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# Acridine 0.75-hydrate

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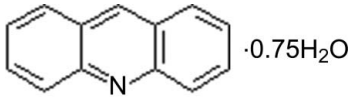
Key indicators: single-crystal X-ray study; $T$ = 197 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.058; $wR$ factor = 0.197; data-to-parameter ratio = 13.3.

The title compound, $C_{13}H_9N\cdot0.75H_2O$ 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 O—H···O and O—H···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 C—H···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 C—H···$\pi$ 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

$C_{13}H_9N\cdot0.75H_2O$
$M_r$ = 192.71
Orthorhombic, *Pbcn*
$a$ = 26.400 (5) Å
$b$ = 8.893 (5) Å
$c$ = 17.492 (5) Å
$V$ = 4107 (3) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 197 K
0.3 × 0.3 × 0.3 mm

### Data collection

Bruker SMART 6000 diffractometer
14504 measured reflections
3606 independent reflections
1733 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C1/C6–C8/C13/N1 and C1–C6 rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2*B*···N2 | 0.933 (3) | 1.942 (2) | 2.873 (4) | 175.2 (2) |
| C7—H7···O1 | 0.93 | 2.35 | 3.271 (4) | 171 |
| O1—H1···O2$^{i}$ | 0.95 (1) | 1.98 (5) | 2.777 (4) | 139 (6) |
| C16—H16···*Cg*1$^{ii}$ | 0.93 | 2.93 | 3.773 (5) | 152 |
| C18—H18···*Cg*2$^{iii}$ | 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: EZ2255).

## References

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# supporting information

*Acta Cryst.* (2011). E**67**, o2761 [https://doi.org/10.1107/S1600536811038220]

## Acridine 0.75-hydrate

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

### S1. 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···O and C—H···O hydrogen bonds (see Table 1).

### S2. 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.

### S3. 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.

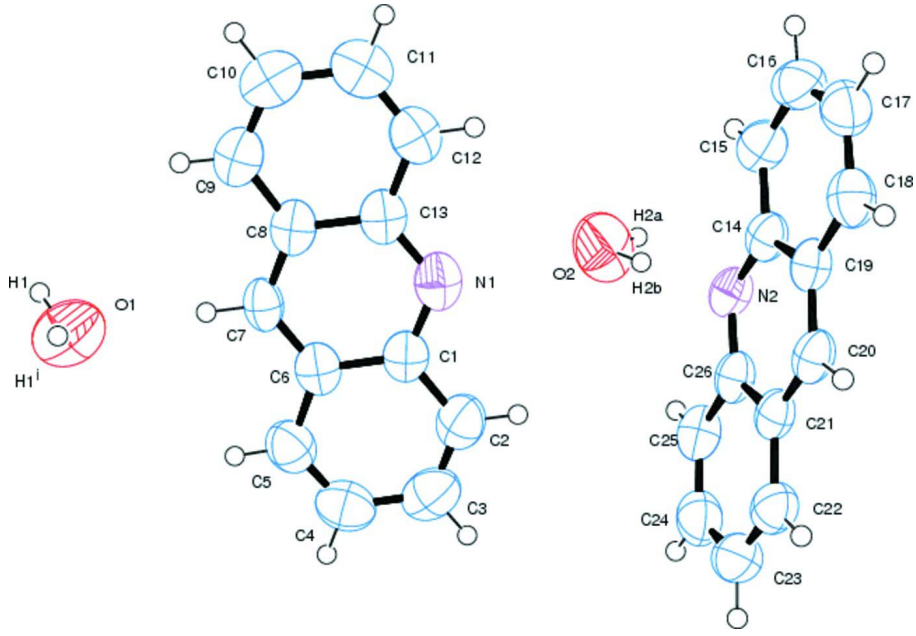


**Figure 1**

The asymmetric unit with atom labels and 50% probability displacement ellipsoids for non-H atoms. Atom H1$^{i}$ is generated by a two-fold axis (-x, y, -z-1/2).

