

Fractional atomic coordinates for C₁₆H₁₄F₃NO

Atom	x/a	y/b	z/c	U(equiv)
N(1)	-0.6645(3)	0.7013(1)	-0.2039(3)	0.0507
C(2)	-0.6151(4)	0.65457(12)	-0.1551(3)	0.0437
C(3)	-0.5144(4)	0.63807(12)	-0.2358(3)	0.0427
C(4)	-0.5668(4)	0.66973(12)	-0.3485(3)	0.0442
C(5)	-0.5368(4)	0.66851(14)	-0.4617(4)	0.0588
C(6)	-0.5948(5)	0.70359(18)	-0.5480(4)	0.0708
C(7)	-0.6800(5)	0.73901(16)	-0.5208(4)	0.0740
C(8)	-0.7117(5)	0.74067(13)	-0.4085(4)	0.0620
C(9)	-0.6532(4)	0.70568(12)	-0.3225(3)	0.0455
C(10)	-0.5370(4)	0.65461(12)	-0.0153(3)	0.0421
C(11)	-0.5491(4)	0.61663(13)	0.0565(3)	0.0546
C(12)	-0.4749(5)	0.61723(16)	0.1856(4)	0.0667
C(13)	-0.3911(5)	0.65547(18)	0.2422(3)	0.0662
C(14)	-0.3804(5)	0.69362(15)	0.1707(3)	0.0612
C(15)	-0.4524(4)	0.69305(13)	0.0430(3)	0.0532
C(16)	-0.7881(5)	0.72296(16)	-0.1695(4)	0.0668
O(17)	-0.3556(3)	0.6446(1)	-0.1771(2)	0.0587
C(18)	-0.5418(5)	0.58696(14)	-0.2707(4)	0.0584
F(19)	-0.5036(3)	0.55945(8)	-0.1691(2)	0.0837
F(20)	-0.4590(3)	0.57203(9)	-0.3414(3)	0.0865
F(21)	-0.6865(3)	0.57734(8)	-0.3344(2)	0.0761
N(101)	0.1404(4)	0.5556(1)	0.2410(3)	0.0537
C(102)	0.0889(4)	0.60205(11)	0.2612(3)	0.0440
C(103)	-0.0052(4)	0.61882(11)	0.1259(3)	0.0413
C(104)	0.0557(4)	0.58768(11)	0.0446(3)	0.0422
C(105)	0.0279(4)	0.58843(13)	-0.0843(3)	0.0521
C(106)	0.0915(5)	0.55324(15)	-0.1376(4)	0.0612
C(107)	0.1770(5)	0.51841(14)	-0.0629(4)	0.0613
C(108)	0.2019(4)	0.51660(12)	0.0645(4)	0.0555
C(109)	0.1390(4)	0.55175(11)	0.1177(3)	0.0463
C(110)	0.0055(4)	0.60178(12)	0.3578(3)	0.0474
C(111)	0.0256(5)	0.63802(14)	0.4434(4)	0.0608
C(112)	-0.0465(6)	0.63650(19)	0.5342(4)	0.0776
C(113)	-0.1411(6)	0.5999(2)	0.5392(4)	0.0854
C(114)	-0.1613(6)	0.56461(19)	0.4543(5)	0.0822
C(115)	-0.0888(5)	0.56484(15)	0.3634(4)	0.0666
C(116)	0.2622(5)	0.53467(16)	0.3426(4)	0.0759
O(117)	-0.1657(2)	0.61156(8)	0.0934(2)	0.0489
C(118)	0.0209(4)	0.67025(12)	0.1087(3)	0.0516
F(119)	-0.0220(3)	0.69645(8)	0.1907(2)	0.0719
F(120)	-0.0557(3)	0.68569(8)	-0.0049(2)	0.0722
F(121)	0.1678(3)	0.68034(7)	0.1281(2)	0.0679

