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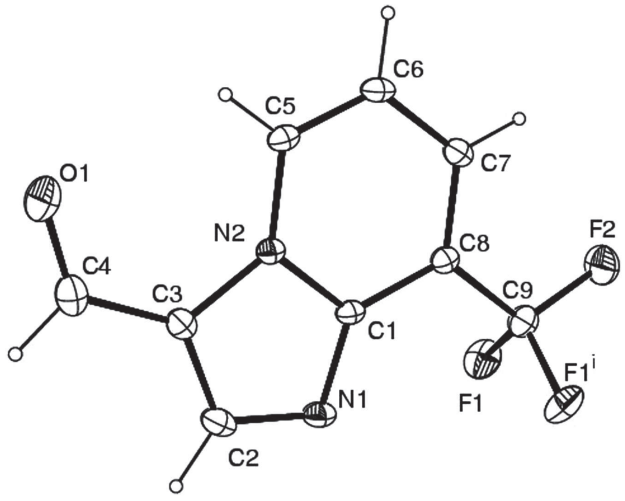
Crystal structure of 8-(trifluoromethyl)imidazo [1,2-*a*]pyridine-3-carbaldehyde, $C_9H_5F_3N_2O$



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Abstract

$C_9H_5F_3N_2O$, orthorhombic, *Pnma* (no. 62), $a = 7.276(2)$ Å, $b = 6.7773(19)$ Å, $c = 17.613(5)$ Å, $V = 868.5(4)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0399$, $wR_{ref}(F^2) = 0.1122$, $T = 293(2)$ K.

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The crystal structure is shown in the figure (i = x, $-y$, z). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title compound was prepared from 8-(trifluoromethyl) imidazo[1,2-*a*]pyridine, according to the procedure of McKenna et al. [5]. The intermediate of 8-(trifluoromethyl) imidazo[1,2-*a*]pyridine was prepared according to the procedure of Mu et al. [6].

Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.65×0.32 × 0.25 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.15 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ_{max}, completeness:	25.01°, 100.0%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3447, 839, 0.0184
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 729
$N(param)_{refined}$:	89
Programs:	Bruker programs [1], SHELX [2, 3], WinGX and ORTEP [4]

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

Atom	x	y	z	U_{iso}*/U_{eq}
O(1)	0.5672(4)	0.2500	0.3061(1)	103(1)
N(1)	0.1282(2)	0.2500	0.4931(1)	0.062(1)
N(2)	0.4273(2)	0.2500	0.4624(1)	0.046(1)
F(1)	0.1184(2)	0.0932(2)	0.6568(1)	0.100(1)
F(2)	0.3077(3)	0.2500	0.7259(1)	110(1)
C(1)	0.2995(3)	0.2500	0.5202(1)	0.047(1)
C(2)	0.1488(4)	0.2500	0.4175(2)	0.069(1)
H(2)	0.0505	0.2500	0.3838	0.083*
C(3)	0.3284(3)	0.2500	0.3951(1)	0.058(1)
C(4)	0.4055(5)	0.2500	0.3204(2)	0.080(1)
H(4)	0.3243	0.2500	0.2796	0.096*
C(5)	0.6134(3)	0.2500	0.4759(1)	0.052(1)
H(5)	0.6963	0.2500	0.4357	0.063*
C(6)	0.6736(3)	0.2500	0.5473(1)	0.058(1)
H(6)	0.7993	0.2500	0.5569	0.069*
C(7)	0.5492(3)	0.2500	0.6082(1)	0.057(1)
H(7)	0.5934	0.2500	0.6577	0.068*
C(8)	0.3642(3)	0.2500	0.5957(1)	0.051(1)
C(9)	0.2287(4)	0.2500	0.6586(1)	0.069(1)

Experimental details

H atoms were positioned geometrically and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 times the equivalent isotropic displacement parameters of their parent atoms, and C—H distances were set equal to 0.93 Å.

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Comment

Imidazo[1,2-a]pyridine derivatives have a high potential for biological activity [7]. In continuation of our work on the structure and biological activity of heterocycles derivatives [8–13], we obtained a colourless crystalline compound prepared from 8-(trifluoromethyl)imidazo[1,2-*a*]pyridine. The structural identity was resolved using single-crystal X-ray diffraction.

The title molecule consists of the imidazo[1,2-a]pyridine core moiety, and one trifluoromethyl and one carbaldehyde group, which confirms the synthesis of the title compound. The imidazo[1,2-a]pyridine ring (C1/C2/C3/C5/C6/C7/C8/N1/N2) and atoms C9/F2/C4/O1 are coplanar due to the crystallographically imposed mirror plane. At least one non-classical intermolecular C4′-H4′$\cdots$O1 hydrogen bond exists between two imidazo[1,2-a]pyridine of neighbouring molecules with a C–H$\cdots$O angle of 168.4° ($' = -1/2 + x$, $1/2 - y$, $1/2 - z$).

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