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N′-(4-Hydroxybenzylidene)benzohydrazide dimethylformamide solvate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.149
Data-to-parameter ratio = 15.7

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

The components of the title solvate structure, $C_{14}H_{12}N_2O_2\cdot C_3H_7NO$, are connected *via* N—H···O, O—H···N and O—H···O hydrogen bonds, leading to a chain motif.

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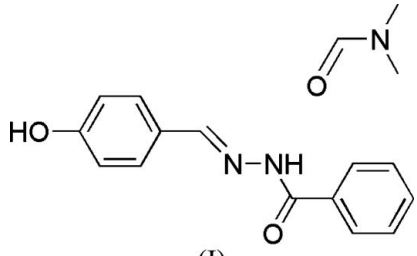
Comment

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, the present study details the crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) comprises one moelcule each of *N*′-(4-hydroxybenzylidene)benzohydrazide and dimethylformamide (Fig. 1). The key N1—N2, N1═C7 and C6—C7 bond lengths are 1.384 (3), 1.274 (3) and 1.465 (3) Å, respectively, which are consistent with those found in 2-hydroxy-3-methoxybenzaldehyde 2,4-dinitrophenylhydrazone (Jing *et al.*, 2005). The non-H atoms of the phenol group are coplanar, with an r.m.s. deviation of 0.017 Å, and similarly the r.m.s. deviation of the N1/N2/C8–C14/O2 atoms from their least-squares plane is 0.073 Å. The dihedral angle between the

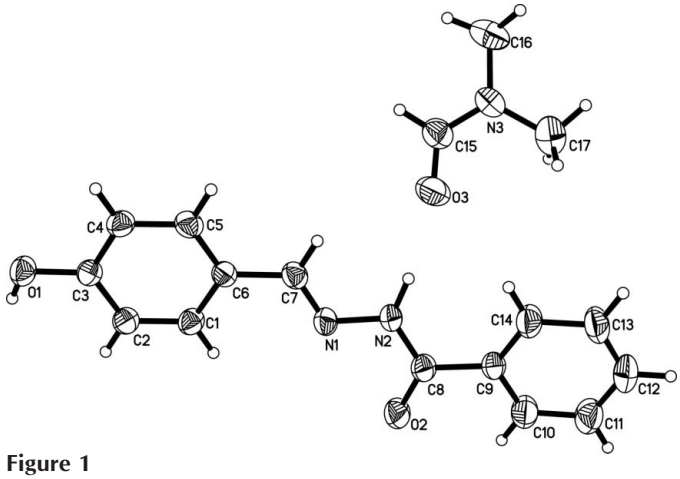


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level.

aformentioned planes is 8.17 (10)°. Intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds stabilize the crystal packing (Fig. 2). As detailed in Table 1, the H atom on O1 forms a strong interaction with atom O2^{i} and these extend along the *b* axis to form a chain [symmetry code: (i) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$]. Additional stabilization of the chain is afforded by somewhat weaker O1—H···N2^{i} interactions. In this sense, the hydroxyl H atom might be thought of as being bifurcated. The dimethylformamide molecules are connected to this chain *via* N—H···O3 interactions.

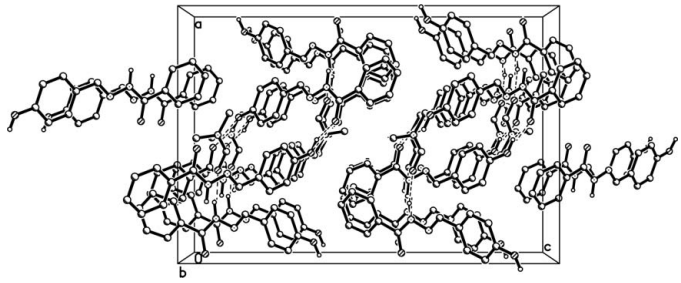


Figure 2
A view of the crystal packing in (I); hydrogen-bonding interactions are shown as dashed lines.

Experimental

An anhydrous ethanol solution of 4-hydroxybenzaldehyde (1.22 g, 10 mmol) was added to an anhydrous ethanol solution of benzohydrazide (1.36 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, whereupon a yellow precipitate appeared. The product was isolated, recrystallized from ethanol and then dried *in vacuo* to give pure compound (I) in 87% yield; m.p. 504 K, literature 502 K (Kaupp *et al.*, 2000). Bright-yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution.

Crystal data

$C_{14}H_{12}N_2O_2\cdot C_3H_7NO$
$M_r = 313.35$
Orthorhombic, *Pbca*
$a = 15.518$ (3) Å
$b = 9.3215$ (18) Å
$c = 22.942$ (5) Å
$V = 3318.4$ (11) Å^3
$Z = 8$
$D_x = 1.254$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2528 reflections
$\theta = 2.7$–$22.5°$
$\mu = 0.09$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.30 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1997)
$T_{min} = 0.932$, $T_{max} = 0.983$
17730 measured reflections
3424 independent reflections
1576 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 26.5°$
$h = -19 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.149$
$S = 0.98$
3424 reflections
218 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.9554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0099 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.91 (3)	2.64 (4)	3.316 (3)	132 (3)
O1—H1···O2^{i}	0.91 (3)	1.81 (4)	2.677 (3)	158 (3)
N2—H2···O3	0.97 (3)	1.91 (3)	2.864 (3)	166 (2)

Symmetry code: (i) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

C-bound H atoms were included in the riding-model approximation, with C—H bond lengths of 0.93 (aromatic) and 0.96 Å (methyl), and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C), respectively. The O- and N-bound H atoms were refined freely (see Table 1).

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, 1999); software used to prepare material for publication: *SHELXTL*.

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