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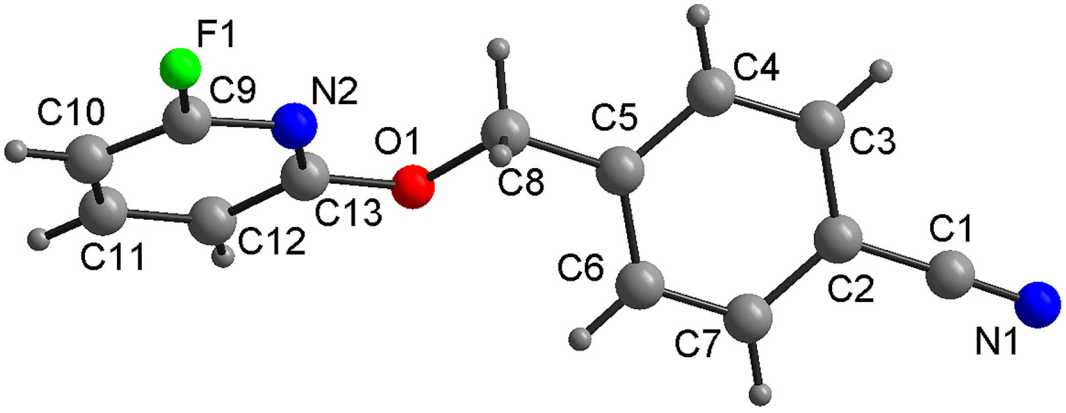
The crystal structure of 4-((6-fluoropyridin-2-yloxy)methyl)benzonitrile, $C_{13}H_9FN_2O$



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Abstract

$C_{13}H_9FN_2O$, triclinic, $P\bar{1}$ (no. 2), a = 7.4664(8) Å, b = 8.2700(7) Å, c = 10.0709(11) Å, α = 76.991(8)°, β = 88.403(9)°, γ = 63.619(10)° V = 540.93(10) Å^3, Z = 2, R_{gt}(F) = 0.0534, w$R_{ref}(F^2)$ = 0.1644, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.29 × 0.25 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.10 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω
θ_{max}, completeness:	29.7°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6733, 2638, 0.040
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1752
$N(param)_{refined}$:	154
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], Olex2 [4]

Source of material

The title compound was prepared according to the synthetic method reported in the literature [5]. The crude product was recrystallized from ethanol to afford crystals suitable for single crystal X-ray diffraction.

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors are U_{iso}(H) = 1.2 times U_{eq}(C, aromatic ring), U_{iso}(H) = 1.2 times U_{eq}(CH_2). The final refinement were performed using geometrical restraints, with C–H = 0.93 Å (aromatic ring), C–H = 0.97 Å (CH_2).

Comment

Both O-alkylation and N-alkylation of 2-pyridone are all an important molecular scaffold for there biological and pharmaceutical properties [6–8]. However, based on the Hard–Soft Acid–Base theory, the softer nitrogen atom will tends to bond the softer carbon atom than oxygen. And, the N-alkylation compound is more thermodynamic stable than O-alkylation. Thus, there are a large amount of methods for N-alkylation for the 2-pyridone moiety, but the absolute selective synthesis of O-alkylation is even rarer. We have

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7909 (3)	0.9542 (2)	0.58876 (17)	0.0581 (4)
C2	0.7672 (2)	0.8284 (2)	0.52019 (15)	0.0481 (4)
C3	0.7570 (2)	0.6697 (2)	0.59588 (16)	0.0520 (4)
H3	0.7621	0.6452	0.6908	0.062*
C4	0.7391 (2)	0.5491 (2)	0.52725 (15)	0.0493 (4)
H4	0.7337	0.4423	0.5772	0.059*
C5	0.7292 (2)	0.5844 (2)	0.38584 (15)	0.0447 (4)
C6	0.7376 (2)	0.7450 (2)	0.31186 (15)	0.0511 (4)
H6	0.7296	0.7712	0.2168	0.061*
C7	0.7578 (2)	0.8649 (2)	0.37889 (16)	0.0532 (4)
H7	0.7651	0.9707	0.3289	0.064*
C8	0.6972 (3)	0.4562 (2)	0.31601 (16)	0.0541 (4)
H8A	0.7392	0.3358	0.3788	0.065*
H8B	0.5559	0.5061	0.2881	0.065*
C9	0.5895 (2)	0.2195 (2)	0.04884 (16)	0.0533 (4)
C10	0.6903 (3)	0.1790 (2)	−0.06295 (18)	0.0593 (4)
H10	0.6582	0.1204	−0.1205	0.071*
C11	0.8433 (3)	0.2299 (2)	−0.08584 (18)	0.0626 (5)
H11	0.9178	0.2055	−0.1608	0.075*
C12	0.8864 (3)	0.3166 (2)	0.00158 (17)	0.0584 (4)
H12	0.9886	0.3522	−0.0130	0.070*
C13	0.7714 (2)	0.3489 (2)	0.11230 (15)	0.0467 (4)
F1	0.43556 (17)	0.17571 (15)	0.07788 (11)	0.0776 (4)
N1	0.8131 (3)	1.0545 (2)	0.64069 (17)	0.0803 (5)
N2	0.62283 (19)	0.30163 (17)	0.13730 (12)	0.0497 (4)
O1	0.81120 (16)	0.43601 (16)	0.19823 (11)	0.0552 (3)

reported the syntheses and the structures of some related compounds [5, 9–11].

Single crystal structure analysis reveals that the title compound crystallizes in the triclinic $P\bar{1}$ space group with one crystallographically independent molecule in the asymmetric unit (see the figure). All bond lengths and angles are in the expected ranges. The title compound consists of one cyanophenyl and a pyridyl moiety, and the dihedral angle between the two planes is 48.1°.

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