2-(4-(Dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide

Supplementary material

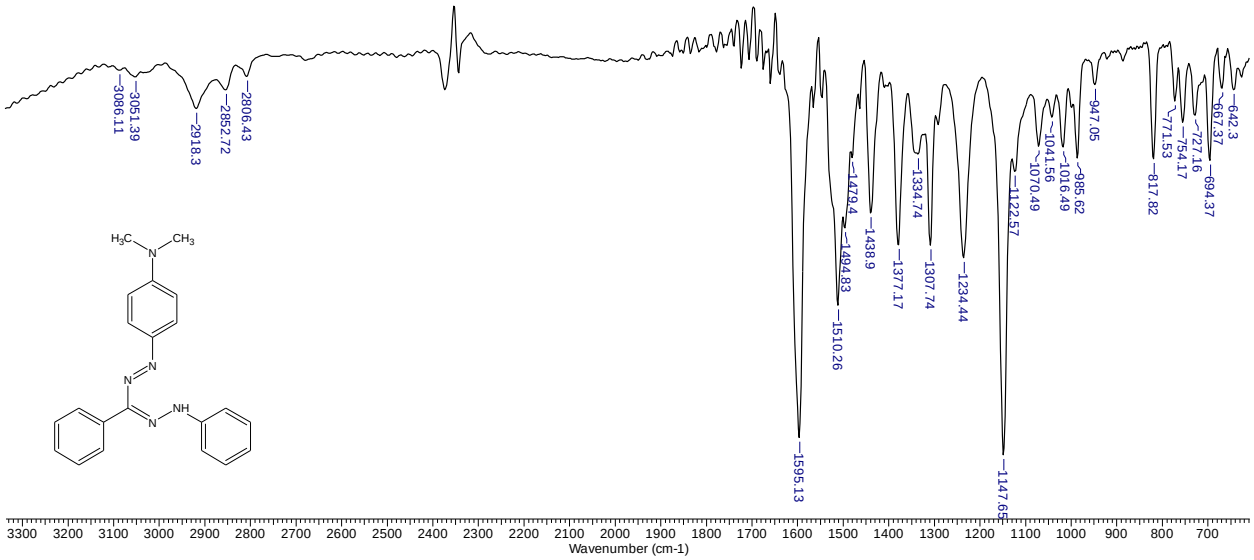

Figure S1. IR-spectrum 1-(4-(dimethylamino)phenyl)-3,5-diphenylformazan **17**

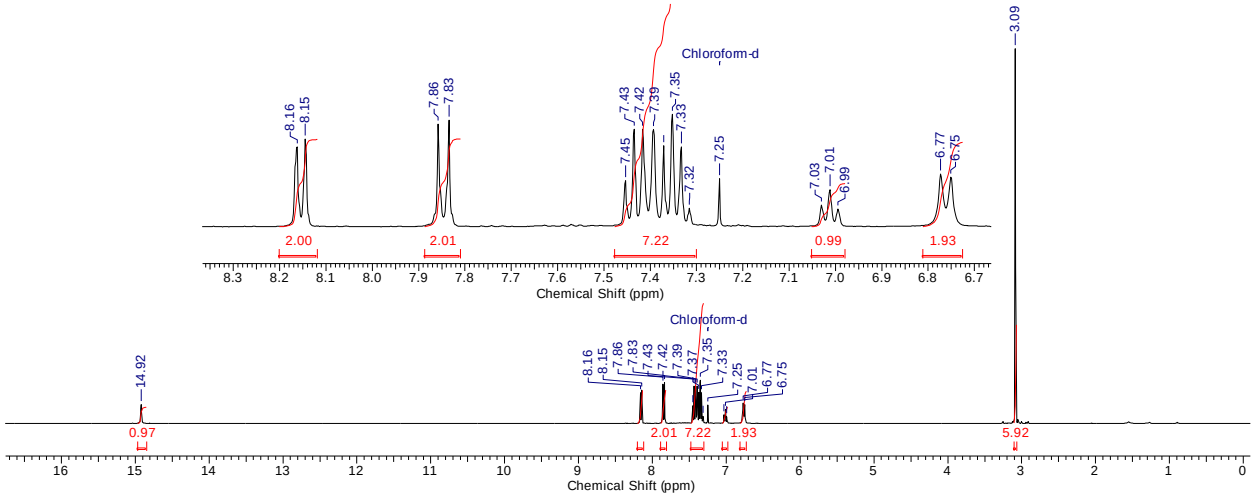

Figure S2.^{1}H NMR 1-(4-(dimethylamino)phenyl)-3,5-diphenylformazan **17**

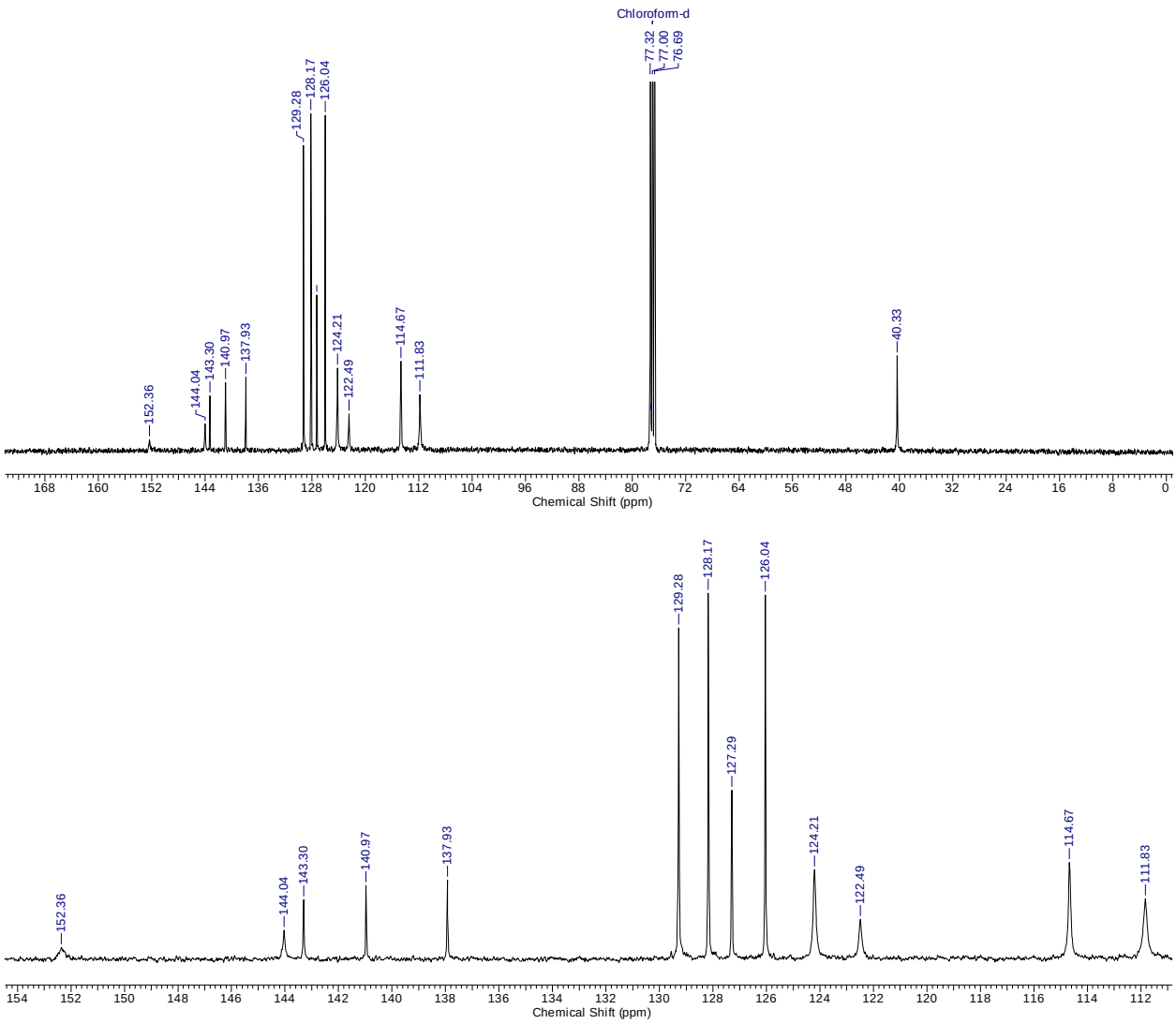

Figure S3.^{13}C NMR 1-(4-(dimethylamino)phenyl)-3,5-diphenylformazan **17**

