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2′-(2-Hydroxy-3,5-diiodobenzylidene)isonicotinohydrazide methanol solvate

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In the title compound, $C_{13}H_9I_2N_3O_2 \cdot CH_3OH$, the Schiff base molecule displays a *trans* configuration with respect to the C═N double bond. The dihedral angle between the benzene and pyridine rings is 24.6 (2)°. The crystal structure is stabilized by intermolecular N—H⋯O, O—H⋯N and C—H⋯O hydrogen bonds, forming a network.

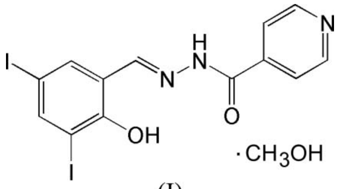
Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.093
Data-to-parameter ratio = 17.5

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

Comment

Compounds derived from the condensation reaction of aromatic carbaldehydes with hydrazides exhibit a wide range of biological activities and applications (Tarafder *et al.*, 2002; Cukurovali *et al.*, 2002; Ali *et al.*, 2002). The crystal structure of 2′-(2-hydroxy-3,5-diiodobenzylidene)isonicotinohydrazide methanol solvate, (I), is reported here.



(I)

The asymmetric unit of (I) comprises a Schiff base molecule and a methanol solvent molecule (Fig. 1), in which the bond lengths and bond angles are within normal ranges (Allen *et al.*, 1987) and comparable with those observed in similar compounds (Qiu *et al.*, 2006; Yang & Guo, 2006; Yang, 2006). The C7═N1 bond length of 1.275 (6) Å conforms to the value for a double bond, and is comparable with that in other Schiff bases (Qian *et al.*, 2006; Zhao, 2006). The C8—N2 bond length of 1.362 (6) Å is intermediate between those typical for the corresponding single and double bonds, suggesting some degree of delocalization in the acetohydrazide system. The molecule displays a *trans* configuration about the C═N and C—N bonds. The dihedral angle between the benzene ring and the pyridine ring is 24.6 (2)°.

The molecular structure is stabilized by an intramolecular O—H⋯N hydrogen bond (Table 1). In the crystal structure, molecules are linked through intermolecular O—H⋯N, N—H⋯O and C—H⋯O hydrogen bonds (Table 1), forming a network (Fig. 2).

Experimental

3,5-Diiodosalicylaldehyde (0.1 mmol, 36.9 mg) and pyridine-4-carboxylic acid hydrazide (0.1 mmol, 13.7 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for

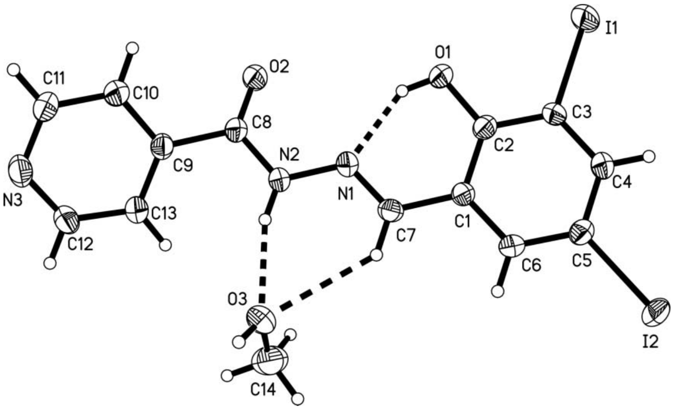


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown as dashed lines.

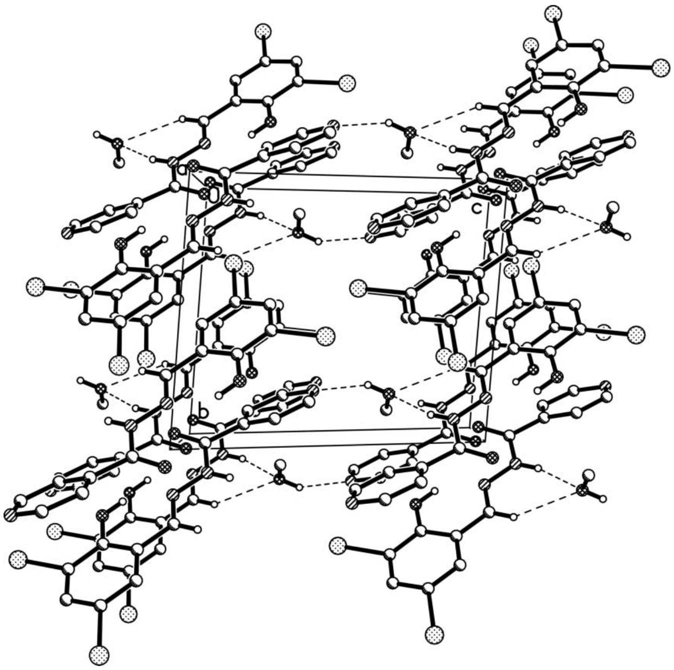


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

10 min to give a clear yellow solution. Crystals of (I) were formed by gradual evaporation of the solvent over 10 d at room temperature (yield 82.3%). Analysis found: C 32.17, H 2.59, N 7.87%; calculated for $C_{14}H_{13}I_2N_3O_3$: C 32.02, H 2.50, N 8.00%.

Crystal data

$C_{13}H_9I_2N_3O_2 \cdot CH_3OH$
$M_r = 525.07$
Triclinic, $P\overline{1}$
$a = 8.977$ (2) Å
$b = 9.114$ (3) Å
$c = 11.387$ (3) Å
$\alpha = 92.099$ (2)°
$\beta = 111.455$ (3)°
$\gamma = 95.638$ (2)°
$V = 860.2$ (4) Å^3
$Z = 2$
$D_x = 2.027$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.67$ mm^{-1}
$T = 298$ (2) K
Block, yellow
0.23 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.486$, $T_{\max} = 0.558$
(expected range = 0.450–0.517)
4887 measured reflections
3490 independent reflections
2579 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.093$
$S = 1.05$
3490 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 1.1556P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.96$ e Å^{-3}
$\Delta\rho_{\min} = -1.09$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯N1	0.82	1.84	2.555 (5)	146
N2—H2⋯O3	0.86	1.98	2.814 (6)	163
O3—H3⋯N3$^{\rm i}$	0.82	2.04	2.786 (6)	152
C7—H7⋯O3	0.93	2.56	3.305 (5)	138

Symmetry code: (i) $-x, -y, -z + 1$.

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with O—H = 0.82, N—H = 0.86 and C—H = 0.93–0.96 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C,N) or $1.5U_{\rm eq}$(methyl C and O). The deepest residual electron density hole is located 0.91 Å from atom I1.

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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