Fractional atomic coordinates for C₁₆H₁₄F₃NO

Atom	x/a	y/b	z/c	U(iso)
H(16)	-0.8100	0.7547	-0.2091	0.087(3)
H(17)	-0.7579	0.7262	-0.0763	0.087(3)
H(18)	-0.8821	0.7032	-0.2003	0.087(3)
H(21)	-0.7013	0.6322	-0.1636	0.087(3)
H(51)	-0.4746	0.6427	-0.4807	0.087(3)
H(61)	-0.5749	0.7031	-0.6304	0.087(3)
H(71)	-0.7203	0.7644	-0.5841	0.087(3)
H(81)	-0.7745	0.7665	-0.3905	0.087(3)
H(111)	-0.6106	0.5887	0.0161	0.087(3)
H(121)	-0.4831	0.5896	0.2377	0.087(3)
H(131)	-0.3374	0.6555	0.3349	0.087(3)
H(141)	-0.3203	0.7217	0.2115	0.087(3)
H(151)	-0.4437	0.7208	-0.0086	0.087(3)
H(116)	0.2873	0.5031	0.3167	0.087(3)
H(117)	0.3559	0.5550	0.3622	0.087(3)
H(118)	0.2300	0.5319	0.4189	0.087(3)
H(1021)	0.1733	0.6248	0.3001	0.087(3)
H(1051)	-0.0363	0.6136	-0.1378	0.087(3)
H(1061)	0.0755	0.5533	-0.2299	0.087(3)
H(1071)	0.2226	0.4936	-0.1025	0.087(3)
H(1081)	0.2634	0.4909	0.1170	0.087(3)
H(1111)	0.0922	0.6652	0.4397	0.087(3)
H(1121)	-0.0295	0.6624	0.5971	0.087(3)
H(1131)	-0.1944	0.5993	0.6041	0.087(3)
H(1141)	-0.2303	0.5379	0.4571	0.087(3)
H(1151)	-0.1041	0.5383	0.3025	0.087(3)

