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X-ray Crystallographic Data

Compound **3**	Triclinic modification **A**	Monoclinic modification **B**
unit cell parameters	a = 5.1110 b = 8.6350 c = 13.7710 →= 96.808 β = 96.563 γ = 95.869	a = 26.6810(10) b = 7.4550(10) c = 12.4780(10) →= 90.000(3) β = 102.903(4) γ = 90.000(3)
standard deviation for C, N	0.003 ❹	0.0025 ❹
formula	$C_{12}H_9N_4F_3$	$C_{12}H_9N_4F_3$
molecular weight	266.196	266.196
units/unit cell	2	8
D (calc), g/cm^3	1.481	1.466
space group	P-1	C2/C
wavelenght ❹(CuKa)	1.54060	1.54060
no reflections	1996 (7.2% weak)	2007 (8.8% weak)
final R value	0.0667	0.0878

A Nonius CAD4 automatic diffractometer was used with CuKa radiation and a graphite monochromator. The structures were solved by direct methods (SHELXS). The parameters were refined by full-matrix least square calculations (SHELXL) with anisotropic displacement parameters for all non-H atoms. In both structural modifications a subsequent difference Fourier map showed all hydrogen atoms. Hydrogen atom parameters were idealized and not refined. The F atoms of the trifluoromethyl group have a rotational disorder and were difficult to refine. The variation of the bond lenghts in the phenyl ring are larger than expected and may be due to effects from the disorder.

MODIFICATION A

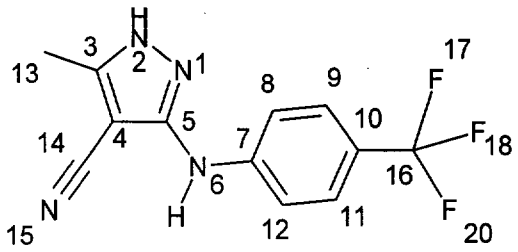

Table 1. Bond lengths in Angstroms

N(1)	-N(2)	1.385(4)	C(9)	-C(10)	1.344(6)
N(1)	-C(5)	1.324(4)	C(10)	-C(11)	1.367(6)
N(2)	-C(3)	1.331(4)	C(10)	-C(16)	1.486(6)
C(3)	-C(4)	1.377(4)	C(11)	-C(12)	1.376(6)
C(3)	-C(13)	1.497(5)	C(14)	-N(15)	1.152(5)
C(4)	-C(5)	1.424(4)	C(16)	-F(17)	1.282(10)
C(4)	-C(14)	1.408(4)	C(16)	-F(18)	1.416(11)
C(5)	-N(6)	1.370(4)	C(16)	-F(19)	1.326(10)
N(6)	-C(7)	1.400(4)	C(16)	-F(20)	1.331(11)
C(7)	-C(8)	1.379(5)	C(16)	-F(21)	1.316(11)
C(7)	-C(12)	1.367(5)	C(16)	-F2(2)	1.198(13)
C(8)	-C(9)	1.394(6)			

Table 2. Bond angles in degrees

C(5)	-N(1)	-N(2)	104.41(24)	N(15)	-C(14)	-C(4)	179.0(4)
C(3)	-N(2)	-N(1)	112.9(3)	F(17)	-C(16)	-C(10)	114.5(5)
C(4)	-C(3)	-N(2)	106.3(3)	F(18)	-C(16)	-C(10)	110.8(5)
C(13)	-C(3)	-N(2)	122.4(3)	F(18)	-C(16)	-F(17)	108.6(7)
C(13)	-C(3)	-C(4)	131.2(3)	F(19)	-C(16)	-C(10)	113.1(5)
C(5)	-C(4)	-C(3)	105.8(3)	F(19)	-C(16)	-F(17)	110.2(7)
C(4)	-C(5)	-N(1)	110.5 (3)	F(19)	-C(16)	-F(18)	98.3(6)
C(14)	-C(4)	-C(3)	126.6(3)	F(20)	-C(16)	-C(10)	112.9(6)
C(14)	-C(4)	-C(5)	127.6(3)	F(20)	-C(16)	-F(17)	80.3(6)
N(6)	-C(5)	-N(1)	125.3(3)	F(20)	-C(16)	-F(18)	125.9(7)
N(6)	-C(5)	-C(4)	124.2(3)	F(20)	-C(16)	-F(19)	34.8(6)
C(7)	-N(6)	-C(5)	128.4(3)	F(21)	-C(16)	-C(10)	114.1(6)
C(8)	-C(7)	-N(6)	124.5(3)	F(21)	-C(16)	-F(17)	27.9(6)
C(12)	-C(7)	-N(6)	117.6(3)	F(21)	-C(16)	-F(18)	83.9(6)
C(12)	-C(7)	-C(8)	117.9(3)	F(21)	-C(16)	-F(19)	128.2(7)
C(9)	-C(8)	-C(7)	120.1(4)	F(21)	-C(16)	-F(20)	105.3(7)
C(10)	-C(9)	-C(8)	121.4(4)	F2(2)	-C(16)	-C(10)	115.2(7)
C(11)	-C(10)	-C(9)	118.6(4)	F2(2)	-C(16)	-F(17)	121.8(8)
C(16)	-C(10)	-C(9)	121.2(4)	F2(2)	-C(16)	-F(18)	24.0(7)
C(16)	-C(10)	-C(11)	120.1(4)	F2(2)	-C(16)	-F(19)	75.0(7)
C(12)	-C(11)	-C(10)	120.9(4)	F2(2)	-C(16)	-F(20)	105.7(8)
C(11)	-C(12)	-C(7)	121.1(4)	F2(2)	-C(16)	-F(21)	102.5(8)

