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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.039
 wR factor = 0.107
Data-to-parameter ratio = 14.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-Hydroxy-4-methoxybenzaldehyde
(pyridine-2-carbonyl)hydrazoneThe molecule of the title compound, $\text{C}_{14}\text{H}_{13}\text{N}_3\text{O}_3$, is nearly planar. The crystal structure is stabilized mainly through intermolecular $\text{O}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds

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Comment

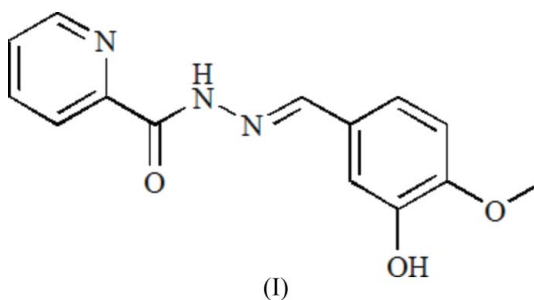
Schiff bases have received considerable attention because of their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). A series of carboxyl hydrazone complexes, similar to the title compound, has been reported previously (Yu *et al.*, 2005; Pan & Yang, 2005*a,b*).

Fig. 1 shows the molecular structure of (I). The molecule is nearly planar, with an r.m.s. deviation of 0.0462 (2) Å, which means that there is extensive $p-\pi$ and $\pi-\pi$ conjugation through the whole molecule. An intermolecular $\text{O}2-\text{H}2\text{B}\cdots\text{O}1^{\text{ii}}$ [(ii): $1-x, 2-y, 1-z$] hydrogen bond exists between the hydroxy H atom and the carbonyl O atom, resulting in a centrosymmetric dimer. An intramolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bond (Fig. 1) also promotes planarity of the molecular backbone. In addition, intermolecular $\text{N}2-\text{H}2\text{A}\cdots\text{O}3^{\text{i}}$ and $\text{C}7-\text{H}7\cdots\text{O}3^{\text{i}}$ [(i): $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$] hydrogen bonds involving the methoxy atom (Table 2) form a six-membered ring described by the graph-set descriptor $R_2^1(6)$, linking the dimers in the bc plane (Fig. 2).

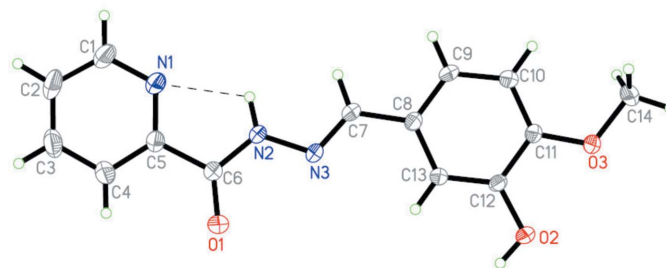


Figure 1

A view of the molecule of (I), showing the atom-labelling scheme and an intramolecular hydrogen bond (dashed line). Displacement ellipsoids are drawn at the 30% probability level.

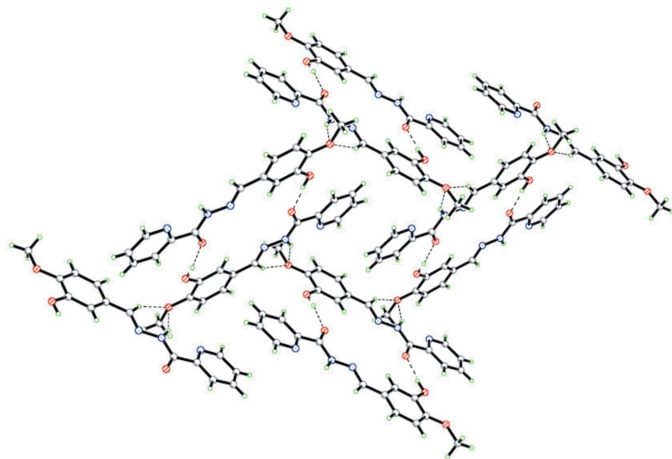


Figure 2
The packing of (I), viewed along the *a* axis, showing the intermolecular hydrogen bonding interactions (dashed lines).

Experimental

The title compound was synthesized according to the method of Yu *et al.* (2005). Single crystals of (I), suitable for X-ray diffraction, were obtained by recrystallization from an ethanol-water solution (2:1 *v/v*).

Crystal data

$C_{14}H_{13}N_3O_3$	$D_x = 1.344 \text{ Mg m}^{-3}$
$M_r = 271.27$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3286 reflections
$a = 7.515$ (3) Å	$\theta = 2.2\text{--}26.4^\circ$
$b = 13.590$ (5) Å	$\mu = 0.10 \text{ mm}^{-1}$
$c = 13.172$ (5) Å	$T = 294$ (2) K
$\beta = 94.689$ (7)°	Block, colourless
$V = 1340.6$ (9) Å ³	$0.24 \times 0.22 \times 0.18 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2744 independent reflections
φ and ω scans	2124 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{\text{int}} = 0.028$
$T_{\text{min}} = 0.970$, $T_{\text{max}} = 0.983$	$\theta_{\text{max}} = 26.5^\circ$
7403 measured reflections	$h = -9 \rightarrow 4$
	$k = -16 \rightarrow 16$
	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.4125P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
2744 reflections	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
191 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.072 (4)

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.2286 (18)	N3—C7	1.2745 (19)
N2—N3	1.3881 (17)	C7—C8	1.457 (2)
C6—N2—N3	121.83 (13)	N3—C7—C8	123.17 (13)
C7—N3—N2	113.58 (12)	C6—N2—N3—C7	−177.77 (14)
C6—N2—N3—C7	−177.77 (14)	N1—C5—C6—O1	171.67 (15)
C5—N1—C1—C2	−0.8 (3)	N2—N3—C7—C8	179.82 (13)
N3—N2—C6—O1	−2.8 (2)	N3—C7—C8—C13	6.5 (2)
N3—N2—C6—C5	176.80 (13)		

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

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N2—H2A \cdots O3 ⁱ	0.89 (2)	2.26 (2)	3.093 (2)	155 (2)
O2—H2B \cdots O1 ⁱⁱ	0.87 (2)	1.85 (2)	2.722 (2)	173 (2)
C7—H7 \cdots O3 ⁱ	0.93	2.33	3.203 (2)	155
N2—H2A \cdots N1 ⁱⁱⁱ	0.89 (2)	2.18 (2)	2.629 (2)	110 (1)

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) x, y, z .

All H atoms bound to C were positioned geometrically and allowed to ride on their parent atoms, with $d(C\text{—}H) = 0.93$ Å for aromatic C and $d(C\text{—}H) = 0.96$ Å for methyl C, $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ for aromatic C and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$ for methyl C. The H atoms attached to the amido N atom and the hydroxy O atom were located in a difference map, and refined as riding with $N2\text{—}H2A = 0.892$ Å and $O2\text{—}H2B = 0.871$ Å. The U_{iso} values for H2A and H2B were refined freely.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

References

- Bruker (1997). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Hadjoudis, E., Vittorakis, M. & Moustakali-Mavridis, J. (1987). *Tetrahedron*, **43**, 1345–1360.
- Pan, F. Y. & Yang, J. G. (2005a). *Acta Cryst.* **E61**, o354–o355.
- Pan, F. Y. & Yang, J. G. (2005b). *Acta Cryst.* **E61**, o352–o353.
- Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
- Yu, M., Chen, X. & Jing, Z. L. (2005). *Acta Cryst.* **E61**, o1345–o1346.