Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-*N*′-(4-Benzoyloxy-3-methoxybenzylidene)-2-methoxybenzohydrazide monohydrate

Jian-Rong Han,[a]* Xiao-Feng Wang,[b] Xiao-Li Zhen,[a] Xia Tian[a] and Shou-Xin Liu[c]‡

[a]College of Sciences, Hebei University of Science & Technology, Shijiazhuang 050018, People's Republic of China, [b]Shijiazhuang Pharmaceutical Group Ouyi Pharmaceutical Co Ltd, Shijiazhuang 050051, People's Republic of China, and [c]College of Chemical & Pharmaceutical Engineering, Hebei University of Science & Technology, Shijiazhuang 050018, People's Republic of China

‡ Additional contact author, e-mail address liu_shouxin@163.com

Correspondence e-mail: han_jianrong@163.com

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.114
Data-to-parameter ratio = 15.2

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

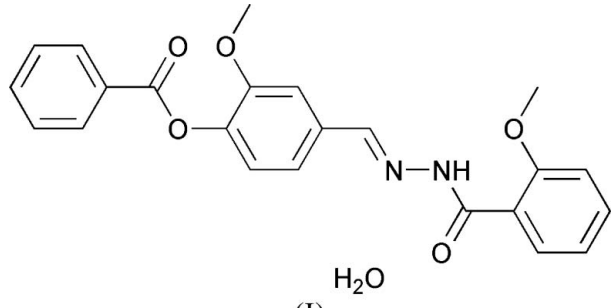
© 2006 International Union of Crystallography
All rights reserved

Received 7 November 2006
Accepted 8 November 2006

In the title compound, $C_{23}H_{22}N_2O_6$, the vanillin group makes dihedral angles of 81.15 (6) and 23.52 (7)°, respectively, with the phenyl ring and the benzohydrazide mean plane. An intramolecular N—H···O hydrogen bond helps to stabilize the molecular conformation, while the water molecule interacts with the organic molecule by way of a bifurcated O—H···(O,N) interaction.

Comment

There has been a steady growth of interest in the synthesis, structure, and reactivity of Schiff bases due to their potential applications in areas such as biological modelling, catalysis, and as molecular magnets (Jones *et al.*, 1979; Larson & Pecoraro, 1991). 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).



(I)

In (I) (Fig. 1), the vanillin group (atoms C8–C13/C15/O2/O3) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.015 Å. This plane makes dihedral angles of 23.52 (7) and 81.15 (6)°, respectively, with the benzohydrazide ring (atoms C17–C22) and the C1–C6 phenyl ring. The dihedral angle between the C1–C6 and C17–C22 mean planes is 59.63 (8)°. All other bond lengths and angles for (I) are within their normal ranges (Allen *et al.*, 1987).

An intramolecular hydrogen bond links the NH group to O5, thereby influencing the molecular conformation. A bifurcated O—H···(N,O) intermolecular hydrogen bond links the water molecule to the organic molecule (Table 1). The other water H atom participates in an O—H···O hydrogen bond to an adjacent organic molecule, resulting in dimeric associations of two organic molecules and two water mol-

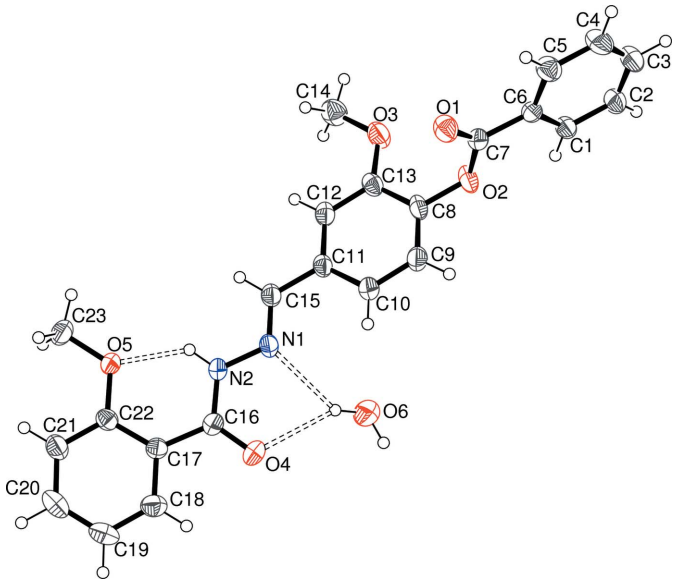


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level and hydrogen bonds indicated by dashed lines.

ecules (Fig. 2). A weak intermolecular C—H···O interaction is also present.

Experimental

An anhydrous ethanol solution (50 ml) of 4-formyl-2-methoxyphenyl benzoate (2.56 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 2-methoxybenzohydrazide (1.66 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a pale-yellow precipitate. The product was isolated, recrystallized from acetonitrile and then dried in a vacuum to give the pure compound in 78% yield. Pale-yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{23}H_{20}N_2O_5\cdot H_2O$
M_r = 422.43
Monoclinic, $P2_1/c$
a = 7.9685 (15) Å
b = 18.584 (3) Å
c = 14.205 (3) Å
β = 91.045 (4)°
V = 2103.2 (7) Å^3
Z = 4
D_x = 1.334 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, pale yellow
0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.981
11792 measured reflections
4281 independent reflections
1915 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
S = 1.03
4281 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

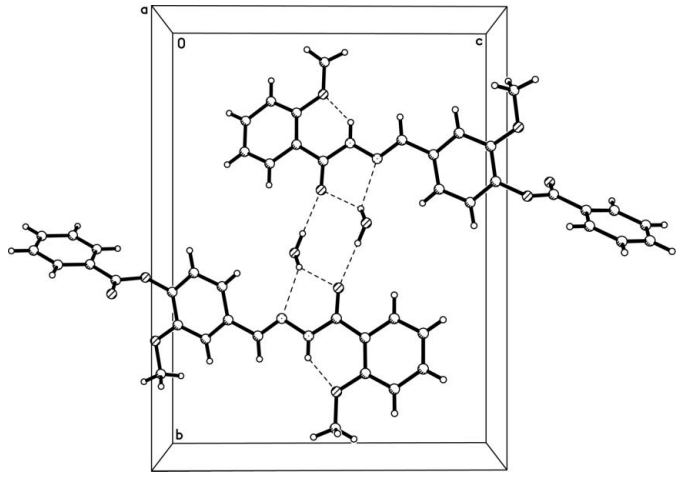


Figure 2
A packing diagram for (I), with hydrogen bonds shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O5	0.86	1.95	2.617 (2)	133
O6—H6A···O4^{i}	0.87	1.95	2.814 (2)	179
O6—H6B···N1	0.86	2.32	3.050 (2)	142
O6—H6B···O4	0.86	2.34	3.108 (3)	148
C15—H15···O1^{ii}	0.93	2.52	3.380 (3)	155

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

The H atoms were included in calculated positions (C—H = 0.93–0.96 Å, O—H = 0.85 Å and N—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N,O) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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*.

The project was supported by the Foundation of the Education Department of Hebei Province (grant No. 606022).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
Jones, R. D., Summerville, D. A. & Basolo, F. (1979). *Chem. Rev.* **17**, 139–179.
Larson, E. J. & Pecoraro, V. L. (1991). *J. Am. Chem. Soc.* **113**, 3810–3818.
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. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.