

Shu-Sheng Zhang, Yong-Hong Wen,* Mao-Jie Li and Xue-Mei Li

College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.063
 wR factor = 0.142
Data-to-parameter ratio = 8.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N'*-(2-Hydroxybenzylidene)-2-(quinolin-8-yloxy)-acetohydrazide monohydrate

In the title compound, $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_3 \cdot \text{H}_2\text{O}$, the dihedral angle between the planes of the benzene ring and the quinoline ring system is $26.6(2)^\circ$. Each solvent water molecule is linked to two acetohydrazide molecules *via* intermolecular $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, forming chains along $[010]$.

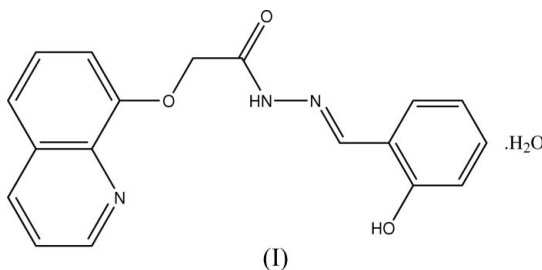
Received 29 September 2005

Accepted 10 October 2005

Online 15 October 2005

Comment

Recently, we have reported the structure of *N'*-(2-fluorobenzylidene)-2-(quinolin-8-yloxy)acetohydrazide methanol solvate (Wen *et al.*, 2005). We now report here the crystal structure of the title compound, (I).



The bond lengths and angles in (I) (Table 1) are comparable with those in the above fluoro-derivative (Wen *et al.*, 2005). The $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_3$ molecule is non-planar (Fig. 1). The dihedral angle between the planes of the benzene ring and the quinoline ring system is $26.6(2)^\circ$.

Intramolecular $\text{O}3-\text{H}3 \cdots \text{N}3$ and $\text{N}2-\text{H}2 \cdots \text{O}1$ hydrogen bonds generate rings of graph-set motifs $S(6)$ and $S(5)$, respectively (Bernstein *et al.*, 1995). Each water molecule is linked to two $\text{C}_{18}\text{H}_{15}\text{N}_3\text{O}_3$ molecules *via* intermolecular $\text{N}2-\text{H}2 \cdots \text{O}1\text{W}$, $\text{O}1\text{W}-\text{H}2\text{W}1 \cdots \text{N}1$ and $\text{O}1\text{W}-\text{H}1\text{W}1 \cdots \text{O}2^i$ hydrogen bonds [symmetry code: (i) $-x, y - \frac{1}{2}, \frac{1}{2} - z$; Table 2], to form chains along $[010]$ (Fig. 2).

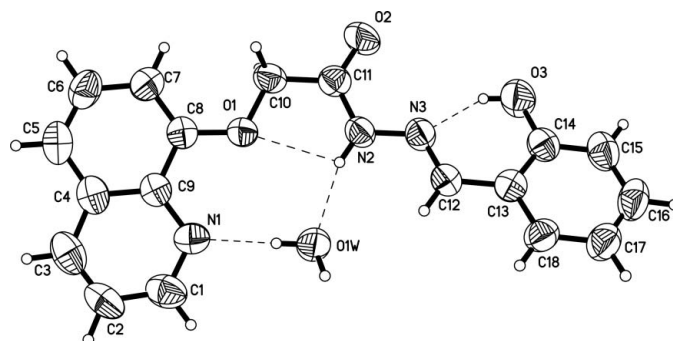


Figure 1

The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines represent hydrogen bonds.

Experimental

Compound (I) was prepared according to the method of Wen *et al.* (2005). Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a tetrahydrofuran–methanol (1:2 *v/v*) solution over a period of 7 d.

