

Yong-Hong Wen, Mao-Jie Li,
Shu-Sheng Zhang* and
Xue-Mei LiCollege 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
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.032
 wR factor = 0.083
Data-to-parameter ratio = 8.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*N*-(4-Methoxyphenyl)-2-(quinolin-8-yloxy)-
acetamide monohydrate

In the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$, all bond lengths and angles are within normal ranges. The dihedral angle formed by the benzene ring with the quinoline moiety is $67.06(7)^\circ$. Molecules are linked into chains along the a axis by intermolecular $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds involving the solvent water molecule. The packing is further stabilized by $\pi-\pi$ interactions.

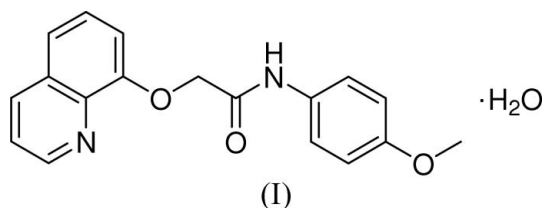
Received 5 September 2005

Accepted 3 October 2005

Online 12 October 2005

Comment

Recently, we have reported the structure of an amide-type acyclic compound with 8-hydroxyquinoline as the skeleton, namely *N*-phenyl-2-(quinolin-8-yloxy)acetamide hemihydrate, (II) (Li *et al.*, 2005). We have synthesized and carried out the structure determination of the title compound, (I), reported here.



All bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compound (II). The dihedral angle formed by the benzene ring with the quinoline moiety is $67.06(7)^\circ$. There is one intramolecular hydrogen bond, *viz.* $\text{C}13-\text{H}13\text{A} \cdots \text{O}2$, forming a six-membered ring. In the crystal structure, molecules are linked into chains along the a axis by intermolecular $\text{N}2-\text{H}2\text{A} \cdots \text{O}1\text{W}^i$, $\text{O}1\text{W}-\text{H}2\text{W}1 \cdots \text{O}2^{\text{ii}}$ and $\text{O}1\text{W}-\text{H}1\text{W}1 \cdots \text{N}1^{\text{ii}}$ hydrogen bonds (Table 2 and Fig. 2) involving the solvent water molecule. The packing is further stabilized by $\pi-\pi$ interactions involving the benzene rings ($\text{C}g2$ is the centroid of the $\text{C}12-\text{C}17$ benzene ring): $\text{C}g3 \cdots \text{C}g3(-\frac{1}{2} + x, \frac{1}{2} - y, -z) = 3.737$ Å.

Experimental

To a solution of 8-hydroxyquinoline (2.9 g, 20 mmol) in acetone (40 ml) were added 2-chloro-*N*-(4-methoxyphenyl)acetamide (3.99 g, 20 mmol), K_2CO_3 (3.04 g, 22 mmol) and KI (0.5 g), and the resulting mixture was stirred at 333 K for 5 h. After cooling to room temperature, the mixture was washed three times with water and then filtered. The title compound was obtained after drying the yellow powder at room temperature for 48 h. Yellow single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a petroleum ether–ethyl acetate (1:3 *v/v*) solution over a period of 6 d.

Crystal data

$C_{18}H_{16}N_2O_3 \cdot H_2O$
 $M_r = 326.34$
 Orthorhombic, $P2_12_12_1$
 $a = 6.8814$ (13) Å
 $b = 11.627$ (2) Å
 $c = 20.468$ (4) Å
 $V = 1637.6$ (5) Å³
 $Z = 4$
 $D_x = 1.324$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 4023 reflections
 $\theta = 2.6$ – 25.8°
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
 Plate, yellow
 $0.42 \times 0.42 \times 0.12$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.961$, $T_{\max} = 0.989$
 9310 measured reflections

1901 independent reflections
 1737 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\max} = 26.1^\circ$
 $h = -8 \rightarrow 8$
 $k = -13 \rightarrow 14$
 $l = -25 \rightarrow 24$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.084$
 $S = 1.12$
 1901 reflections
 225 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.1826P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.13$ e Å⁻³
 $\Delta\rho_{\min} = -0.14$ e Å⁻³

Table 1

Selected bond lengths (Å).

O1—C8	1.371 (2)	N2—C11	1.340 (2)
O1—C10	1.418 (2)	N2—C12	1.426 (2)
O2—C11	1.223 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2A \cdots O1W^i$	0.86	2.01	2.853 (2)	166
$O1W-H1W1 \cdots N1^{ii}$	0.87 (3)	2.02 (3)	2.886 (3)	176 (3)
$O1W-H2W1 \cdots O2^{ii}$	0.84 (3)	1.93 (3)	2.762 (2)	173 (2)
$C13-H13A \cdots O2^{ii}$	0.93	2.41	2.889 (3)	112

Symmetry code: (i) $x - 1, y, z$; (ii) x, y, z .

All H atoms were located in difference Fourier maps and all except water H atoms, which were refined freely, were constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The Friedel reflections were merged before the final refinement because of the absence of any significant anomalous scattering effects.

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 Program for New Century Excellent Talents in Universities (No. NCET-04-

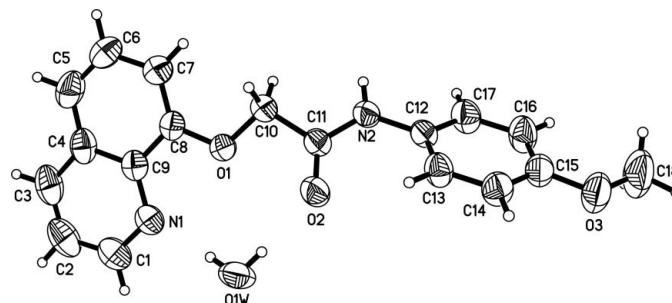


Figure 1

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

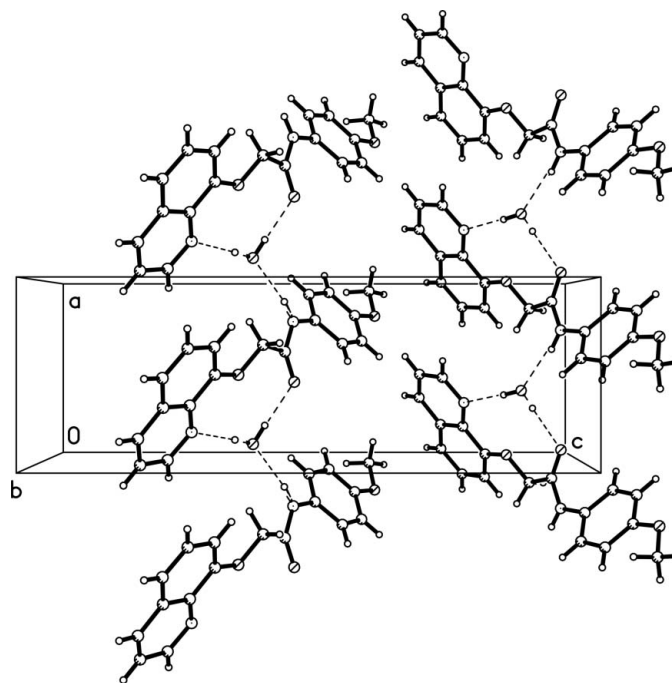


Figure 2

Packing diagram of (I), showing the intermolecular hydrogen bonds (dashed lines), viewed down the b axis.

0649), and by the Project of Educational Administration of Shandong Province (No. J04B12).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, S1–19.
 Li, X.-M., Wen, Y.-H., Li, M.-J. & Zhang, S.-S. (2005). *Acta Cryst. E* **61**, o2389–o2390.
 Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.