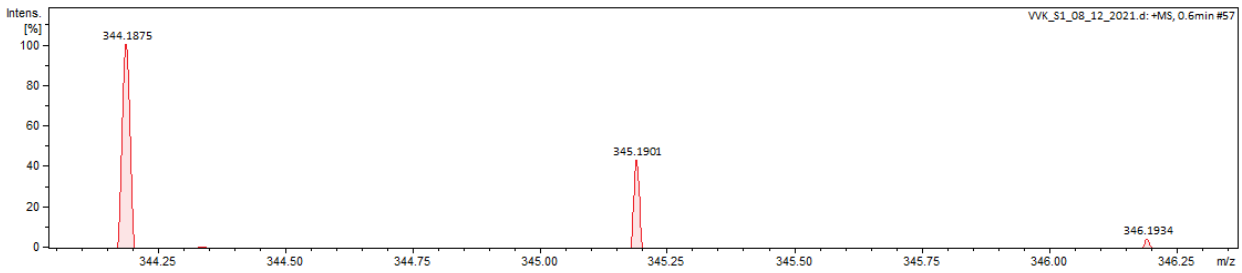

Figure S4. HRMS 1-(4-(dimethylamino)phenyl)-3,5-diphenylformazan **17**

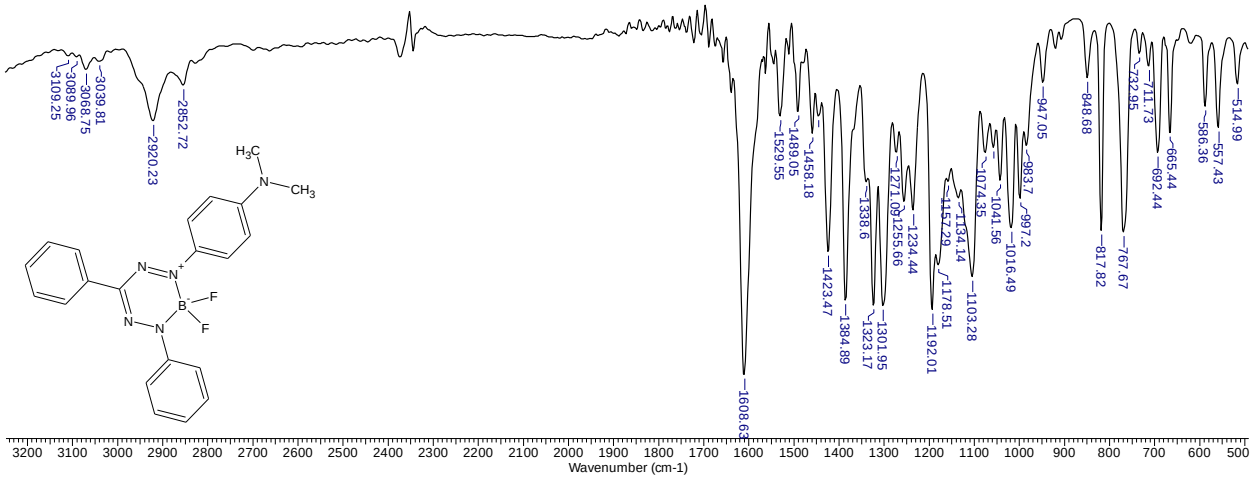

Figure S5. IR-spectrum 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

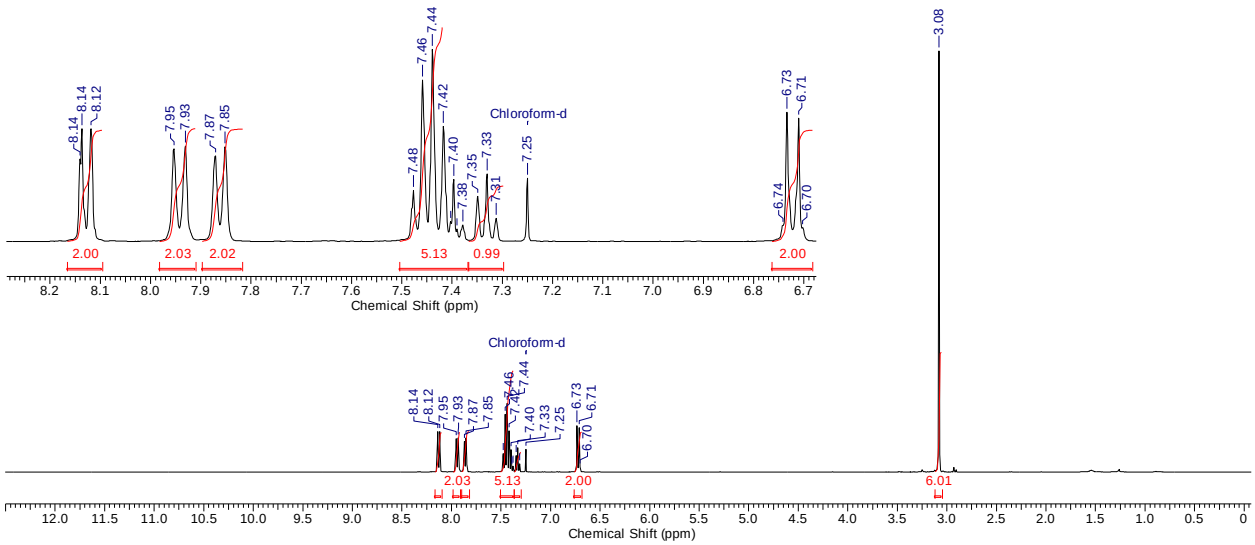

Figure S6. ^{1}H NMR 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

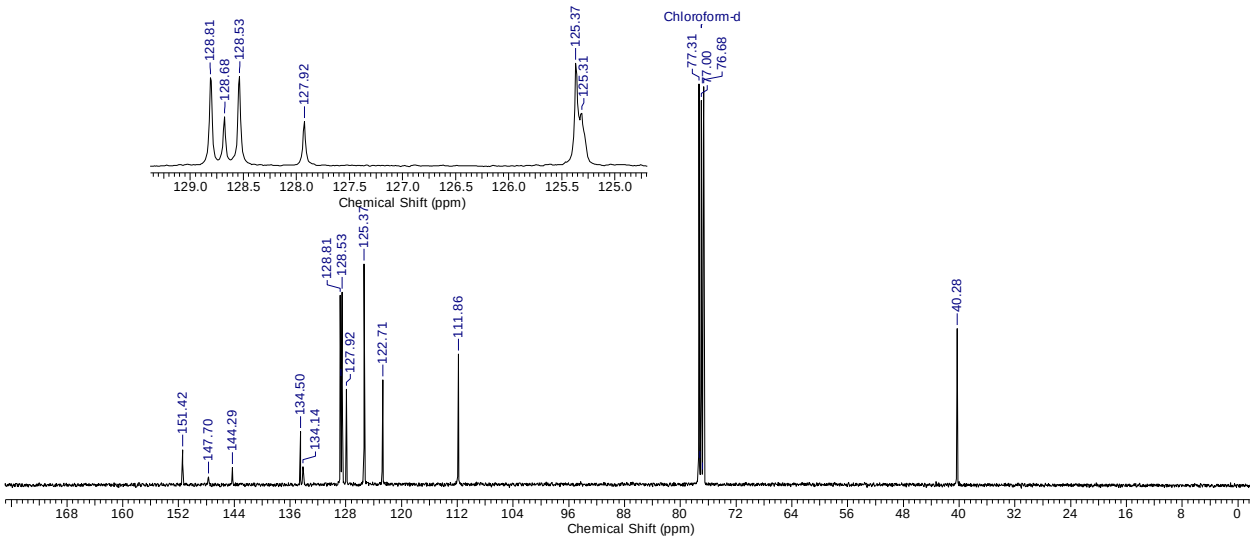