Table 3. Torsion angles in degrees

C(5)	-N(1)	-N(2)	-C(3)	0.7(3)	N(6)	-C(7)	-C(12)	-C(11)	-179.8(4)
N(2)	-N(1)	-C(5)	-C(4)	-0.6(3)	C(8)	-C(7)	-C(12)	-C(11)	-1.2(6)
N(2)	-N(1)	-C(5)	-N(6)	-179.6(3)	C(7)	-C(8)	-C(9)	-C(10)	-0.8(7)
N(1)	-N(2)	-C(3)	-C(4)	-0.3(4)	C(8)	-C(9)	-C(10)	-C(11)	-0.5(7)
N(1)	-N(2)	-C(3)	-C(13)	-179.4(3)	C(8)	-C(9)	-C(10)	-C(16)	179.3(4)
N(2)	-C(3)	-C(4)	-C(5)	0.0(3)	C(9)	-C(10)	-C(11)	-C(12)	1.2(7)
N(2)	-C(3)	-C(4)	-C(14)	-178.9(3)	C(16)	-C(10)	-C(11)	-C(12)	-178.7(4)
C(13)	-C(3)	-C(4)	-C(5)	178.9(4)	C(9)	-C(10)	-C(16)	-F(17)	-22.4(7)
C(13)	-C(3)	-C(4)	-C(14)	0.0(6)	C(9)	-C(10)	-C(16)	-F(18)	100.8(6)
C(3)	-C(4)	-C(5)	-N(1)	0.5(4)	C(9)	-C(10)	-C(16)	-F(19)	-149.8(6)
C(3)	-C(4)	-C(5)	-N(6)	179.6(3)	C(9)	-C(10)	-C(16)	-F(20)	-111.9(6)
C(14)	-C(4)	-C(5)	-N(1)	179.5(3)	C(9)	-C(10)	-C(16)	-F(21)	8.2(8)
C(14)	-C(4)	-C(5)	-N(6)	-1.4(5)	C(9)	-C(10)	-C(16)	-F2(2)	126.4(8)
C(3)	-C(4)	-C(14)	-N(15)	173(19)	C(11)	-C(10)	-C(16)	-F(17)	157.4(6)
C(5)	-C(4)	-C(14)	-N(15)	-4(20)	C(11)	-C(10)	-C(16)	-F(18)	-79.2(6)
N(1)	-C(5)	-N(6)	-C(7)	-8.6(5)	C(11)	-C(10)	-C(16)	-F(19)	30.0(7)
C(4)	-C(5)	-N(6)	-C(7)	172.4(3)	C(11)	-C(10)	-C(16)	-F(20)	67.9(7)
C(5)	-N(6)	-C(7)	-C(8)	2.8(5)	C(11)	-C(10)	-C(16)	-F(21)	-171.8(6)
C(5)	-N(6)	-C(7)	-C(12)	-178.6(3)	C(11)	-C(10)	-C(16)	-F2(2)	-53.6(8)
N(6)	-C(7)	-C(8)	-C(9)	-179.6(4)	C(10)	-C(11)	-C(12)	-C(7)	-0.1(7)
C(12)	-C(7)	-C(8)	-C(9)	1.8(6)					

