−10(2)	2(2)	0(2)
C64	27(2)	29(2)	30(2)	1(2)	6(2)	1(2)
C65	20(2)	23(2)	23(2)	0(2)	−3(2)	−3(1)
C66	24(2)	24(2)	24(2)	2(2)	−4(2)	−5(2)
C67	26(2)	35(2)	17(2)	−6(2)	1(2)	−7(2)
C68	26(2)	42(3)	18(2)	2(2)	−3(2)	−5(2)
C69	28(2)	26(2)	29(2)	3(2)	−5(2)	−1(2)
C70	19(2)	29(2)	19(2)	4(2)	1(1)	−4(2)
C71	28(2)	22(2)	22(2)	6(2)	−2(2)	1(2)
C72	27(2)	28(2)	26(2)	2(2)	1(2)	−1(2)
C73	38(2)	27(2)	29(2)	2(2)	−2(2)	−5(2)
C74	52(3)	25(2)	30(2)	−2(2)	0(2)	12(2)
C75	25(2)	43(3)	22(2)	4(2)	4(2)	5(2)
C76	32(2)	31(2)	20(2)	6(2)	−3(2)	0(2)
B41	20(2)	20(2)	26(2)	−1(2)	−9(2)	−1(2)
F41	33(1)	28(1)	37(1)	6(1)	−13(1)	−3(1)
F42	63(2)	34(1)	53(2)	3(1)	−37(1)	−16(1)
F43	69(2)	27(1)	59(2)	3(1)	−31(1)	−20(1)
F44	47(1)	22(1)	39(1)	2(1)	−14(1)	−3(1)
F45	30(1)	25(1)	30(1)	5(1)	−2(1)	−6(1)
F46	41(1)	27(1)	23(1)	2(1)	−7(1)	1(1)
F47	37(1)	34(1)	35(1)	−2(1)	−17(1)	−3(1)
F48	28(1)	29(1)	44(1)	5(1)	−8(1)	−11(1)

F49	26(1)	26(1)	29(1)	−1(1)	2(1)	−6(1)
F50	42(1)	30(1)	50(2)	−15(1)	−5(1)	−10(1)
F51	53(2)	38(1)	32(1)	−15(1)	−3(1)	6(1)
F52	45(1)	34(1)	27(1)	2(1)	11(1)	5(1)
F53	44(1)	36(1)	28(1)	4(1)	−3(1)	6(1)
F54	65(2)	29(1)	40(2)	11(1)	10(1)	5(1)
F55	50(2)	33(2)	75(2)	2(1)	18(1)	−11(1)
F56	36(1)	45(2)	69(2)	−5(1)	−7(1)	−9(1)
F57	34(1)	37(1)	39(1)	5(1)	−9(1)	−1(1)
F58	42(1)	25(1)	26(1)	−3(1)	0(1)	2(1)
F59	38(1)	40(1)	23(1)	−9(1)	1(1)	−4(1)
F60	45(1)	51(2)	21(1)	9(1)	−2(1)	−2(1)
F61	46(1)	30(1)	29(1)	11(1)	−3(1)	3(1)
F62	28(1)	32(1)	38(1)	0(1)	4(1)	−8(1)
F63	60(2)	31(1)	48(2)	−6(1)	−2(1)	−11(1)
F64	77(2)	37(2)	47(2)	−8(1)	15(1)	11(1)
F65	34(1)	63(2)	38(2)	6(1)	8(1)	12(1)
F66	26(1)	43(1)	34(1)	7(1)	−1(1)	−11(1)
N41	24(2)	21(2)	22(2)	0(1)	2(1)	−4(1)
C81	50(3)	51(3)	54(3)	5(2)	−8(2)	1(2)
Cl81	54(1)	73(1)	54(1)	−4(1)	−8(1)	−9(1)
Cl82	45(1)	48(1)	48(1)	4(1)	2(1)	7(1)
C83	70(3)	43(3)	41(3)	4(2)	22(2)	9(2)
Cl83	64(1)	75(1)	54(1)	3(1)	−14(1)	13(1)
Cl84	79(1)	49(1)	43(1)	9(1)	10(1)	18(1)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H1A	49	6836	1576	25	1
H1B	206	7732	1860	25	1
H41A	9819	2456	3037	27	1
H41B	10012	3335	3332	27	1
H81A	7901	9500	1281	62	1
H81B	7033	9765	1877	62	1
H83A	1119	349	3745	65	1
H83B	708	–423	3327	65	1

Table 6. Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
N1–H1A···F9	0.92	2.17	2.826(3)	127.5
N1–H1B···F18	0.92	2.07	2.760(3)	130.6
N41–H41B···F49	0.92	2.13	2.778(4)	127.0
N41–H41A···F58	0.92	2.09	2.766(4)	129.7

Symmetry transformations used to generate equivalent atoms:

Crystal and structure refinement data for $[Ph_3C][N\{CN\text{-}B(C_6F_5)_3\}_2]$,

Compound **4b**

Identification code	markh8
Elemental formula	C19 H15, C38 B2 F30 N3
Formula weight	1333.3
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 20.132(4) Å α = 90 ° b = 9.1300(18) Å β = 107.92(3) ° c = 28.525(6) Å γ = 90 °
Cell volume, V	4988.6(17) $Å^3$
No. of formula units/cell, Z	4
Density (calculated)	1.775 Mg/m^3
F(000)	2632
Absorption coefficient	0.183 mm^{-1}
Temperature	140(1) K
Wavelength	0.71073 Å
Crystal colour, shape	yellow block
Crystal size	0.45 x 0.35 x 0.10 mm
Crystal mounting	on a glass fibre, in oil, fixed in cold N_2 stream
On the diffractometer:	
Theta range for data collection	1.5 - 25.4 °
Index ranges for h, k, l	-22/21, -10/10, -34/31
Crystal degradation	0 %
Absorption correction	None
Total no. of reflections measured (not including absences)	7531
No. of unique reflections	5117 (Rint for equivalents = 0.071)
No. of 'observed' reflections ($I > 2\sigma_I$)	2271
Structure determined by:	direct methods, in SHELXS
Refinement:	Full-matrix least-squares on F^2, in SHELXL

Data / restraints / parameters	5117 / 0 / 829
Goodness-of-fit on F^2, S	0.943
Final R indices ('observed' data)	R1 = 0.065, wR2 = 0.146
Final R indices (all data)	R1 = 0.159, wR2 = 0.188
Reflections weighted: $w = [\sigma^2(Fo^2)+(0.0924P)^2]^{-1}$ where $P=(Fo^2+2Fc^2)/3$	
Largest diff. peak and hole	0.25 and -0.28 e.Å^{-3}
Location of largest difference peak	close to H(85)

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)
N(1)	3247(5)	69(9)	2283(3)	63(2)
N(2)	4016(4)	-817(7)	3053(3)	49(2)
N(3)	2086(5)	1109(7)	2133(2)	48(2)
C(1)	3626(6)	-370(10)	2706(4)	56(3)
C(2)	2645(6)	633(10)	2233(3)	51(3)
B(1)	4444(6)	-1437(10)	3547(3)	41(3)
B(2)	1368(6)	1831(11)	1961(3)	46(3)
C(11)	5242(5)	-1236(8)	3583(3)	43(2)
C(12)	5524(5)	-209(8)	3336(3)	47(3)
C(13)	6205(5)	-129(9)	3367(3)	47(2)
C(14)	6669(5)	-1053(9)	3668(3)	43(2)
C(15)	6424(5)	-2043(9)	3925(3)	49(2)
C(16)	5742(6)	-2101(9)	3885(3)	46(2)
F(12)	5094(3)	803(5)	3052(2)	62(2)
F(13)	6431(3)	887(5)	3102(2)	62(2)
F(14)	7335(3)	-944(5)	3691(2)	63(2)
F(15)	6887(3)	-2963(5)	4230(2)	60(2)
F(16)	5546(3)	-3091(5)	4173(2)	56(1)
C(21)	4250(5)	-3174(9)	3525(3)	46(2)
C(22)	4015(5)	-3961(9)	3841(4)	56(3)
C(23)	3833(6)	-5394(11)	3797(4)	69(3)
C(24)	3864(6)	-6138(10)	3398(4)	64(3)
C(25)	4104(6)	-5468(10)	3060(4)	61(3)
C(26)	4290(5)	-4009(10)	3132(3)	53(3)
F(22)	3986(3)	-3325(5)	4269(2)	71(2)
F(23)	3599(3)	-6066(5)	4137(2)	82(2)
F(24)	3660(3)	-7563(5)	3336(2)	91(2)
F(25)	4158(4)	-6202(5)	2671(2)	103(3)
F(26)	4530(3)	-3385(5)	2794(2)	70(2)
C(31)	4185(5)	-532(9)	3940(3)	42(2)
C(32)	3514(6)	-544(9)	3935(3)	47(3)
C(33)	3241(6)	248(10)	4242(4)	54(3)
C(34)	3667(6)	1089(10)	4597(4)	57(3)
C(35)	4327(6)	1191(10)	4620(3)	59(3)
C(36)	4594(6)	388(9)	4309(3)	48(3)
F(32)	3041(3)	-1324(5)	3598(2)	58(2)
F(33)	2571(3)	184(5)	4222(2)	68(2)
F(34)	3411(3)	1862(5)	4908(2)	66(2)
F(35)	4780(3)	2051(5)	4952(2)	66(2)
F(36)	5272(3)	526(5)	4354(2)	62(2)
C(41)	987(5)	1719(9)	2377(3)	43(2)
C(42)	340(6)	2371(10)	2299(3)	53(3)
C(43)	-50(6)	2373(9)	2611(3)	48(3)
C(44)	211(6)	1656(10)	3050(4)	57(3)
C(45)	832(6)	1001(10)	3154(3)	53(3)
C(46)	1220(6)	1051(10)	2836(3)	55(3)
F(42)	56(3)	3064(5)	1870(2)	58(2)
F(43)	-683(3)	2954(5)	2501(2)	66(2)
F(44)	-158(3)	1620(5)	3367(2)	64(2)
F(45)	1101(3)	342(5)	3589(2)	69(2)
F(46)	1827(3)	342(5)	2956(2)	65(2)

C(51)	991(5)	901(8)	1465(3)	46(3)
C(52)	388(5)	77(9)	1366(3)	46(2)
C(53)	99(6)	-669(10)	938(4)	56(3)
C(54)	440(6)	-703(9)	600(3)	52(3)
C(55)	1040(6)	74(11)	669(3)	53(3)
C(56)	1294(5)	790(10)	1093(3)	50(3)
F(52)	21(3)	10(5)	1692(2)	56(2)
F(53)	-490(3)	-1408(5)	868(2)	65(2)
F(54)	181(3)	-1454(5)	180(2)	63(2)
F(55)	1372(3)	62(5)	321(2)	58(2)
F(56)	1900(3)	1535(5)	1140(2)	57(1)
C(61)	1512(5)	3530(9)	1863(3)	48(3)
C(62)	1960(5)	4341(9)	2215(3)	50(3)
C(63)	2117(5)	5799(10)	2171(4)	58(3)
C(64)	1819(6)	6488(9)	1747(4)	64(3)
C(65)	1383(5)	5741(10)	1374(3)	49(3)
C(66)	1222(5)	4306(10)	1445(3)	52(3)
F(62)	2271(3)	3710(5)	2653(2)	65(2)
F(63)	2570(3)	6502(5)	2542(2)	68(2)
F(64)	1987(3)	7894(5)	1682(2)	72(2)
F(65)	1088(3)	6425(5)	954(2)	67(2)
F(66)	760(3)	3685(5)	1058(2)	58(2)
C(4)	2234(5)	7813(9)	-112(3)	49(3)
C(71)	2074(5)	8674(9)	-547(4)	56(3)
C(72)	2210(5)	10225(9)	-504(3)	61(3)
C(73)	2052(6)	11059(10)	-914(4)	77(4)
C(74)	1781(6)	10449(11)	-1363(4)	77(4)
C(75)	1662(6)	8965(11)	-1414(3)	70(3)
C(76)	1787(5)	8097(10)	-1003(3)	63(3)
C(81)	2803(6)	8157(9)	284(3)	55(3)
C(82)	3429(6)	8620(8)	218(4)	57(3)
C(83)	4007(6)	8846(10)	597(4)	68(3)
C(84)	3944(7)	8737(10)	1069(5)	84(4)
C(85)	3334(7)	8348(9)	1147(3)	65(3)
C(86)	2770(5)	8028(9)	754(4)	55(3)
C(91)	1818(6)	6555(9)	-92(3)	55(3)
C(92)	2115(5)	5334(9)	182(3)	53(3)
C(93)	1718(6)	4090(9)	198(3)	61(3)
C(94)	1034(6)	4087(9)	-59(3)	58(3)
C(95)	718(6)	5295(10)	-324(3)	62(3)
C(96)	1116(6)	6502(9)	-348(3)	62(3)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

