Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Fluorobenzaldehyde picoloylhydrazone

Si-Chang Shao,[a] Zhong-Lu You,[b] Shao-Hua Fan,[a] Lu-Lu Tang,[c] Yong-Shan Lin[c] and Hai-Liang Zhu[a]*

[a]Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and [c]Department of Chemistry, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China

Correspondence e-mail: hailiang_zhu@163.com

Received 5 October 2004
Accepted 27 October 2004
Online 6 November 2004

Key indicators

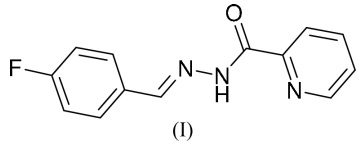
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.145
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, 4-fluorobenzaldehyde (pyridine-2-carbonyl)hydrazone, $C_{13}H_{10}FN_3O$, is roughly planar and displays a *trans* configuration with respect to the C=N double bond.

Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

In the title compound, (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C7=N1 bond length of 1.266 (3) Å conforms to the value for a double bond. The bond length of 1.345 (3) Å between atoms C8 and N2 is greater than the value for a double bond, and less than the value for a single bond, because of conjugation effects in the molecule. The dihedral angle between the pyridine and benzene rings is 0.7 (2)°.

Experimental

Pyridine-2-carboxylic acid hydrazide (0.2 mmol, 27.4 mg) and 2-fluorobenzaldehyde (0.2 mmol, 28.1 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. After keeping the solution in air for 10 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

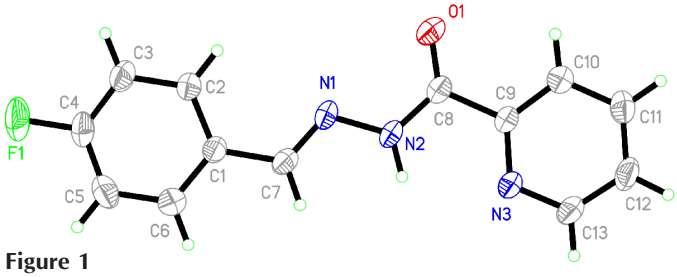


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Crystal data

$C_{13}H_{10}FN_3O$
$M_r = 243.24$
Monoclinic, $P2_1/n$
$a = 5.812\ (3)$ Å
$b = 14.276\ (8)$ Å
$c = 13.878\ (7)$ Å
$\beta = 98.344\ (8)^\circ$
$V = 1139.3\ (11)$ Å^3
$Z = 4$
$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1485 reflections
$\theta = 2.9$–23.4°
$\mu = 0.11$ mm^{-1}
$T = 298\ (2)$ K
Block, yellow
0.38 × 0.28 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.961$, $T_{max} = 0.976$
6467 measured reflections
2342 independent reflections
1493 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.5^\circ$
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 17$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.145$
$S = 1.04$
2342 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.1645P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Atom H2A was located in a difference Fourier map and refined isotropically, with the U_{iso}(H) value fixed at 0.08 Å^2 and the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, Peoples Republic of China, for research grant No. 2004kj300zd.

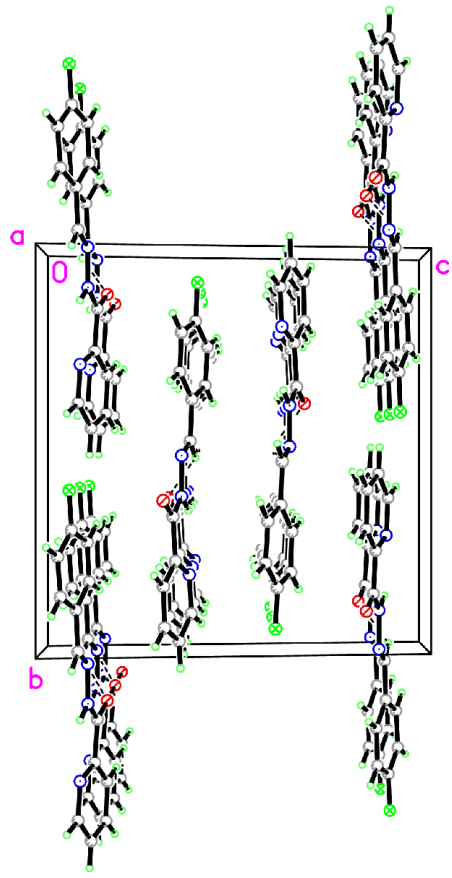


Figure 2
The crystal packing of (I), viewed along the *a* axis.

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