Figure S7. ^{13}C NMR 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

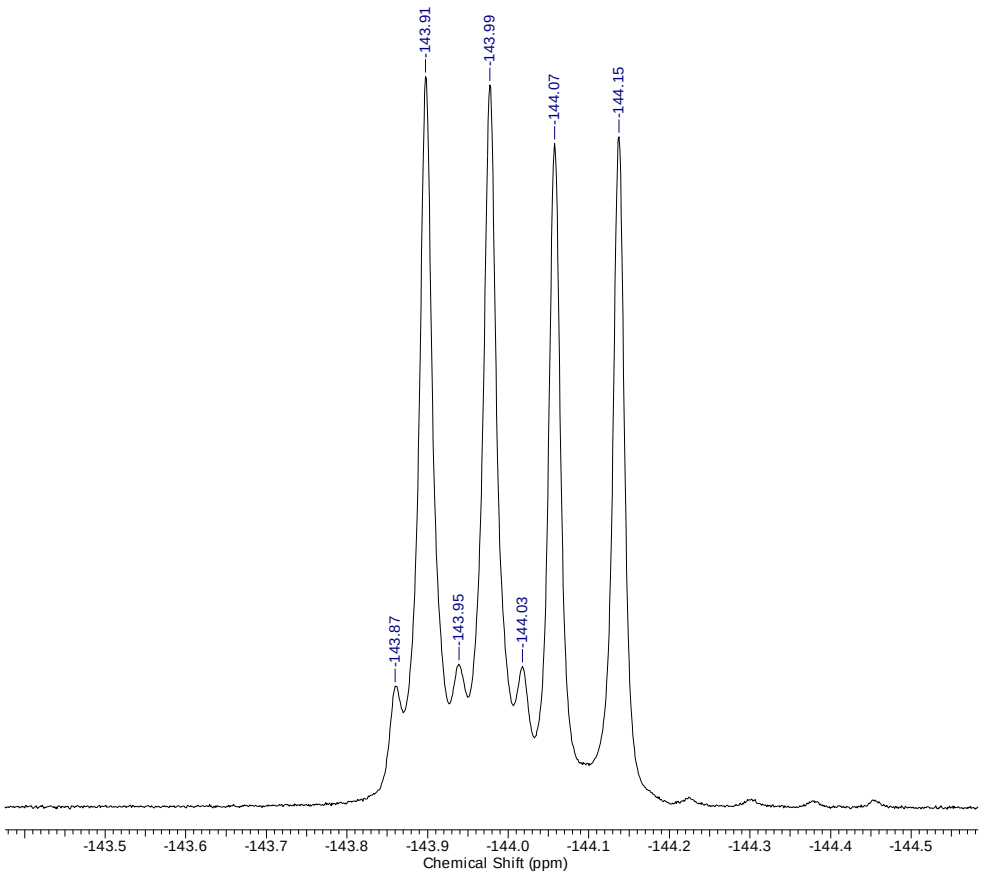

Figure S8. ^{19}F NMR 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

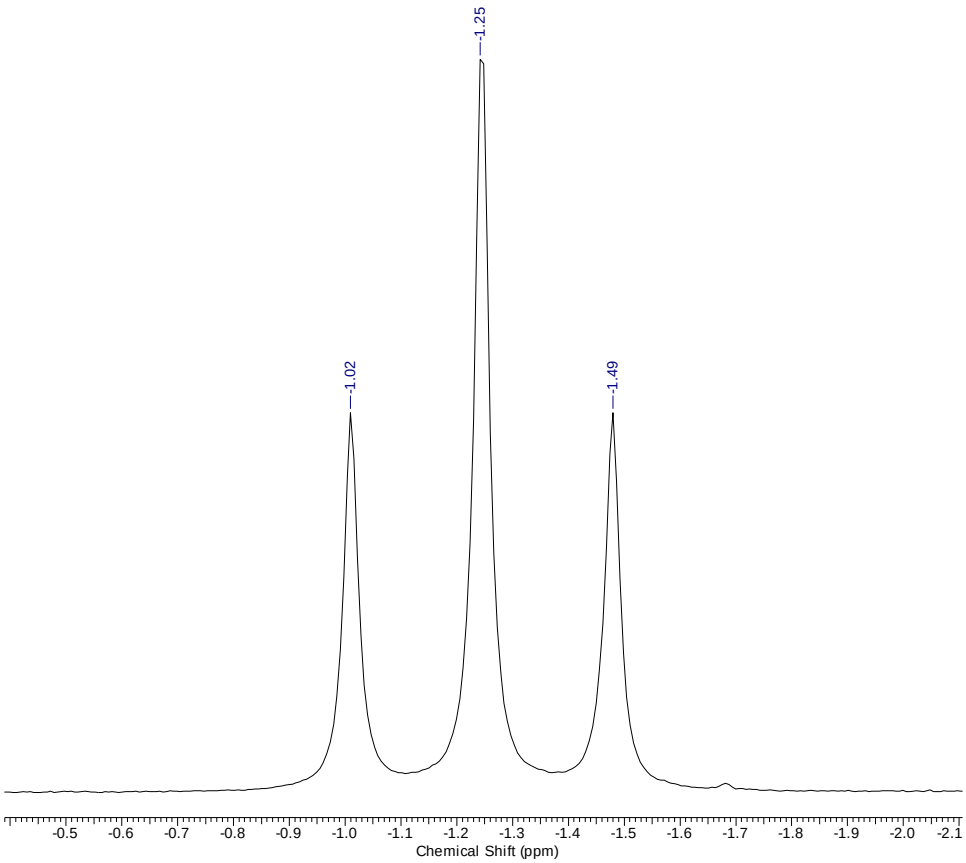

Figure S9. ^{11}B NMR 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

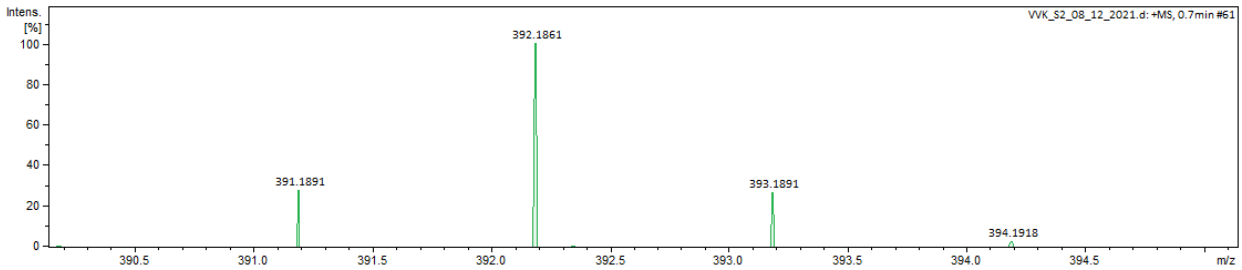

Figure S10. HRMS 2-(4-(dimethylamino)phenyl)-3,3-difluoro-4,6-diphenyl-3,4-dihydro-1,2,4,5,3-tetrazaborinin-2-ium-3-ide **18**

