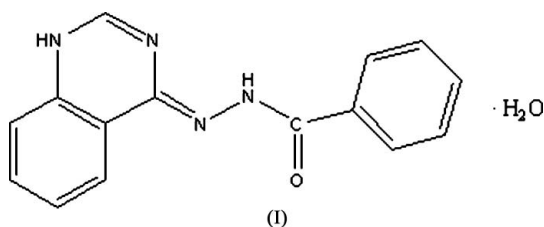


4-Benzoylhydrazono-1,4-dihydroquinazoline
monohydrateXiu-Wen Li, Zhang-Lan Qin* and
Ting WanDepartment of Chemistry, Central China Normal
University, Wuhan, Hubei 430079, People's
Republic of ChinaCorrespondence e-mail:
mingmou2289@tom.com

Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.051
 wR factor = 0.149
Data-to-parameter ratio = 15.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the crystal structure of the title compound,
 $\text{C}_{15}\text{H}_{12}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$, molecules are linked by N—H...O
hydrogen bonds and π – π and C—H... π interactions.Received 17 March 2006
Accepted 2 April 2006

Comment

The quinazoline ring system is found widely in alkaloids and
many biologically active compounds which find uses as
fungicides, anti-inflammatory, anticancer, antimicrobial and
antihypertensive agents (Alexandre *et al.*, 2003; Cobb *et al.*,
1999). Here we report the crystal structure of 4-(benzoyl-
hydrazono)-1,4-dihydroquinazoline as its monohydrate, (I)
(Fig. 1).The structure of (I) shows the quinazoline ring system and
benzamido groups to be linked through a C=N double bond.
The dihedral angle between the quinazoline unit and the
phenyl ring is $20.1(1)^\circ$. Selected bond lengths are given in
Table 1. The crystal structure exhibits both π – π and C—H– π
interactions (Table 1 and Fig. 2). The distance between the
centroids of parallel pairs of quinazoline ring systems, related
by inversion centers, is $3.652(1)$ Å; the perpendicular distance
is $3.455(1)$ Å. Hydrogen bonding is also observed, further
strengthening the crystal structure (Table 2).

Experimental

The title compound, (I), was prepared according to the procedure of
Liu & Song (2004). Crystals suitable for X-ray diffraction were
obtained by vapor diffusion of dioxane into a dimethylformamide
solution at room temperature (m.p. 519 K). Analysis calculated for
 $\text{C}_{15}\text{H}_{14}\text{N}_4\text{O}_2$: C 63.82, H 5.00, N 19.85%; found: C 62.79, H 5.01, N
19.87%.

Crystal data

 $\text{C}_{15}\text{H}_{12}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$
 $M_r = 282.30$
Monoclinic, $C2/c$
 $a = 16.9865(14)$ Å
 $b = 7.2085(6)$ Å
 $c = 22.1444(18)$ Å
 $\beta = 92.0220(10)^\circ$
 $V = 2709.8(4)$ Å³ $Z = 8$
 $D_x = 1.384$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 292(2)$ K
Block, yellow
 $0.20 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.972$, $T_{\max} = 0.981$

15045 measured reflections
 3091 independent reflections
 2643 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.150$
 $S = 1.05$
 3091 reflections
 202 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0936P)^2 + 0.5569P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.32 \text{ e } \text{Å}^{-3}$

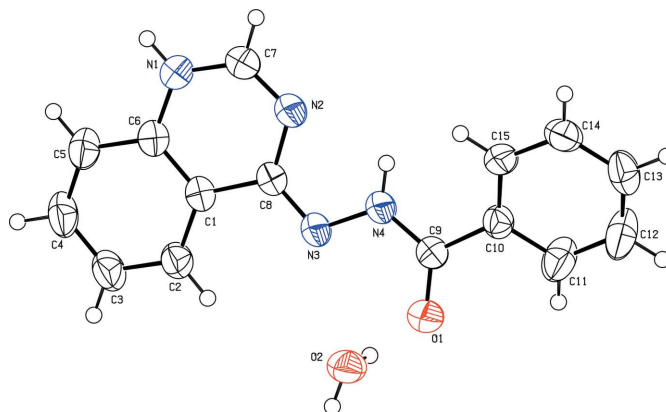


Figure 1 The molecular structure of (I), showing the atom labeling and 50% probability ellipsoids for the non-H atoms.

