Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Nitrobenzaldehyde picoloylhydrazone

Si-Chang Shao,[a] Zhong-Lu You,[b] Shao-Hua Fan,[a] Lu-Lu Tang,[c] Zhong-Duo Xiong[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

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.122
Data-to-parameter ratio = 13.5

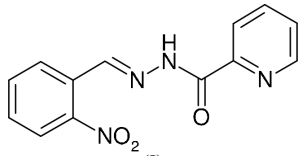
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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

The molecule of the title compound, 2-nitrobenzaldehyde (pyridine-2-carbonyl)hydrazone, $C_{13}H_{10}N_4O_3$, is roughly planar and displays a *trans* configuration with respect to the C=N double bond. In the crystal structure, the molecules are linked through weak intermolecular N—H···O hydrogen bonds, forming discrete dimers.

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=N2 bond length of 1.263 (2) Å conforms to the value for a double bond. The bond length of 1.349 (2) Å between atoms C8 and N3 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 1.3 (2)°. The dihedral between the nitryl plane and the benzene ring is 27.3 (2)°.

In the crystal structure, the molecules are linked through weak intermolecular N—H···O hydrogen bonds, forming discrete dimers (Table 1 and Fig. 2).

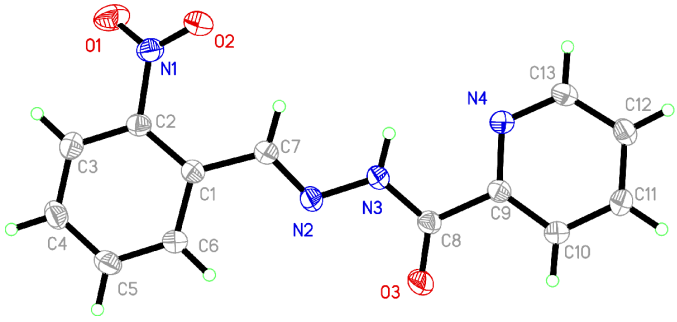


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

Pyridine-2-carboxylic acid hydrazide (0.2 mmol, 27.4 mg) and 2-nitrobenzaldehyde (0.2 mmol, 30.2 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 8 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$C_{13}H_{10}N_4O_3$
M_r = 270.25
Monoclinic, $C2/c$
a = 12.191 (3) Å
b = 9.398 (3) Å
c = 21.624 (6) Å
β = 103.415 (4)°
V = 2410.0 (11) Å^3
Z = 8
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2674 reflections
θ = 2.8–27.9°
μ = 0.11 mm^{-1}
T = 298 (2) K
Block, yellow
0.32 × 0.30 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.987
6729 measured reflections
2486 independent reflections
2022 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.5°
$h = -14 \rightarrow 15$
$k = -11 \rightarrow 10$
$l = -25 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.05
2486 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.5995P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{i}	0.889 (9)	2.363 (15)	3.1384 (18)	145.8 (19)

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

Atom H3A 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).

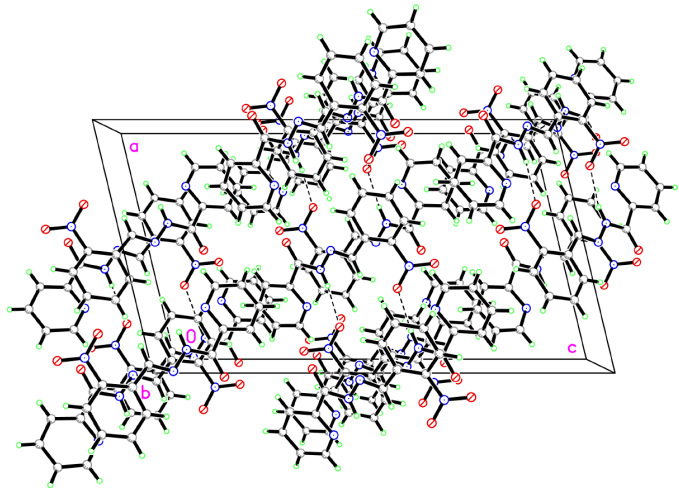


Figure 2
The crystal packing of (I), viewed along the b axis. Dashed lines indicate hydrogen bonds.

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.

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