

**(E)-N-Benzoyl-N'-(3-hydroxy-4-methoxybenzylidene)hydrazine****Jun Shi**

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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 = 0.045  
 $wR$  factor = 0.120  
 Data-to-parameter ratio = 15.3

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

The molecule of the title compound,  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_3$ , is non-planar. The asymmetric unit contains two independent molecules which are quite distinct from each other. Two bifurcated intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds help to establish the molecular conformation and consolidate the crystal packing.

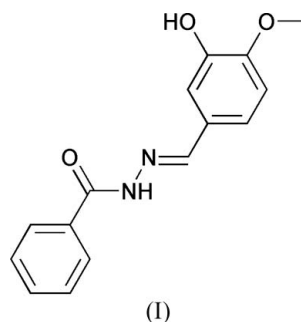
Received 18 October 2005

Accepted 25 October 2005

Online 31 October 2005

**Comment**

Metal complexes based on Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.*, 2001). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I) (Fig. 1).



The asymmetric unit of (I) contains two independent molecules which are quite distinct from each other. In molecule 1, the isovanillin group (C2–C8/O1/O2) is planar, with an r.m.s. deviation,  $\delta$ , from the mean plane of 0.020 (2) Å, and it makes a dihedral angle of 74.12 (5)° with the benzene C10–C15 ring. In molecule 2, the isovanillin group (C2–C8/O1/O2) is also planar, with  $\delta = 0.020$  (2) Å, but it makes a dihedral angle of 24.34 (8)° with the C25–C30 benzene ring. The isovanillin groups of the two independent molecules are almost perpendicular to each other, with a dihedral angle of 87.72 (4)°, while the dihedral angle between the two benzene rings is 14.05 (10)°.

Two bifurcated intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and two intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds are found (Table 1), which help to establish the molecular conformation and consolidate the crystal packing (Fig. 2).

**Experimental**

An anhydrous ethanol solution of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added to an anhydrous ethanol solution of benzoylhydrazine (1.36 g, 10 mmol) and the mixture

stirred at 350 K for 5 h under nitrogen, whereupon a pale-yellow precipitate appeared. The product was then isolated, recrystallized from ethanol, and dried in vacuum to give the pure compound in 86% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{15}H_{14}N_2O_3$   
 $M_r = 270.28$   
 Monoclinic,  $P2_1/c$   
 $a = 7.5209(10) \text{ \AA}$   
 $b = 19.221(3) \text{ \AA}$   
 $c = 18.971(3) \text{ \AA}$   
 $\beta = 96.265(2)^\circ$   
 $V = 2726.1(7) \text{ \AA}^3$   
 $Z = 8$

$D_x = 1.317 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 4256 reflections  
 $\theta = 2.4\text{--}26.3^\circ$   
 $\mu = 0.09 \text{ mm}^{-1}$   
 $T = 294(2) \text{ K}$   
 Block, colorless  
 $0.28 \times 0.20 \times 0.16 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.968, T_{\max} = 0.985$   
 15237 measured reflections

5591 independent reflections  
 3644 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$   
 $\theta_{\text{max}} = 26.4^\circ$   
 $h = -8 \rightarrow 9$   
 $k = -19 \rightarrow 24$   
 $l = -21 \rightarrow 23$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.121$   
 $S = 1.01$   
 5591 reflections  
 365 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.3319P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2\cdots O3^i$	0.82	1.85	2.6739 (17)	180
$O5-H5\cdots O6^{ii}$	0.82	1.94	2.7521 (18)	175
$N2-H2A\cdots O4^{iii}$	0.86	2.21	2.867 (2)	133
$N2-H2A\cdots O5^{iii}$	0.86	2.51	3.326 (2)	158
$N4-H4\cdots O1^{iv}$	0.86	2.26	3.0206 (19)	147
$N4-H4\cdots O2^{iv}$	0.86	2.60	3.309 (2)	140

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

All H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C—H, O—H and N—H bond lengths and  $U_{\text{iso}}(\text{H})$  values are as follows: aromatic C—H = 0.93  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ; methyl C—H = 0.96  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ ; O—H = 0.82  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ ; N—H = 0.86  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ .

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

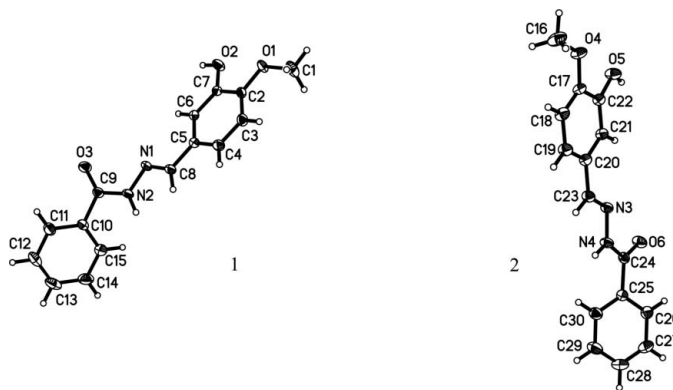


Figure 1 The structure of the asymmetric unit of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

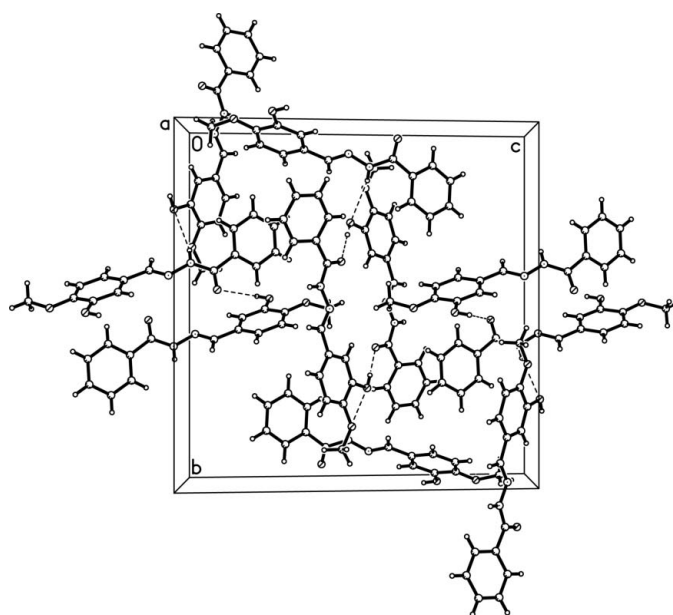


Figure 2 Packing diagram of (I), showing intermolecular hydrogen bonds (dashed lines).

References

Bruker (1999). SMART (Version 5.0) and SAINT (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.  
 Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997b). SHELXTL for Windows NT. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.