

2-Phenylpyrrolo[2,3-*h*]quinoline dihydrateDaniel E. Lynch<sup>a\*</sup> and Ian McClenaghan<sup>b</sup><sup>a</sup>School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and <sup>b</sup>Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, EnglandCorrespondence e-mail:  
apx106@coventry.ac.uk

## Key indicators

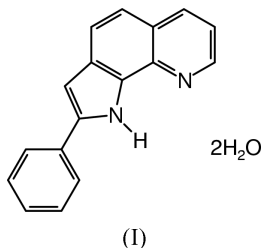
Single-crystal X-ray study  
*T* = 150 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.048  
*wR* factor = 0.093  
Data-to-parameter ratio = 8.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The crystal structure of the title compound,  $\text{C}_{17}\text{H}_{12}\text{N}_2 \cdot 2\text{H}_2\text{O}$ , comprises an essentially flat molecule, with the phenyl ring being inclined at  $18.7(1)^\circ$  to the plane of the pyrrolo[2,3-*h*]quinoline moiety, packed with two water molecules per asymmetric unit, all in a tetragonal lattice. One water molecule is involved in hydrogen-bonding associations with both pyrrolo-NH and quinoline-N sites while, as part of the overall hydrogen-bonding network, both water molecules and their symmetry equivalents construct a 'Chinese lantern' arrangement.

Received 28 August 2002  
Accepted 23 September 2002  
Online 27 September 2002

## Comment

The title compound, (I), was prepared from a two-stage procedure starting with the reaction of 8-hydrazinoquinoline dihydrochloride hydrate and acetophenone, followed by the cyclization of the intermediate product (*E*)-2-acetylbenzene-8-quinonylhydrozone. A structural example of this intermediate, as the thiophene derivative, has been previously published (Lynch & McClenaghan, 2001*a*). Furthermore, the structure of 2-(4-pyridyl)pyrrolo[3,2-*h*]quinoline, a product analogous to the title compound, has also been reported (Lynch & McClenaghan, 2001*b*). We are currently studying the structural aspects of derivatives of both 8-quinonylhydrozone and pyrrolo[3,2-*h*]quinoline before studying their potential as metal-chelating agents.



The molecule of (I) (Fig. 1) is essentially flat, with the phenyl ring being inclined at  $18.7(1)^\circ$  to the plane of the pyrrolo[2,3-*h*]quinoline moiety. It crystallizes with two water molecules per asymmetric unit. One O—H site from one water molecule resides in a hydrogen-bonded triangular arrangement with both pyrrolo-NH and quinoline-N sites. The other O—H site, in conjunction with the second water molecule and their symmetry-related analogues, then forms a hydrogen-bonded 'Chinese lantern' arrangement (Fig. 2).

## Experimental

The title compound was obtained from Key Organics Ltd and crystals were grown from an ethanol solution.

## Crystal data

$C_{17}H_{12}N_2 \cdot 2H_2O$   
 $M_r = 280.32$   
 Tetragonal,  $I\bar{4}$   
 $a = 24.758(4) \text{ \AA}$   
 $c = 4.6952(9) \text{ \AA}$   
 $V = 2878.1(8) \text{ \AA}^3$   
 $Z = 8$   
 $D_x = 1.294 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 5959 reflections  
 $\theta = 2.9\text{--}27.5^\circ$   
 $\mu = 0.09 \text{ mm}^{-1}$   
 $T = 150(2) \text{ K}$   
 Block, colourless  
 $0.20 \times 0.10 \times 0.10 \text{ mm}$

## Data collection

Bruker–Nonius KappaCCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SORTAV; Blessing, 1995)  
 $T_{\min} = 0.983$ ,  $T_{\max} = 0.991$   
 8208 measured reflections