(a) In the anion

N(1) - C(1)	1.279(11)	N(1) - C(2)	1.285(13)
N(2) - C(1)	1.133(11)	N(3) - C(2)	1.157(12)
N(2) - B(1)	1.517(11)	N(3) - B(2)	1.526(13)
B(1) - C(11)	1.590(14)	B(2) - C(41)	1.601(14)
B(1) - C(21)	1.629(12)	B(2) - C(51)	1.625(12)
B(1) - C(31)	1.602(12)	B(2) - C(61)	1.618(12)
C(11) - C(12)	1.394(11)	C(41) - C(42)	1.386(13)
C(11) - C(16)	1.360(11)	C(41) - C(46)	1.390(11)
C(12) - F(12)	1.351(9)	C(42) - F(42)	1.338(9)
C(12) - C(13)	1.348(12)	C(42) - C(43)	1.356(13)
C(13) - F(13)	1.361(9)	C(43) - F(43)	1.325(11)
C(13) - C(14)	1.353(11)	C(43) - C(44)	1.367(12)
C(14) - C(15)	1.350(12)	C(44) - F(44)	1.336(11)
C(14) - F(14)	1.324(10)	C(44) - C(45)	1.335(14)
C(15) - F(15)	1.355(9)	C(45) - F(45)	1.335(9)
C(15) - C(16)	1.343(12)	C(45) - C(46)	1.365(13)
C(16) - F(16)	1.358(9)	C(46) - F(46)	1.332(11)
C(21) - C(22)	1.349(12)	C(51) - C(52)	1.381(13)
C(21) - C(26)	1.376(11)	C(51) - C(56)	1.381(13)
C(22) - F(22)	1.369(9)	C(52) - F(52)	1.357(10)
C(22) - C(23)	1.354(12)	C(52) - C(53)	1.362(12)
C(23) - F(23)	1.347(11)	C(53) - F(53)	1.325(11)
C(23) - C(24)	1.344(12)	C(53) - C(54)	1.343(13)
C(24) - F(24)	1.359(9)	C(54) - F(54)	1.340(9)
C(24) - C(25)	1.351(13)	C(54) - C(55)	1.361(14)
C(25) - F(25)	1.329(10)	C(55) - F(55)	1.356(10)
C(25) - C(26)	1.381(12)	C(55) - C(56)	1.333(11)
C(26) - F(26)	1.333(9)	C(56) - F(56)	1.368(10)
C(31) - C(32)	1.346(13)	C(61) - C(62)	1.346(11)
C(31) - C(36)	1.400(11)	C(61) - C(66)	1.355(10)
C(32) - F(32)	1.333(9)	C(62) - F(62)	1.343(9)
C(32) - C(33)	1.373(12)	C(62) - C(63)	1.383(11)
C(33) - F(33)	1.335(11)	C(63) - F(63)	1.331(10)
C(33) - C(34)	1.348(13)	C(63) - C(64)	1.332(12)
C(34) - F(34)	1.353(10)	C(64) - F(64)	1.354(9)
C(34) - C(35)	1.314(14)	C(64) - C(65)	1.339(12)
C(35) - F(35)	1.347(10)	C(65) - F(65)	1.319(8)
C(35) - C(36)	1.380(12)	C(65) - C(66)	1.380(11)
C(36) - F(36)	1.338(11)	C(66) - F(66)	1.330(9)

C(1)-N(1)-C(2)	119.9(9)		
N(2)-C(1)-N(1)	171.7(12)	N(3)-C(2)-N(1)	172.4(10)
C(1)-N(2)-B(1)	171.2(11)	C(2)-N(3)-B(2)	174.1(9)
N(2)-B(1)-C(11)	106.8(7)	N(3)-B(2)-C(41)	110.8(7)
N(2)-B(1)-C(21)	105.5(7)	N(3)-B(2)-C(51)	101.3(7)
N(2)-B(1)-C(31)	104.0(7)	N(3)-B(2)-C(61)	105.5(8)
C(11)-B(1)-C(21)	109.9(7)	C(41)-B(2)-C(51)	114.2(9)
C(11)-B(1)-C(31)	115.8(7)	C(41)-B(2)-C(61)	110.1(8)
C(31)-B(1)-C(21)	113.9(8)	C(61)-B(2)-C(51)	114.2(7)
C(12)-C(11)-B(1)	127.4(8)	C(42)-C(41)-B(2)	119.6(8)
C(16)-C(11)-B(1)	120.7(9)	C(46)-C(41)-B(2)	128.9(9)
C(16)-C(11)-C(12)	111.9(9)	C(42)-C(41)-C(46)	111.5(8)
F(12)-C(12)-C(11)	118.5(9)	F(42)-C(42)-C(41)	117.8(8)
C(13)-C(12)-C(11)	124.6(8)	C(43)-C(42)-C(41)	126.9(9)

C(13)-C(12)-F(12)	116.9(8)	F(42)-C(42)-C(43)	115.4(9)
C(12)-C(13)-F(13)	120.6(8)	F(43)-C(43)-C(42)	123.7(9)
C(12)-C(13)-C(14)	119.9(9)	C(42)-C(43)-C(44)	117.7(10)
C(14)-C(13)-F(13)	119.6(9)	F(43)-C(43)-C(44)	118.5(9)
F(14)-C(14)-C(13)	118.4(8)	F(44)-C(44)-C(43)	119.7(10)
C(15)-C(14)-C(13)	117.7(10)	C(45)-C(44)-C(43)	119.2(9)
F(14)-C(14)-C(15)	123.9(8)	C(45)-C(44)-F(44)	121.1(10)
C(14)-C(15)-F(15)	118.0(10)	F(45)-C(45)-C(44)	119.5(9)
C(16)-C(15)-C(14)	121.1(9)	C(44)-C(45)-C(46)	121.7(10)
C(16)-C(15)-F(15)	120.8(9)	F(45)-C(45)-C(46)	118.7(10)
C(15)-C(16)-C(11)	124.6(9)	C(45)-C(46)-C(41)	123.0(10)
F(16)-C(16)-C(11)	118.2(10)	F(46)-C(46)-C(41)	118.1(9)
C(15)-C(16)-F(16)	117.1(8)	F(46)-C(46)-C(45)	118.7(9)
C(22)-C(21)-B(1)	128.4(8)	C(52)-C(51)-B(2)	127.5(9)
C(26)-C(21)-B(1)	119.9(8)	C(56)-C(51)-B(2)	120.6(10)
C(22)-C(21)-C(26)	111.7(8)	C(56)-C(51)-C(52)	111.8(8)
C(21)-C(22)-F(22)	119.4(7)	F(52)-C(52)-C(51)	120.9(8)
C(21)-C(22)-C(23)	126.5(10)	C(53)-C(52)-C(51)	124.2(9)
C(23)-C(22)-F(22)	114.0(9)	F(52)-C(52)-C(53)	114.8(9)
F(23)-C(23)-C(22)	121.2(10)	F(53)-C(53)-C(52)	120.3(9)
C(24)-C(23)-C(22)	119.0(10)	C(54)-C(53)-C(52)	118.8(11)
C(24)-C(23)-F(23)	119.8(9)	F(53)-C(53)-C(54)	120.8(10)
C(23)-C(24)-F(24)	120.2(10)	F(54)-C(54)-C(53)	120.5(11)
C(23)-C(24)-C(25)	119.7(9)	C(53)-C(54)-C(55)	120.7(9)
C(25)-C(24)-F(24)	120.1(9)	F(54)-C(54)-C(55)	118.6(10)
F(25)-C(25)-C(24)	120.4(8)	F(55)-C(55)-C(54)	120.4(10)
C(24)-C(25)-C(26)	118.1(9)	C(56)-C(55)-C(54)	117.5(9)
F(25)-C(25)-C(26)	121.5(9)	C(56)-C(55)-F(55)	122.0(10)
C(21)-C(26)-C(25)	125.0(9)	C(55)-C(56)-C(51)	126.6(10)
F(26)-C(26)-C(21)	118.5(8)	F(56)-C(56)-C(51)	118.9(9)
F(26)-C(26)-C(25)	116.5(9)	C(55)-C(56)-F(56)	114.4(9)
C(32)-C(31)-B(1)	122.0(8)	C(62)-C(61)-B(2)	120.8(8)
C(36)-C(31)-B(1)	126.4(10)	C(66)-C(61)-B(2)	127.0(8)
C(32)-C(31)-C(36)	111.6(9)	C(62)-C(61)-C(66)	112.1(8)
F(32)-C(32)-C(31)	120.2(9)	F(62)-C(62)-C(61)	118.1(8)
C(31)-C(32)-C(33)	125.9(10)	C(61)-C(62)-C(63)	125.6(9)
F(32)-C(32)-C(33)	113.8(10)	F(62)-C(62)-C(63)	116.3(8)
F(33)-C(33)-C(32)	123.3(10)	F(63)-C(63)-C(62)	120.8(9)
C(34)-C(33)-C(32)	119.4(12)	C(64)-C(63)-C(62)	119.1(9)
F(33)-C(33)-C(34)	117.2(10)	F(63)-C(63)-C(64)	120.1(8)
C(33)-C(34)-F(34)	120.5(11)	C(63)-C(64)-F(64)	120.6(9)
C(35)-C(34)-C(33)	118.5(10)	C(63)-C(64)-C(65)	118.9(8)
C(35)-C(34)-F(34)	120.9(10)	C(65)-C(64)-F(64)	120.3(9)
C(34)-C(35)-F(35)	122.1(10)	F(65)-C(65)-C(64)	118.8(8)
C(34)-C(35)-C(36)	121.2(10)	C(64)-C(65)-C(66)	119.6(9)
F(35)-C(35)-C(36)	116.6(11)	F(65)-C(65)-C(66)	121.5(8)
C(35)-C(36)-C(31)	123.1(11)	C(61)-C(66)-C(65)	124.7(9)
F(36)-C(36)-C(31)	118.4(9)	F(66)-C(66)-C(61)	120.6(8)
F(36)-C(36)-C(35)	118.5(9)	F(66)-C(66)-C(65)	114.8(8)

(b) In the cation

C(4) - C(71)	1.420(11)	C(82) - C(83)	1.339(13)
C(4) - C(81)	1.374(12)	C(83) - C(84)	1.392(13)
C(4) - C(91)	1.433(12)	C(84) - C(85)	1.361(16)
C(71) - C(72)	1.441(11)	C(85) - C(86)	1.359(12)
C(71) - C(76)	1.355(11)	C(91) - C(92)	1.388(10)
C(72) - C(73)	1.350(10)	C(91) - C(96)	1.377(13)
C(73) - C(74)	1.348(11)	C(92) - C(93)	1.397(11)
C(74) - C(75)	1.377(12)	C(93) - C(94)	1.346(13)
C(75) - C(76)	1.373(11)	C(94) - C(95)	1.378(11)

C(81) - C(82)	1.397(14)	C(95) - C(96)	1.376(12)
C(81) - C(86)	1.368(11)		

C(81)-C(4)-C(71)	120.0(9)	C(83)-C(82)-C(81)	122.2(11)
C(71)-C(4)-C(91)	120.0(8)	C(82)-C(83)-C(84)	117.1(13)
C(81)-C(4)-C(91)	120.0(9)	C(85)-C(84)-C(83)	122.2(11)
C(4)-C(71)-C(72)	118.8(8)	C(86)-C(85)-C(84)	119.1(11)
C(76)-C(71)-C(4)	122.6(8)	C(85)-C(86)-C(81)	120.7(11)
C(76)-C(71)-C(72)	118.6(8)	C(92)-C(91)-C(4)	120.7(9)
C(73)-C(72)-C(71)	119.4(9)	C(96)-C(91)-C(4)	121.7(8)
C(74)-C(73)-C(72)	120.6(9)	C(96)-C(91)-C(92)	117.7(8)
C(73)-C(74)-C(75)	120.9(9)	C(91)-C(92)-C(93)	121.3(9)
C(76)-C(75)-C(74)	119.8(9)	C(94)-C(93)-C(92)	118.9(9)
C(71)-C(76)-C(75)	120.4(9)	C(93)-C(94)-C(95)	121.3(9)
C(4)-C(81)-C(82)	121.0(10)	C(96)-C(95)-C(94)	119.4(10)
C(86)-C(81)-C(4)	120.5(11)	C(95)-C(96)-C(91)	121.4(9)
C(86)-C(81)-C(82)	118.4(9)		

