

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Acridine 0.75-hydrate

Einat Schur,* Joel Bernstein, Andreas Lemmerer and Radion Vainer

Ben Gurion University of the Negev, Beer Sheva, Israel 84105

Correspondence e-mail: schur@bgu.ac.il

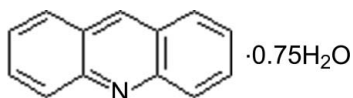
Received 29 June 2011; accepted 19 September 2011

Key indicators: single-crystal X-ray study; $T = 197$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.058; wR factor = 0.197; data-to-parameter ratio = 13.3.

The title compound, $\text{C}_{13}\text{H}_9\text{N}\cdot 0.75\text{H}_2\text{O}$ was obtained during a study of the polymorphic system of acridine, by slow evaporation from an ethanol–water solution. There are two acridine molecules (indicated by I and II, respectively) and one and a half water molecules in the asymmetric unit. The half-molecule of water is located on a crystallographic twofold axis. The crystal structure is built up from two threads of molecule II sewn together with water molecules through $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds from one side and with $\pi-\pi$ interactions [centroid–centroid distance = 3.640 (3) and 3.7431 (3) Å] between overlapping molecules II on the other side. Molecule I is attached to this thread from both sides by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. The threads are connected to each other by $\pi-\pi$ interactions [centroid–centroid distances = 3.582 (3) and 3.582 (3) Å] between the inner side of molecule I and stabilized by a $\text{C}-\text{H}\cdots\pi$ interaction on the other side of molecule I. This thread with rows of molecule I hanging on its sides is generated by translation perpendicular to the a axis.

Related literature

For the five anhydrous polymorphs of acridine, see: Phillips (1954, 1956), Phillips *et al.* (1960) and Mei & Wolf (2004) for monoclinic forms VI and VII, and Braga *et al.* (2010) for orthorhombic form IV and monoclinic forms II and III. For further crystallographic studies of acridine hydrate, see: Groth (1919); Lowde *et al.* (1953).



Experimental

Crystal data

 $\text{C}_{13}\text{H}_9\text{N}\cdot 0.75\text{H}_2\text{O}$ $M_r = 192.71$ Orthorhombic, $Pbcn$ $a = 26.400$ (5) Å $b = 8.893$ (5) Å $c = 17.492$ (5) Å $V = 4107$ (3) Å³ $Z = 16$ Mo $K\alpha$ radiation $\mu = 0.08$ mm⁻¹ $T = 197$ K $0.3 \times 0.3 \times 0.3$ mm

Data collection

Bruker SMART 6000 diffractometer
14504 measured reflections3606 independent reflections
1733 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$ $wR(F^2) = 0.197$ $S = 1.00$

3606 reflections

272 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C1/C6–C8/C13/N1 and C1–C6 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2B}\cdots\text{N2}$	0.933 (3)	1.942 (2)	2.873 (4)	175.2 (2)
$\text{C7}-\text{H7}\cdots\text{O1}$	0.93	2.35	3.271 (4)	171
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.95 (1)	1.98 (5)	2.777 (4)	139 (6)
$\text{C16}-\text{H16}\cdots\text{Cg1}^{\text{ii}}$	0.93	2.93	3.773 (5)	152
$\text{C18}-\text{H18}\cdots\text{Cg2}^{\text{iii}}$	0.93	2.93	3.848 (5)	168

Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $x, -y + 1, z + \frac{1}{2}$; (iii) $-x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZZ255).

