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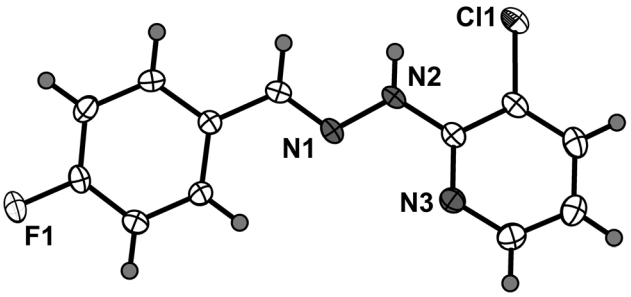
The crystal structure of (*E*)-3-chloro-2-(2-(4-fluorobenzylidene)hydrazinyl)pyridine, $C_{12}H_9Cl_FN_3$



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Abstract

$C_{12}H_9Cl_FN_3$, monoclinic, $P2_1/n$ (no. 14), a = 10.120(4) Å, b = 13.823(6) Å, c = 16.480(7) Å, β = 91.744(8)°, V = 2304.4(17) Å^3, Z = 8, $R_{gt}(F)$ = 0.0402, $wR_{ref}(F^2)$ = 0.0932, T = 113.15 K.

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Only one of the two crystallographically independent moleules of the title 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.

Source of material

According to the our previous work [4], the 3-chloro-2-hydrazinylpyridine (1.43 g, 0.1 mol) and 4-fluorobenzaldehyde (1.24 g, 0.1 mol) was dissolved in EtOH (50 mL) and stirred at room temperature for 24 h. Then a solid was obtained, which was filtered and dried with 85% yield. The solid was recrystallized from ethanol as colorless block crystals.

Table 1: Data collection and handling.

Crystal:	Colorless prism
Size:	0.20 × 0.20 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.32 mm^{-1}
Diffractometer, scan mode:	ω
θ_{max}, completeness:	27.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	22,536, 5483, 0.044
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 4604
$N(param)_{refined}$:	307
Programs:	Olex2 [1], SHELX [2, 3]

Experimental details

Hydrogen atoms were added using riding models. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program and refined with the ShelXL [3] refinement package.

Comment

Pyridine is an attractive heterocycle because of the excellent biological activity of some derivatives, such as insecticidal activity [5], fungicidal activity [6], herbicidal activity [7]. On the other hand, the hydrazone group is an active group in many bioactive molecules [8].

The asymmetric unit of the title pyridine compound consists of two molecule, which is the same as reported work [4, 9]. Geometric parameters (bond lengths and bond angles) are all in the normal ranges [10–12]. The title compound shows an E configuration around the C7=N1 bond. The C7=N1 and N4=C19 bond lengths (1.289(2), 1.282(2) Å) are typical for a C=N double bond [13]. In the title compound, the phenyl ring is nearly in the same plane with the pyridine ring in both independent molecules.

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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}
Cl1	−0.38845 (4)	−0.19073 (3)	0.08628 (3)	0.03236 (12)
F1	0.20724 (9)	0.40525 (6)	0.24092 (6)	0.0338 (2)
N1	−0.22853 (13)	0.08362 (8)	0.17193 (8)	0.0222 (3)
N2	−0.29329 (13)	−0.00277 (8)	0.15728 (8)	0.0245 (3)
H2	−0.2525	−0.0582	0.1662	0.029*
N3	−0.49118 (13)	0.08102 (8)	0.13412 (8)	0.0233 (3)
C1	0.12947 (15)	0.32514 (10)	0.23167 (10)	0.0234 (3)
C2	−0.00248 (16)	0.33696 (11)	0.21119 (11)	0.0279 (4)
H2A	−0.0389	0.3998	0.2036	0.033*
C3	−0.08082 (15)	0.25556 (10)	0.20191 (10)	0.0261 (4)
H3	−0.1722	0.2627	0.1882	0.031*
C4	−0.02774 (14)	0.16277 (10)	0.21239 (9)	0.0198 (3)
C5	0.10637 (15)	0.15427 (11)	0.23368 (10)	0.0251 (3)
H5	0.1440	0.0919	0.2415	0.030*
C6	0.18574 (15)	0.23591 (11)	0.24358 (10)	0.0281 (4)
H6	0.2769	0.2299	0.2583	0.034*
C7	−0.10802 (15)	0.07601 (10)	0.19870 (10)	0.0221 (3)
H7	−0.0713	0.0139	0.2096	0.026*
C8	−0.42223 (15)	−0.00121 (10)	0.12863 (9)	0.0210 (3)
C9	−0.48146 (16)	−0.08549 (10)	0.09531 (10)	0.0243 (3)
C10	−0.61163 (16)	−0.08396 (11)	0.06917 (10)	0.0291 (4)
H10	−0.6525	−0.1405	0.0474	0.035*
C11	−0.68249 (16)	0.00173 (11)	0.07515 (10)	0.0303 (4)
H11	−0.7727	0.0053	0.0577	0.036*
C12	−0.61782 (16)	0.08122 (11)	0.10706 (10)	0.0274 (4)
H12	−0.6658	0.1401	0.1102	0.033*
Cl2	0.05702 (4)	0.58235 (2)	0.16911 (2)	0.02695 (11)
F2	−0.23767 (11)	1.13806 (7)	0.56619 (6)	0.0448 (3)
N4	−0.09219 (12)	0.83511 (8)	0.29660 (8)	0.0208 (3)
N5	−0.05299 (12)	0.75652 (8)	0.25234 (8)	0.0219 (3)
H5A	−0.0418	0.6997	0.2756	0.026*
N6	−0.06113 (13)	0.85439 (8)	0.13699 (8)	0.0257 (3)
C13	−0.20850 (16)	1.05980 (11)	0.51954 (11)	0.0288 (4)
C14	−0.23277 (15)	1.06506 (11)	0.43733 (11)	0.0275 (4)
H14	−0.2710	1.1216	0.4137	0.033*
C15	−0.20081 (14)	0.98696 (10)	0.38954 (10)	0.0236 (3)
H15	−0.2186	0.9893	0.3326	0.028*
C16	−0.14204 (14)	0.90391 (10)	0.42449 (10)	0.0212 (3)
C17	−0.12203 (15)	0.90098 (10)	0.50860 (10)	0.0248 (3)
H17	−0.0854	0.8445	0.5332	0.030*
C18	−0.15470 (15)	0.97917 (11)	0.55715 (10)	0.0281 (4)
H18	−0.1404	0.9771	0.6144	0.034*
C19	−0.09868 (15)	0.82341 (10)	0.37355 (10)	0.0222 (3)
H19	−0.0756	0.7630	0.3975	0.027*
C20	−0.03169 (14)	0.76864 (10)	0.17111 (10)	0.0205 (3)
C21	0.02210 (14)	0.69337 (10)	0.12411 (10)	0.0219 (3)
C22	0.04700 (16)	0.70789 (12)	0.04390 (10)	0.0307 (4)
H22	0.0824	0.6573	0.0121	0.037*
C23	0.01954 (19)	0.79819 (12)	0.00960 (11)	0.0384 (4)
H23	0.0375	0.8116	−0.0455	0.046*
C24	−0.03450 (17)	0.86693 (12)	0.05883 (11)	0.0344 (4)
H24	−0.0545	0.9282	0.0354	0.041*

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