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Isonicotinic acid (2-hydroxy-3-methoxybenzylidene)hydrazide

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The title compound, $C_{14}H_{13}N_3O_3$, was prepared using 2-hydroxy-3-methoxybenzaldehyde and 4-pyridinecarboxylic acid hydrazide. In the crystal structure, an intramolecular O—H···N hydrogen bond [H···N = 1.83 (2) Å] appears to stabilize the planar conformation of the molecule, while intermolecular N—H···N hydrogen bonds [H···N = 2.213 (15) Å] link molecules into extended chains along [001].

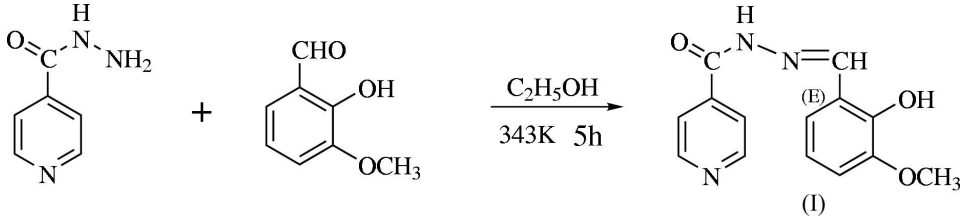
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.116
Data-to-parameter ratio = 13.6

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

Comment

Schiff bases have received considerable attention in the literature because of their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). The crystal structure determination of the title compound was undertaken as part of a study to investigate the physical and chemical properties of the compound.



(I)

A view of (I) is shown in Fig. 1. The C7—C8, C7—N3 and N2—N3 bond lengths of 1.451 (3) Å, 1.279 (3) Å and 1.370 (2) Å, respectively, are consistent with those in a related structure we determined recently (Jing *et al.*, 2005). The pyridine ring (C1—C2—C3—C4—C5—N1) is planar, the r.m.s. deviation of the fitted atoms being 0.0105 Å, and the C6—O1—N2—N3 portion of the structure is planar with an r.m.s. of 0.0082 Å. In addition, the *O*-vanillin moiety (O2—O3—C7—C8—C9—C10—C11—C12—C13) is also essentially

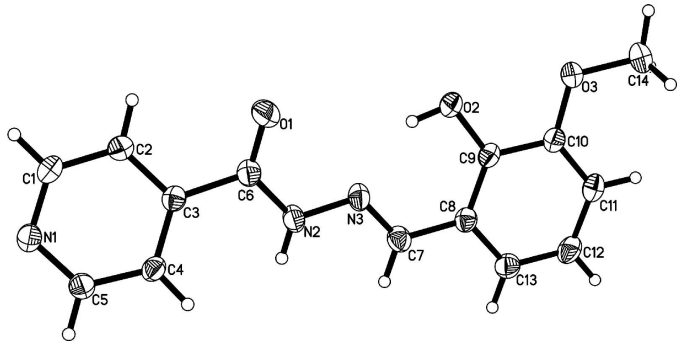


Figure 1
A view of the title compound, with 30% probability displacement ellipsoids.

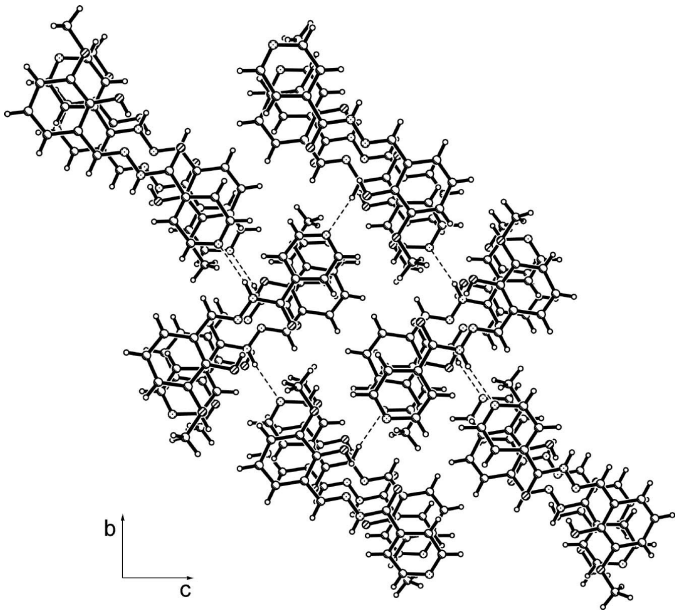


Figure 2
Intermolecular hydrogen bonding interactions (dashed lines) in (I).

planar, with an r.m.s. deviation of 0.0244 Å. The dihedral angles between the pyridine group and the *O*-vanillin group with the C6—O1—N2—N3 portion are 22.86 (1)° and 7.49 (1)°, respectively. The latter value suggests that the intramolecular O—H···N hydrogen bond (Table 1) stabilizes the planar conformation of part of the molecule. In the crystal structure, N—H···N intermolecular hydrogen bonds link molecules into extended chains along [001] (see Fig. 2).

Experimental

An anhydrous ethanol solution of 2-hydroxy-3-methoxybenzaldehyde (1.52 g, 10 mmol) was added to an anhydrous ethanol solution of 4-pyridinecarboxylic acid hydrazide (1.37 g, 10 mmol), and the mixture was stirred at 343 K for 5 h under nitrogen. A yellow precipitate appeared. The product was isolated and recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 78% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a solution in ethanol.

Crystal data

$C_{14}H_{13}N_3O_3$
M_r = 271.27
Monoclinic, $P2_1/c$
a = 7.671 (2) Å
b = 16.268 (5) Å
c = 10.884 (3) Å
β = 110.415 (5)°
V = 1273.0 (6) Å^3
Z = 4
D_x = 1.415 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 981 reflections
θ = 2.8–24.1°
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, yellow
0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.968, T_{max} = 0.984
7239 measured reflections
2603 independent reflections
1752 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.4°
$h = -9 \rightarrow 9$
$k = -20 \rightarrow 19$
$l = -13 \rightarrow 6$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.116
S = 1.06
2603 reflections
191 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.2950P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0053 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N3	0.859 (10)	1.826 (17)	2.591 (2)	147 (3)
N2—H2B···N1^{i}	0.863 (9)	2.214 (10)	3.068 (3)	171 (2)

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

H atoms bonded to C atoms were included in calculated positions [C—H = 0.93–0.96 Å] and refined using a riding-model approximation with $U_{iso} = 1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C). The H atoms bonded to N and O atoms were refined independently with isotropic displacement parameters.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); 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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