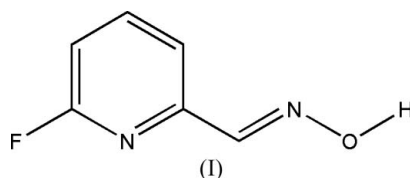


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Key indicatorsSingle-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.061
 wR factor = 0.135
Data-to-parameter ratio = 13.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(E)-6-Fluoropyridine-2-carbaldehyde oxime**The title compound, $\text{C}_6\text{H}_5\text{FN}_2\text{O}$, exists as the *E* isomer. The crystal structure is stabilized by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding.Received 27 June 2006
Accepted 15 August 2006**Comment**

The title compound, (I), is an important intermediate in drug synthesis (Frey & Marcantonio, 2001).



The molecular structure of (I) is shown in Fig. 1. The molecule is planar and similar to (*E*)-3-fluoropyridine-4-carbaldehyde oxime (Sorof *et al.*, 1985). In the crystal structure, molecules are connected by hydrogen bonds between the hydroxy group and the pyridine N atom (Table 1), forming one-dimensional supramolecular chains. The chains are arranged in an anti-parallel fashion and pack in a typical herringbone motif (Fig. 2).

Experimental

Oxalyl chloride (1.24 ml, 14 mmol) in dichloromethane (30 ml) was placed in a three-necked flask fitted with two addition funnels. Dimethyl sulfoxide (2.1 ml, 30 mmol) in dichloromethane (6 ml) was placed in one funnel and 6-fluoro-2-pyridinemethanol (1.52 g, 12 mmol) in dichloromethane (12 ml) in the other. The flask was cooled to 213 K and dimethyl sulfoxide was added over a period of 20 min. Stirring was continued for a further 20 min, followed by addition of the alcohol solution over 20 min. After the mixture had been stirred at 213 K for 20 min, triethylamine (8.4 ml, 60 mmol) was added. The cooling bath was removed and the suspension was allowed to warm to room temperature. Water (36 ml) was added, the yellow organic layer was separated, and the aqueous layer was extracted with dichloromethane (3×7.5 ml). The combined organic solution was dried and concentrated to give 6-fluoropyridine-2-carbaldehyde as an orange–yellow liquid (yield 85%). Hydroxylamine hydrochloride (0.828 g, 12 mmol) was dissolved in 7.5 ml of water and then neutralized by 6 M aqueous solution of NaOH. 6-Fluoro-2-pyridinecarbaldehyde (1 g) in 2.5 ml ethanol was added to this mixture with stirring. The reaction mixture was refluxed for 2 h. The precipitate was collected by suction filtration and washed with cold water; after being dried under reduced pressure, the title compound (I) was obtained as a white solid (yield 85%). Single crystals of (I) were obtained by recrystallization from an ethyl acetate solution at room temperature.

Crystal data

$C_6H_5FN_2O$
 $M_r = 140.12$
 Monoclinic, $P2_1/c$
 $a = 8.006 (2) \text{ \AA}$
 $b = 8.525 (2) \text{ \AA}$
 $c = 9.260 (2) \text{ \AA}$
 $\beta = 91.998 (5)^\circ$
 $V = 631.6 (3) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.474 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.12 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Prism, colorless
 $0.13 \times 0.11 \times 0.07 \text{ mm}$

Data collection

Bruker SMART APEX CCD
 detector diffractometer
 φ and ω scans
 Absorption correction: none
 3566 measured reflections

1250 independent reflections
 582 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.067$
 $\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.135$
 $S = 0.98$
 1250 reflections
 91 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0465P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.24 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots N1^i$	1.04	1.84	2.865 (3)	165

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

The hydroxy H atom was located in a difference Fourier map and refined as riding in its as-found relative position, $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were placed in calculated positions ($C-H = 0.93 \text{ \AA}$) and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

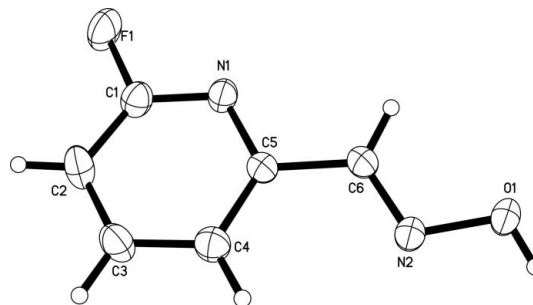


Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

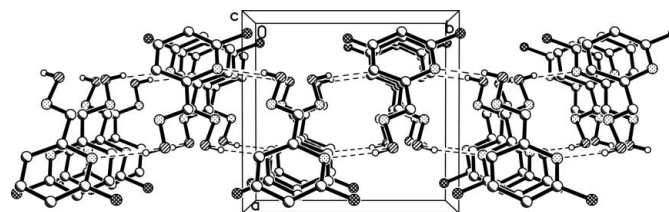


Figure 2

Perspective view of the hydrogen bonding (dashed lines) in (I). H atoms not involved in hydrogen bonding have been omitted.

This work is supported by the National Analytical Research Center of Electrochemistry and Spectroscopy, Changchun Institute of Applied Chemistry, China.

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