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# 2′-(4-Methoxybenzylidene)isonicotinohydrazide monohydrate

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**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.034
*wR* factor = 0.097
Data-to-parameter ratio = 16.5

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

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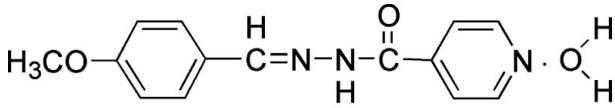
The title compound, $C_{14}H_{13}N_3O_2\cdot H_2O$, was prepared from pyridine-4-carboxylic acid hydrazide and 4-methoxybenzaldehyde. In the crystal structure, the water molecules participate in O—H···O, O—H···N and N—H···O hydrogen bonds with the hydrazide molecules; these interactions contribute to the stability of the structure.

## Comment

The syntheses and structures of Schiff bases have attracted much attention, because their metal complexes have been studied extensively as model compounds of active centres in various proteins and enzymes (Santos *et al.*, 2001). As part of an investigation of physical and chemical properties, we report the synthesis and molecular structure of the title compound, (I) (Fig. 1).



(I)

The C7—C8, C7—N3 and N2—N3 bond lengths of 1.4623 (14), 1.2734 (14) and 1.3881 (12) Å, respectively, are consistent with those in related structures (Jing *et al.*, 2005; Yu *et al.*, 2005). The system (C7–C14/N2/N3/O2) is planar, the r.m.s. deviation of fitted atoms being 0.0308 Å, and the pyridine ring (C1–C6/N1) is planar with an r.m.s. deviation of 0.0214 Å. The dihedral angle between the two planes is 36.78 (3)°. It should be noted that the water molecules participate in O—H···O, O—H···N and N—H···O hydrogen

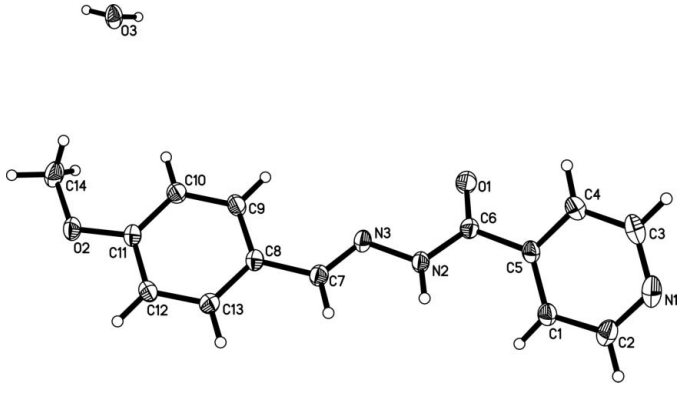



**Figure 1**
An view of the title compound, with 30% probability displacement ellipsoids.

bonds with the hydrazide molecules (Table 1); these interactions play a key role in stabilization of the crystal structure (Fig. 2).

## Experimental

An anhydrous ethanol solution of pyridine-4-carboxylic acid hydrazide (1.37 g, 10 mmol) was added to an anhydrous ethanol solution of 4-methoxybenzaldehyde (1.36 g, 10 mmol), and the mixture was stirred at 350 K for 5 h under nitrogen. A white precipitate appeared. The product was isolated and recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 89% yield. Bright-white single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

*Crystal data*

$C_{14}H_{15}N_3O_3$
$M_r$ = 273.29
Monoclinic, $P2_1/c$
$a$ = 7.3660 (15) Å
$b$ = 12.422 (3) Å
$c$ = 14.785 (3) Å
$\beta$ = 96.699 (2)°
$V$ = 1343.6 (5) Å$^3$
$Z$ = 4
$D_x$ = 1.351 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3520 reflections
$\theta$ = 2.8–27.8°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 294 (2) K
Block, white
0.24 × 0.14 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.960, $T_{max}$ = 0.990
8826 measured reflections
3186 independent reflections
2585 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014
$\theta_{max}$ = 27.9°
$h = -7 \rightarrow 9$
$k = -16 \rightarrow 14$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
$S$ = 1.04
3186 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.2087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.032 (3)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$B$···O1$^{i}$ | 0.86 (2) | 2.02 (2) | 2.8794 (14) | 177 (2) |
| O3—H3$A$···N1$^{ii}$ | 0.91 (2) | 1.90 (2) | 2.8071 (14) | 180 (2) |
| N2—H2$A$···O3$^{iii}$ | 0.90 (1) | 2.04 (2) | 2.9324 (15) | 172 (1) |

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

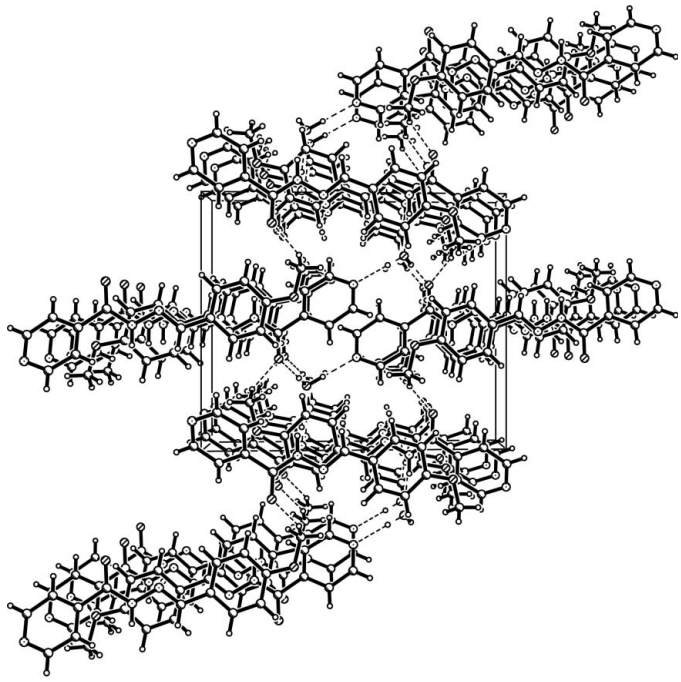


**Figure 2**
Intermolecular hydrogen bonds in (I), shown as dashed lines.

Atom H2*A* attached to N2 and atoms H3*A* and H3*B* attached to O3 were located in a difference Fourier map. Atom H2*A* was refined freely, while for H3*A* and H3*B* the positions were refined with $U_{iso}$(H) = $U_{eq}$(O). Other H atoms were included in calculated positions (C—H = 0.93–0.96 Å) and refined using the riding-model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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