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N′-(4-Hydroxybenzylidene)isonicotinohydrazide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.111
Data-to-parameter ratio = 16.0

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

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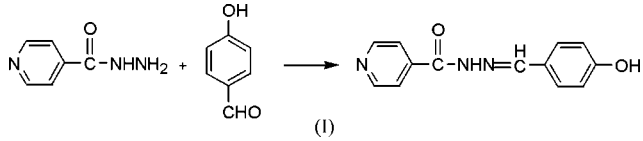
The title compound, $C_{13}H_{11}N_3O_2$, was prepared by the reaction of pyridine-4-carboxylic acid hydrazide and *p*-hydroxybenzaldehyde in ethanol. In the crystal structure, all non-H atoms are coplanar, with an r.m.s. deviation of 0.096 Å. N—H···N, O—H···N and O—H···O intermolecular hydrogen bonds stabilize the structure.

Comment

The synthesis and structure of Schiff bases have attracted much attention because of their pharmacological activity (Parashar *et al.*, 1988) and photochromic properties (Hadjoudis *et al.*, 1987). We report here the synthesis and crystal structure of the title compound, (I).



(I)

The C7—C8, C7═N3 and N2—N3 bond lengths are 1.452 (2), 1.273 (2) and 1.382 (2) Å, respectively; these values are in good agreement with those in a similar system (Jing *et al.*, 2005). All the non-H atoms are coplanar, with an r.m.s. deviation of 0.096 Å.

Intermolecular N—H···N, O—H···N and O—H···O hydrogen bonds are found in the crystal structure (Table 1 and Fig. 2). These stabilize the structure, forming a supramolecular network pattern.

Experimental

An anhydrous ethanol solution (50 ml) of pyridine-4-carboxylic acid hydrazide (1.37 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of *p*-hydroxybenzaldehyde (1.22 g, 10 mmol), and the mixture was stirred at 343 K for 5 h under nitrogen, producing a yellow precipitate. The product was isolated, recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 82% yield. Bright-yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{13}H_{11}N_3O_2$
M_r = 241.25
Monoclinic, $P2_1/c$
a = 8.4553 (14) Å
b = 10.1812 (16) Å
c = 13.408 (2) Å
β = 98.646 (2)°
V = 1141.1 (3) Å^3
Z = 4
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1357 reflections
θ = 2.4–24.5°
μ = 0.10 mm^{-1}
T = 294 (2) K
Plate, yellow
0.32 × 0.26 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.950, T_{max} = 0.990
7461 measured reflections
2731 independent reflections
1779 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 28.0°
$h = -7 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.111
S = 1.08
2731 reflections
171 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.0289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N1^{i}	0.87 (2)	2.40 (2)	3.2350 (17)	160 (2)
O2—H2···N3^{ii}	0.90 (2)	2.46 (2)	3.1177 (15)	130 (2)
O2—H2···O1^{ii}	0.90 (2)	2.00 (2)	2.8340 (14)	155 (2)

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

C-bound H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier atom). H atoms attached to N and O atoms were located in a difference Fourier map and refined freely.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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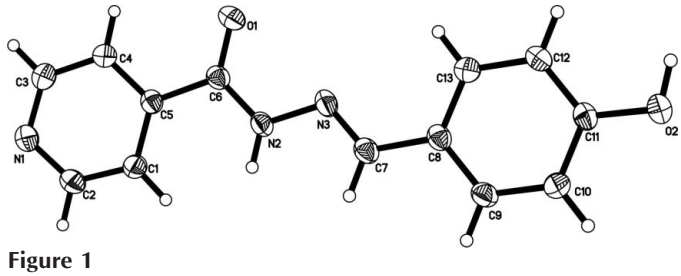

Figure 1
A view of the title compound, shown with 30% probability displacement ellipsoids.

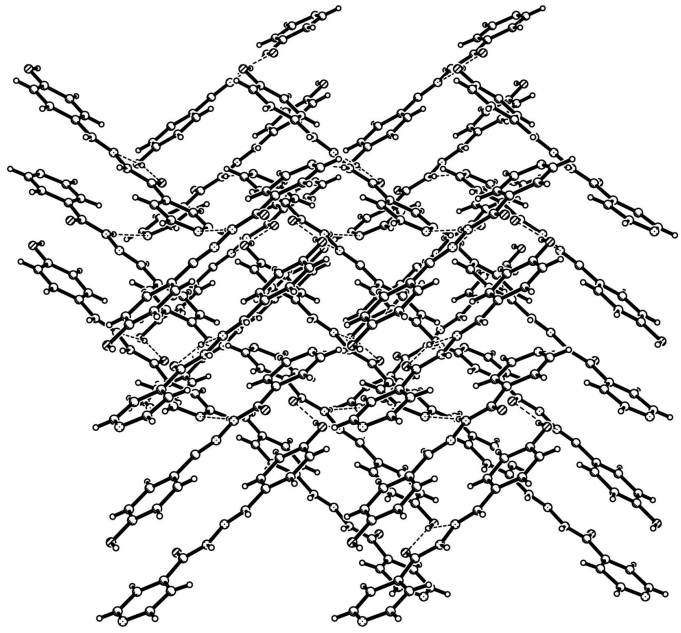

Figure 2
The intermolecular hydrogen-bonding interactions (dashed lines) in (I)..

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