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2′-(4-Hydroxybenzylidene)isonicotinohydrazide monohydrate

Xi-Shi Tai,[a,b]* Fan-Yuan Kong[a] and Jie Yin[c]

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, [b]NingXia Natural Gas Transfering Key Laboratory, NingXia University, Yinchuan 750021, People's Republic of China, and [c]College of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, People's Republic of China

Correspondence e-mail: taixishi@lzu.edu.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.108
Data-to-parameter ratio = 13.7

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

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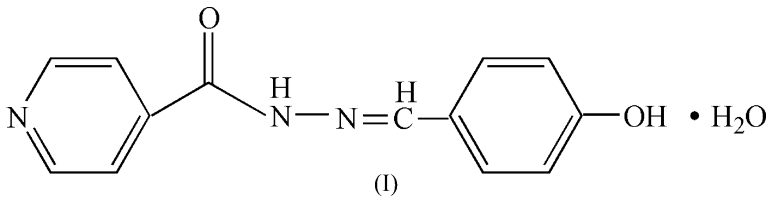
The bond lengths in the title compound, $C_{13}H_{11}N_3O_2\cdot H_2O$ indicate that the organic molecule exists in the keto form. A network of O—H···O, O—H···N and N—H···O hydrogen bonds helps to consolidate the crystal packing.

Comment

As part of our ongoing studies of the coordination chemistry of aroylhydrazone ligands (Tai *et al.*, 2003, 2004), the synthesis and structure of the title compound, (I), are now reported.



(I)

In the molecule of (I) (Fig. 1), the C6—O1 bond length of 1.238 (2) Å clearly corresponds to a C=O double bond, *i.e.* the molecule exists in the keto form. The dihedral angle between the N1/C1–C5 and C8–C13 mean planes is 12.58 (10)°. This twisting of the molecule may arise from its hydrogen-bonding requirement.

The component species of (I) interact by way of O—H···O, N—H···O and O—H···N hydrogen bonds (Table 1), leading to [001] columns of the organic species cross-linked by the water molecules.

Experimental

4-Hydroxybenzaldehyde (10 mmol) was added to a solution of isonicotinyl hydrazine (10 mmol) in ethanol (30 ml). The mixture was stirred continuously for 3 h under reflux, evaporating some ethanol. The product was then collected by filtration and dried *in vacuo* (yield 86%). Elemental analysis calculated for $C_{13}H_{13}N_3O_3$: C 60.23, H 5.02, N 16.26%; found: C 60.46, H 5.18, N 16.00%. IR (KBr disk): 3436 (*w*, N—H), 3280 (*m*, O—H), 1628 (*s*, C=O), 1553 (*m*, py-C=N). MS (FAB): 260 (*M*+1). Single crystals of (I) suitable for X-ray determination were obtained by evaporation of an ethanol solution over two weeks.

Crystal data

$C_{13}H_{11}N_3O_2\cdot H_2O$
M_r = 259.26
Orthorhombic, *Pbca*
a = 7.0488 (15) Å
b = 12.150 (3) Å
c = 28.649 (6) Å
V = 2453.6 (9) Å^3
Z = 8
D_x = 1.404 Mg m^{-3}
Mo *Kα* radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.972, T_{max} = 0.980
12855 measured reflections
2512 independent reflections
1253 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 0.96
2512 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O1^{i}	0.89 (3)	1.97 (3)	2.833 (2)	163 (2)
O3—H3A···N3^{ii}	0.83 (3)	2.49 (3)	3.212 (3)	146 (2)
O3—H3A···O1^{ii}	0.83 (3)	2.21 (3)	2.914 (2)	142 (2)
O2—H2···N1^{iii}	0.86 (3)	1.92 (3)	2.769 (2)	169 (3)
N2—H2B···O3	0.90 (2)	2.01 (2)	2.893 (3)	166.5 (19)

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

The O- and N-bound H atoms were located in difference maps and their positions were freely refined with the constraint U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O). The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); software used to prepare material for publication: *SHELXTL*.

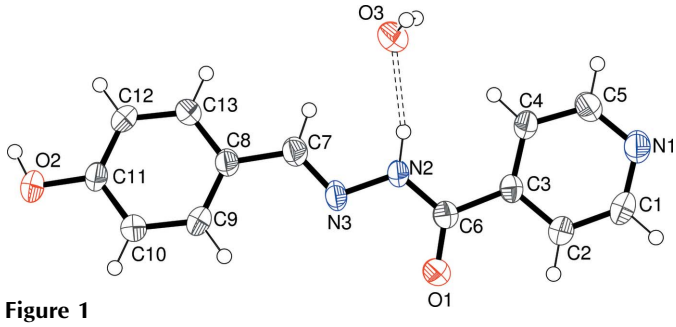


Figure 1
The molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). The dashed lines indicate a hydrogen bond.

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