References

- Braga, D., Grepioni, F., Maini, L., Mazzeo, P. P. & Rubini, K. (2010). *Thermochimica Acta*, **507–508**, 1–8.
- Bruker (2003). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2005). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Groth, P. (1919). *Chem. Kristallogr.* **5**, 816–817.
- Lowde, R. D., Phillips, D. C. & Wood, R. G. (1953). *Acta Cryst.* **6**, 553–556.
- Mei, X. & Wolf, C. (2004). *Cryst. Growth Des.* **4**, 1099–1103.
- Phillips, D. C. (1954). *Acta Cryst.* **7**, C649, abstract No. 25.
- Phillips, D. C. (1956). *Acta Cryst.* **9**, 237–250.
- Phillips, D. C., Ahmed, F. R. & Barnes, W. H. (1960). *Acta Cryst.* **13**, 365–377.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2011). E67, o2761 [doi:10.1107/S1600536811038220]

Acridine 0.75-hydrate

E. Schur, J. Bernstein, A. Lemmerer and R. Vainer

Comment

Acridine hydrate is the hydrated form of the very rich polymorphic system of acridine. There are five anhydrous polymorphs of acridine with fully analyzed structures: an orthorhombic form and four monoclinic forms. For the orthorhombic form (form IV) cell parameters were first published by Phillips (1954), and the full solution was recently published by Braga *et al.* (2010). The monoclinic forms are designated II, III, VI and VII. The crystal structure of forms III and II respectively were determined by Phillips (1956) and Phillips *et al.* (1960) and redetermined by Mei and Wolf (2004) and by Braga *et al.* (2010). Forms VI and VII were reported by Mei and Wolf (2004). The form described in this paper was initially thought to be one of the first polymorphs of acridine and known historically as the orthorhombic form of Groth (1919) and subsequently labeled as acridine I. Lowde *et al.* (1953) established the unit cell parameters, the space group and the density. From analysis using the Karl Fischer reagent, it was concluded that acridine I is in fact the monohydrate and not a polymorph of acridine.

There are two acridine molecules and one and a half water molecules in the asymmetric unit (see Fig. 1). In the packing diagram (see Fig. 2), molecule I is colored in green, molecule II is colored in blue, the water molecule that is sitting on a two fold axis is red and the other one is in yellow. The molecules are linked by O—H \cdots O and C—H \cdots O hydrogen bonds (see Table 1).

Experimental

The title compound was obtained by slow evaporation from an ethanol-water solution in 3:1 and 2:1 ratio at 4°C. The crystals are unstable at room temperature and transform to the anhydrous form III. The common habit of acridine hydrate is thick yellow needles but other habits may be obtained as well.

Refinement

The water H atoms were located in a difference map and refined with distance restraints of O—H = 0.94 (2) Å. Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.930 (1) Å.

Figures

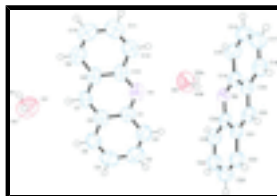


Fig. 1. The asymmetric unit with atom labels and 50% probability displacement ellipsoids for non-H atoms. Atom H1¹ is generated by a two-fold axis (-x, y, -z-1/2).

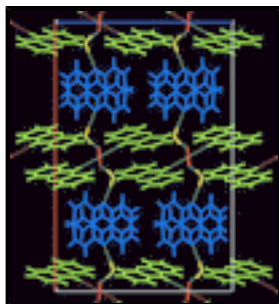


Fig. 2. The packing of acridine hydrate viewed down the *b* axis. Hydrogen bonds are marked in dashed lines.

Acridine 0.75-hydrate

Crystal data

$C_{13}H_9N \cdot 0.75H_2O$

$M_r = 192.71$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 26.400 (5) \text{ \AA}$

$b = 8.893 (5) \text{ \AA}$

$c = 17.492 (5) \text{ \AA}$

$V = 4107 (3) \text{ \AA}^3$

$Z = 16$

$F(000) = 1632$

$D_x = 1.247 \text{ Mg m}^{-3}$

$D_m = 1.247 \text{ Mg m}^{-3}$

D_m measured by not measured

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1764 reflections

$\theta = 2.3\text{--}21.8^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 197 \text{ K}$

Cube, yellow

$0.3 \times 0.3 \times 0.3 \text{ mm}$

Data collection

Bruker SMART 6000
diffractometer

Radiation source: fine-focus sealed tube
graphite

phi and ω scans

14504 measured reflections

3606 independent reflections

1733 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.068$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 3.3^\circ$

$h = -31 \rightarrow 22$

$k = -10 \rightarrow 9$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.058$

