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(*E*)-*N*′-(2-Methoxybenzylidene)isonicotinohydrazide dihydrate

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The title compound, $C_{14}H_{13}N_3O_2\cdot 2H_2O$, displays a *trans* configuration with respect to the C=N double bond. In the crystal structure, the molecules are linked through weak intermolecular O—H···O and O—H···N hydrogen bonds, forming a network structure.

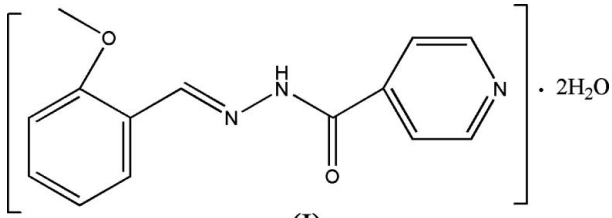
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.133
Data-to-parameter ratio = 13.1

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

Comment

Recently, we have reported the structures of a few Schiff base complexes (Qiu *et al.*, 2004; Zhu *et al.*, 2003). As an extension of our work on the structural characterization of Schiff base compounds, the title compound, (I), is reported here.



(I)

In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987). The C7=N2 bond length of 1.277 (2) Å conforms to the value for a double bond and agrees with the value of 1.269 (7) Å observed by us in a similar compound (Yang *et al.*, 2006). The N1—C8 bond length of 1.350 (2) Å is greater than the value for a double bond and less than the value for a single bond, owing to the effects of conjugation in the molecule. The dihedral angle [8.5 (2)°] between the benzene and pyridine ring planes is smaller than the values found in the structure cited above [39.1 (4) and 19.7 (4)°; Yang *et al.*, 2006]

In the crystal structure, the molecules are linked through weak intermolecular O—H···O and O—H···N hydrogen bonds, forming a network structure (Table 2 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. 2-Methoxybenzaldehyde (0.1 mmol, 14.2 mg) and isonicotinohydrazide (0.1 mmol, 13.4 mg) were dissolved in ethanol (95%, 10 ml). The reaction mixture was stirred for 20 min to give a clear solution. After allowing this solution to stand at room temperature in air for 10 d, large colourless crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator, using anhydrous $CaCl_2$ (yield 61%).

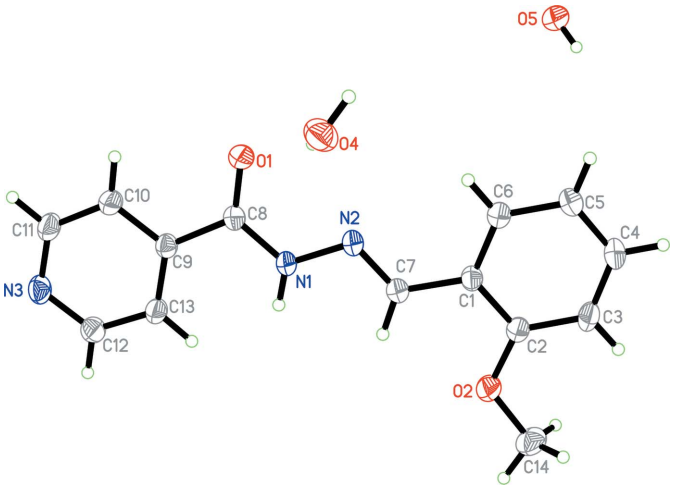


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

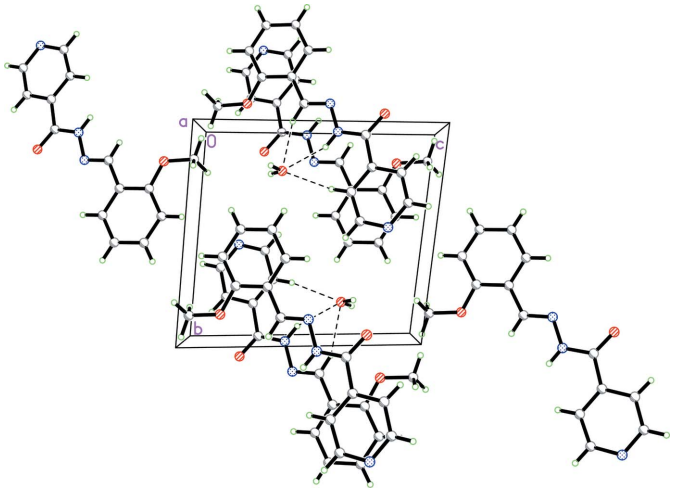


Figure 2
The crystal packing of (I), viewed approximately along the *a* axis. Dashed lines indicate intermolecular hydrogen bonds.

Crystal data

$C_{14}H_{13}N_3O_2\cdot 2H_2O$
$M_r = 291.31$
Triclinic, $P\overline{1}$
$a = 7.5279\ (5)$ Å
$b = 9.6929\ (6)$ Å
$c = 10.3980\ (7)$ Å
$\alpha = 92.308\ (3)^\circ$
$\beta = 100.340\ (3)^\circ$
$\gamma = 107.928\ (2)^\circ$
$V = 706.44\ (8)$ Å^3
$Z = 2$
$D_x = 1.369$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 298\ (2)$ K
Block, colourless
0.42 × 0.36 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.955$, $T_{max} = 0.981$
3933 measured reflections
2716 independent reflections
1966 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.133$
$S = 1.03$
2716 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.1327P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected torsion angles (°).

C8—N1—N2—C7	−178.75 (17)	C7—C1—C2—O2	−5.1 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···O4^{i}	0.81 (3)	1.98 (3)	2.786 (3)	175 (3)
O5—H5A···O1^{ii}	0.83 (3)	2.23 (3)	3.012 (3)	157 (3)
O4—H4B···O1	0.86 (3)	2.29 (3)	3.072 (3)	152 (3)
O4—H4A···N3^{iii}	0.84 (3)	2.14 (3)	2.922 (2)	154 (3)
N1—H1···O5^{iv}	0.86	2.16	2.965 (2)	157

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y-1, z$; (iv) $x, y+1, z$.

The water H atoms were located in a difference Fourier map and refined isotropically. All other H atoms were positioned geometrically and constrained to ride on their parent atoms, with Csp^2—H = 0.93 Å, C_{methyl}—H = 0.96 Å, N—H = 0.86 Å, and U_{iso}(H) = $1.2U_{eq}$(Csp^2, N) or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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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