

***N*-Phenyl-2-(quinolin-8-yloxy)acetamide hemihydrate****Xue-Mei Li, Yong-Hong Wen,  
Mao-Jie Li and  
Shu-Sheng Zhang\***College of Chemistry and Molecular  
Engineering, Qingdao University of Science and  
Technology, 266042 Qingdao, Shandong,  
People's Republic of China

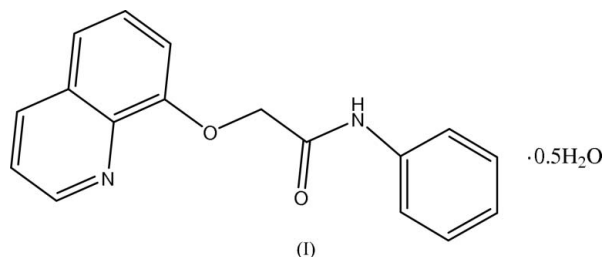
Correspondence e-mail: shushzhang@126.com

**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.049  
 $wR$  factor = 0.126  
Data-to-parameter ratio = 10.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{17}\text{H}_{14}\text{N}_2\text{O}_2 \cdot 0.5\text{H}_2\text{O}$ , all bond lengths and angles are within normal ranges. The dihedral angle formed by the phenyl ring with the quinoline moiety is  $27.30(9)^\circ$ . The crystal packing is stabilized by intermolecular  $\text{N}-\text{H} \cdots \text{O}$ ,  $\text{C}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonds involving the solvent water molecule.

**Comment**

Recently, we have reported the structure of an amide-type acyclic compound with an 8-hydroxyquinolinate skeleton, namely *N,N*-diphenyl-2-(quinolin-8-yloxy)acetamide monohydrate, (II) (Wen *et al.*, 2005). In order to investigate the effect of the substituent groups of the acyclic compounds on the coordination selectivity and extractability for metal ions, we have synthesized and carried out the structure determination of the title compound, (I).



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 phenyl ring with the quinoline moiety is  $27.30(9)^\circ$ . There are two intramolecular hydrogen bonds, *viz.*  $\text{N}2-\text{H}1\text{N}2 \cdots \text{O}1$  and  $\text{C}17-\text{H}17 \cdots \text{O}2$ , forming a five- and six-membered ring, respectively. The crystal packing is stabilized by intermolecular  $\text{N}2-\text{H}1\text{N}2 \cdots \text{O}1\text{W}$ ,  $\text{C}13-\text{H}13 \cdots \text{O}1\text{W}$  and  $\text{O}1\text{W}-\text{H}1\text{W}1 \cdots \text{N}1$  hydrogen bonds (Table 2 and Fig. 2) involving the solvent water molecule.

**Experimental**

2-Chloro-*N*-phenylacetamide was prepared by the reaction of phenylamine and chloroacetyl chloride in the presence of triethylamine, according to the literature method of Wen *et al.* (2004). To a solution of 8-hydroxyquinoline (1.45 g, 10 mmol) in acetone (40 ml) were added 2-chloro-*N*-phenylacetamide (1.69 g, 10 mmol),  $\text{K}_2\text{CO}_3$  (1.52 g, 11 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. Colorless single crystals suitable for an X-ray diffraction study were obtained by slow evaporation of a petroleum ether–ethyl acetate (1:2, *v/v*) solution over a period of 3 d.

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Crystal data

C<sub>17</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>·0.5H<sub>2</sub>O  
*M<sub>r</sub>* = 287.31  
 Monoclinic, C2/c  
*a* = 11.093 (5) Å  
*b* = 12.944 (6) Å  
*c* = 19.584 (9) Å  
 β = 91.855 (9)°  
*V* = 2811 (2) Å<sup>3</sup>  
*Z* = 8

*D<sub>x</sub>* = 1.358 Mg m<sup>-3</sup>  
 Mo Kα radiation  
 Cell parameters from 1582 reflections  
 θ = 2.4–21.7°  
 μ = 0.09 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, colorless  
 0.39 × 0.17 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 ω scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.965, *T<sub>max</sub>* = 0.989  
 7758 measured reflections

2766 independent reflections  
 1883 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.029  
 θ<sub>max</sub> = 26.1°  
*h* = -13 → 10  
*k* = -14 → 15  
*l* = -24 → 23

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.049  
*wR* (*F*<sup>2</sup>) = 0.126  
*S* = 1.03  
 2766 reflections  
 255 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.2335P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 (Δ/σ)<sub>max</sub> < 0.001  
 Δρ<sub>max</sub> = 0.15 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.17 e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

O1—C8	1.370 (2)	N2—C11	1.342 (2)
O1—C10	1.424 (2)	N2—C12	1.415 (2)
O2—C11	1.224 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1W1...N1 <sup>i</sup>	0.91 (2)	1.99 (3)	2.853 (3)	157 (2)
N2—H1N2...O1 <sup>ii</sup>	0.87 (2)	2.35 (2)	2.722 (2)	106 (2)
N2—H1N2...O1W <sup>ii</sup>	0.87 (2)	2.26 (2)	3.109 (2)	170 (2)
C13—H13...O1W <sup>ii</sup>	0.95 (2)	2.55 (2)	3.359 (3)	143 (2)
C17—H17...O2 <sup>ii</sup>	0.96 (2)	2.16 (2)	2.824 (3)	125 (2)

Symmetry codes: (i) -*x*, *y*, -*z* + ½; (ii) *x*, *y*, *z*.

All H atoms were located in difference Fourier maps and refined freely. The C—H distances are in the range 0.93 (2)–1.01 (2) Å.

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).

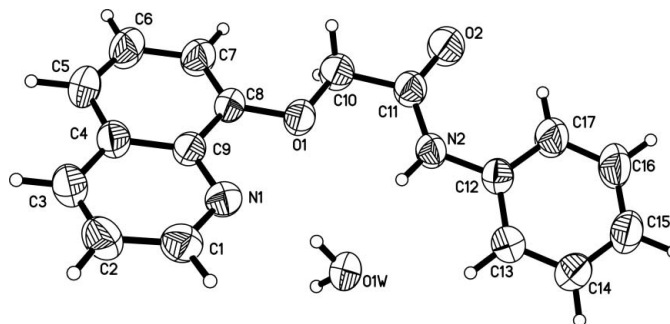


Figure 1

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

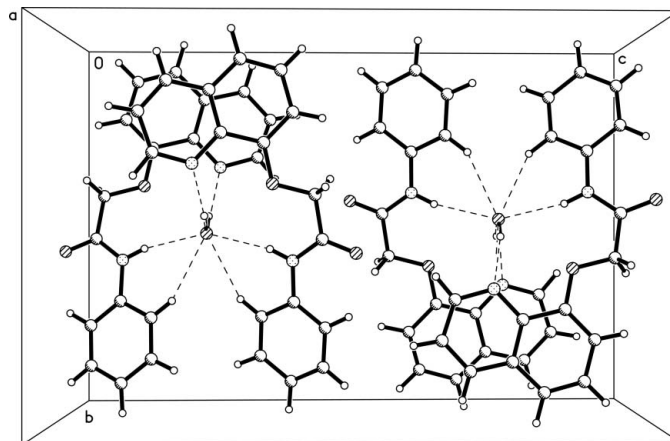


Figure 2

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

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