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3) for the expression:
$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$
E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	50(7)	90(6)	54(6)	13(5)	22(5)	23(5)
N(2)	64(7)	50(4)	30(5)	3(4)	8(4)	-6(4)
N(3)	74(7)	41(4)	29(5)	4(3)	18(4)	1(4)
C(1)	65(9)	60(6)	52(8)	-10(6)	31(6)	-8(5)
C(2)	74(10)	53(6)	25(6)	6(4)	15(6)	-9(6)
B(1)	51(9)	52(6)	22(6)	3(5)	12(5)	12(5)
B(2)	50(9)	50(6)	33(7)	4(5)	5(5)	5(5)
C(11)	48(7)	40(5)	41(6)	-9(4)	15(5)	10(4)
C(12)	58(9)	40(5)	42(7)	5(5)	15(5)	0(5)
C(13)	35(8)	44(5)	70(7)	7(5)	27(5)	4(4)
C(14)	45(8)	47(5)	39(6)	-2(5)	17(5)	4(5)
C(15)	49(8)	50(6)	51(7)	4(5)	18(5)	9(5)
C(16)	63(9)	34(5)	45(6)	-16(4)	23(5)	0(5)
F(12)	64(5)	60(3)	62(4)	21(3)	17(3)	2(3)
F(13)	69(5)	68(3)	50(4)	8(3)	19(3)	-9(3)
F(14)	51(5)	71(3)	70(4)	3(3)	21(3)	-2(3)
F(15)	59(4)	62(3)	57(4)	15(3)	13(3)	6(3)
F(16)	58(4)	57(3)	55(3)	16(3)	19(3)	1(2)
C(21)	43(7)	48(5)	45(6)	-4(5)	10(4)	-8(4)
C(22)	66(9)	39(6)	64(8)	-7(5)	20(5)	-2(5)
C(23)	74(10)	66(7)	67(8)	12(6)	23(6)	-6(6)
C(24)	83(10)	47(6)	50(8)	-1(6)	5(6)	3(5)
C(25)	86(10)	46(6)	45(7)	-4(5)	13(6)	8(5)
C(26)	57(8)	59(6)	45(7)	4(5)	20(5)	-5(5)
F(22)	104(6)	55(3)	65(4)	3(3)	42(3)	0(3)
F(23)	96(6)	60(3)	105(5)	16(3)	54(4)	1(3)
F(24)	125(6)	44(3)	87(5)	6(3)	7(4)	-2(3)
F(25)	189(8)	50(3)	60(4)	-13(3)	20(4)	9(4)
F(26)	104(6)	66(3)	46(4)	-4(3)	31(3)	4(3)
C(31)	46(8)	48(5)	36(6)	7(4)	19(5)	8(4)
C(32)	58(9)	47(6)	37(6)	8(5)	16(5)	2(5)
C(33)	62(9)	56(6)	50(8)	11(5)	25(6)	3(6)
C(34)	67(10)	69(7)	45(7)	8(5)	29(6)	9(6)
C(35)	75(10)	56(6)	41(7)	-1(5)	12(6)	5(6)
C(36)	50(8)	54(6)	46(7)	8(5)	23(5)	8(5)
F(32)	51(4)	63(3)	59(4)	-7(3)	13(3)	-5(3)
F(33)	80(6)	60(3)	72(4)	-7(3)	35(3)	2(3)
F(34)	72(5)	71(3)	62(4)	-11(3)	31(3)	5(3)
F(35)	75(5)	70(3)	51(4)	-17(3)	17(3)	-2(3)
F(36)	70(5)	65(3)	49(4)	-9(3)	14(3)	-7(3)
C(41)	49(8)	48(5)	34(6)	-9(4)	15(4)	-4(4)
C(42)	48(8)	70(7)	44(7)	9(5)	17(5)	3(5)
C(43)	63(9)	50(6)	33(6)	-6(5)	16(5)	1(5)
C(44)	46(9)	71(7)	64(8)	-14(6)	31(6)	-11(5)
C(45)	48(9)	72(7)	40(7)	9(5)	14(5)	-11(5)
C(46)	61(9)	49(6)	48(7)	-2(5)	6(6)	-5(5)
F(42)	57(4)	69(3)	50(4)	6(3)	18(3)	5(3)
F(43)	55(5)	74(3)	73(4)	5(3)	26(3)	5(3)
F(44)	66(5)	64(3)	73(4)	-6(3)	40(3)	-7(3)
F(45)	76(5)	88(4)	43(4)	14(3)	19(3)	-2(3)
F(46)	65(5)	76(4)	59(4)	21(3)	24(3)	8(3)

C(51)	72(9)	34(5)	31(6)	-2(4)	13(5)	5(5)
C(52)	58(8)	51(6)	26(6)	-1(4)	11(5)	-3(5)
C(53)	40(8)	68(7)	62(8)	6(6)	17(6)	3(5)
C(54)	75(10)	36(5)	36(7)	-4(5)	2(6)	-3(5)
C(55)	61(9)	77(7)	30(7)	17(5)	26(5)	12(6)
C(56)	49(8)	65(6)	38(7)	8(5)	14(5)	6(5)
F(52)	59(5)	61(3)	52(4)	-3(2)	24(3)	-10(3)
F(53)	61(5)	74(3)	60(4)	-6(3)	20(3)	-8(3)
F(54)	68(5)	69(3)	46(3)	0(3)	10(3)	-3(3)
F(55)	68(5)	66(3)	45(3)	-3(3)	24(3)	-2(3)
F(56)	61(5)	62(3)	52(4)	1(3)	22(3)	-6(3)
C(61)	57(8)	47(5)	40(6)	1(5)	12(5)	2(4)
C(62)	59(8)	52(6)	42(7)	3(5)	20(5)	7(5)
C(63)	59(8)	56(6)	59(8)	-16(6)	17(6)	0(5)
C(64)	105(11)	33(5)	56(7)	-14(5)	27(6)	0(5)
C(65)	69(8)	56(6)	25(6)	1(5)	19(5)	8(5)
C(66)	80(9)	58(6)	21(6)	-3(5)	19(5)	0(5)
F(62)	87(5)	58(3)	44(3)	-6(3)	13(3)	-6(3)
F(63)	79(5)	60(3)	63(4)	-8(3)	21(3)	-11(3)
F(64)	94(5)	44(3)	84(4)	-3(3)	36(3)	-5(3)
F(65)	85(5)	60(3)	54(4)	18(3)	19(3)	3(3)
F(66)	59(4)	54(3)	51(3)	5(3)	4(3)	8(2)
C(4)	52(8)	54(6)	48(7)	-13(5)	26(5)	5(5)
C(71)	69(9)	57(6)	47(7)	-1(5)	24(5)	-2(5)
C(72)	95(10)	45(5)	46(7)	9(5)	24(5)	-12(5)
C(73)	123(12)	43(6)	70(9)	11(6)	38(7)	1(6)
C(74)	107(11)	62(7)	67(9)	29(6)	34(7)	7(6)
C(75)	94(10)	74(7)	38(7)	10(6)	15(5)	3(6)
C(76)	82(10)	64(6)	44(7)	0(6)	20(5)	8(5)
C(81)	72(9)	64(6)	28(6)	-6(5)	14(6)	-11(5)
C(82)	53(9)	48(5)	70(8)	6(5)	21(6)	6(5)
C(83)	47(9)	73(7)	88(9)	5(6)	24(7)	-2(5)
C(84)	112(14)	55(7)	79(10)	-6(6)	21(8)	-11(7)
C(85)	120(12)	46(6)	34(7)	2(5)	29(7)	1(6)
C(86)	58(8)	51(6)	54(7)	-1(5)	13(6)	-6(5)
C(91)	58(8)	49(6)	54(7)	7(5)	12(5)	-1(5)
C(92)	65(8)	52(6)	42(6)	0(5)	17(5)	-5(5)
C(93)	79(10)	50(6)	53(7)	3(5)	22(6)	-8(5)
C(94)	64(9)	62(6)	47(7)	0(5)	15(5)	-12(5)
C(95)	78(9)	62(6)	43(7)	11(5)	11(5)	-1(6)
C(96)	74(10)	49(6)	66(8)	6(5)	26(6)	-4(5)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) of the parent carbon atom.

	x	y	z	U(iso)
H(72)	2406	10648	-195	74
H(73)	2131	12064	-887	92
H(74)	1673	11040	-1642	93
H(75)	1498	8550	-1726	84
H(76)	1673	7107	-1037	76
H(82)	3445	8778	-101	68
H(83)	4432	9065	549	82
H(84)	4331	8937	1339	101
H(85)	3304	8302	1466	79
H(86)	2358	7719	806	66
H(92)	2588	5343	359	63
H(93)	1923	3278	383	73
H(94)	770	3253	-57	70
H(95)	240	5294	-487	75
H(96)	906	7299	-539	74

Crystal and structure refinement data for **$(CPh_3)[FB(C_6F_4\text{-}C_6F_5\text{-}2)_3]$, CPh_3[F-PBB]**

Identification code	markh11
Empirical formula	C19 H15, C36 B F28
Formula weight	1218.5
Crystal system	Triclinic
Space group	P-1 (no. 2)
Unit cell dimensions	a = 9.788(2) Å α = 90.21(3) ° b = 18.682(4) Å β = 92.34(3) ° c = 27.788(6) Å γ = 104.52(3) °
Volume	4914.3(17) $Å^3$
No. of formula units, Z	4
Calculated density	1.647 Mg/m^3
F(000)	2408
Absorption coefficient	0.170 mm^{-1}
Temperature	140(1) K
Wavelength	0.71073 Å
Crystal colour, shape	yellow prisms
Crystal size	0.25 x 0.15 x 0.10 mm
Crystal mounting	on a glass fibre, in oil, fixed in cold N_2 stream
On the diffractometer:	
Theta range for data collection	1.3 to 22.5 °
Limiting indices	-10<=h<=10, -20<=k<=20, -29<=l<=29
Completeness to theta = 22.5	91.8%
Absorption correction	Not applied
Reflections collected (not including absences)	19145
No. of unique reflections	11805 [R(int) for equivalents = 0.211]
No. of 'observed' reflections ($I > 2\sigma_I$)	4916
Structure determined by:	direct methods, in SHELXS
Refinement:	Full-matrix-block least-squares on F^2, in SHELXL

Data / restraints / parameters	11805 / 0 / 1506
Goodness-of-fit on F^2	0.887
Final R indices ('observed' data)	R1 = 0.097, wR2 = 0.216
Final R indices (all data)	R1 = 0.202, wR2 = 0.257
Reflections weighted: $w = [\sigma^2(Fo^2)+(0.1234P)^2]^{-1}$ where $P=(Fo^2+2Fc^2)/3$	
Largest diff. peak and hole	0.51 and -0.47 e.Å^{-3}
Location of largest difference peak	close to C(109)

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. E.s.ds are in parentheses.

	x	y	z	U(eq)	S.o.f.#
C(1)	4440(9)	6531(5)	1084(3)	49(2)	
C(11)	5371(9)	7234(5)	966(3)	48(2)	
C(12)	5098(9)	7630(5)	546(3)	53(2)	
C(13)	6038(10)	8310(5)	435(4)	62(3)	
C(14)	7268(10)	8569(5)	744(4)	64(3)	
C(15)	7531(10)	8182(5)	1160(3)	54(2)	
C(16)	6590(9)	7521(5)	1278(3)	60(3)	
C(21)	4973(8)	5978(5)	1366(3)	42(2)	
C(22)	4106(10)	5555(5)	1710(3)	55(3)	
C(23)	4637(10)	5069(5)	2002(3)	56(2)	
C(24)	5947(10)	4947(5)	1924(3)	61(3)	
C(25)	6777(9)	5352(5)	1588(4)	54(3)	
C(26)	6349(9)	5880(5)	1311(3)	49(2)	
C(31)	2958(9)	6343(5)	932(3)	51(2)	
C(32)	2232(9)	5626(5)	792(3)	53(2)	
C(33)	873(10)	5455(6)	634(3)	65(3)	
C(34)	132(10)	6008(6)	589(3)	65(3)	
C(35)	761(9)	6735(6)	741(3)	63(3)	
C(36)	2189(10)	6914(5)	890(3)	56(3)	
C(4)	789(9)	2594(5)	3851(3)	56(3)	
C(41)	-297(8)	1942(5)	3995(3)	44(2)	
C(42)	-160(10)	1561(5)	4413(4)	62(3)	
C(43)	-1211(12)	924(6)	4539(4)	75(3)	
C(44)	-2358(12)	679(6)	4218(4)	71(3)	
C(45)	-2551(10)	1049(6)	3794(4)	69(3)	
C(46)	-1514(9)	1680(5)	3666(4)	58(3)	
C(51)	442(9)	3196(5)	3582(3)	47(2)	
C(52)	-870(11)	3374(6)	3628(4)	67(3)	
C(53)	-1176(10)	3941(6)	3368(4)	68(3)	
C(54)	-244(11)	4327(6)	3029(3)	63(3)	
C(55)	1022(11)	4149(5)	2965(4)	62(3)	
C(56)	1383(9)	3602(6)	3252(3)	61(3)	
C(61)	2268(10)	2583(6)	3982(3)	64(3)	
C(62)	2687(10)	1902(7)	3971(3)	66(3)	
C(63)	4089(12)	1933(7)	4058(4)	83(3)	
C(64)	5060(13)	2558(10)	4183(4)	96(4)	
C(65)	4669(12)	3239(9)	4200(4)	95(5)	
C(66)	3267(10)	3261(6)	4109(3)	68(3)	
F(7)	3420(5)	7713(3)	3569(2)	56(1)	
B(7)	2715(10)	6938(6)	3446(4)	50(3)	
C(71)	1674(9)	6974(5)	2962(3)	51(2)	
C(72)	1471(8)	6426(5)	2600(3)	45(2)	
F(72)	2028(5)	5835(3)	2636(2)	54(1)	
C(73)	678(9)	6466(5)	2165(3)	43(2)	
F(73)	548(5)	5916(3)	1827(2)	59(1)	
C(74)	48(9)	7015(5)	2085(3)	48(2)	
F(74)	-751(5)	7057(3)	1675(2)	67(2)	
C(75)	160(10)	7576(5)	2446(3)	51(3)	
F(75)	-531(5)	8106(3)	2363(2)	62(1)	

