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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.043
 wR factor = 0.114
Data-to-parameter ratio = 7.2

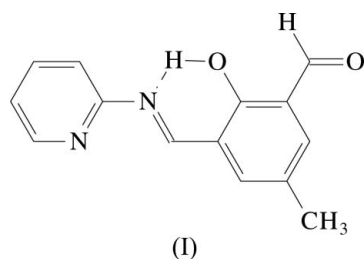
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

(*E*)-2-Hydroxy-5-methyl-3-[(2-pyridylimino)-methyl]benzaldehyde

The title compound, $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$, is stabilized in the solid state as an enol–imine tautomer, with a strong intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond, one $\text{C}-\text{H}\cdots\text{N}$ and three $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds, generating edge-fused $[S(6)R_2^2(8)R_2^2(8)R_1^2(6)]$ motifs. The molecule is approximately planar, with a dihedral angle of $4.40(10)^\circ$ between the two aromatic rings.

Comment

Schiff bases are used as substrates in the preparation of a number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Moreover, Schiff bases are also known to have biological activities, such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh & Dash, 1988), antitumour (Hodnett & Dunn, 1970; Desai *et al.*, 2001) and herbicidal properties (Holla *et al.*, 2000). Schiff bases have also been employed as ligands for the complexation of metal ions (Odabaşoğlu *et al.*, 2007; Aydoğan *et al.*, 2001). On the industrial scale, they have a wide range of applications, such as dyes and pigments (Taggi *et al.*, 2002). In continuation of our work on Schiff bases (Yathirajan *et al.*, 2007; Odabaşoğlu *et al.*, 1999, 2003, 2004, 2005*a,b*, 2006, 2007; Ersanlı *et al.*, 2003), the title new Schiff base, (I), was synthesized and its crystal structure is reported (Fig. 1, Table 1).



There are two possible types of intramolecular hydrogen bonds in salicylaldehyde Schiff bases, as exhibited by the keto–amine ($\text{N}\cdots\text{H}-\text{O}$) and enol–imine ($\text{N}-\text{H}\cdots\text{O}$) tautomeric forms. Salicylaldehyde Schiff bases have been found in the keto form (Odabaşoğlu *et al.*, 2003), in the enol form (Leardini *et al.*, 1998; Odabaşoğlu *et al.*, 2005*b*) and as enol/keto mixtures (Nazır *et al.*, 2000). The present X-ray crystallographic investigation shows that compound (I) prefers the enol–imine tautomeric form.

Compound (I) displays a strong intramolecular hydrogen bond (Table 2) involving atoms N1 and O1, a common feature of salicylidene systems. In (I), molecules are linked through an $\text{O}-\text{H}\cdots\text{N}$ intramolecular hydrogen bond, and molecules are

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linked through three C—H...O and one C—H...N intermolecular hydrogen bonds. These hydrogen bonds generate edge-fused $[S(6)R_2^2(8)R_2^2(8)R_2^1(6)]$ motifs (Etter, 1990) (Fig. 2 and Table 2). The molecule is almost planar, with dihedral angles of $0.47(8)^\circ$ between the C1–C6 ring and the intramolecularly hydrogen-bonded ring, and $4.40(10)^\circ$ between the hydrogen-bonded ring and the pyridyl ring.

Experimental

A mixture of 5-hydroxy-2-methylisophthalaldehyde (2.58 g, 0.01 mol) and pyridin-2-amine (0.94 g, 0.01 mol) in absolute ethanol (20 ml) containing two drops of 4 M sulfuric acid was refluxed for about 4 h. On cooling, the solid which separated was filtered off and recrystallized from ethanol (m.p. 393–395 K). Analysis for $C_{14}H_{12}N_2O_2$: found (calculated): C 69.83 (69.99), H 4.96 (5.03), N 11.52% (11.66%).