Anisotropic thermal parameters for C₁₆H₁₄F₃NO

Atom	u(11)	u(22)	u(33)	u(23)	u(13)	u(12)
N(1)	0.0522(18)	0.0551(19)	0.0441(17)	0.0025(13)	0.0143(13)	0.0165(14)
C(2)	0.0407(19)	0.048(2)	0.0413(18)	0.0018(15)	0.0114(15)	0.0003(15)
C(3)	0.0344(18)	0.051(2)	0.0407(19)	-0.0002(15)	0.0098(14)	0.0042(14)
C(4)	0.0398(19)	0.053(2)	0.0401(19)	-0.0005(15)	0.0125(16)	-0.0024(15)
C(5)	0.049(2)	0.078(3)	0.050(2)	0.001(2)	0.0162(18)	-0.0025(19)
C(6)	0.068(3)	0.097(4)	0.046(2)	0.013(2)	0.017(2)	-0.006(3)
C(7)	0.082(3)	0.076(3)	0.052(3)	0.020(2)	0.005(2)	-0.001(3)
C(8)	0.072(3)	0.053(2)	0.051(2)	0.0071(19)	0.006(2)	0.0096(19)
C(9)	0.043(2)	0.046(2)	0.039(2)	0.0013(15)	0.0019(15)	-0.0007(15)
C(10)	0.0372(18)	0.047(2)	0.0416(18)	0.0026(15)	0.0122(15)	0.0052(14)
C(11)	0.047(2)	0.063(2)	0.054(2)	0.0076(18)	0.0153(18)	-0.0058(18)
C(12)	0.056(2)	0.092(3)	0.054(2)	0.026(2)	0.020(2)	0.008(2)
C(13)	0.061(3)	0.095(3)	0.040(2)	-0.000(2)	0.0140(19)	0.018(2)
C(14)	0.066(3)	0.064(3)	0.049(2)	-0.0101(19)	0.0117(19)	0.004(2)
C(15)	0.060(2)	0.052(2)	0.046(2)	-0.0011(16)	0.0136(18)	0.0036(17)
C(16)	0.063(3)	0.077(3)	0.061(2)	-0.003(2)	0.020(2)	0.025(2)
O(17)	0.0330(13)	0.089(2)	0.0533(15)	0.0027(13)	0.0126(11)	0.0064(12)
C(18)	0.057(3)	0.060(3)	0.061(2)	0.005(2)	0.023(2)	0.0171(19)
F(19)	0.110(2)	0.0568(15)	0.0889(18)	0.0197(13)	0.0380(16)	0.0279(13)
F(20)	0.1030(19)	0.0745(17)	0.0988(19)	-0.0128(14)	0.0557(16)	0.0231(14)
F(21)	0.0770(18)	0.0647(15)	0.0833(17)	-0.0178(12)	0.0207(14)	-0.0095(12)
N(101)	0.065(2)	0.0480(18)	0.0494(19)	0.0068(14)	0.0195(15)	0.0114(15)
C(102)	0.049(2)	0.0360(19)	0.0450(19)	0.0006(14)	0.0126(16)	-0.0028(14)
C(103)	0.0412(18)	0.0410(19)	0.0427(19)	0.0034(14)	0.0147(15)	-0.0007(14)
C(104)	0.0397(19)	0.0393(19)	0.048(2)	-0.0007(15)	0.0150(15)	-0.0073(14)
C(105)	0.050(2)	0.059(2)	0.048(2)	0.0006(17)	0.0162(18)	-0.0060(17)
C(106)	0.063(3)	0.075(3)	0.050(2)	-0.014(2)	0.024(2)	-0.012(2)
C(107)	0.063(3)	0.059(3)	0.069(3)	-0.019(2)	0.031(2)	-0.009(2)
C(108)	0.058(2)	0.041(2)	0.072(3)	-0.0032(17)	0.026(2)	0.0013(17)
C(109)	0.048(2)	0.0381(19)	0.056(2)	0.0018(16)	0.0202(17)	-0.0043(16)
C(110)	0.050(2)	0.047(2)	0.0409(19)	0.0027(15)	0.0082(16)	0.0029(16)
C(111)	0.058(2)	0.068(3)	0.051(2)	-0.0090(19)	0.0097(19)	0.0052(19)
C(112)	0.076(3)	0.104(4)	0.047(2)	-0.010(2)	0.013(2)	0.025(3)
C(113)	0.075(3)	0.137(5)	0.049(3)	0.020(3)	0.025(2)	0.025(3)
C(114)	0.084(3)	0.097(4)	0.071(3)	0.028(3)	0.034(3)	-0.006(3)
C(115)	0.085(3)	0.063(3)	0.057(2)	0.0041(19)	0.030(2)	-0.011(2)
C(116)	0.083(3)	0.080(3)	0.063(3)	0.024(2)	0.021(2)	0.026(2)
O(117)	0.0391(13)	0.0532(14)	0.0526(15)	0.0030(11)	0.0123(11)	-0.000(1)
C(118)	0.047(2)	0.050(2)	0.055(2)	0.0007(18)	0.0124(18)	-0.0011(17)
F(119)	0.0888(17)	0.0464(13)	0.0889(16)	-0.0087(12)	0.0401(14)	0.0015(11)
F(120)	0.0798(16)	0.0581(14)	0.0674(15)	0.0226(11)	0.0078(12)	0.0033(11)
F(121)	0.0596(15)	0.0575(14)	0.0866(16)	0.0059(11)	0.0235(12)	-0.013(1)