C(76)	975(9)	7538(5)	2862(3)	45(2)	
C(77)	1044(9)	8172(5)	3223(3)	52(2)	
C(78)	2070(9)	8848(5)	3203(3)	56(3)	
F(78)	3036(5)	8919(3)	2856(2)	68(2)	
C(79)	2161(10)	9411(5)	3521(3)	57(3)	
F(79)	3193(6)	10046(3)	3489(2)	75(2)	
C(7A)	1154(11)	9328(6)	3865(4)	62(3)	
F(7A)	1245(6)	9901(3)	4186(2)	80(2)	
C(7B)	128(10)	8680(6)	3904(4)	61(3)	
F(7B)	-812(6)	8624(3)	4247(2)	85(2)	
C(7C)	97(9)	8126(5)	3573(3)	57(3)	
F(7C)	-948(5)	7493(3)	3619(2)	73(2)	
C(81)	3938(8)	6517(5)	3349(3)	45(2)	
C(82)	3973(10)	5809(5)	3515(3)	55(3)	
F(82)	2896(5)	5415(3)	3786(2)	67(2)	
C(83)	4977(11)	5449(5)	3419(3)	56(3)	
F(83)	4929(6)	4754(3)	3590(2)	80(2)	
C(84)	6071(9)	5780(6)	3124(4)	61(3)	
F(84)	7067(5)	5415(3)	3009(2)	76(2)	
C(85)	6111(9)	6479(6)	2952(4)	58(3)	
F(85)	7170(5)	6778(3)	2648(2)	73(2)	
C(86)	5098(9)	6843(5)	3048(3)	57(3)	
C(87)	5255(9)	7604(5)	2827(4)	51(3)	
C(88)	4786(9)	7690(5)	2364(4)	54(3)	
F(88)	4124(5)	7086(3)	2095(2)	60(1)	
C(89)	4934(10)	8369(6)	2141(4)	55(3)	
F(89)	4429(6)	8448(3)	1685(2)	70(2)	
C(8A)	5639(11)	9013(6)	2399(5)	75(3)	
F(8A)	5755(6)	9690(3)	2197(2)	86(2)	
C(8B)	6113(10)	8933(6)	2870(5)	68(3)	
F(8B)	6763(6)	9551(3)	3134(2)	88(2)	
C(8C)	5949(10)	8255(6)	3075(4)	60(3)	
F(8C)	6466(5)	8202(3)	3531(2)	75(2)	
C(91)	1699(14)	6689(11)	3917(4)	9(7)*	0.37(3)
C(92)	359(16)	6218(12)	3846(4)	21(7)*	0.37(3)
C(93)	-529(13)	6049(12)	4230(6)	54(8)*	0.37(3)
C(94)	-77(15)	6352(13)	4684(5)	34(8)*	0.37(3)
C(95)	1263(16)	6823(13)	4754(4)	43(8)*	0.37(3)
C(96)	2151(13)	6992(11)	4371(5)	25(7)*	0.37(3)
F(92)	-101(5)	5839(3)	3440(2)	79(2)	
F(93)	-1820(30)	5577(16)	4179(10)	73(9)*	0.37(3)
F(94)	-850(40)	6150(20)	5068(15)	119(14)	0.37(3)
F(95)	1570(40)	7030(30)	5228(18)	109(16)	0.37(3)
C(91X)	1767(14)	6533(9)	3952(4)	83(10)*	0.63(3)
C(92X)	462(14)	6029(10)	3879(3)	67(7)*	0.63(3)
C(93X)	-335(11)	5754(9)	4271(5)	61(5)*	0.63(3)
C(94X)	171(12)	5983(10)	4736(4)	74(6)*	0.63(3)
C(95X)	1476(12)	6488(10)	4808(4)	55(5)*	0.63(3)
C(96X)	2273(10)	6763(8)	4416(5)	50(5)*	0.63(3)
F(93X)	-1619(15)	5275(10)	4194(5)	78(5)	0.63(3)
F(94X)	-710(30)	5760(14)	5123(6)	120(10)	0.63(3)
F(95X)	1940(20)	6746(16)	5252(10)	107(9)	0.63(3)
C(97)	3625(10)	7388(6)	4517(3)	58(3)	
C(98)	3722(11)	8097(7)	4606(3)	67(3)	
F(98)	2521(6)	8394(3)	4572(2)	87(2)	
C(99)	4969(11)	8636(6)	4721(4)	65(3)	
F(99)	5010(6)	9361(3)	4800(2)	81(2)	
C(9A)	6173(11)	8405(6)	4762(3)	62(3)	
F(9A)	7420(6)	8884(3)	4896(2)	78(2)	
C(9B)	6148(10)	7655(6)	4691(3)	61(3)	
F(9B)	7323(5)	7414(3)	4741(2)	68(2)	

C(9C)	4887(10)	7156(6)	4564(3)	54(2)
F(9C)	4852(5)	6444(3)	4518(2)	70(2)
F(10)	1560(4)	1594(2)	1319(2)	50(1)
B(10)	2273(10)	2335(6)	1494(4)	48(3)
C(101)	1038(8)	2714(5)	1660(3)	46(2)
C(102)	928(9)	3461(5)	1562(3)	47(2)
F(102)	2036(5)	3926(3)	1335(2)	63(1)
C(103)	-126(10)	3763(5)	1703(3)	53(2)
F(103)	-102(6)	4469(3)	1591(2)	77(2)
C(104)	-1206(9)	3346(6)	1963(3)	58(3)
F(104)	-2248(5)	3657(3)	2102(2)	75(2)
C(105)	-1161(9)	2643(6)	2071(3)	57(3)
F(105)	-2227(5)	2241(3)	2355(2)	76(2)
C(106)	-112(9)	2311(5)	1937(3)	54(3)
C(107)	-194(9)	1539(5)	2109(4)	52(3)
C(108)	277(9)	1414(5)	2561(3)	46(2)
F(108)	933(5)	1992(3)	2852(2)	59(1)
C(109)	67(9)	718(5)	2758(4)	54(3)
F(109)	563(6)	617(3)	3223(2)	75(2)
C(10A)	-636(10)	126(5)	2473(5)	65(3)
F(10A)	-751(6)	-583(3)	2668(2)	90(2)
C(10B)	-1054(10)	215(7)	2027(5)	68(3)
F(10B)	-1736(6)	-389(3)	1743(2)	97(2)
C(10C)	-883(9)	912(6)	1838(3)	52(3)
F(10C)	-1454(5)	995(3)	1386(2)	72(2)
C(111)	3301(8)	2229(5)	1946(3)	44(2)
C(112)	3785(9)	2800(5)	2311(3)	47(2)
F(112)	3355(5)	3448(3)	2235(2)	61(1)
C(113)	4633(9)	2760(6)	2714(4)	53(2)
F(113)	5021(5)	3362(3)	3013(2)	67(2)
C(114)	5079(9)	2168(6)	2790(3)	48(2)
F(114)	5975(5)	2109(3)	3185(2)	70(2)
C(115)	4703(9)	1572(6)	2478(4)	56(3)
F(115)	5222(5)	966(3)	2563(2)	67(2)
C(116)	3835(9)	1592(5)	2062(3)	47(2)
C(117)	3523(8)	908(5)	1737(3)	45(2)
C(118)	2753(9)	228(5)	1892(3)	54(3)
F(118)	2351(5)	166(3)	2362(2)	64(2)
C(119)	2395(10)	-398(5)	1613(4)	63(3)
F(119)	1668(6)	-1046(3)	1785(2)	82(2)
C(11A)	2803(10)	-357(5)	1136(4)	62(3)
F(11A)	2478(6)	-972(3)	853(2)	85(2)
C(11B)	3566(10)	317(6)	963(3)	59(3)
F(11B)	3986(6)	349(3)	499(2)	72(2)
C(11C)	3917(9)	937(5)	1262(3)	51(2)
F(11C)	4670(5)	1572(3)	1069(2)	65(2)
C(121)	3106(8)	2782(5)	1026(3)	43(2)
C(122)	4472(10)	3234(5)	1051(3)	57(3)
F(122)	5301(5)	3265(3)	1471(2)	66(2)
C(123)	5064(9)	3665(5)	661(4)	52(3)
F(123)	6443(5)	4084(3)	733(2)	74(2)
C(124)	4352(11)	3670(5)	239(3)	60(3)
F(124)	4928(6)	4095(3)	-136(2)	74(2)
C(125)	2988(9)	3204(5)	195(3)	54(3)
F(125)	2287(5)	3211(3)	-255(2)	59(1)
C(126)	2377(9)	2779(5)	571(3)	52(3)
C(127)	839(9)	2336(5)	470(3)	53(3)
C(128)	-246(10)	2667(6)	464(3)	53(3)
F(128)	-17(5)	3408(3)	538(2)	63(1)
C(129)	-1680(10)	2271(7)	376(4)	66(3)

F(129)	-2706(5)	2618(3)	396(2)	81(2)
C(12A)	-1914(10)	1520(6)	292(3)	62(3)
F(12A)	-3270(6)	1132(4)	215(2)	94(2)
C(12B)	-851(11)	1176(6)	281(4)	65(3)
F(12B)	-1120(5)	435(3)	195(2)	78(2)
C(12C)	574(10)	1572(6)	372(3)	59(3)
F(12C)	1571(5)	1217(3)	355(2)	63(2)

- site occupancy, if different from 1.
* - U(iso) ($Å^2$ x 10^3)

Table 2. Molecular dimensions. Bond lengths are in Ångstroms, angles in degrees. E.s.ds are in parentheses.

(a) In the cations

C(1)-C(11)	1.445(11)	C(4)-C(51)	1.453(13)
C(1)-C(31)	1.449(12)	C(4)-C(41)	1.471(12)
C(1)-C(21)	1.484(12)	C(4)-C(61)	1.484(13)
C(11)-C(12)	1.434(12)	C(41)-C(42)	1.385(13)
C(11)-C(16)	1.434(12)	C(41)-C(46)	1.452(12)
C(12)-C(13)	1.413(12)	C(42)-C(43)	1.419(13)
C(13)-C(14)	1.427(13)	C(43)-C(44)	1.388(14)
C(14)-C(15)	1.414(13)	C(44)-C(45)	1.398(15)
C(15)-C(16)	1.393(11)	C(45)-C(46)	1.407(12)
C(21)-C(22)	1.412(11)	C(51)-C(56)	1.411(12)
C(21)-C(26)	1.417(11)	C(51)-C(52)	1.416(13)
C(22)-C(23)	1.401(13)	C(52)-C(53)	1.370(14)
C(23)-C(24)	1.383(13)	C(53)-C(54)	1.411(13)
C(24)-C(25)	1.363(12)	C(54)-C(55)	1.379(13)
C(25)-C(26)	1.390(13)	C(55)-C(56)	1.402(14)
C(31)-C(32)	1.394(12)	C(61)-C(66)	1.426(13)
C(31)-C(36)	1.455(13)	C(61)-C(62)	1.431(14)
C(32)-C(33)	1.343(12)	C(62)-C(63)	1.370(14)
C(33)-C(34)	1.407(14)	C(63)-C(64)	1.343(15)
C(34)-C(35)	1.398(13)	C(64)-C(65)	1.418(18)
C(35)-C(36)	1.399(12)	C(65)-C(66)	1.396(16)

C(11)-C(1)-C(31)	121.4(9)	C(23)-C(24)-H(24)	120.2
C(11)-C(1)-C(21)	120.9(8)	C(24)-C(25)-C(26)	122.4(9)
C(31)-C(1)-C(21)	117.6(7)	C(24)-C(25)-H(25)	118.8
C(12)-C(11)-C(16)	120.9(8)	C(26)-C(25)-H(25)	118.8
C(12)-C(11)-C(1)	121.2(8)	C(25)-C(26)-C(21)	118.5(8)
C(16)-C(11)-C(1)	117.9(8)	C(25)-C(26)-H(26)	120.7
C(13)-C(12)-C(11)	120.0(9)	C(21)-C(26)-H(26)	120.7
C(13)-C(12)-H(12)	120.0	C(32)-C(31)-C(1)	122.3(9)
C(11)-C(12)-H(12)	120.0	C(32)-C(31)-C(36)	117.1(8)
C(12)-C(13)-C(14)	117.8(10)	C(1)-C(31)-C(36)	120.4(8)
C(12)-C(13)-H(13)	121.1	C(33)-C(32)-C(31)	122.5(9)
C(14)-C(13)-H(13)	121.1	C(33)-C(32)-H(32)	118.8
C(15)-C(14)-C(13)	122.2(9)	C(31)-C(32)-H(32)	118.8
C(15)-C(14)-H(14)	118.9	C(32)-C(33)-C(34)	120.4(9)
C(13)-C(14)-H(14)	118.9	C(32)-C(33)-H(33)	119.8
C(16)-C(15)-C(14)	120.3(9)	C(34)-C(33)-H(33)	119.8
C(16)-C(15)-H(15)	119.8	C(35)-C(34)-C(33)	120.8(9)
C(14)-C(15)-H(15)	119.8	C(35)-C(34)-H(34)	119.6
C(15)-C(16)-C(11)	118.8(10)	C(33)-C(34)-H(34)	119.6
C(15)-C(16)-H(16)	120.6	C(34)-C(35)-C(36)	118.3(9)
C(11)-C(16)-H(16)	120.6	C(34)-C(35)-H(35)	120.9
C(22)-C(21)-C(26)	119.1(9)	C(36)-C(35)-H(35)	120.9
C(22)-C(21)-C(1)	119.2(8)	C(35)-C(36)-C(31)	120.6(8)
C(26)-C(21)-C(1)	121.7(8)	C(35)-C(36)-H(36)	119.7
C(23)-C(22)-C(21)	119.5(9)	C(31)-C(36)-H(36)	119.7
C(23)-C(22)-H(22)	120.2	C(51)-C(4)-C(41)	122.3(8)
C(21)-C(22)-H(22)	120.2	C(51)-C(4)-C(61)	122.3(8)
C(24)-C(23)-C(22)	120.4(9)	C(41)-C(4)-C(61)	115.4(9)
C(24)-C(23)-H(23)	119.8	C(42)-C(41)-C(46)	120.1(8)
C(22)-C(23)-H(23)	119.8	C(42)-C(41)-C(4)	122.6(8)
C(25)-C(24)-C(23)	119.6(10)	C(46)-C(41)-C(4)	117.3(9)
C(25)-C(24)-H(24)	120.2	C(41)-C(42)-C(43)	121.4(10)