Table 1

Selected bond lengths (Å).

C6—N1	1.3853 (17)	C9—O1	1.2344 (16)
C7—N2	1.2972 (18)	C9—N4	1.3331 (17)
C7—N1	1.3320 (17)	C9—C10	1.4969 (17)
C8—N3	1.2976 (16)	N3—N4	1.3858 (14)
C8—N2	1.3885 (16)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4A \cdots N2	0.86 (1)	2.12 (2)	2.5526 (15)	111 (1)
O2—H2B \cdots O1	0.83 (1)	2.08 (1)	2.9071 (18)	174 (2)
O2—H2A \cdots N3 ⁱ	0.83 (1)	2.36 (1)	3.1400 (15)	158 (2)
O2—H2A \cdots O1 ⁱ	0.83 (1)	2.31 (2)	2.9048 (15)	130 (2)
N1—H1 \cdots O2 ⁱⁱ	0.86 (1)	2.01 (1)	2.8524 (16)	168 (2)
C12—H12 \cdots Cg1 ⁱⁱⁱ	0.93	2.78	3.522 (2)	138

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $-x, -y + 2, -z + 1$; (iii) $x, -y - 1, z - \frac{1}{2}$. Cg1 is the centroid of atoms C10–C15.

All aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $C-H = 0.93 \text{ Å}$ and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. The N and the water H atoms were located in a difference map, and were refined with the constraints $N-H = 0.86 (1) \text{ Å}$ and $O-H = 0.82 (1) \text{ Å}$. The U_{iso} values were set at 1.2 and 1.5 times U_{eq} of their carrier atoms for H4A and water H atoms, respectively.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

The authors acknowledge financial support from the Science Foundation of Hubei Province (grant No. 99 J059).

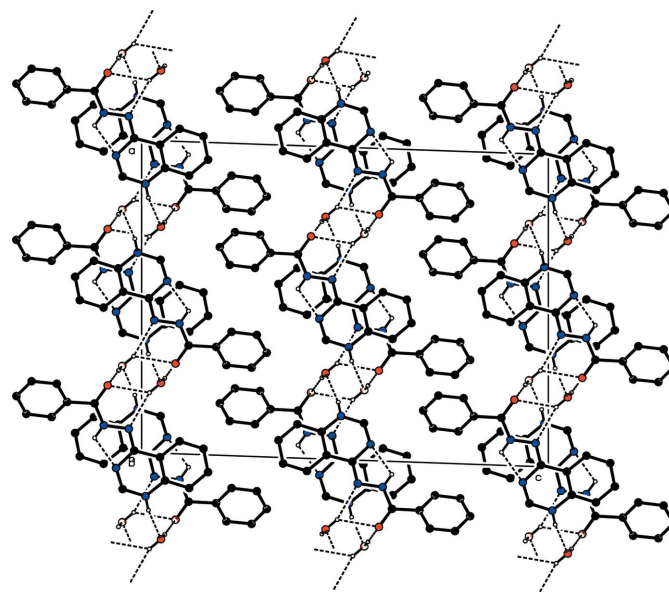


Figure 2 Plot of the crystal packing, showing the formation of chains. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

References

Alexandre, F.-R., Berecibar, A., Wrighlesworth, R. & Besson, T. (2003). *Tetrahedron*, **59**, 1413–1419.
 Bruker (2001). SAINT-Plus (Version 6.45) and SMART (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
 Cobb, J. M., Fiorini, M. T., Goddard, C. R., Theoclitou, M.-E. & Abell, C. (1999). *Tetrahedron Lett.* **40**, 1045–1048.
 Liu, G. & Song, B. A. (2004). *Chin. Org. Chem.* **10**, 1296–1299.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (2003). SADABS. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.