Table 4. Fractional Coordinates of atoms with Standard Deviations

	x	y	z	Ueq
N(1)	-0.2312(5)	0.1267(3)	0.03107(18)	0.0543(15)
N(2)	-0.3409(6)	0.0997(3)	-0.06702(18)	0.0594(16)
C(3)	-0.2043(7)	0.1818(4)	-0.12446(22)	0.0558(19)
C(4)	0.0054(6)	0.2687(3)	-0.06359(22)	0.0505(18)
C(5)	-0.0211(6)	0.2308(3)	0.03293(21)	0.0473(17)
N(6)	0.1507(6)	0.2924(3)	0.11536(18)	0.0550(15)
C(7)	0.1268(7)	0.2761(3)	0.21399(21)	0.0510(18)
C(8)	-0.0784(9)	0.1861(6)	0.2450(3)	0.085(3)
C(9)	-0.0845(10)	0.1782(6)	0.3452(3)	0.088(3)
C(10)	0.1086(8)	0.2555(4)	0.4134(3)	0.0661(22)
C(11)	0.3152(10)	0.3419(6)	0.3826(3)	0.092(3)
C(12)	0.3238(9)	0.3523(5)	0.2841(3)	0.083(3)
C(13)	-0.2867(10)	0.1727(5)	-0.23302(24)	0.0836(24)
C(14)	0.2013(7)	0.3750(4)	-0.09178(22)	0.0545(19)
N(15)	0.3632(7)	0.4627(4)	-0.11337(24)	0.0775(21)
C(16)	0.1001(11)	0.2483(6)	0.5203(3)	0.087(3)
F(17)	-0.1321(17)	0.2121(12)	0.5435(6)	0.128(3)
F(18)	0.2689(24)	0.1410(9)	0.5549(7)	0.139(3)
F(19)	0.2176(19)	0.3774(11)	0.5768(5)	0.127(3)
F(20)	0.0632(24)	0.3850(11)	0.5694(6)	0.143(3)
F(21)	-0.0900(22)	0.1462(9)	0.5396(7)	0.125(3)
F(22)	0.2941(24)	0.2090(14)	0.5635(8)	0.152(3)

Table 5. Fractional Coordinates of hydrogens with Standard Deviations
# indicates AFIXed atom, * indicates DFIXed atom

	x	y	z	Uiso	
H(2A)	-0.5185(6)	0.0205(3)	-0.09407(18)	0.0534(16)	#
H(6A)	0.3276(6)	0.3626(3)	0.10259(18)	0.0536(15)	#
H(8A)	-0.2344(9)	0.1215(6)	0.1916(3)	0.055(3)	#
H(9A)	-0.2478(10)	0.1085(6)	0.3686(3)	0.062(3)	#
H(11A)	0.4738(10)	0.4030(6)	0.4364(3)	0.057(3)	#
H(12A)	0.4890(9)	0.4216(5)	0.2617(3)	0.059(3)	#
H(13A)	-0.1473(10)	0.2487(5)	-0.26428(24)	0.056(3)	#
H(13B)	-0.4821(10)	0.2094(5)	-0.24576(24)	0.056(3)	#
H(13C)	-0.2903(10)	0.0532(5)	-0.26735(24)	0.056(3)	#

