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## Key indicators

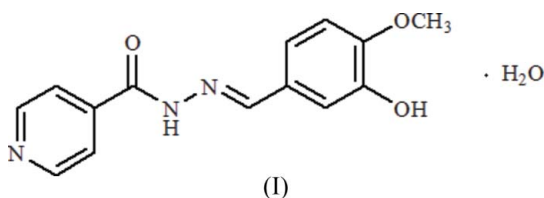
Single-crystal X-ray study  
 $T = 294\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.039  
 $wR$  factor = 0.107  
Data-to-parameter ratio = 14.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.3-Hydroxy-4-methoxybenzaldehyde  
isonicotinoylhydrazone monohydrate

The asymmetric unit of the title compound,  $\text{C}_{14}\text{H}_{13}\text{N}_3\text{O}_3 \cdot \text{H}_2\text{O}$ , consists of one isonicotinic acid (3-hydroxy-4-methoxybenzylidene)hydrazide (IBH) molecule and one water molecule connected through an  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bond. Further  $\text{O}-\text{H} \cdots \text{O}$ ,  $\text{O}-\text{H} \cdots \text{N}$  and  $\text{N}-\text{H} \cdots \text{O}$  hydrogen bonds result in the formation of an intricate three-dimensional supramolecular network.

Received 7 October 2005  
Accepted 17 October 2005  
Online 22 October 2005

## Comment

Benzoylhydrazone derivatives have received considerable attention, owing to their bacteriostatic activity and wide application in tuberculosis treatments (Edwards *et al.*, 1975). Carbonylhydrazone is a structural motif showing bioactivity (Zhi *et al.*, 2003). Pyridine-type carbonylhydrazone compounds are well known as ligands capable of coordinating to a metal centre through their O/N atoms (Puri & Agarwala, 1998). As part of our ongoing research into the coordination chemistry of metal ions, the title compound, (I), was prepared using 3-hydroxy-4-methoxybenzaldehyde and isonicotinic acid hydrazide, and its crystal structure is reported here.



Compound (I) contains one isonicotinic acid (3-hydroxy-4-methoxybenzylidene)hydrazide (IBH) molecule and one water molecule, which are connected by an  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bond, as shown in Fig. 1. The IBH molecule adopts

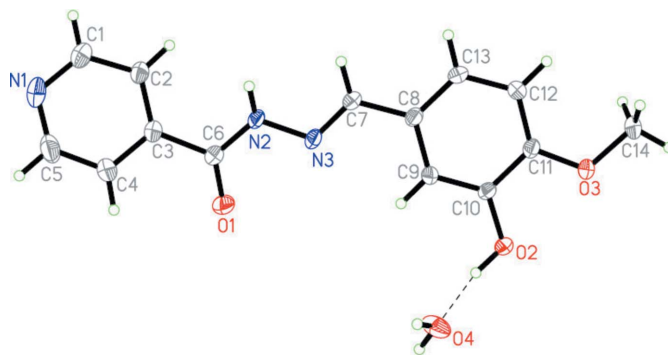
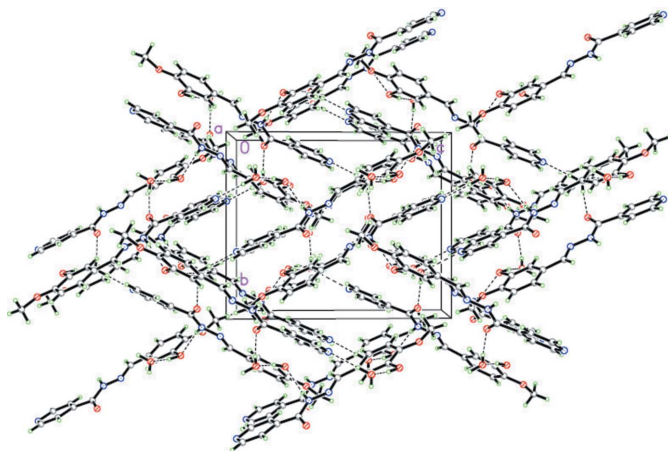


Figure 1

A view of the asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level. The dashed line indicates a hydrogen bond.