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **18**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	3296.4(7)	5277.7(11)	-1357.7(15)	50.8(4)
F2	3262.7(7)	4264.5(9)	893.8(17)	50.4(4)
N1	3238.8(9)	6072.3(12)	1254.9(19)	28.5(4)
N2	2847.3(9)	6903.0(11)	1155.5(19)	27.9(4)
N3	1782.4(9)	6040.8(11)	-78.1(19)	27.6(4)
N4	2152.1(9)	5175.6(11)	24.0(19)	29.1(4)
N5	5896.0(9)	6405.4(12)	5208(2)	33.5(4)
C1	2166.9(10)	6868.5(14)	332(2)	26.9(4)
C2	3892.2(11)	6111.7(14)	2315(2)	28.9(4)
C3	4504.6(11)	5490.8(15)	2046(2)	30.4(4)
C4	5162.7(11)	5580.7(14)	2999(2)	30.2(5)
C5	5240.2(11)	6287.6(14)	4284(2)	30.4(4)
C6	4608.3(11)	6889.5(15)	4574(3)	34.6(5)
C7	3958.1(11)	6803.4(15)	3607(3)	33.5(5)
C8	6556.0(11)	5827.2(17)	4867(3)	38.8(5)
C9	5970.8(12)	7179.8(15)	6472(3)	39.1(5)
C10	1781.5(10)	7844.2(13)	58(2)	25.1(4)
C11	2047.3(11)	8712.5(14)	850(2)	30.2(4)
C12	1662.6(12)	9614.4(15)	626(3)	33.6(5)
C13	1018.9(12)	9660.0(15)	-389(3)	34.6(5)
C14	760.3(11)	8804.3(14)	-1215(3)	33.6(5)
C15	1143.4(11)	7905.5(14)	-1010(2)	30.1(4)
C16	1686.5(11)	4306.4(14)	-161(2)	29.1(4)
C17	957.0(12)	4339.1(14)	304(2)	32.9(5)
C18	496.4(12)	3515.5(15)	49(3)	37.1(5)
C19	759.9(13)	2650.0(15)	-664(3)	39.1(5)
C20	1486.5(13)	2613.3(15)	-1116(3)	39.7(5)
C21	1957.7(12)	3434.4(15)	-862(3)	36.0(5)
B1	3010.4(13)	5141.5(18)	163(3)	32.9(5)