Table 6. Anisotropic temperature factors with Standard Deviations

	U11	U22	U33	U23	U13	U12
N(1)	0.0533(15)	0.0662(16)	0.0390(14)	0.0113(11)	0.0056(12)	-0.0177(13)
N(2)	0.0570(16)	0.0744(17)	0.0422(15)	0.0135(12)	0.0066(12)	-0.0199(14)
C(3)	0.0590(20)	0.0636 (18)	0.0421(16)	0.0126(14)	0.0108(15)	-0.0074(17)
C(4)	0.0473(18)	0.0575(17)	0.0447(17)	0.0137(14)	0.0112(14)	-0.0051(15)
C(5)	0.0433(16)	0.0535(16)	0.0428(16)	0.0093(13)	0.0095(13)	-0.0037(14)
N(6)	0.0524(15)	0.0659(16)	0.0429(14)	0.0127(12)	0.0069(12)	-0.0151(13)
C(7)	0.0547(19)	0.0540(16)	0.0416(16)	0.0100(13)	0.0066(14)	-0.0041(15)
C(8)	0.087(3)	0.117(3)	0.0412(18)	0.0156(19)	0.0039(19)	-0.044(3)
C(9)	0.097(3)	0.112(3)	0.0485(21)	0.0238(21)	0.0074(21)	-0.038(3)
C(10)	0.082(3)	0.0683(20)	0.0438(18)	0.0095(16)	0.0055(18)	-0.0039(20)
C(11)	0.101(3)	0.115(3)	0.0498(20)	0.0071(21)	-0.0013(22)	-0.040(3)
C(12)	0.092(3)	0.098(3)	0.0496(21)	0.0119(20)	0.0037(20)	-0.0418(24)
C(13)	0.116(3)	0.090(3)	0.0397(18)	0.0161(18)	0.0090(21)	-0.011(3)
C(14)	0.0562(19)	0.0598(18)	0.0450(18)	0.0115(14)	0.0097(15)	-0.0032(17)
N(15)	0.0756(21)	0.0833(21)	0.0697(20)	0.0239(16)	0.0199(17)	-0.0236(18)
C(16)	0.102(3)	0.102(3)	0.0518(22)	0.0189(22)	0.0041(24)	-0.011(3)
F(17)	0.105(3)	0.228(3)	0.042(3)	0.021(4)	0.019(3)	-0.025(3)
F(18)	0.203(3)	0.135(3)	0.075(4)	0.063(3)	-0.009(3)	0.014(3)
F(19)	0.190(3)	0.124(3)	0.051(3)	-0.010(3)	0.014(3)	-0.067(3)
F(20)	0.248(3)	0.115(3)	0.063(3)	-0.001(3)	0.050(3)	0.036(3)
F(21)	0.170(3)	0.134(3)	0.067(3)	0.027(3)	0.039(3)	-0.021(3)
F2(2)	0.157(3)	0.220(3)	0.080(3)	0.070(3)	0.009(3)	0.045(3)

MODIFICATION B

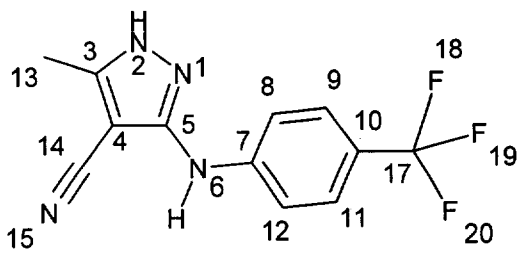

Table 1. Bond lengths in Angstroms

N(1)	-N(2)	1.373(3)	C(7)	-C(12)	1.396(4)
N(1)	-C(5)	1.320(3)	C(8)	-C(9)	1.378(4)
N(2)	-C(3)	1.344(3)	C(9)	-C(10)	1.381(4)
C(3)	-C(4)	1.384(4)	C(10)	-C(11)	1.380(4)
C(3)	-C(13)	1.482(4)	C(10)	-C(16)	1.492(4)
C(4)	-C(5)	1.421(3)	C(11)	-C(12)	1.376(4)
C(4)	-C(14)	1.416(4)	C(14)	-N(15)	1.138(4)
C(5)	-N(6)	1.392(3)	C(16)	-F(18)	1.322(4)
N(6)	-C(7)	1.377(3)	C(16)	-F(19)	1.339(4)
C(7)	-C(8)	1.416(4)	C(16)	-F1(7)	1.331(4)

Table 2. Bond angles in degrees

C(5)	-N(1)	-N(2)	104.19(21)	C(9)	-C(8)	-C(7)	120.8(3)
C(3)	-N(2)	-N(1)	113.60(22)	C(10)	-C(9)	-C(8)	120.1(3)
C(4)	-C(3)	-N(2)	105.37(22)	C(11)	-C(10)	-C(9)	119.9(3)
C(13)	-C(3)	-N(2)	123.23(24)	C(16)	-C(10)	-C(9)	118.8(3)
C(13)	-C(3)	-C(4)	131.40(24)	C(16)	-C(10)	-C(11)	121.4(3)
C(5)	-C(4)	-C(3)	105.65(21)	C(12)	-C(11)	-C(10)	120.8(3)
C(4)	-C(5)	-N(1)	111.19(22)	C(11)	-C(12)	-C(7)	120.7(3)
C(14)	-C(4)	-C(3)	126.10(24)	N(15)	-C(14)	-C(4)	178.9(3)
C(14)	-C(4)	-C(5)	128.23(23)	F(18)	-C(16)	-C(10)	113.4(3)
N(6)	-C(5)	-N(1)	124.44(23)	F(19)	-C(16)	-C(10)	112.2(3)
N(6)	-C(5)	-C(4)	124.37(22)	F(19)	-C(16)	-F(18)	106.2(3)
C(7)	-N(6)	-C(5)	128.33(23)	F1(7)	-C(16)	-C(10)	113.0(3)
C(8)	-C(7)	-N(6)	116.16(23)	F1(7)	-C(16)	-F(18)	106.1(3)
C(12)	-C(7)	-N(6)	126.11(24)	F1(7)	-C(16)	-F(19)	105.3(3)
C(12)	-C(7)	-C(8)	117.72(24)				