**Figure 2**  
The packing of (I), viewed down the *a* axis, showing the extended hydrogen-bonding network (dashed lines).

an *E* configuration with respect to the C=N bond. The bond lengths and angles in IBH (Table 1) are within normal ranges (Allen *et al.*, 1987). The C7–C8, C7=N3 and N2–N3 bond lengths are comparable with those observed in some related compounds (Yu *et al.*, 2005; Jing *et al.*, 2005; Deng *et al.*, 2005). Excluding the H atoms, the IBH molecule is roughly planar, and the pyridyl and benzene rings are only slightly twisted, with a dihedral angle of 10.4 (6)°.

The crystal packing of (I) is characterized by many intermolecular hydrogen-bonding interactions, as summarized in Table 2. Each O–H group of the water molecule is hydrogen bonded to a carboxy O1 or pyridyl N1 acceptor to form O–H...N and O–H...O hydrogen bonds. At the same time, the N–H group forms bifurcated hydrogen bonds with the hydroxy atom O2 and the methoxy atom O3. These interactions stabilize the structure, forming a supramolecular network pattern (Fig. 2).

## Experimental

An ethanol solution (50 ml) of isonicotinic acid hydrazide (1.37 g, 10 mmol) was added to an ethanol solution (50 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol), and the mixture was stirred at 343 K for 5 h, producing a light-yellow precipitate. The product was isolated, recrystallized from ethanol–water (2:1 *v/v*) and then dried *in vacuo* to give the pure title compound in 82% yield. Single crystals of (I) suitable for X-ray diffraction were obtained by the slow evaporation of the mother liquor.

### Crystal data

C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>O<sub>3</sub>·H<sub>2</sub>O  
*M<sub>r</sub>* = 289.29  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 9.1684 (16) Å  
*b* = 11.489 (2) Å  
*c* = 13.889 (2) Å  
 $\beta$  = 93.688 (3)°  
*V* = 1459.9 (4) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.316 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 2154 reflections  
 $\theta$  = 2.3–26.1°  
 $\mu$  = 0.10 mm<sup>-1</sup>  
*T* = 294 (2) K  
 Block, colourless  
 0.26 × 0.24 × 0.22 mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.960, *T<sub>max</sub>* = 0.979  
 8023 measured reflections

2977 independent reflections  
 1964 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.032  
 $\theta_{\text{max}}$  = 26.4°  
*h* = -9 → 11  
*k* = -11 → 14  
*l* = -17 → 16

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.039  
*wR*(*F*<sup>2</sup>) = 0.107  
*S* = 1.01  
 2977 reflections  
 208 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.2089P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97 (Sheldrick, 1997)  
 Extinction coefficient: 0.025 (2)

**Table 1**

Selected geometric parameters (Å, °).

O1–C6	1.2297 (18)	N1–C1	1.328 (2)
O2–C10	1.3637 (18)	N2–C6	1.336 (2)
O3–C11	1.3650 (17)	N2–N3	1.385 (2)
O3–C14	1.4310 (19)	N3–C7	1.272 (2)
N1–C5	1.326 (3)	C7–C8	1.463 (2)
C6–N2–N3	119.43 (14)	O1–C6–N2	123.15 (15)
C7–N3–N2	115.37 (13)	N3–C7–C8	120.16 (14)
C6–N2–N3–C7	177.55 (15)	N3–N2–C6–C3	177.24 (13)
N3–N2–C6–O1	-2.6 (2)	N2–N3–C7–C8	179.00 (14)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O2–H2A...O4	0.95 (2)	1.66 (2)	2.5956 (18)	169 (2)
N2–H2B...O2 <sup>i</sup>	0.83 (2)	2.12 (2)	2.8715 (19)	151 (2)
N2–H2B...O3 <sup>i</sup>	0.83 (2)	2.63 (2)	3.3193 (19)	141 (2)
O4–H4A...N1 <sup>ii</sup>	0.88 (3)	1.97 (3)	2.841 (2)	170 (3)
O4–H4B...O1 <sup>iii</sup>	0.79 (3)	2.00 (3)	2.783 (2)	171 (2)

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

The H atoms attached to the amido N atom, the hydroxyl O atom and the water O atom were located in a difference map and refined freely with an isotropic model. All C-bound H atoms were positioned geometrically and refined as riding, with C–H = 0.93–0.96 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic CH})$  or  $1.5U_{\text{eq}}(\text{CH}_3)$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); 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, 1997); software used to prepare material for publication: SHELXTL.

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