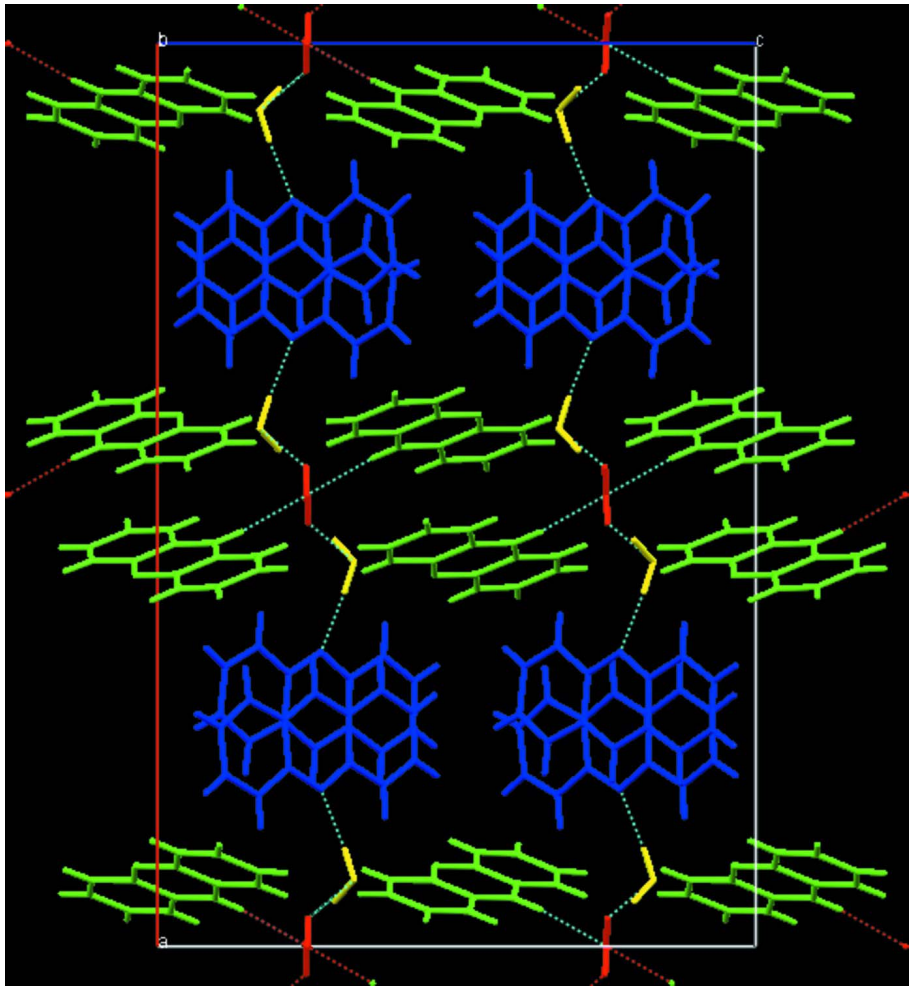


**Figure 2**

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

## Acridine 0.75-hydrate

*Crystal data*

$C_{13}H_9N·0.75H_2O$
$M_r$ = 192.71
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
*a* = 26.400 (5) Å
*b* = 8.893 (5) Å
*c* = 17.492 (5) Å
*V* = 4107 (3) Å$^3$
*Z* = 16
*F*(000) = 1632

$D_x$ = 1.247 Mg m$^{-3}$
$D_m$ = 1.247 Mg m$^{-3}$
$D_m$ measured by not measured
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1764 reflections
$\theta$ = 2.3–21.8°
$\mu$ = 0.08 mm$^{-1}$
*T* = 197 K
Cube, yellow
0.3 × 0.3 × 0.3 mm

*Data collection*

Bruker SMART 6000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator

phi and $\omega$ scans
14504 measured reflections
3606 independent reflections
1733 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.068
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.3°
$h$ = −31→22
$k$ = −10→9
$l$ = −20→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
272 parameters
2 restraints
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.035
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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) |
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |
| 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 (Å, º)*

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*B*···N2 | 0.933 (3) | 1.942 (2) | 2.873 (4) | 175.2 (2) |
| C7—H7···O1 | 0.93 | 2.35 | 3.271 (4) | 171 |
| O1—H1···O2$^{i}$ | 0.95 (1) | 1.98 (5) | 2.777 (4) | 139 (6) |

| | | | | |
|---|---|---|---|---|
| C16—H16···*Cg*1$^{ii}$ | 0.93 | 2.93 | 3.773 (5) | 152 |
| C18—H18···*Cg*2$^{iii}$ | 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.