Table 3. Torsion angles in degrees

C(5)	-N(1)	-N(2)	-C(3)	0.5(3)	C(5)	-N(6)	-C(7)	-C(12)	8.8(4)
N(2)	-N(1)	-C(5)	-C(4)	0.0(3)	N(6)	-C(7)	-C(8)	-C(9)	-179.7(3)
N(2)	-N(1)	-C(5)	-N(6)	179.45(23)	C(12)	-C(7)	-C(8)	-C(9)	-0.6(4)
N(1)	-N(2)	-C(3)	-C(4)	-0.6(3)	N(6)	-C(7)	-C(12)	-C(11)	180.0(3)
N(1)	-N(2)	-C(3)	-C(13)	-179.63(24)	C(8)	-C(7)	-C(12)	-C(11)	1.1(4)
N(2)	-C(3)	-C(4)	-C(5)	0.6(3)	C(7)	-C(8)	-C(9)	-C(10)	0.4(4)
N(2)	-C(3)	-C(4)	-C(14)	178.9(3)	C(8)	-C(9)	-C(10)	-C(11)	-0.3(4)
C(13)	-C(3)	-C(4)	-C(5)	179.4(3)	C(8)	-C(9)	-C(10)	-C(16)	-179.2(3)
C(13)	-C(3)	-C(4)	-C(14)	-2.1(5)	C(9)	-C(10)	-C(11)	-C(12)	0.8(4)
C(3)	-C(4)	-C(5)	-N(1)	-0.2(3)	C(16)	-C(10)	-C(11)	-C(12)	179.5(3)
C(3)	-C(4)	-C(5)	-N(6)	-179.83(24)	C(9)	-C(10)	-C(16)	-F(18)	51.6(4)
C(14)	-C(4)	-C(5)	-N(1)	-178.5(3)	C(9)	-C(10)	-C(16)	-F(19)	-68.6(4)
C(14)	-C(4)	-C(5)	-N(6)	1.8(4)	C(9)	-C(10)	-C(16)	-F1(7)	172.4(3)
C(3)	-C(4)	-C(14)	-N(15)	-147(15)	C(11)	-C(10)	-C(16)	-F(18)	-127.1(3)
C(5)	-C(4)	-C(14)	-N(15)	30(15)	C(11)	-C(10)	-C(16)	-F(19)	112.5(3)
N(1)	-C(5)	-N(6)	-C(7)	3.9(4)	C(11)	-C(10)	-C(16)	-F1(7)	-6.3(4)
C(4)	-C(5)	-N(6)	-C(7)	-176.66(25)	C(10)	-C(11)	-C(12)	-C(7)	-1.0(4)
C(5)	-N(6)	-C(7)	-C(8)	-172.32(25)					

Table 4. Fractional Coordinates of atoms with Standard Deviations

	x	y	z	Ueq
N(1)	0.48657(8)	0.2231(3)	0.87111(18)	0.0488(15)
N(2)	0.53609(8)	0.2675(3)	0.86731(18)	0.0511(15)
C(3)	0.56610(9)	0.3062(4)	0.96626(20)	0.0424(16)
C(4)	0.53461(9)	0.2886(3)	1.04006(20)	0.0388(15)
C(5)	0.48580(9)	0.2363(3)	0.97625(20)	0.0379(15)
N(6)	0.44270(9)	0.2044(3)	1.01897(18)	0.0464(15)
C(7)	0.39485(10)	0.1456(3)	0.96460(20)	0.0414(15)
C(8)	0.35612(10)	0.1463(4)	1.02589(22)	0.0481(16)
C(9)	0.30695(11)	0.0893(4)	0.9793(3)	0.0510(17)
C(10)	0.29495(10)	0.0294(3)	0.87187(24)	0.0467(17)
C(11)	0.33222(11)	0.0278(4)	0.81099(23)	0.0496(17)
C(12)	0.38157(10)	0.0834(4)	0.85639(21)	0.0452(16)
C(13)	0.62085(10)	0.3586(4)	0.98234(24)	0.0554(18)
C(14)	0.54948(10)	0.3134(4)	1.15534(23)	0.0473(16)
N(15)	0.56085(10)	0.3312(5)	1.24816(20)	0.0682(19)
C(16)	0.24121(11)	-0.0291(4)	0.8234(3)	0.0602(20)
F(18)	0.20620(8)	0.0903(4)	0.8351(3)	0.1118(20)
F(19)	0.22901(9)	-0.1810(4)	0.86893(22)	0.1069(20)
F(17)	0.23296(8)	-0.0632(4)	0.71623(19)	0.0916(18)