Crystal data

$C_{14}H_{12}N_2O_2$	$V = 606.72(10) \text{ \AA}^3$
$M_r = 240.26$	$Z = 2$
Monoclinic, Pc	Mo $K\alpha$ radiation
$a = 7.4049(8) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 4.2957(3) \text{ \AA}$	$T = 296 \text{ K}$
$c = 20.154(2) \text{ \AA}$	$0.56 \times 0.27 \times 0.18 \text{ mm}$
$\beta = 108.847(8)^\circ$	

Data collection

Stoe IPDSII diffractometer	10246 measured reflections
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	1184 independent reflections
$T_{\min} = 0.954$, $T_{\max} = 0.989$	853 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.100$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$	2 restraints
$wR(F^2) = 0.114$	H-atom parameters constrained
$S = 0.99$	$\Delta\rho_{\max} = 0.18 \text{ e \AA}^{-3}$
1184 reflections	$\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$
164 parameters	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1–C9	1.432 (5)	C9–N1	1.282 (4)
C2–O1	1.349 (4)	C10–N1	1.422 (4)
N1–C9–C1	121.9 (3)	C9–N1–C10	120.5 (3)
C1–C9–N1–C10	−177.8 (3)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1...N1	0.82	1.85	2.585 (3)	148
C9–H9...O2 ⁽ⁱ⁾	0.93	2.79	3.620 (4)	150
C14–H14...O1 ⁽ⁱ⁾	0.93	2.71	3.546 (5)	151
C6–H6...O2 ⁽ⁱ⁾	0.93	2.77	3.612 (4)	152
C7–H7...N2 ⁽ⁱⁱ⁾	0.93	2.73	3.606 (5)	158

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

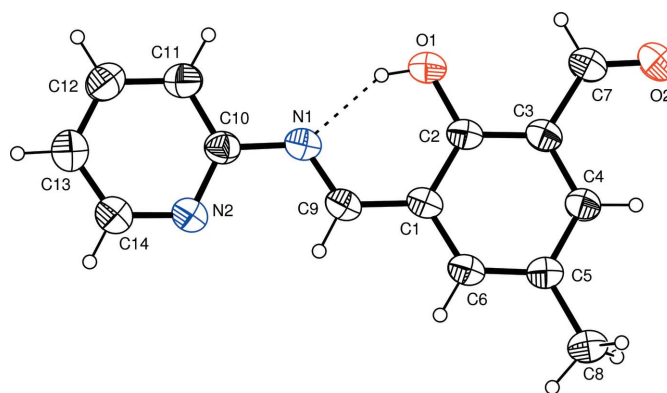


Figure 1

The molecular structure of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

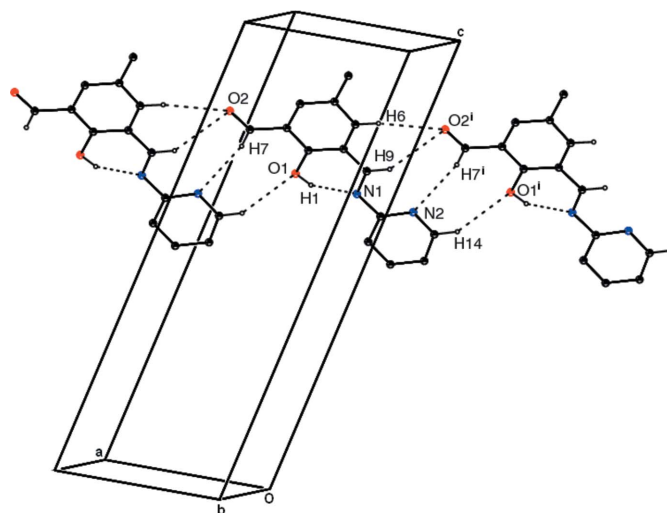


Figure 2

Part of the crystal structure of (I). For the sake of clarity, H atoms not involved in the hydrogen-bonding motifs have been omitted. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) $1 - x, 1 - y, z$.]

In the absence of significant anomalous scattering effects, 160 Friedel pairs were merged. All H atoms were treated as riding on their parent atoms, with C–H = 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ for aromatic, aldehydic and imino H, with C–H = 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H, and with O–H = 0.82 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ for the H atom of the hydroxyl group.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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