Interatomic distances (Å) for C₁₆H₁₄F₃NO

N(1) - C(2)	1.464(4)	N(1) - C(9)	1.375(4)
N(1) - C(16)	1.455(5)	C(2) - C(3)	1.564(4)
C(2) - C(10)	1.504(5)	C(3) - C(4)	1.506(5)
C(3) - O(17)	1.415(4)	C(3) - C(18)	1.516(5)
C(4) - C(5)	1.386(5)	C(4) - C(9)	1.389(5)
C(5) - C(6)	1.381(6)	C(6) - C(7)	1.377(6)
C(7) - C(8)	1.384(6)	C(8) - C(9)	1.377(5)
C(10) - C(11)	1.380(5)	C(10) - C(15)	1.388(5)
C(11) - C(12)	1.392(5)	C(12) - C(13)	1.374(6)
C(13) - C(14)	1.378(6)	C(14) - C(15)	1.375(5)
C(18) - F(19)	1.338(4)	C(18) - F(20)	1.336(4)
C(18) - F(21)	1.328(4)		
N(101) - C(102)	1.456(4)	N(101) - C(109)	1.385(4)
N(101) - C(116)	1.452(5)	C(102) - C(103)	1.566(4)
C(102) - C(110)	1.518(5)	C(103) - C(104)	1.507(5)
C(103) - O(117)	1.424(4)	C(103) - C(118)	1.515(5)
C(104) - C(105)	1.389(5)	C(104) - C(109)	1.387(5)
C(105) - C(106)	1.394(5)	C(106) - C(107)	1.378(6)
C(107) - C(108)	1.376(5)	C(108) - C(109)	1.389(5)
C(110) - C(111)	1.387(5)	C(110) - C(115)	1.384(5)
C(111) - C(112)	1.386(6)	C(112) - C(113)	1.377(7)
C(113) - C(114)	1.362(7)	C(114) - C(115)	1.388(6)
C(118) - F(119)	1.342(4)	C(118) - F(120)	1.322(4)
C(118) - F(121)	1.335(4)		

Bond angles (°) for C₁₆H₁₄F₃NO

C(2) - N(1) - C(9)	109.6(3)	C(2) - N(1) - C(16)	117.9(3)
C(9) - N(1) - C(16)	121.8(3)	N(1) - C(2) - C(3)	103.4(2)
N(1) - C(2) - C(10)	112.3(3)	C(3) - C(2) - C(10)	115.4(3)
C(2) - C(3) - C(4)	102.4(3)	C(2) - C(3) - O(17)	114.2(3)
C(4) - C(3) - O(17)	108.6(3)	C(2) - C(3) - C(18)	111.1(3)
C(4) - C(3) - C(18)	112.5(3)	O(17) - C(3) - C(18)	108.1(3)
C(3) - C(4) - C(5)	130.7(3)	C(3) - C(4) - C(9)	108.8(3)
C(5) - C(4) - C(9)	120.5(3)	C(4) - C(5) - C(6)	118.7(4)
C(5) - C(6) - C(7)	120.1(4)	C(6) - C(7) - C(8)	122.0(4)
C(7) - C(8) - C(9)	117.7(4)	N(1) - C(9) - C(4)	111.2(3)
N(1) - C(9) - C(8)	127.7(3)	C(4) - C(9) - C(8)	121.0(3)
C(2) - C(10) - C(11)	120.6(3)	C(2) - C(10) - C(15)	120.2(3)
C(11) - C(10) - C(15)	119.2(3)	C(10) - C(11) - C(12)	119.7(4)
C(11) - C(12) - C(13)	120.6(4)	C(12) - C(13) - C(14)	119.8(3)
C(13) - C(14) - C(15)	119.8(4)	C(10) - C(15) - C(14)	120.9(4)
C(3) - C(18) - F(19)	111.8(3)	C(3) - C(18) - F(20)	112.5(3)
F(19) - C(18) - F(20)	105.9(3)	C(3) - C(18) - F(21)	113.3(3)
F(19) - C(18) - F(21)	106.5(3)	F(20) - C(18) - F(21)	106.3(3)

