organic papers

# N′-(3-Hydroxybenzylidene)-2-methoxy-benzohydrazide

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Key indicators

Single-crystal X-ray study
$T = 294$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 12.7

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

In the crystal structure of the title compound, $C_{15}H_{14}N_2O_3$, molecules are connected *via* weak intermolecular O—H···O and C—H···O hydrogen-bonding interactions, forming a zigzag form.

Comment

Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). A knowledge of the ligand structure is important in understanding the coordination potential of these ligands. Investigation of their crystal structures may provide useful information concerning their physical and chemical properties. In the present study, we report the synthesis and structure of the title compound, (I).

(I)
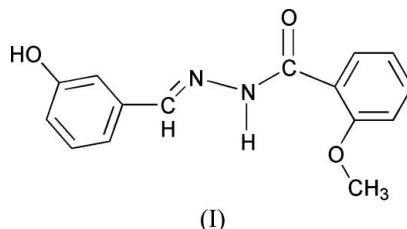
In the molecular structure of (I) (Fig. 1), the values of the geometric parameters of (I) are normal. The Schiff base is nearly planar, with deviations of −0.178 (1), −0.140 (1), 0.168 (2), 0.133 (2), −0.111 (1), 0.100 (1) and 0.100 (1) Å for O1, O2, C4, C5, C8, C9 and C(10, respectively. The benzene rings (C2–C7) and (C10–C15) make a dihedral angle of 2.08 (7)° with each other. An intramolecular N—H···O hydrogen-bonding interaction stabilizes the molecular conformation, while intermolecular O—H···O and C—H···O hydrogen-bonding interactions stabilize the crystal structure (Table 1). The molecules associate in a zigzag pattern along the *b* axis, forming a supramolecular structure, as illustrated in Fig. 2.

Experimental

An anhydrous ethanol solution (50 ml) of 3-hydroxybenzaldehyde (1.22 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 2-methoxybenzhydrazide (1.66 g, 10 mmol) and the mixture was stirred at 330 K for 8 h under N_2, yielding a yellow solution. The solvent was removed and the residue recrystallized from *N,N*-dimethylformamide. The product was isolated and then dried *in vacuo* to give pure (I) in 93% yield. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an *N,N*-dimethylformamide solution.
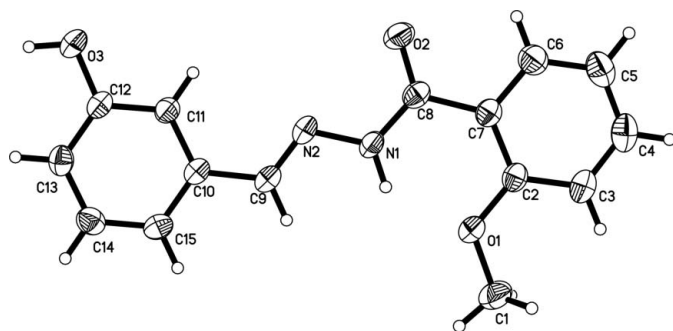
Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_{15}H_{14}N_2O_3$	$Z = 4$
$M_r = 270.27$	$D_x = 1.316$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.2127$ (12) Å	$\mu = 0.09$ mm^{-1}
$b = 7.9412$ (7) Å	$T = 294$ (2) K
$c = 14.4446$ (13) Å	Block, yellow
$\beta = 115.8150$ (10)°	$0.36 \times 0.28 \times 0.12$ mm
$V = 1364.3$ (2) Å^3	

Data collection

|	
Bruker SMART CCD area detector diffractometer	7204 measured reflections
φ and ω scans	2407 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1780 reflections with $I > 2\sigma(I)$
$T_{min} = 0.967$, $T_{max} = 0.989$	$R_{int} = 0.018$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.0805P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.098$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.12$ e Å^{-3}
2407 reflections	$\Delta\rho_{min} = -0.19$ e Å^{-3}
189 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1⋯O1	0.904 (15)	1.933 (15)	2.6355 (14)	133.2 (12)
O3—H3⋯O2^i	0.93 (2)	1.83 (2)	2.7294 (15)	162.2 (19)
O3—H3⋯N2^i	0.93 (2)	2.58 (2)	3.1244 (15)	117.7 (16)
C9—H9⋯O3^{ii}	0.93	2.54	3.3430 (17)	146

Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.
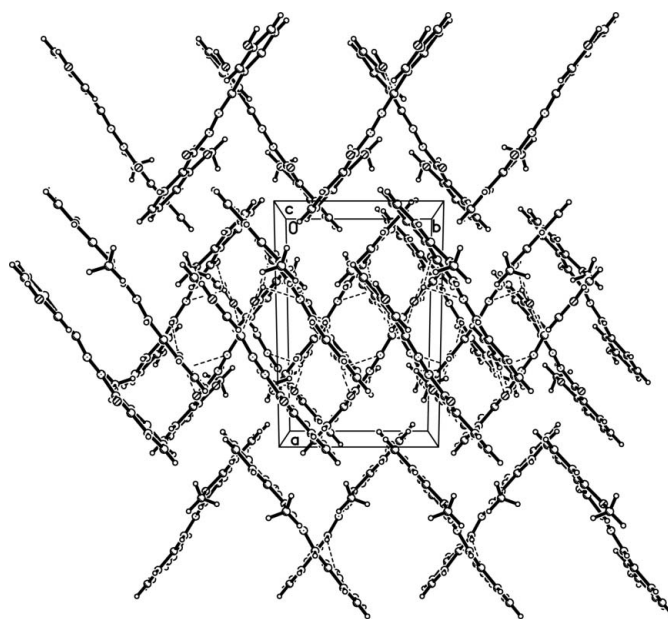
Figure 2
Packing view of (I) along the *c* axis, showing intermolecular hydrogen bonds (dashed lines).

H atoms bonded to C atoms were included in calculated positions and refined using a riding-model approximation with C—H(aromatic) = 0.93 Å, C—H(methyl) = 0.96 Å, and with U_{iso}(H) = $1.2U_{eq}$(C) for aromatic H and U_{iso}(H) = $1.5U_{eq}$(C) for methyl H. The atoms of the NH and OH groups were found a difference Fourier map and refined freely.

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

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