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N,*N*-Diphenyl-2-(quinolin-8-yloxy)acetamide monohydrate

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In the title compound, $C_{23}H_{18}N_2O_2{\cdot}H_2O$, all bond lengths and angles are within normal ranges. The dihedral angles formed by the two phenyl rings with the quinoline moiety are 61.40 (9) and 85.66 (8)°. The crystal packing is stabilized by intermolecular C—H···O and O—H···O hydrogen bonds involving the solvent water molecule.

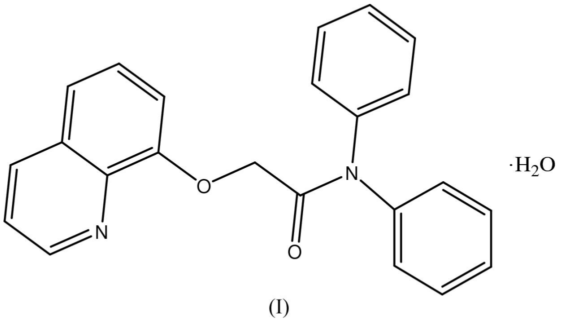
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.120
Data-to-parameter ratio = 14.5

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

Comment

8-Hydroxyquinoline and its derivatives have found extensive application as analytical reagents, *e.g.* in absorption spectrophotometry, fluorimetry, solvent extraction and partition chromatography, due to their ability to form stable complexes with many metallic ions (Bratzel *et al.*, 1972). Some 8-hydroxyquinoline derivatives and their complexes with transition metals demonstrate antibacterial activity (Patel & Patel, 1999). In continuation of our search for good extractants of metal ions, fluorescent materials and analytical reagents, we obtained the title compound, (I) (Fig. 1), the monohydrate of a new amide-based 8-hydroxyquinoline derivative, and we report its crystal structure here.



(I)

All bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987). The sum of the angles around atom N2 is 359.99°, implying a planar configuration. The dihedral angles formed by the two phenyl rings with the quinoline moiety are 61.40 (9) and 85.66 (8)°. The dihedral angle between the two phenyl rings is 67.57 (10)°.

The crystal packing (Fig. 2) of (I) is stabilized by intermolecular C—H···O and O—H···O hydrogen bonds (Table 2) involving the solvent water molecule.

Experimental

N,*N*-Diphenyl-2-chloroacetamide was prepared by the reaction of diphenylamine 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*,*N*-diphenylacetamide (2.45 g, 10 mmol), K_2CO_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 filtered. Colourless single crystals of (I) suitable for X-ray diffraction study were obtained by slow evaporation of a petroleum ether–ethyl acetate solution (1:2 *v*/*v*) over a period of 7 d.

Crystal data

$C_{23}H_{18}N_2O_2 \cdot H_2O$
$M_r = 372.41$
Triclinic, $P\overline{1}$
$a = 9.1761\ (8)$ Å
$b = 9.5962\ (8)$ Å
$c = 11.9113\ (10)$ Å
$\alpha = 72.5260\ (10)^\circ$
$\beta = 78.339\ (2)^\circ$
$\gamma = 82.942\ (2)^\circ$
$V = 977.63\ (14)$ Å^3

$Z = 2$
$D_x = 1.265$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 1838 reflections
$\theta = 2.4$–24.9°
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Column, colourless
0.40 × 0.20 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.967$, $T_{\max} = 0.992$
5557 measured reflections

3773 independent reflections
2805 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 26.0^\circ$
$h = -8 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.120$
$S = 1.04$
3773 reflections
261 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.1798P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.3716 (18)	N2—C11	1.354 (2)
O1—C10	1.4128 (19)	N2—C12	1.449 (2)
O2—C11	1.2188 (19)	N2—C18	1.449 (2)
C8—O1—C10	116.23 (12)	C11—N2—C18	124.10 (13)
C11—N2—C12	118.94 (13)	C12—N2—C18	116.95 (12)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2$^{\rm i}$	0.89 (2)	1.93 (2)	2.817 (2)	174 (3)
O1*W*—H2*W*1···N1$^{\rm i}$	0.89 (3)	1.98 (3)	2.872 (2)	175 (3)
C5—H5*A*···O1*W*$^{\rm ii}$	0.93	2.58	3.502 (3)	169
C23—H23*A*···O1*W*$^{\rm iii}$	0.93	2.47	3.383 (3)	166

Symmetry codes: (i) x, y, z; (ii) $x, y-1, z$; (iii) $-x+1, -y+2, -z$.

All H atoms were located in a difference Fourier map. The two H atoms of the water molecule were refined isotropically. Carbon-bound H atoms were constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

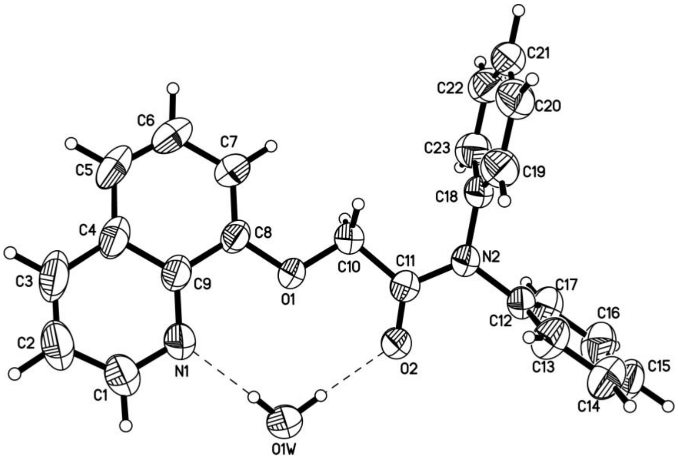


Figure 1
A view of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds.

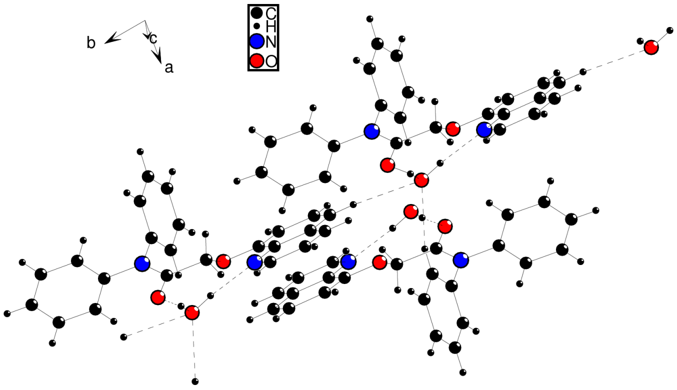


Figure 2
A packing diagram for (I), showing the intermolecular hydrogen bonds (dashed lines), viewed approximately down the *c* axis.

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* and *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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