C(102) - N(101) - C(109)	109.2(3)	C(102) - N(101) - C(116)	117.6(3)
C(109) - N(101) - C(116)	120.8(3)	N(101) - C(102) - C(103)	103.7(3)
N(101) - C(102) - C(110)	111.8(3)	C(103) - C(102) - C(110)	116.4(3)
C(102) - C(103) - C(104)	102.0(3)	C(102) - C(103) - O(117)	114.4(2)
C(104) - C(103) - O(117)	108.5(3)	C(102) - C(103) - C(118)	111.1(3)
C(104) - C(103) - C(118)	113.2(3)	O(117) - C(103) - C(118)	107.7(3)
C(103) - C(104) - C(105)	130.0(3)	C(103) - C(104) - C(109)	108.9(3)
C(105) - C(104) - C(109)	120.8(3)	C(104) - C(105) - C(106)	118.3(3)
C(105) - C(106) - C(107)	120.0(3)	C(106) - C(107) - C(108)	122.2(3)
C(107) - C(108) - C(109)	117.8(4)	N(101) - C(109) - C(104)	111.1(3)
N(101) - C(109) - C(108)	128.0(3)	C(104) - C(109) - C(108)	120.8(3)
C(102) - C(110) - C(111)	120.4(3)	C(102) - C(110) - C(115)	120.4(3)
C(111) - C(110) - C(115)	119.2(4)	C(110) - C(111) - C(112)	119.8(4)
C(111) - C(112) - C(113)	120.9(4)	C(112) - C(113) - C(114)	118.9(4)
C(113) - C(114) - C(115)	121.4(4)	C(110) - C(115) - C(114)	119.7(4)
C(103) - C(118) - F(119)	111.2(3)	C(103) - C(118) - F(120)	113.0(3)
F(119) - C(118) - F(120)	106.9(3)	C(103) - C(118) - F(121)	112.6(3)
F(119) - C(118) - F(121)	105.9(3)	F(120) - C(118) - F(121)	106.8(3)

Crystal data for C₁₆H₁₄F₃N₁O₁

Formula	C ₁₆ H ₁₄ F ₃ N ₁ O ₁		
Crystal Class	Monoclinic		
Space Group	P 2 ₁ /a		
a (Å)	9.232 (5)	alpha	90
b (Å)	28.647 (19)	beta	108.61 (5)
c (Å)	11.234 (7)	gamma	90
Volume	2816 (3)		
Z	8		
Radiation type	Mo Kα		
Wavelength (Å)	0.710690		
Density	1.38		
M (g.mol ⁻¹)	293.29		
μ (mm ⁻¹)	0.113		
Temperature (K)	295		
Size (mm)	0.6 x 0.4 x 0.3		
Colour	colourless		
Shape	parallelepiped		
Diffractometer	Enraf-Nonius Mach-3		
Scan type	2 Theta/Omega		
Reflections measured	5400		
Independent reflections	4949		
Rint	0.05		
Theta min, max	1 25.00		
Hmin, Hmax	0 10		
Kmin, Kmax	0 34		
Lmin, Lmax	-13 12		
Secondary extinction coefficient	100		
Decay	0.07		
Refinement on F			
R-factor	0.0480	$R = \sum F_o - F_c / \sum F_o $	
Weighted R-factor	0.0593	$R_w = [\sum w (F_o - F_c)^2 / \sum w F_o^2]^{1/2}$	
Delta Rho min (e/Å ³)	-0.76		
Delta Rho max (e/Å ³)	0.68		
Reflections used	2503		
sigma(I) limit	3.00		
Number of parameters	381		
Goodness of fit	1.048		

Weighting scheme of the form $w = w' [1 - (||F_o| - |F_c||) / 6\sigma(F_o)]^2$ with $w' = 1 / \sum_r A_r T_r(X)$ with coefficients 1.55, 0.985 and 0.93 for a Chebychev series for which $X = F_c / F_c(\max)$