C(41)-C(42)-H(42)	119.3	C(53)-C(54)-H(54)	120.2
C(43)-C(42)-H(42)	119.3	C(54)-C(55)-C(56)	119.3(9)
C(44)-C(43)-C(42)	117.5(10)	C(54)-C(55)-H(55)	120.4
C(44)-C(43)-H(43)	121.2	C(56)-C(55)-H(55)	120.4
C(42)-C(43)-H(43)	121.2	C(55)-C(56)-C(51)	121.6(9)
C(43)-C(44)-C(45)	123.1(10)	C(55)-C(56)-H(56)	119.2
C(43)-C(44)-H(44)	118.4	C(51)-C(56)-H(56)	119.2
C(45)-C(44)-H(44)	118.4	C(66)-C(61)-C(62)	120.7(10)
C(44)-C(45)-C(46)	119.7(10)	C(66)-C(61)-C(4)	118.9(10)
C(44)-C(45)-H(45)	120.2	C(62)-C(61)-C(4)	120.3(9)
C(46)-C(45)-H(45)	120.2	C(63)-C(62)-C(61)	117.8(10)
C(45)-C(46)-C(41)	118.1(10)	C(63)-C(62)-H(62)	121.1
C(45)-C(46)-H(46)	121.0	C(61)-C(62)-H(62)	121.1
C(41)-C(46)-H(46)	121.0	C(64)-C(63)-C(62)	123.2(13)
C(56)-C(51)-C(52)	117.7(10)	C(64)-C(63)-H(63)	118.4
C(56)-C(51)-C(4)	120.9(9)	C(62)-C(63)-H(63)	118.4
C(52)-C(51)-C(4)	121.3(8)	C(63)-C(64)-C(65)	119.9(12)
C(53)-C(52)-C(51)	120.3(9)	C(63)-C(64)-H(64)	120.0
C(53)-C(52)-H(52)	119.9	C(65)-C(64)-H(64)	120.0
C(51)-C(52)-H(52)	119.9	C(66)-C(65)-C(64)	120.6(12)
C(52)-C(53)-C(54)	121.2(10)	C(66)-C(65)-H(65)	119.7
C(52)-C(53)-H(53)	119.4	C(64)-C(65)-H(65)	119.7
C(54)-C(53)-H(53)	119.4	C(65)-C(66)-C(61)	117.5(12)
C(55)-C(54)-C(53)	119.7(11)	C(65)-C(66)-H(66)	121.2
C(55)-C(54)-H(54)	120.2	C(61)-C(66)-H(66)	121.2

(b) In the anions

F(7)-B(7)	1.472(11)	C(85)-C(86)	1.369(13)
B(7)-C(81)	1.619(14)	C(85)-F(85)	1.373(10)
B(7)-C(71)	1.667(15)	C(86)-C(87)	1.525(13)
B(7)-C(91)	1.671(14)	C(87)-C(88)	1.373(13)
B(7)-C(91X)	1.780(13)	C(87)-C(8C)	1.398(12)
C(71)-C(72)	1.403(11)	C(88)-F(88)	1.357(9)
C(71)-C(76)	1.416(13)	C(88)-C(89)	1.390(13)
C(72)-F(72)	1.350(10)	C(89)-F(89)	1.363(11)
C(72)-C(73)	1.423(12)	C(89)-C(8A)	1.405(14)
C(73)-C(74)	1.337(12)	C(8A)-F(8A)	1.366(13)
C(73)-F(73)	1.368(9)	C(8A)-C(8B)	1.391(16)
C(74)-F(74)	1.368(10)	C(8B)-F(8B)	1.364(10)
C(74)-C(75)	1.430(12)	C(8B)-C(8C)	1.367(14)
C(75)-F(75)	1.349(11)	C(8C)-F(8C)	1.359(12)
C(75)-C(76)	1.389(13)	C(91)-C(92)	1.3900
C(76)-C(77)	1.535(11)	C(92)-F(92)	1.331(11)
C(77)-C(7C)	1.360(11)	C(92)-C(93)	1.3900
C(77)-C(78)	1.405(11)	C(93)-F(93)	1.35(3)
C(78)-C(79)	1.356(11)	C(94)-F(94)	1.34(4)
C(78)-F(78)	1.360(9)	C(94)-C(95)	1.3900
C(79)-F(79)	1.358(10)	C(94)-C(93)	1.3900
C(79)-C(7A)	1.382(12)	C(95)-F(95)	1.37(5)
C(7A)-C(7B)	1.373(12)	C(95)-C(96)	1.3900
C(7A)-F(7A)	1.374(10)	C(96)-C(91)	1.3900
C(7B)-F(7B)	1.338(9)	C(96)-C(97)	1.486(13)
C(7B)-C(7C)	1.375(12)	C(91X)-C(92X)	1.3900
C(7C)-F(7C)	1.367(9)	C(92X)-F(92)	1.329(10)
C(81)-C(82)	1.410(13)	C(92X)-C(93X)	1.3900
C(81)-C(86)	1.448(11)	C(93X)-F(93X)	1.355(13)
C(82)-C(83)	1.356(13)	C(94X)-C(95X)	1.3900
C(82)-F(82)	1.378(10)	C(94X)-C(93X)	1.3900
C(83)-F(83)	1.375(11)	C(94X)-F(94X)	1.40(2)
C(83)-C(84)	1.394(13)	C(95X)-F(95X)	1.34(3)
C(84)-F(84)	1.369(11)	C(95X)-C(96X)	1.3900
C(84)-C(85)	1.385(14)	C(96X)-C(91X)	1.3900

C(96X)-C(97)	1.545(13)	C(112)-F(112)	1.392(10)
C(97)-C(98)	1.326(14)	C(113)-C(114)	1.300(12)
C(97)-C(9C)	1.410(14)	C(113)-F(113)	1.361(10)
C(98)-C(99)	1.398(13)	C(114)-C(115)	1.375(12)
C(98)-F(98)	1.420(12)	C(114)-F(114)	1.400(10)
C(99)-C(9A)	1.354(14)	C(115)-F(115)	1.370(11)
C(99)-F(99)	1.363(11)	C(115)-C(116)	1.412(13)
C(9A)-F(9A)	1.358(10)	C(116)-C(117)	1.521(11)
C(9A)-C(9B)	1.408(14)	C(117)-C(118)	1.385(11)
C(9B)-F(9B)	1.337(11)	C(117)-C(11C)	1.387(12)
C(9B)-C(9C)	1.379(12)	C(118)-C(119)	1.364(12)
C(9C)-F(9C)	1.327(10)	C(118)-F(118)	1.375(10)
F(10)-B(10)	1.457(10)	C(119)-F(119)	1.341(10)
B(10)-C(111)	1.623(14)	C(119)-C(11A)	1.396(13)
B(10)-C(101)	1.627(13)	C(11A)-F(11A)	1.352(10)
B(10)-C(121)	1.674(13)	C(11A)-C(11B)	1.392(13)
C(101)-C(106)	1.439(11)	C(11B)-F(11B)	1.366(10)
C(101)-C(102)	1.452(12)	C(11B)-C(11C)	1.386(12)
C(102)-C(103)	1.364(12)	C(11C)-F(11C)	1.356(9)
C(102)-F(102)	1.385(9)	C(121)-C(122)	1.389(11)
C(103)-F(103)	1.351(10)	C(121)-C(126)	1.425(13)
C(103)-C(104)	1.379(12)	C(122)-F(122)	1.386(11)
C(104)-C(105)	1.359(13)	C(122)-C(123)	1.408(12)
C(104)-F(104)	1.361(10)	C(123)-C(124)	1.340(13)
C(105)-C(106)	1.390(13)	C(123)-F(123)	1.386(9)
C(105)-F(105)	1.397(10)	C(124)-F(124)	1.367(10)
C(106)-C(107)	1.505(13)	C(124)-C(125)	1.399(12)
C(107)-C(108)	1.362(13)	C(125)-C(126)	1.379(12)
C(107)-C(10C)	1.397(12)	C(125)-F(125)	1.402(10)
C(108)-F(108)	1.355(9)	C(126)-C(127)	1.539(11)
C(108)-C(109)	1.383(12)	C(127)-C(128)	1.356(12)
C(109)-C(10A)	1.375(14)	C(127)-C(12C)	1.407(13)
C(109)-F(109)	1.393(12)	C(128)-F(128)	1.360(10)
C(10A)-C(10B)	1.314(15)	C(128)-C(129)	1.423(12)
C(10A)-F(10A)	1.411(12)	C(129)-F(129)	1.327(11)
C(10B)-C(10C)	1.380(14)	C(129)-C(12A)	1.381(14)
C(10B)-F(10B)	1.383(10)	C(12A)-F(12A)	1.352(10)
C(10C)-F(10C)	1.378(11)	C(12A)-C(12B)	1.355(14)
C(111)-C(112)	1.445(11)	C(12B)-F(12B)	1.360(11)
C(111)-C(116)	1.447(12)	C(12B)-C(12C)	1.417(12)
C(112)-C(113)	1.379(13)	C(12C)-F(12C)	1.313(11)

F(7)-B(7)-C(81)	107.3(7)	F(74)-C(74)-C(75)	117.4(9)
F(7)-B(7)-C(71)	105.3(8)	F(75)-C(75)-C(76)	124.2(8)
C(81)-B(7)-C(71)	113.6(7)	F(75)-C(75)-C(74)	118.0(9)
F(7)-B(7)-C(91)	101.8(8)	C(76)-C(75)-C(74)	117.8(10)
C(81)-B(7)-C(91)	118.8(11)	C(75)-C(76)-C(71)	124.9(8)
C(71)-B(7)-C(91)	108.5(8)	C(75)-C(76)-C(77)	113.6(9)
F(7)-B(7)-C(91X)	108.3(8)	C(71)-C(76)-C(77)	121.5(8)
C(81)-B(7)-C(91X)	108.8(9)	C(7C)-C(77)-C(78)	115.5(7)
C(71)-B(7)-C(91X)	113.2(8)	C(7C)-C(77)-C(76)	122.5(8)
C(91)-B(7)-C(91X)	10.3(9)	C(78)-C(77)-C(76)	121.9(7)
C(72)-C(71)-C(76)	114.2(9)	C(79)-C(78)-F(78)	119.5(8)
C(72)-C(71)-B(7)	120.0(9)	C(79)-C(78)-C(77)	122.9(8)
C(76)-C(71)-B(7)	125.7(8)	F(78)-C(78)-C(77)	117.5(7)
F(72)-C(72)-C(71)	122.7(8)	C(78)-C(79)-F(79)	120.2(8)
F(72)-C(72)-C(73)	115.5(7)	C(78)-C(79)-C(7A)	118.3(9)
C(71)-C(72)-C(73)	121.8(9)	F(79)-C(79)-C(7A)	121.5(8)
C(74)-C(73)-F(73)	120.1(8)	C(7B)-C(7A)-F(7A)	120.4(8)
C(74)-C(73)-C(72)	121.8(8)	C(7B)-C(7A)-C(79)	121.4(8)
F(73)-C(73)-C(72)	118.2(8)	F(7A)-C(7A)-C(79)	118.2(9)
C(73)-C(74)-F(74)	123.1(8)	F(7B)-C(7B)-C(7A)	119.1(8)
C(73)-C(74)-C(75)	119.5(9)	F(7B)-C(7B)-C(7C)	123.3(9)