1838 independent reflections  
 1205 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.079$   
 $\theta_{\max} = 27.5^\circ$   
 $h = -32 \rightarrow 32$   
 $k = -32 \rightarrow 32$   
 $l = -6 \rightarrow 5$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.093$   
 $S = 1.05$   
 1838 reflections  
 206 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0339P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N9-H1 \cdots O1W$	0.88 (3)	2.36 (3)	3.145 (3)	148 (3)
$O2W-H3W \cdots O2W^i$	0.83 (2)	1.99 (2)	2.807 (3)	168 (3)
$O2W-H4W \cdots O1W^{ii}$	0.85 (2)	1.90 (2)	2.744 (3)	175 (3)
$O1W-H1W \cdots N1$	0.87 (2)	1.94 (2)	2.801 (3)	172 (3)
$O1W-H2W \cdots O2W$	0.83 (2)	2.02 (2)	2.840 (3)	170 (3)

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

All aromatic H atoms were included in the refinement, at calculated positions, as riding models, with C–H set to 0.95  $\text{\AA}$ . All water H atoms were initially located in a difference synthesis, but were then restrained to a distance of 0.83  $\text{\AA}$ , with riding displacement parameters. The remaining N-attached H atom was located in a difference synthesis; its positional and displacement parameters were refined. In the absence of significant anomalous scattering effects, the absolute structure can not be determined; Friedel pairs were merged.

Data collection: DENZO (Otwinowski & Minor, 1997) and COLLECT (Hooft, 1998); cell refinement: DENZO and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLUTON94 (Spek, 1994) and PLATON97 (Spek, 1997); software used to prepare material for publication: SHELXL97.

The authors thank the EPSRC National Crystallography Service (Southampton).

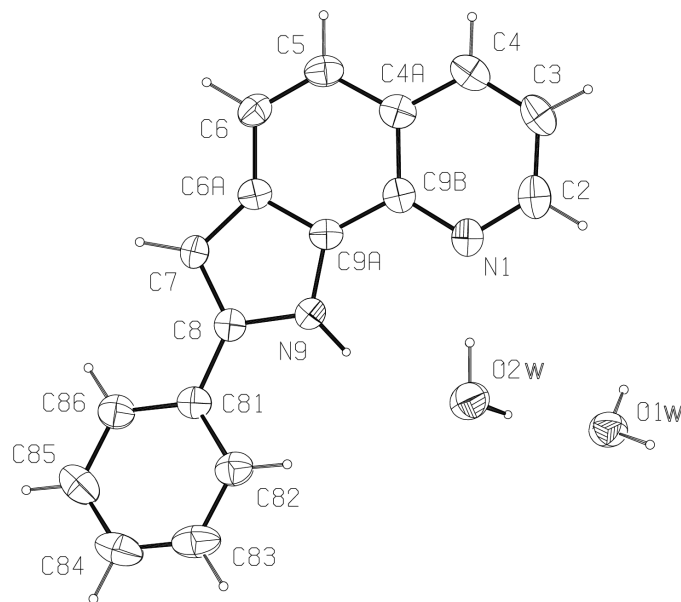


Figure 1

The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

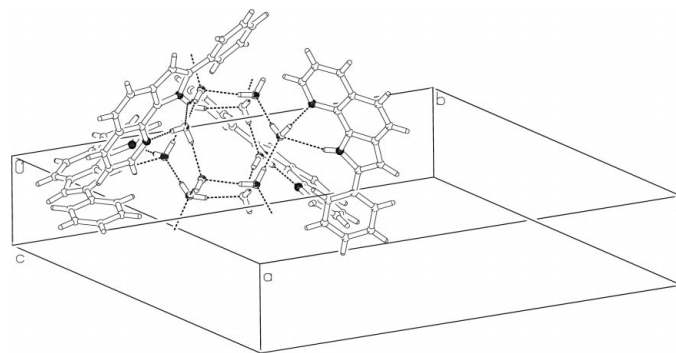


Figure 2

Partial packing diagram, showing the hydrogen-bonded 'Chinese lantern' arrangement of the water molecules. Hydrogen-bonding associations are shown as dotted lines.

## References

- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–37.  
 Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.  
 Lynch, D. E. & McClenaghan I. (2001a). *Acta Cryst.* **E57**, o52–o53.  
 Lynch, D. E. & McClenaghan I. (2001b). *Acta Cryst.* **E57**, o56–o57.  
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Spek, A. L. (1994). *PLUTON94*. University of Utrecht, The Netherlands.  
 Spek, A. L. (1997). *PLATON97*. Version of May 1997. University of Utrecht, The Netherlands.