$wR(F^2) = 0.197$

$S = 1.00$

3606 reflections

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 1.779P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.035$

272 parameters

$$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$$

2 restraints

$$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.08797 (12)	0.6902 (4)	-0.0316 (2)	0.0579 (9)
C2	0.10417 (14)	0.8419 (5)	-0.0350 (2)	0.0746 (11)
H2	0.1166	0.8883	0.0088	0.090*
C3	0.10180 (15)	0.9206 (5)	-0.1017 (3)	0.0846 (13)
H3	0.1125	1.0202	-0.1031	0.102*
C4	0.08311 (15)	0.8515 (6)	-0.1688 (3)	0.0839 (13)
H4	0.0813	0.9066	-0.2140	0.101*
C5	0.06791 (14)	0.7066 (5)	-0.1681 (2)	0.0741 (11)
H5	0.0563	0.6625	-0.2130	0.089*
C6	0.06934 (11)	0.6201 (5)	-0.0995 (2)	0.0581 (9)
C7	0.05310 (11)	0.4738 (4)	-0.09624 (19)	0.0551 (9)
H7	0.0409	0.4271	-0.1401	0.066*
C8	0.05470 (11)	0.3952 (4)	-0.0281 (2)	0.0571 (9)
C9	0.03850 (13)	0.2431 (5)	-0.0214 (2)	0.0703 (11)
H9	0.0268	0.1922	-0.0644	0.084*
C10	0.03996 (14)	0.1718 (5)	0.0472 (3)	0.0789 (12)
H10	0.0293	0.0724	0.0507	0.095*
C11	0.05760 (14)	0.2473 (6)	0.1135 (2)	0.0798 (12)
H11	0.0583	0.1969	0.1601	0.096*
C12	0.07325 (13)	0.3910 (5)	0.1097 (2)	0.0689 (11)
H12	0.0843	0.4392	0.1538	0.083*
C13	0.07305 (11)	0.4701 (4)	0.0390 (2)	0.0578 (9)
C14	0.19756 (12)	0.7990 (4)	0.28030 (18)	0.0503 (8)
C15	0.16763 (13)	0.7107 (4)	0.3315 (2)	0.0628 (10)
H15	0.1325	0.7115	0.3271	0.075*
C16	0.18986 (15)	0.6257 (4)	0.3863 (2)	0.0716 (11)
H16	0.1697	0.5686	0.4189	0.086*
C17	0.24310 (16)	0.6224 (4)	0.3950 (2)	0.0708 (11)
H17	0.2577	0.5645	0.4334	0.085*
C18	0.27294 (14)	0.7039 (4)	0.3470 (2)	0.0638 (10)