C(7A)-C(7B)-C(7C)	117.6(8)	C(93X)-C(92X)-C(91X)	120.0
C(77)-C(7C)-F(7C)	119.9(7)	F(93X)-C(93X)-C(92X)	119.4(10)
C(77)-C(7C)-C(7B)	124.2(9)	F(93X)-C(93X)-C(94X)	120.6(10)
F(7C)-C(7C)-C(7B)	115.9(7)	C(92X)-C(93X)-C(94X)	120.0
C(82)-C(81)-C(86)	113.3(8)	C(95X)-C(94X)-C(93X)	120.0
C(82)-C(81)-B(7)	125.9(7)	C(95X)-C(94X)-F(94X)	120.5(11)
C(86)-C(81)-B(7)	120.7(8)	C(93X)-C(94X)-F(94X)	119.2(11)
C(83)-C(82)-F(82)	114.7(9)	F(95X)-C(95X)-C(94X)	120.5(12)
C(83)-C(82)-C(81)	125.6(9)	F(95X)-C(95X)-C(96X)	119.4(13)
F(82)-C(82)-C(81)	119.8(8)	C(94X)-C(95X)-C(96X)	120.0
C(82)-C(83)-F(83)	122.2(9)	C(91X)-C(96X)-C(95X)	120.0
C(82)-C(83)-C(84)	119.4(10)	C(91X)-C(96X)-C(97)	122.4(9)
F(83)-C(83)-C(84)	118.4(9)	C(95X)-C(96X)-C(97)	117.2(9)
F(84)-C(84)-C(85)	121.5(9)	C(98)-C(97)-C(9C)	116.6(9)
F(84)-C(84)-C(83)	120.3(10)	C(98)-C(97)-C(96)	110.9(13)
C(85)-C(84)-C(83)	118.2(9)	C(9C)-C(97)-C(96)	132.4(13)
C(86)-C(85)-F(85)	120.6(10)	C(98)-C(97)-C(96X)	128.0(11)
C(86)-C(85)-C(84)	122.5(9)	C(9C)-C(97)-C(96X)	115.1(11)
F(85)-C(85)-C(84)	116.7(8)	C(96)-C(97)-C(96X)	18.4(9)
C(85)-C(86)-C(81)	121.0(10)	C(97)-C(98)-C(99)	125.8(10)
C(85)-C(86)-C(87)	117.1(8)	C(97)-C(98)-F(98)	121.6(10)
C(81)-C(86)-C(87)	121.9(8)	C(99)-C(98)-F(98)	112.5(10)
C(88)-C(87)-C(8C)	115.8(10)	C(9A)-C(99)-F(99)	119.9(9)
C(88)-C(87)-C(86)	122.0(8)	C(9A)-C(99)-C(98)	116.8(10)
C(8C)-C(87)-C(86)	122.1(10)	F(99)-C(99)-C(98)	123.3(10)
F(88)-C(88)-C(87)	119.7(9)	C(99)-C(9A)-F(9A)	120.7(10)
F(88)-C(88)-C(89)	116.0(9)	C(99)-C(9A)-C(9B)	120.8(9)
C(87)-C(88)-C(89)	124.4(9)	F(9A)-C(9A)-C(9B)	118.4(10)
F(89)-C(89)-C(88)	123.7(8)	F(9B)-C(9B)-C(9C)	119.1(10)
F(89)-C(89)-C(8A)	117.8(10)	F(9B)-C(9B)-C(9A)	121.5(9)
C(88)-C(89)-C(8A)	118.5(10)	C(9C)-C(9B)-C(9A)	119.4(10)
F(8A)-C(8A)-C(8B)	122.3(10)	F(9C)-C(9C)-C(9B)	119.4(9)
F(8A)-C(8A)-C(89)	119.9(12)	F(9C)-C(9C)-C(97)	119.9(9)
C(8B)-C(8A)-C(89)	117.7(11)	C(9B)-C(9C)-C(97)	120.5(10)
F(8B)-C(8B)-C(8C)	119.1(11)	F(10)-B(10)-C(111)	106.3(8)
F(8B)-C(8B)-C(8A)	119.0(11)	F(10)-B(10)-C(101)	106.3(7)
C(8C)-C(8B)-C(8A)	121.9(10)	C(111)-B(10)-C(101)	111.6(7)
F(8C)-C(8C)-C(8B)	119.9(9)	F(10)-B(10)-C(121)	106.5(7)
F(8C)-C(8C)-C(87)	118.4(10)	C(111)-B(10)-C(121)	114.9(7)
C(8B)-C(8C)-C(87)	121.7(10)	C(101)-B(10)-C(121)	110.8(8)
C(96)-C(91)-C(92)	120.0	C(106)-C(101)-C(102)	111.9(8)
C(96)-C(91)-B(7)	120.2(9)	C(106)-C(101)-B(10)	121.2(8)
C(92)-C(91)-B(7)	119.7(9)	C(102)-C(101)-B(10)	126.9(7)
F(92)-C(92)-C(93)	115.6(10)	C(103)-C(102)-F(102)	116.7(8)
F(92)-C(92)-C(91)	124.0(10)	C(103)-C(102)-C(101)	125.7(8)
C(93)-C(92)-C(91)	120.0	F(102)-C(102)-C(101)	117.4(7)
F(93)-C(93)-C(92)	121.7(15)	F(103)-C(103)-C(102)	120.0(9)
F(93)-C(93)-C(94)	118.2(15)	F(103)-C(103)-C(104)	120.4(9)
C(92)-C(93)-C(94)	120.0	C(102)-C(103)-C(104)	119.6(9)
F(94)-C(94)-C(95)	118(2)	C(105)-C(104)-F(104)	123.5(9)
F(94)-C(94)-C(93)	121(2)	C(105)-C(104)-C(103)	117.7(9)
C(95)-C(94)-C(93)	120.0	F(104)-C(104)-C(103)	118.8(10)
F(95)-C(95)-C(96)	128(2)	C(104)-C(105)-C(106)	124.9(9)
F(95)-C(95)-C(94)	112(2)	C(104)-C(105)-F(105)	116.9(8)
C(96)-C(95)-C(94)	120.0	C(106)-C(105)-F(105)	118.2(9)
C(95)-C(96)-C(91)	120.0	C(105)-C(106)-C(101)	120.2(9)
C(95)-C(96)-C(97)	113.7(9)	C(105)-C(106)-C(107)	117.6(8)
C(91)-C(96)-C(97)	125.4(9)	C(101)-C(106)-C(107)	122.1(8)
C(96X)-C(91X)-C(92X)	120.0	C(108)-C(107)-C(10C)	116.0(9)
C(96X)-C(91X)-B(7)	120.2(9)	C(108)-C(107)-C(106)	121.3(8)
C(92X)-C(91X)-B(7)	119.6(9)	C(10C)-C(107)-C(106)	122.4(9)
F(92)-C(92X)-C(93X)	118.3(10)	F(108)-C(108)-C(107)	119.9(8)
F(92)-C(92X)-C(91X)	121.6(10)	F(108)-C(108)-C(109)	116.5(8)

C(107)-C(108)-C(109)	123.6(8)	F(11B)-C(11B)-C(11C)	121.0(8)
C(10A)-C(109)-C(108)	117.3(11)	F(11B)-C(11B)-C(11A)	118.8(8)
C(10A)-C(109)-F(109)	121.1(10)	C(11C)-C(11B)-C(11A)	120.1(8)
C(108)-C(109)-F(109)	121.6(8)	F(11C)-C(11C)-C(11B)	116.8(8)
C(10B)-C(10A)-C(109)	121.3(11)	F(11C)-C(11C)-C(117)	121.6(8)
C(10B)-C(10A)-F(10A)	121.9(10)	C(11B)-C(11C)-C(117)	121.6(8)
C(109)-C(10A)-F(10A)	116.5(12)	C(122)-C(121)-C(126)	114.4(8)
C(10A)-C(10B)-C(10C)	121.0(9)	C(122)-C(121)-B(10)	124.7(8)
C(10A)-C(10B)-F(10B)	120.5(12)	C(126)-C(121)-B(10)	120.6(7)
C(10C)-C(10B)-F(10B)	118.4(12)	F(122)-C(122)-C(121)	119.7(8)
F(10C)-C(10C)-C(10B)	119.9(9)	F(122)-C(122)-C(123)	117.9(8)
F(10C)-C(10C)-C(107)	119.4(10)	C(121)-C(122)-C(123)	122.4(9)
C(10B)-C(10C)-C(107)	120.6(10)	C(124)-C(123)-F(123)	121.1(8)
C(112)-C(111)-C(116)	110.1(8)	C(124)-C(123)-C(122)	122.5(8)
C(112)-C(111)-B(10)	121.5(8)	F(123)-C(123)-C(122)	116.5(9)
C(116)-C(111)-B(10)	128.4(8)	C(123)-C(124)-F(124)	122.2(9)
C(113)-C(112)-F(112)	118.5(8)	C(123)-C(124)-C(125)	116.9(9)
C(113)-C(112)-C(111)	126.1(9)	F(124)-C(124)-C(125)	120.9(9)
F(112)-C(112)-C(111)	115.4(8)	C(126)-C(125)-C(124)	121.9(9)
C(114)-C(113)-F(113)	121.9(9)	C(126)-C(125)-F(125)	122.8(8)
C(114)-C(113)-C(112)	120.0(9)	C(124)-C(125)-F(125)	115.3(8)
F(113)-C(113)-C(112)	118.0(9)	C(125)-C(126)-C(121)	121.9(8)
C(113)-C(114)-C(115)	121.1(10)	C(125)-C(126)-C(127)	115.0(8)
C(113)-C(114)-F(114)	122.2(8)	C(121)-C(126)-C(127)	123.1(8)
C(115)-C(114)-F(114)	116.7(9)	C(128)-C(127)-C(12C)	119.9(9)
F(115)-C(115)-C(114)	119.5(9)	C(128)-C(127)-C(126)	121.5(9)
F(115)-C(115)-C(116)	119.9(9)	C(12C)-C(127)-C(126)	118.5(9)
C(114)-C(115)-C(116)	120.5(9)	C(127)-C(128)-F(128)	121.3(9)
C(115)-C(116)-C(111)	122.2(8)	C(127)-C(128)-C(129)	122.9(9)
C(115)-C(116)-C(117)	115.8(9)	F(128)-C(128)-C(129)	115.8(8)
C(111)-C(116)-C(117)	122.0(8)	F(129)-C(129)-C(12A)	123.6(9)
C(118)-C(117)-C(11C)	116.2(8)	F(129)-C(129)-C(128)	120.3(10)
C(118)-C(117)-C(116)	121.4(8)	C(12A)-C(129)-C(128)	116.0(9)
C(11C)-C(117)-C(116)	122.2(8)	F(12A)-C(12A)-C(12B)	120.4(10)
C(119)-C(118)-F(118)	117.1(8)	F(12A)-C(12A)-C(129)	117.0(10)
C(119)-C(118)-C(117)	124.2(9)	C(12B)-C(12A)-C(129)	122.6(9)
F(118)-C(118)-C(117)	118.7(8)	C(12A)-C(12B)-F(12B)	121.0(9)
F(119)-C(119)-C(118)	121.7(9)	C(12A)-C(12B)-C(12C)	121.1(10)
F(119)-C(119)-C(11A)	119.7(8)	F(12B)-C(12B)-C(12C)	117.9(10)
C(118)-C(119)-C(11A)	118.6(9)	F(12C)-C(12C)-C(127)	123.6(8)
F(11A)-C(11A)-C(11B)	121.0(9)	F(12C)-C(12C)-C(12B)	119.0(9)
F(11A)-C(11A)-C(119)	119.8(8)	C(127)-C(12C)-C(12B)	117.4(10)
C(11B)-C(11A)-C(119)	119.2(9)		

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3) for the expression:
$\exp\{-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})\}$
E.s.ds are in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	51(6)	50(6)	45(5)	-6(5)	13(4)	8(5)
C(11)	55(6)	50(6)	38(5)	2(5)	-17(5)	14(5)
C(12)	34(5)	64(7)	57(6)	1(5)	2(4)	8(5)
C(13)	73(7)	51(6)	67(7)	1(5)	19(6)	20(6)
C(14)	49(6)	54(6)	81(8)	-6(6)	3(6)	-2(5)
C(15)	58(6)	54(6)	48(6)	5(5)	-8(5)	14(5)
C(16)	57(6)	52(6)	65(6)	-9(5)	14(5)	0(5)
C(21)	29(5)	46(6)	49(5)	-3(5)	-7(4)	8(4)
C(22)	52(6)	48(6)	53(6)	-6(5)	-10(5)	-7(5)
C(23)	59(7)	46(6)	61(6)	2(5)	-1(5)	7(5)
C(24)	66(7)	56(6)	56(6)	4(5)	-15(5)	12(5)
C(25)	42(5)	54(6)	70(7)	-14(6)	5(5)	17(5)
C(26)	46(6)	42(6)	57(6)	-3(5)	5(4)	10(5)
C(31)	34(5)	59(7)	63(6)	1(5)	9(4)	14(5)
C(32)	41(6)	66(7)	56(6)	7(5)	1(5)	21(5)
C(33)	49(7)	69(7)	69(7)	-6(6)	4(5)	1(6)
C(34)	37(6)	90(9)	63(7)	9(6)	-12(5)	10(6)
C(35)	35(6)	80(8)	75(7)	-11(6)	6(5)	15(5)
C(36)	56(7)	55(6)	52(6)	10(5)	3(5)	2(5)
C(4)	47(6)	66(7)	50(6)	-16(5)	7(5)	7(5)
C(41)	35(5)	43(6)	51(6)	-3(5)	0(4)	5(4)
C(42)	52(6)	65(7)	73(7)	13(6)	11(5)	17(5)
C(43)	92(9)	79(8)	56(7)	14(6)	12(7)	23(7)
C(44)	77(8)	75(8)	66(7)	11(6)	8(6)	28(6)
C(45)	39(6)	73(7)	87(8)	-9(7)	-6(5)	1(5)
C(46)	46(6)	51(6)	76(7)	-1(5)	14(5)	9(5)
C(51)	48(6)	41(6)	49(6)	-4(5)	-3(5)	7(5)
C(52)	67(7)	58(7)	74(7)	-7(6)	30(6)	9(6)
C(53)	53(6)	67(8)	85(8)	-15(7)	7(6)	14(6)
C(54)	70(7)	72(7)	42(6)	-14(5)	-12(5)	11(6)
C(55)	73(8)	50(6)	62(7)	9(5)	11(5)	13(6)
C(56)	39(5)	79(8)	48(6)	-20(6)	-5(5)	-15(5)
C(61)	48(6)	88(8)	45(6)	10(5)	-2(5)	-1(6)
C(62)	54(7)	91(9)	52(6)	6(6)	6(5)	14(6)
C(63)	44(7)	116(10)	94(9)	8(7)	0(6)	27(7)
C(64)	46(8)	171(15)	66(8)	7(9)	5(6)	18(10)
C(65)	43(8)	155(14)	59(7)	12(8)	-2(5)	-28(8)
C(66)	47(7)	90(8)	58(6)	-1(6)	1(5)	1(6)
F(7)	48(3)	53(3)	59(3)	-11(3)	5(2)	-4(2)
B(7)	38(6)	58(8)	53(7)	1(6)	8(5)	8(5)
C(71)	45(5)	51(6)	53(6)	-8(5)	12(5)	5(5)
C(72)	35(5)	50(6)	51(6)	2(5)	6(4)	10(5)
F(72)	50(3)	45(3)	68(3)	-8(3)	1(2)	12(3)
C(73)	49(5)	38(5)	44(6)	10(5)	-1(5)	17(5)
F(73)	55(3)	60(3)	61(3)	-20(3)	-8(3)	16(3)
C(74)	36(5)	62(7)	40(6)	13(5)	-9(4)	3(5)
F(74)	56(3)	72(4)	71(4)	-9(3)	-3(3)	16(3)
C(75)	57(6)	45(6)	41(6)	5(5)	13(5)	-7(5)
F(75)	50(3)	56(3)	86(4)	-14(3)	0(3)	24(3)
C(76)	45(5)	48(6)	41(6)	2(4)	6(4)	8(5)
C(77)	48(6)	49(6)	56(6)	-12(5)	10(5)	5(5)