Crystal data

$C_{18}H_{15}N_3O_3 \cdot H_2O$
 $M_r = 339.35$
 Orthorhombic, $P2_12_12_1$
 $a = 4.6661$ (12) Å
 $b = 15.110$ (4) Å
 $c = 23.314$ (6) Å
 $V = 1643.7$ (7) Å³
 $Z = 4$
 $D_x = 1.371$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 1233 reflections
 $\theta = 2.7$ – 20.9°
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
 Rod, colourless
 $0.43 \times 0.11 \times 0.09$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.959$, $T_{\max} = 0.991$
 9129 measured reflections

1924 independent reflections
 1317 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.116$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -5 \rightarrow 5$
 $k = -18 \rightarrow 18$
 $l = -19 \rightarrow 28$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.143$
 $S = 1.12$
 1924 reflections
 235 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.0947P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1–C8	1.366 (5)	N2–C11	1.354 (5)
O1–C10	1.426 (5)	N2–N3	1.376 (5)
O2–C11	1.219 (5)	N3–C12	1.278 (5)
O3–C14	1.364 (5)	C10–C11	1.491 (6)
C8–O1–C10	117.1 (3)	O2–C11–N2	123.0 (4)
C11–N2–N3	117.3 (3)	N2–C11–C10	117.7 (4)
C12–N3–N2	117.5 (3)		
C11–N2–N3–C12	169.5 (4)	O1–C10–C11–N2	−1.5 (6)
C10–O1–C8–C7	−7.2 (6)	N2–N3–C12–C13	179.2 (3)
C8–O1–C10–C11	176.8 (3)	N3–C12–C13–C14	−5.4 (6)
N3–N2–C11–C10	179.2 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3–H3 ⁱ ···N3 ⁱ	0.82	1.89	2.610 (5)	146
N2–H2 ⁱ ···O1 ⁱ	0.86	2.33	2.687 (5)	105
N2–H2 ⁱ ···O1W ⁱ	0.86	1.96	2.789 (5)	162
O1W–H1W1 ⁱ ···O2 ⁱⁱ	0.84 (4)	2.01 (3)	2.824 (4)	166 (6)
O1W–H2W1 ⁱ ···N1 ⁱ	0.84 (4)	1.91 (4)	2.755 (5)	178 (4)

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

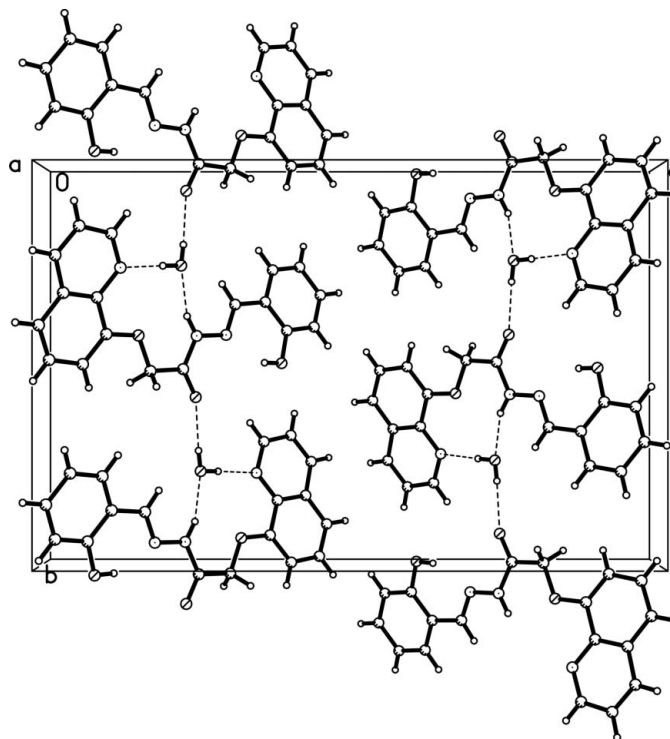


Figure 2

A packing diagram for (I), showing the hydrogen-bonded (dashed lines) chains along the *b* axis.

The water H atoms were located in a difference Fourier map, while the other H atoms were positioned geometrically. The water H atoms were refined with O–H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. All other H atoms were constrained to ride on their parent atoms, with O–H = 0.82 Å, N–H = 0.86 Å and C–H = 0.93 or 0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ – $1.5 U_{\text{eq}}(\text{parent atom})$. Owing to the absence of any significant anomalous scatterers in the molecules, Friedel pairs were merged before the final refinement.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

This project was supported by the Programme for New Century Excellent Talents in Universities (grant No. NCET-04-0649) and the Project of Educational Administration of Shandong Province (grant No. J04B12).

References

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
 Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXTL. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
 Siemens (1996). SMART and SAINT. Versions 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Wen, Y.-H., Zhang, S.-S., Li, M.-J. & Li, X.-M. (2005). *Acta Cryst. E* **61**, o2045–o2046.