supplementary materials

H18	0.3079	0.7009	0.3530	0.077*
C19	0.25146 (12)	0.7941 (4)	0.28769 (18)	0.0514 (8)
C20	0.28036 (11)	0.8773 (4)	0.23658 (18)	0.0524 (8)
H20	0.3155	0.8749	0.2398	0.063*
C21	0.25709 (12)	0.9640 (4)	0.18072 (18)	0.0504 (8)
C22	0.28402 (14)	1.0520 (4)	0.1261 (2)	0.0639 (10)
H22	0.3192	1.0524	0.1271	0.077*
C23	0.25950 (17)	1.1351 (4)	0.0727 (2)	0.0737 (11)
H23	0.2779	1.1914	0.0376	0.088*
C24	0.20596 (17)	1.1363 (4)	0.0705 (2)	0.0734 (11)
H24	0.1893	1.1932	0.0336	0.088*
C25	0.17860 (13)	1.0551 (4)	0.1217 (2)	0.0632 (10)
H25	0.1434	1.0584	0.1199	0.076*
C26	0.20288 (12)	0.9648 (4)	0.17826 (18)	0.0514 (8)
N1	0.08930 (10)	0.6160 (4)	0.03670 (17)	0.0675 (9)
N2	0.17409 (9)	0.8829 (3)	0.22676 (15)	0.0528 (7)
O1	0.0000	0.3361 (6)	-0.2500	0.1183 (16)
O2	0.07381 (11)	0.8227 (5)	0.17081 (17)	0.1234 (14)
H2A	0.0499	0.9004	0.2031	0.137 (18)*
H2B	0.1071	0.8385	0.1869	0.137 (18)*
H1	-0.0308 (14)	0.280 (6)	-0.248 (4)	0.205*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0437 (18)	0.066 (2)	0.064 (2)	0.0044 (17)	0.0016 (16)	-0.010 (2)
C2	0.065 (2)	0.075 (3)	0.084 (3)	-0.003 (2)	0.015 (2)	-0.021 (3)
C3	0.074 (3)	0.071 (3)	0.110 (3)	-0.002 (2)	0.029 (3)	-0.009 (3)
C4	0.077 (3)	0.095 (4)	0.080 (3)	0.006 (3)	0.017 (2)	0.008 (3)
C5	0.066 (2)	0.093 (3)	0.064 (2)	-0.002 (2)	0.0025 (18)	-0.005 (2)
C6	0.0389 (17)	0.073 (3)	0.063 (2)	0.0082 (17)	0.0009 (15)	-0.012 (2)
C7	0.0434 (18)	0.068 (2)	0.054 (2)	0.0046 (18)	-0.0042 (15)	-0.0172 (19)
C8	0.0383 (17)	0.062 (2)	0.071 (2)	0.0124 (17)	-0.0010 (16)	-0.016 (2)
C9	0.056 (2)	0.069 (3)	0.086 (3)	0.005 (2)	0.0002 (19)	-0.016 (2)
C10	0.058 (2)	0.067 (3)	0.112 (3)	0.011 (2)	0.010 (2)	0.003 (3)
C11	0.060 (2)	0.097 (4)	0.082 (3)	0.017 (2)	-0.002 (2)	0.010 (3)
C12	0.053 (2)	0.086 (3)	0.068 (3)	0.010 (2)	-0.0068 (18)	-0.003 (2)
C13	0.0365 (17)	0.071 (3)	0.066 (2)	0.0093 (17)	-0.0025 (15)	-0.011 (2)
C14	0.0470 (18)	0.047 (2)	0.0574 (19)	0.0011 (16)	0.0037 (16)	-0.0130 (17)
C15	0.054 (2)	0.063 (2)	0.072 (2)	-0.0028 (19)	0.0115 (18)	-0.010 (2)
C16	0.087 (3)	0.059 (3)	0.069 (2)	-0.006 (2)	0.013 (2)	-0.003 (2)
C17	0.087 (3)	0.063 (3)	0.063 (2)	0.002 (2)	-0.008 (2)	-0.003 (2)
C18	0.063 (2)	0.063 (2)	0.066 (2)	0.008 (2)	-0.0122 (19)	-0.009 (2)
C19	0.0486 (18)	0.049 (2)	0.0570 (19)	0.0012 (16)	-0.0049 (16)	-0.0135 (18)
C20	0.0380 (17)	0.054 (2)	0.065 (2)	-0.0018 (16)	-0.0014 (15)	-0.0157 (19)
C21	0.0512 (18)	0.0441 (19)	0.0560 (19)	-0.0004 (16)	0.0004 (16)	-0.0157 (17)
C22	0.064 (2)	0.061 (2)	0.066 (2)	-0.0080 (19)	0.0095 (19)	-0.014 (2)
C23	0.099 (3)	0.058 (3)	0.065 (2)	-0.011 (2)	0.011 (2)	-0.005 (2)

C24	0.095 (3)	0.059 (2)	0.066 (2)	-0.001 (2)	-0.015 (2)	-0.005 (2)
C25	0.060 (2)	0.057 (2)	0.073 (2)	0.0022 (19)	-0.0128 (19)	-0.011 (2)
C26	0.0475 (18)	0.047 (2)	0.060 (2)	0.0032 (16)	-0.0039 (16)	-0.0153 (18)
N1	0.0478 (16)	0.082 (2)	0.073 (2)	0.0054 (16)	-0.0043 (14)	-0.0156 (19)
N2	0.0406 (15)	0.0505 (17)	0.0672 (17)	0.0005 (13)	-0.0006 (13)	-0.0101 (15)
O1	0.077 (3)	0.118 (4)	0.160 (4)	0.000	0.014 (3)	0.000
O2	0.0619 (18)	0.204 (4)	0.104 (2)	-0.034 (2)	-0.0056 (17)	-0.013 (3)