C(78)	44(6)	65(7)	56(6)	-17(5)	1(5)	7(5)
F(78)	57(3)	64(4)	81(4)	-6(3)	23(3)	9(3)
C(79)	62(7)	50(7)	52(6)	-10(5)	-17(5)	5(5)
F(79)	75(4)	55(4)	88(4)	-13(3)	3(3)	5(3)
C(7A)	65(7)	64(7)	65(7)	-18(6)	7(6)	30(6)
F(7A)	95(4)	76(4)	71(4)	-25(3)	-4(3)	25(3)
C(7B)	52(6)	72(7)	64(7)	-15(6)	16(5)	21(6)
F(7B)	87(4)	94(4)	73(4)	-5(3)	34(3)	19(3)
C(7C)	46(6)	61(7)	67(7)	-19(6)	11(5)	14(5)
F(7C)	63(3)	63(4)	88(4)	-12(3)	29(3)	2(3)
C(81)	36(5)	51(6)	41(5)	-4(5)	-1(4)	-2(4)
C(82)	51(6)	48(6)	63(7)	-3(5)	-2(5)	5(5)
F(82)	62(3)	59(3)	74(4)	4(3)	12(3)	5(3)
C(83)	78(8)	44(7)	50(6)	-1(5)	-9(5)	25(6)
F(83)	85(4)	62(4)	94(4)	-8(3)	-6(3)	26(3)
C(84)	40(6)	72(8)	72(7)	-14(6)	-16(5)	19(6)
F(84)	61(4)	80(4)	96(4)	-8(3)	0(3)	35(3)
C(85)	35(6)	56(7)	84(8)	-7(6)	-4(5)	18(5)
F(85)	51(3)	77(4)	88(4)	-8(3)	23(3)	9(3)
C(86)	46(6)	49(6)	70(7)	-11(5)	4(5)	-1(5)
C(87)	32(5)	56(7)	57(7)	-5(5)	6(5)	-5(5)
C(88)	51(6)	47(7)	58(7)	-4(6)	19(5)	-2(5)
F(88)	55(3)	54(3)	67(3)	-10(3)	5(3)	4(3)
C(89)	55(6)	58(7)	51(7)	-1(6)	14(5)	13(5)
F(89)	72(4)	70(4)	68(4)	11(3)	16(3)	19(3)
C(8A)	66(7)	61(8)	92(10)	-1(7)	31(7)	1(6)
F(8A)	79(4)	48(4)	132(5)	5(4)	34(4)	13(3)
C(8B)	49(6)	51(8)	94(10)	-19(7)	11(6)	-7(5)
F(8B)	79(4)	56(4)	114(5)	-26(4)	20(4)	-10(3)
C(8C)	45(6)	67(8)	59(7)	-13(6)	-1(5)	-3(5)
F(8C)	54(3)	79(4)	81(4)	-31(3)	-4(3)	-4(3)
F(92)	65(4)	89(4)	62(3)	-16(3)	7(3)	-19(3)
F(94)	63(14)	150(30)	140(30)	40(20)	48(14)	10(20)
F(95)	52(17)	220(40)	55(16)	-60(20)	6(12)	30(16)
F(93X)	53(7)	67(10)	91(8)	0(7)	7(5)	-27(7)
F(94X)	108(14)	160(20)	40(7)	12(10)	26(7)	-65(14)
F(95X)	55(12)	170(20)	59(8)	-23(12)	14(9)	-34(12)
C(97)	54(7)	73(8)	42(6)	-11(5)	0(5)	6(6)
C(98)	54(7)	110(10)	44(6)	-6(6)	-2(5)	36(7)
F(98)	68(4)	103(5)	91(5)	-13(4)	-5(3)	22(4)
C(99)	50(7)	64(8)	76(8)	-8(6)	13(5)	3(6)
F(99)	82(4)	65(4)	94(4)	-14(3)	10(3)	15(3)
C(9A)	61(7)	68(8)	48(6)	-10(5)	11(5)	-2(6)
F(9A)	63(4)	77(4)	79(4)	-23(3)	14(3)	-10(3)
C(9B)	50(7)	81(8)	53(6)	-1(6)	7(5)	16(6)
F(9B)	55(4)	76(4)	70(4)	-13(3)	-11(3)	14(3)
C(9C)	51(7)	52(7)	56(6)	3(5)	-3(5)	10(5)
F(9C)	65(4)	64(4)	74(4)	-8(3)	1(3)	3(3)
F(10)	39(3)	49(3)	55(3)	-8(2)	0(2)	-1(2)
B(10)	39(6)	47(7)	52(7)	4(5)	8(5)	-3(5)
C(101)	38(5)	55(6)	42(5)	-8(5)	2(4)	5(4)
C(102)	45(6)	47(6)	48(6)	-8(5)	-6(4)	12(5)
F(102)	57(3)	54(3)	72(4)	1(3)	4(3)	4(3)
C(103)	64(7)	45(6)	54(6)	4(5)	-5(5)	23(5)
F(103)	82(4)	62(4)	91(4)	-8(3)	6(3)	25(3)
C(104)	47(6)	76(8)	56(6)	-15(6)	8(5)	24(6)
F(104)	60(4)	84(4)	89(4)	-13(3)	-1(3)	35(3)
C(105)	44(6)	57(7)	69(7)	0(5)	2(5)	13(5)
F(105)	43(3)	93(4)	90(4)	-5(3)	25(3)	10(3)
C(106)	47(6)	62(7)	48(6)	-18(5)	6(5)	4(5)
C(107)	40(5)	49(7)	60(7)	-12(5)	2(5)	-4(5)
C(108)	46(5)	45(6)	41(6)	-6(5)	8(5)	0(5)

F(108)	54(3)	56(3)	62(3)	-16(3)	-6(3)	5(3)
C(109)	45(6)	42(7)	80(8)	-1(6)	15(5)	17(5)
F(109)	75(4)	70(4)	83(4)	20(3)	10(3)	20(3)
C(10A)	54(6)	35(7)	104(10)	-2(7)	27(7)	3(5)
F(10A)	91(4)	45(4)	134(5)	-5(4)	41(4)	12(3)
C(10B)	52(6)	68(9)	79(9)	-30(8)	20(6)	4(6)
F(10B)	82(4)	70(4)	122(5)	-47(4)	24(4)	-17(3)
C(10C)	51(6)	59(7)	47(6)	-6(6)	13(5)	13(5)
F(10C)	58(3)	83(4)	64(4)	-12(3)	-8(3)	-5(3)
C(111)	39(5)	44(6)	47(6)	-3(5)	13(4)	4(4)
C(112)	38(5)	57(7)	51(6)	2(5)	11(5)	17(5)
F(112)	57(3)	47(3)	77(4)	-8(3)	-10(3)	9(3)
C(113)	33(5)	54(7)	72(7)	13(6)	-4(5)	9(5)
F(113)	58(3)	74(4)	63(3)	-27(3)	-13(3)	6(3)
C(114)	41(5)	70(7)	35(5)	-7(5)	2(4)	18(5)
F(114)	56(3)	104(4)	52(3)	-2(3)	-6(3)	24(3)
C(115)	40(6)	59(7)	70(7)	21(6)	10(5)	15(5)
F(115)	63(3)	68(4)	76(4)	1(3)	2(3)	28(3)
C(116)	36(5)	43(6)	57(6)	0(5)	13(5)	2(4)
C(117)	39(5)	39(6)	60(6)	-3(5)	7(4)	13(4)
C(118)	51(6)	50(7)	61(7)	5(5)	10(5)	14(5)
F(118)	56(3)	68(4)	68(4)	4(3)	23(3)	13(3)
C(119)	57(6)	42(7)	82(8)	0(6)	12(6)	-3(5)
F(119)	86(4)	56(4)	96(4)	-3(3)	17(3)	0(3)
C(11A)	61(7)	41(6)	84(8)	2(6)	5(6)	13(5)
F(11A)	98(5)	59(4)	87(4)	-17(3)	17(3)	-4(3)
C(11B)	53(6)	65(7)	56(7)	-3(6)	15(5)	5(5)
F(11B)	87(4)	62(4)	63(4)	-14(3)	12(3)	11(3)
C(11C)	47(6)	43(6)	60(7)	7(5)	6(5)	6(5)
F(11C)	72(4)	57(4)	66(3)	-1(3)	16(3)	11(3)
C(121)	32(5)	60(6)	31(5)	-14(4)	3(4)	0(4)
C(122)	64(7)	58(6)	47(6)	-7(5)	13(6)	12(5)
F(122)	52(3)	79(4)	55(3)	8(3)	0(3)	-7(3)
C(123)	41(6)	52(6)	57(7)	-11(5)	6(5)	0(5)
F(123)	54(3)	76(4)	72(4)	-14(3)	15(3)	-19(3)
C(124)	71(7)	60(7)	40(6)	-3(5)	14(6)	-1(6)
F(124)	75(4)	72(4)	66(4)	0(3)	28(3)	-3(3)
C(125)	44(6)	71(7)	46(6)	5(5)	5(5)	11(5)
F(125)	51(3)	80(4)	46(3)	8(3)	2(3)	20(3)
C(126)	41(5)	49(6)	65(7)	-5(5)	8(5)	7(5)
C(127)	42(6)	65(7)	45(6)	-9(5)	6(4)	-2(5)
C(128)	55(7)	68(7)	49(6)	1(5)	2(5)	38(6)
F(128)	55(3)	73(4)	65(3)	-3(3)	-6(3)	25(3)
C(129)	37(6)	91(9)	67(7)	-7(6)	3(5)	12(6)
F(129)	45(3)	123(5)	83(4)	-28(4)	-15(3)	40(3)
C(12A)	40(6)	78(8)	61(7)	-4(6)	-4(5)	3(6)
F(12A)	41(3)	125(5)	99(5)	-30(4)	-2(3)	-11(3)
C(12B)	60(7)	65(8)	64(7)	-7(6)	-1(5)	6(6)
F(12B)	60(4)	67(4)	94(4)	-19(3)	5(3)	-4(3)
C(12C)	40(6)	65(7)	62(7)	-10(5)	9(5)	-6(5)
F(12C)	43(3)	75(4)	70(4)	-16(3)	6(3)	12(3)