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **18**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	33.3(7)	86.9(11)	32.8(7)	17.1(7)	6.8(5)	-14.0(7)
F2	58.1(9)	29.9(7)	59.6(9)	17.7(6)	-22.7(7)	-10.6(6)
N1	29.2(9)	26.4(9)	31.0(9)	5.9(7)	10.0(7)	1.1(7)
N2	27.4(9)	23.9(8)	33.7(9)	3.6(7)	12.0(7)	4.2(7)
N3	34.2(9)	21.4(8)	28.1(8)	6.0(7)	8.2(7)	1.1(7)
N4	36.3(9)	23.2(8)	28.4(8)	5.9(7)	5.8(7)	-0.7(7)
N5	30.0(9)	32.7(9)	38.5(10)	3.4(7)	6.2(7)	-0.8(8)
C1	29.6(10)	23.4(10)	29.0(10)	1.5(8)	12.1(8)	2.5(8)
C2	29.4(10)	28.1(10)	30.3(10)	2.7(8)	10.5(8)	3.1(8)
C3	32.2(11)	28.1(10)	31.8(10)	4.2(8)	10.6(9)	-1.1(8)
C4	30.2(11)	28.0(10)	33.7(10)	6.3(8)	11.1(8)	2.0(8)
C5	30.5(11)	27.2(10)	34.5(11)	1.6(8)	9.8(9)	4.7(9)

C6	33.4(11)	32.2(11)	39.2(12)	4.4(9)	9.3(9)	-7.5(9)
C7	28.6(11)	31.4(11)	41.6(12)	6.6(8)	11.0(9)	-3.2(9)
C8	31.6(12)	47.4(13)	37.9(12)	8.8(10)	5.8(9)	-1.1(10)
C9	39.0(12)	34.4(12)	44.0(13)	2.6(9)	2.4(10)	-3.6(10)
C10	27.3(10)	22.6(9)	26.6(9)	0.1(7)	10.5(8)	2.3(8)
C11	32.4(11)	26.2(10)	32.1(10)	-1.6(8)	2.7(8)	2.7(8)
C12	40.3(12)	23.1(10)	37.5(11)	-1.3(8)	4.7(9)	-1.2(9)
C13	39.4(12)	22.9(10)	42.1(12)	5.6(8)	6.2(10)	3.9(9)
C14	33.1(11)	28.9(11)	38.5(11)	2.4(9)	0.3(9)	3.9(9)
C15	33.4(11)	24.6(10)	32.7(10)	-1.8(8)	6.1(9)	-1.9(8)
C16	39.1(11)	21.6(10)	26.5(10)	4.1(8)	3.0(8)	1.9(8)
C17	43.7(12)	22.7(10)	32.9(11)	5.6(9)	6.3(9)	2.7(8)
C18	41.3(12)	28.3(11)	41.8(12)	3.6(9)	4.5(10)	6.8(9)
C19	46.7(13)	23.7(10)	46.1(13)	-0.1(9)	-3.4(10)	3.2(9)
C20	50.4(14)	24.0(10)	44.2(13)	9.0(9)	-0.4(11)	-4.9(9)
C21	42.9(12)	27.1(11)	38.2(12)	7.9(9)	4.9(10)	-3.2(9)
B1	36.2(13)	31.4(12)	31.0(12)	13.3(10)	1.3(10)	-7.1(10)