Geometric parameters (Å, °)

C1—C2	1.416 (5)	C14—N2	1.348 (4)
C1—C6	1.430 (5)	C15—H15	0.9300
C1—N1	1.365 (4)	C15—C16	1.354 (5)
C2—H2	0.9300	C16—H16	0.9300
C2—C3	1.362 (5)	C16—C17	1.414 (5)
C3—H3	0.9300	C17—H17	0.9300
C3—C4	1.414 (6)	C17—C18	1.359 (5)
C4—H4	0.9300	C18—H18	0.9300
C4—C5	1.350 (6)	C18—C19	1.429 (4)
C5—H5	0.9300	C19—C20	1.389 (4)
C5—C6	1.425 (5)	C20—H20	0.9300
C6—C7	1.371 (5)	C20—C21	1.388 (4)
C7—H7	0.9300	C21—C22	1.425 (5)
C7—C8	1.382 (5)	C21—C26	1.432 (4)
C8—C9	1.423 (5)	C22—H22	0.9300
C8—C13	1.434 (5)	C22—C23	1.356 (5)
C9—H9	0.9300	C23—H23	0.9300
C9—C10	1.358 (5)	C23—C24	1.414 (5)
C10—H10	0.9300	C24—H24	0.9300
C10—C11	1.420 (5)	C24—C25	1.359 (5)
C11—H11	0.9300	C25—H25	0.9300
C11—C12	1.345 (6)	C25—C26	1.426 (4)
C12—H12	0.9300	C26—N2	1.352 (4)
C12—C13	1.423 (5)	O1—H1	0.954 (11)
C13—N1	1.367 (5)	O2—H2A	1.093 (4)
C14—C15	1.430 (5)	O2—H2B	0.933 (3)
C14—C19	1.430 (4)		
C2—C1—C6	118.9 (4)	N2—C14—C19	122.5 (3)
N1—C1—C2	119.3 (3)	C14—C15—H15	119.7
N1—C1—C6	121.7 (3)	C16—C15—C14	120.7 (3)
C1—C2—H2	119.6	C16—C15—H15	119.7
C3—C2—C1	120.8 (4)	C15—C16—H16	119.4
C3—C2—H2	119.6	C15—C16—C17	121.2 (4)
C2—C3—H3	119.9	C17—C16—H16	119.4
C2—C3—C4	120.3 (4)	C16—C17—H17	120.0
C4—C3—H3	119.9	C18—C17—C16	119.9 (4)
C3—C4—H4	119.6	C18—C17—H17	120.0
C5—C4—C3	120.7 (4)	C17—C18—H18	119.4
C5—C4—H4	119.6	C17—C18—C19	121.2 (3)