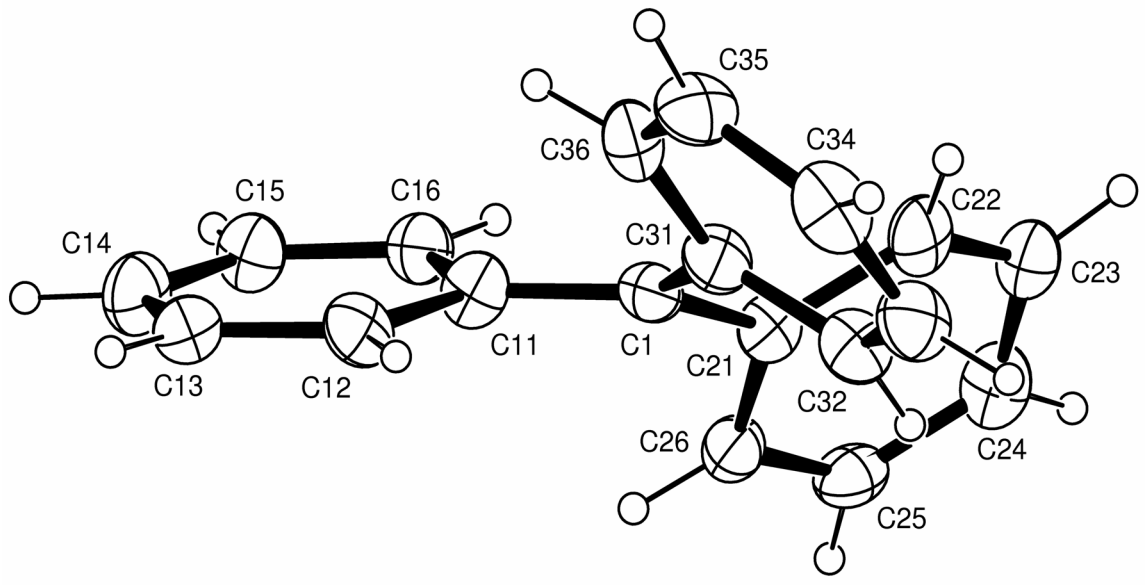
Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3). All hydrogen atoms were included in idealised positions with U(iso)'s set at 1.2*U(eq) of the parent carbon atom.

	x	y	z	U(eq)
H(12)	4302	7438	347	63
H(13)	5862	8581	170	75
H(14)	7917	9005	669	77
H(15)	8336	8371	1356	64
H(16)	6750	7269	1555	72
H(22)	3188	5598	1742	66
H(23)	4106	4827	2251	68
H(24)	6261	4592	2099	73
H(25)	7663	5271	1543	65
H(26)	6951	6164	1095	58
H(32)	2707	5253	809	64
H(33)	418	4967	553	78
H(34)	-786	5890	456	78
H(35)	242	7089	743	75
H(36)	2653	7404	962	67
H(42)	639	1725	4616	75
H(43)	-1134	681	4827	90
H(44)	-3031	249	4288	85
H(45)	-3361	879	3597	83
H(46)	-1606	1923	3379	69
H(52)	-1527	3105	3834	80
H(53)	-2015	4074	3417	82
H(54)	-481	4700	2848	76
H(55)	1630	4389	2735	74
H(56)	2262	3505	3223	73
H(62)	2030	1454	3908	80
H(63)	4383	1499	4028	100
H(64)	5987	2545	4259	115
H(65)	5353	3674	4271	115
H(66)	2994	3702	4131	81

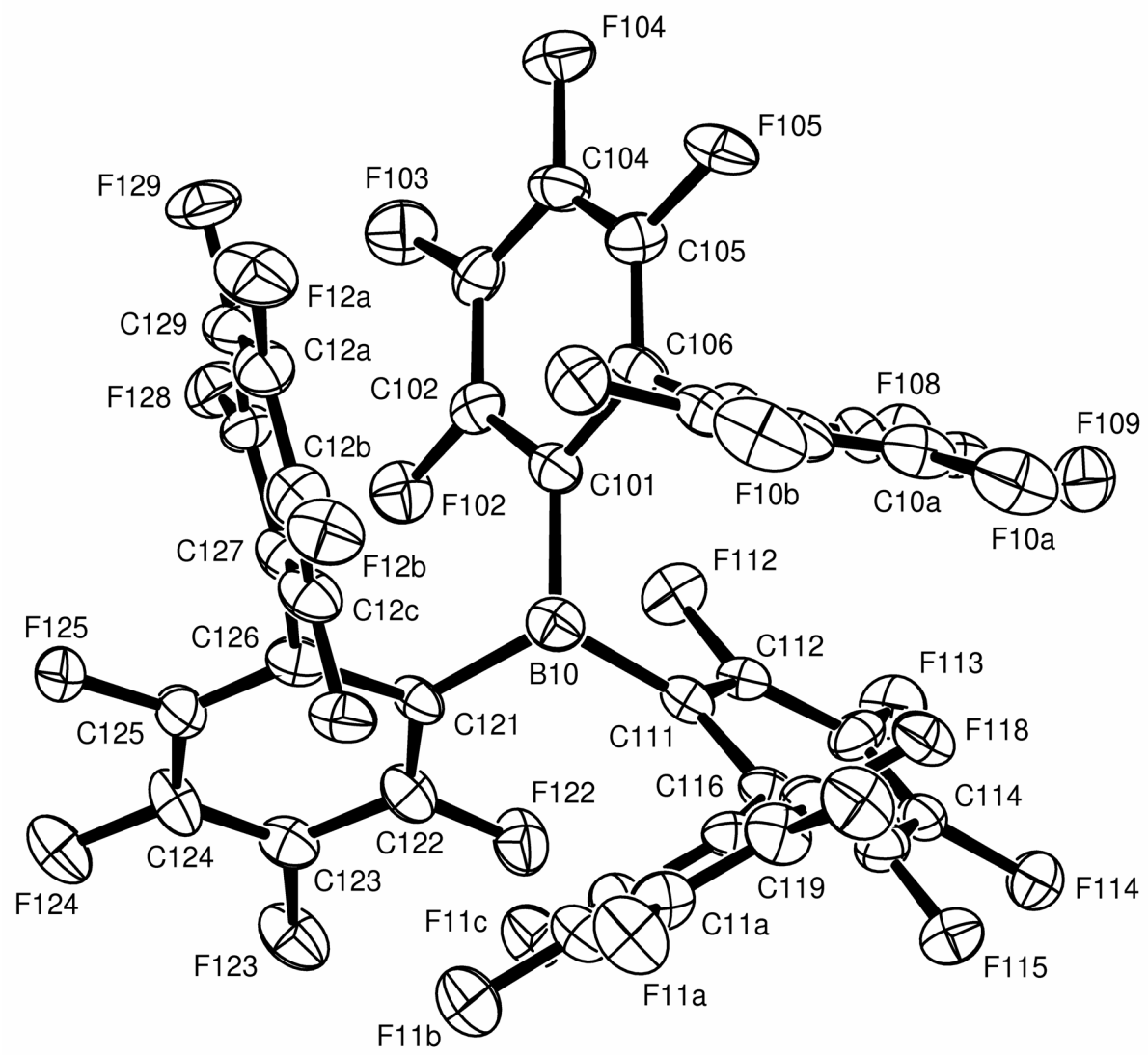
Table 5. Torsion angles, in degrees. E.s.ds are in parentheses.

C(31)-C(1)-C(11)-C(12)	-27.2(11)
C(21)-C(1)-C(11)-C(12)	153.0(8)
C(31)-C(1)-C(11)-C(16)	153.7(8)
C(21)-C(1)-C(11)-C(16)	-26.1(11)
C(11)-C(1)-C(21)-C(22)	142.1(7)
C(31)-C(1)-C(21)-C(22)	-37.8(10)
C(11)-C(1)-C(21)-C(26)	-35.8(11)
C(31)-C(1)-C(21)-C(26)	144.4(8)
C(11)-C(1)-C(31)-C(32)	143.7(8)
C(21)-C(1)-C(31)-C(32)	-36.5(11)
C(11)-C(1)-C(31)-C(36)	-32.1(11)
C(21)-C(1)-C(31)-C(36)	147.7(8)
C(51)-C(4)-C(41)-C(42)	-148.3(9)
C(61)-C(4)-C(41)-C(42)	33.8(11)
C(51)-C(4)-C(41)-C(46)	34.9(11)
C(61)-C(4)-C(41)-C(46)	-142.9(8)
C(41)-C(4)-C(51)-C(56)	-148.1(8)
C(61)-C(4)-C(51)-C(56)	29.6(12)
C(41)-C(4)-C(51)-C(52)	29.1(12)
C(61)-C(4)-C(51)-C(52)	-153.2(9)
C(51)-C(4)-C(61)-C(66)	36.4(12)
C(41)-C(4)-C(61)-C(66)	-145.8(8)
C(51)-C(4)-C(61)-C(62)	-142.3(9)
C(41)-C(4)-C(61)-C(62)	35.6(11)
F(7)-B(7)-C(71)-C(72)	144.3(7)
C(81)-B(7)-C(71)-C(72)	27.2(11)
C(91)-B(7)-C(71)-C(72)	-107.4(11)
C(91X)-B(7)-C(71)-C(72)	-97.6(10)
F(7)-B(7)-C(71)-C(76)	-33.2(10)
C(81)-B(7)-C(71)-C(76)	-150.4(8)
C(91)-B(7)-C(71)-C(76)	75.1(12)
C(91X)-B(7)-C(71)-C(76)	84.9(12)
C(75)-C(76)-C(77)-C(7C)	89.9(11)
C(71)-C(76)-C(77)-C(7C)	-89.1(12)
C(75)-C(76)-C(77)-C(78)	-88.1(11)
C(71)-C(76)-C(77)-C(78)	92.9(11)
F(7)-B(7)-C(81)-C(82)	136.8(8)
C(71)-B(7)-C(81)-C(82)	-107.3(10)
C(91)-B(7)-C(81)-C(82)	22.2(13)
C(91X)-B(7)-C(81)-C(82)	19.8(12)
F(7)-B(7)-C(81)-C(86)	-46.7(10)
C(71)-B(7)-C(81)-C(86)	69.3(10)
C(91)-B(7)-C(81)-C(86)	-161.3(9)
C(91X)-B(7)-C(81)-C(86)	-163.6(8)
C(85)-C(86)-C(87)-C(88)	83.6(11)
C(81)-C(86)-C(87)-C(88)	-96.9(10)
C(85)-C(86)-C(87)-C(8C)	-93.0(10)
C(81)-C(86)-C(87)-C(8C)	86.5(11)
F(7)-B(7)-C(91)-C(96)	-32.7(14)
C(81)-B(7)-C(91)-C(96)	84.8(13)
C(71)-B(7)-C(91)-C(96)	-143.4(11)
F(7)-B(7)-C(91)-C(92)	142.8(10)
C(81)-B(7)-C(91)-C(92)	-99.7(12)
C(71)-B(7)-C(91)-C(92)	32.1(14)
F(7)-B(7)-C(91X)-C(96X)	-32.2(12)
C(81)-B(7)-C(91X)-C(96X)	84.1(10)
C(71)-B(7)-C(91X)-C(96X)	-148.6(8)

F(7)-B(7)-C(91X)-C(92X)	142.8(8)
C(81)-B(7)-C(91X)-C(92X)	-100.9(9)
C(71)-B(7)-C(91X)-C(92X)	26.4(12)
C(95)-C(96)-C(97)-C(98)	-78.1(13)
C(91)-C(96)-C(97)-C(98)	112.9(14)
C(95)-C(96)-C(97)-C(9C)	103.6(13)
C(91)-C(96)-C(97)-C(9C)	-65(2)
C(91X)-C(96X)-C(97)-C(98)	96.3(12)
C(95X)-C(96X)-C(97)-C(98)	-76.4(14)
C(91X)-C(96X)-C(97)-C(9C)	-90.2(12)
C(95X)-C(96X)-C(97)-C(9C)	97.0(10)
F(10)-B(10)-C(101)-C(106)	44.0(11)
C(111)-B(10)-C(101)-C(106)	-71.4(10)
C(121)-B(10)-C(101)-C(106)	159.3(7)
F(10)-B(10)-C(101)-C(102)	-136.0(8)
C(111)-B(10)-C(101)-C(102)	108.5(10)
C(121)-B(10)-C(101)-C(102)	-20.8(12)
C(105)-C(106)-C(107)-C(108)	-81.2(11)
C(101)-C(106)-C(107)-C(108)	96.0(10)
C(105)-C(106)-C(107)-C(10C)	92.0(10)
C(101)-C(106)-C(107)-C(10C)	-90.8(11)
F(10)-B(10)-C(111)-C(112)	-157.8(6)
C(101)-B(10)-C(111)-C(112)	-42.3(10)
C(121)-B(10)-C(111)-C(112)	84.8(10)
F(10)-B(10)-C(111)-C(116)	20.5(11)
C(101)-B(10)-C(111)-C(116)	136.0(8)
C(121)-B(10)-C(111)-C(116)	-96.9(10)
C(115)-C(116)-C(117)-C(118)	64.7(11)
C(111)-C(116)-C(117)-C(118)	-116.5(10)
C(115)-C(116)-C(117)-C(11C)	-119.1(10)
C(111)-C(116)-C(117)-C(11C)	59.7(11)
F(10)-B(10)-C(121)-C(122)	-136.9(8)
C(111)-B(10)-C(121)-C(122)	-19.6(13)
C(101)-B(10)-C(121)-C(122)	107.9(10)
F(10)-B(10)-C(121)-C(126)	49.4(11)
C(111)-B(10)-C(121)-C(126)	166.8(8)
C(101)-B(10)-C(121)-C(126)	-65.7(10)
C(125)-C(126)-C(127)-C(128)	-75.5(11)
C(121)-C(126)-C(127)-C(128)	101.7(12)
C(125)-C(126)-C(127)-C(12C)	103.3(10)
C(121)-C(126)-C(127)-C(12C)	-79.5(11)



View of one of the two trityl cations in crystals of **CPh_3[F-PBB].**



One of the two [F-PBB]$^-$ anions in crystals of **CPh_3[F-PBB]**, viewed down the F-B bond.