Table S3 Bond Lengths for 18.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	B1	1.385(3)	C3	C4	1.376(3)
F2	B1	1.375(3)	C4	C5	1.409(3)
N1	N2	1.310(2)	C5	C6	1.421(3)
N1	C2	1.412(3)	C6	C7	1.370(3)
N1	B1	1.565(3)	C10	C11	1.394(3)
N2	C1	1.355(2)	C10	C15	1.395(3)
N3	N4	1.330(2)	C11	C12	1.392(3)
N3	C1	1.332(2)	C12	C13	1.377(3)
N4	C16	1.430(2)	C13	C14	1.389(3)
N4	B1	1.537(3)	C14	C15	1.385(3)
N5	C5	1.364(3)	C16	C17	1.387(3)
N5	C8	1.455(2)	C16	C21	1.396(3)
N5	C9	1.459(3)	C17	C18	1.381(3)
C1	C10	1.482(2)	C18	C19	1.388(3)
C2	C3	1.404(3)	C19	C20	1.379(3)
C2	C7	1.399(3)	C20	C21	1.390(3)

Table S4 Bond Angles for 18.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	N1	N2	115.27(16)	C6	C7	C2	121.04(18)
B1	N1	N2	120.96(16)	C11	C10	C1	121.06(17)
B1	N1	C2	123.64(15)	C15	C10	C1	120.08(17)
C1	N2	N1	117.64(16)	C15	C10	C11	118.87(17)
C1	N3	N4	116.98(16)	C12	C11	C10	120.26(18)
C16	N4	N3	114.18(16)	C13	C12	C11	120.41(19)
B1	N4	N3	121.56(16)	C14	C13	C12	119.73(19)
B1	N4	C16	124.01(16)	C15	C14	C13	120.23(19)
C8	N5	C5	121.14(17)	C14	C15	C10	120.44(18)
C9	N5	C5	120.53(16)	C17	C16	N4	120.06(17)

C9	N5	C8	118.12(17)	C21	C16	N4	120.00(18)
N3	C1	N2	126.00(17)	C21	C16	C17	119.89(19)
C10	C1	N2	116.18(16)	C18	C17	C16	120.01(19)
C10	C1	N3	117.34(17)	C19	C18	C17	120.4(2)
C3	C2	N1	120.62(17)	C20	C19	C18	119.7(2)
C7	C2	N1	120.78(17)	C21	C20	C19	120.59(19)
C7	C2	C3	118.53(18)	C20	C21	C16	119.4(2)
C4	C3	C2	120.79(18)	F2	B1	F1	111.64(17)
C5	C4	C3	121.17(18)	N1	B1	F1	107.88(19)
C4	C5	N5	121.82(17)	N1	B1	F2	111.10(17)
C6	C5	N5	120.80(18)	N4	B1	F1	110.99(17)
C6	C5	C4	117.37(18)	N4	B1	F2	110.91(19)
C7	C6	C5	121.06(19)	N4	B1	N1	104.02(15)

Table S5 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **18**.

Atom	*x*	*y*	*z*	U(eq)
H3	4464.8(11)	5013.0(15)	1213(2)	36.4(5)
H4	5563.6(11)	5167.7(14)	2791(2)	36.3(5)
H6	4636.8(11)	7349.2(15)	5434(3)	41.6(6)
H7	3554.0(11)	7211.3(15)	3813(3)	40.2(6)
H8a	6431(2)	5127(2)	4811(18)	58.2(8)
H8b	6734(5)	6039(8)	3837(9)	58.2(8)
H8c	6939(3)	5935(9)	5728(10)	58.2(8)
H9a	5894(8)	7828.0(17)	5975(4)	58.7(8)
H9b	5605(5)	7072(6)	7263(10)	58.7(8)
H9c	6462(3)	7149(7)	7012(12)	58.7(8)
H11	2483.4(11)	8689.2(14)	1531(2)	36.3(5)
H12	1841.2(12)	10189.9(15)	1165(3)	40.3(6)
H13	758.7(12)	10261.5(15)	-520(3)	41.6(6)
H14	328.3(11)	8834.7(14)	-1908(3)	40.3(6)
H15	974.1(11)	7339.3(14)	-1588(2)	36.1(5)
H17	778.0(12)	4915.7(14)	787(2)	39.5(6)
H18	6.8(12)	3540.9(15)	358(3)	44.5(6)
H19	447.8(13)	2097.4(15)	-835(3)	46.9(6)
H20	1662.8(13)	2033.9(15)	-1596(3)	47.6(6)
H21	2449.2(12)	3403.3(15)	-1157(3)	43.2(6)