supplementary materials

C4—C5—H5	119.5	C19—C18—H18	119.4
C4—C5—C6	121.0 (4)	C18—C19—C14	118.5 (3)
C6—C5—H5	119.5	C20—C19—C14	118.2 (3)
C5—C6—C1	118.3 (4)	C20—C19—C18	123.3 (3)
C7—C6—C1	119.1 (3)	C19—C20—H20	119.8
C7—C6—C5	122.6 (3)	C21—C20—C19	120.4 (3)
C6—C7—H7	119.8	C21—C20—H20	119.8
C6—C7—C8	120.4 (3)	C20—C21—C22	123.8 (3)
C8—C7—H7	119.8	C20—C21—C26	117.8 (3)
C7—C8—C9	122.8 (3)	C22—C21—C26	118.4 (3)
C7—C8—C13	118.8 (3)	C21—C22—H22	119.2
C9—C8—C13	118.4 (4)	C23—C22—C21	121.5 (3)
C8—C9—H9	119.7	C23—C22—H22	119.2
C10—C9—C8	120.5 (4)	C22—C23—H23	120.0
C10—C9—H9	119.7	C22—C23—C24	120.0 (4)
C9—C10—H10	119.6	C24—C23—H23	120.0
C9—C10—C11	120.7 (4)	C23—C24—H24	119.7
C11—C10—H10	119.6	C25—C24—C23	120.6 (4)
C10—C11—H11	119.7	C25—C24—H24	119.7
C12—C11—C10	120.6 (4)	C24—C25—H25	119.4
C12—C11—H11	119.7	C24—C25—C26	121.2 (3)
C11—C12—H12	119.6	C26—C25—H25	119.4
C11—C12—C13	120.8 (4)	C25—C26—C21	118.2 (3)
C13—C12—H12	119.6	N2—C26—C21	122.7 (3)
C12—C13—C8	118.9 (4)	N2—C26—C25	119.1 (3)
N1—C13—C8	121.5 (3)	C13—N1—C1	118.5 (3)
N1—C13—C12	119.6 (3)	C14—N2—C26	118.4 (3)
C19—C14—C15	118.5 (3)	H2A—O2—H2B	107.1 (3)
N2—C14—C15	119.0 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C1/C6—C8/C13/N1 and C1—C6 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2B \cdots N2	0.933 (3)	1.942 (2)	2.873 (4)	175.2 (2)
C7—H7 \cdots O1	0.93	2.35	3.271 (4)	171.
O1—H1 \cdots O2 ⁱ	0.95 (1)	1.98 (5)	2.777 (4)	139 (6)
C16—H16 \cdots Cg1 ⁱⁱ	0.93	2.93	3.773 (5)	152
C18—H18 \cdots Cg2 ⁱⁱⁱ	0.93	2.93	3.848 (5)	168

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $x, -y+1, z+1/2$; (iii) $-x+1/2, -y+3/2, z+1/2$.

Fig. 1

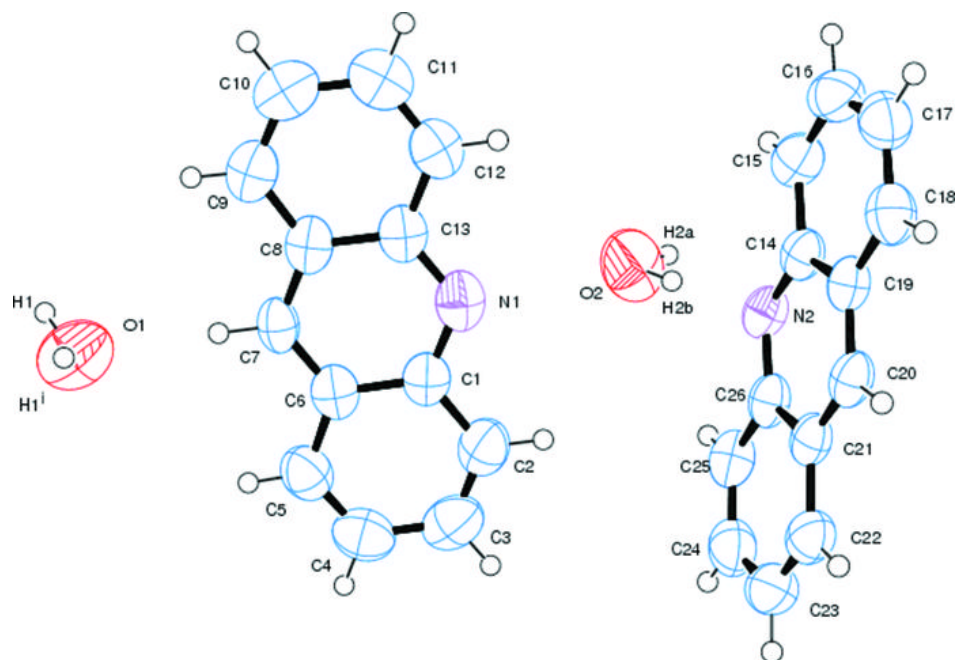


Fig. 2