Table 5. Fractional Coordinates of hydrogens with Standard Deviations
# indicates AFIXed atom, * indicates DFIXed atom

	x	y	z	Uiso
H(2A)	0.54967(8)	0.2714(3)	0.79205(18)	0.0535(14) #
H(6A)	0.44729(9)	0.2297(3)	1.10585(18)	0.0576(15) #
H(8A)	0.36520(10)	0.1912(4)	1.11030(22)	0.0532(15) #
H(9A)	0.27778(11)	0.0916(4)	1.0270(3)	0.0513(16) #
H(11A)	0.32271(11)	-0.0173(4)	0.72664(23)	0.0512(16) #
H(12A)	0.41033(10)	0.0794(4)	0.80775(21)	0.0584(16) #
H(13A)	0.63656(10)	0.3823(4)	1.06870(24)	0.0598(17) #
H(13B)	0.62379(10)	0.4797(4)	0.93658(24)	0.0598(17) #
H(13C)	0.64211(10)	0.2523(4)	0.95383(24)	0.0598(17) #

Table 6. Anisotropic temprature factors with Standard Deviations

	U11	U22	U33	U23	U13	U12
N(1)	0.0522(14)	0.0698(16)	0.0245(13)	0.0035(10)	0.0182(10)	-0.0012(10)
N(2)	0.0524(14)	0.0736(17)	0.0274(14)	0.0073(10)	0.0181(10)	-0.0013(11)
C(3)	0.0507(15)	0.0443(14)	0.0316(16)	0.0063(10)	0.0152(12)	0.0043(10)
C(4)	0.0556(15)	0.0401(14)	0.0206(14)	0.0049(9)	0.0163(11)	0.0050(10)
C(5)	0.0486(15)	0.0410(14)	0.0240(15)	0.0040(10)	0.0160(11)	0.0041(10)
N(6)	0.0567(15)	0.0596(15)	0.0233(13)	-0.0016(9)	0.0195(10)	-0.0009(10)
C(7)	0.0546(15)	0.0387(14)	0.0309(14)	0.0021(10)	0.0194(11)	0.0034(10)
C(8)	0.0558(15)	0.0538(16)	0.0358(15)	-0.0058(12)	0.0253(12)	-0.0031(12)
C(9)	0.0578(16)	0.0517(16)	0.0441(17)	-0.0017(12)	0.0257(13)	-0.0007(11)
C(10)	0.0531(16)	0.0394(14)	0.0467(18)	-0.0048(12)	0.0178(12)	0.0006(11)
C(11)	0.0606(16)	0.0517(16)	0.0350(16)	-0.0094(12)	0.0152(12)	-0.0006(12)
C(12)	0.0521(16)	0.0527(16)	0.0311(15)	-0.0049(11)	0.0203(11)	0.0040(11)
C(13)	0.0569(17)	0.0611(18)	0.0477(18)	0.0105(14)	0.0215(13)	-0.0003(14)
C(14)	0.0467(14)	0.0597(16)	0.0340(17)	0.0039(12)	0.0113(11)	0.0013(11)
N(15)	0.0714(16)	0.1018(23)	0.0294(16)	-0.0073(14)	0.0140(12)	-0.0023(15)
C(16)	0.0578(18)	0.0596(19)	0.0621(21)	-0.0106(15)	0.0222(14)	-0.0074(14)
F(18)	0.0540(13)	0.1182(21)	0.157(3)	-0.0604(18)	0.0200(12)	0.0065(11)
F(19)	0.0964(18)	0.1046(20)	0.1130(21)	0.0130(16)	0.0186(14)	-0.0481(14)
F1(7)	0.0789(15)	0.1263(21)	0.0646(15)	-0.0293(13)	0.0111(11)	-0.0233(12)