

## 5-Hydroxy-3,3,6,6-tetramethyl-9-propyl-1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione monohydrate

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## Key indicators

Single-crystal X-ray study

T = 291 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.039

wR factor = 0.086

Data-to-parameter ratio = 10.1

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

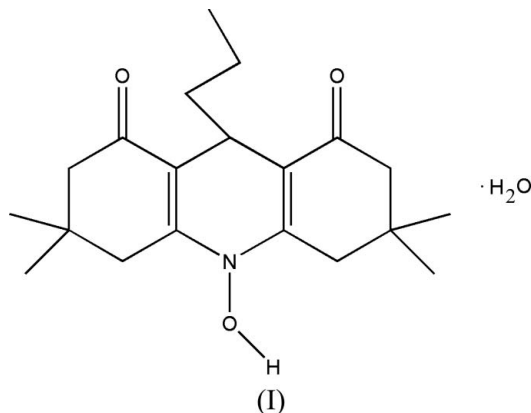
The title compound,  $\text{C}_{20}\text{H}_{29}\text{NO}_3 \cdot \text{H}_2\text{O}$ , has been synthesized by the reaction of hydroxylamine with butyraldehyde and dimidone in ethylene glycol under microwave irradiation. The dihydropyridine ring adopts a boat conformation.

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## Comment

Acridine belongs to a class of compounds which are special not only because of their interesting chemical and physical properties, but also due to their immense utility in the pharmaceutical and dye industries. The discovery of acridines as antimalarial and antitumour agents has attracted the attention of organic chemists and thus led to intense interest in the synthesis of several drugs based on acridine (Khurana *et al.*, 1990; Matsumoto *et al.*, 1983; Nakano *et al.*, 1982). Chemical modification of the acridine ring system, such as the introduction of an aryl group on the N atom, causes laser activity (Murugan *et al.*, 1998). We report here the X-ray crystal structure of the title compound, (I).



In (I), the dihydropyridine ring adopts a boat conformation, with atoms N1 and C7 deviating from the C6/C1/C8/C13 plane by 0.118 (3) and 0.278 (3) Å, respectively (Fig. 1). Both cyclohexene rings adopt an envelope conformation: atom C3 deviates from the C1/C2/C4–C6 plane by 0.657 (4) Å and atom C11 deviates from the C8–C10/C12/C13 plane by 0.635 (4) Å. The C1/C2/C4–C6 and C8–C10/C12/C13 planes form dihedral angles of 11.8 (2) and 12.7 (1)°, respectively, with the C6/C1/C8/C13 plane.

The molecules are connected *via* O–H...O hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2).

## Experimental

Compound (I) was prepared by the reaction of hydroxylamine (2 mmol) with butyraldehyde (2 mmol) and dimidone (4 mmol) in

ethylene glycol (2 ml) under microwave irradiation for 5 min (m.p. 425–426 K). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol (95%) solution.

#### Crystal data

$C_{20}H_{29}NO_3 \cdot H_2O$   
 $M_r = 349.46$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 9.355$  (1) Å  
 $b = 13.046$  (3) Å  
 $c = 16.033$  (3) Å  
 $V = 1956.8$  (6) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.186$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
 Block, colourless  
 $0.50 \times 0.40 \times 0.40$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.960$ ,  $T_{\max} = 0.968$

2550 measured reflections  
 2430 independent reflections  
 1428 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.012$   
 $\theta_{\text{max}} = 27.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.086$   
 $S = 0.85$   
 2430 reflections  
 241 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.12$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.14$  e Å<sup>-3</sup>  
 Extinction correction: SHELXL97 (Sheldrick, 1997)  
 Extinction coefficient: 0.0096 (11)

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1O \cdots O4^i$	0.82	1.83	2.611 (3)	158
$O4-H4OB \cdots O2^{ii}$	0.828 (10)	1.921 (12)	2.742 (3)	171 (4)
$O4-H4OA \cdots O3$	0.824 (10)	1.929 (13)	2.740 (3)	168 (4)

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

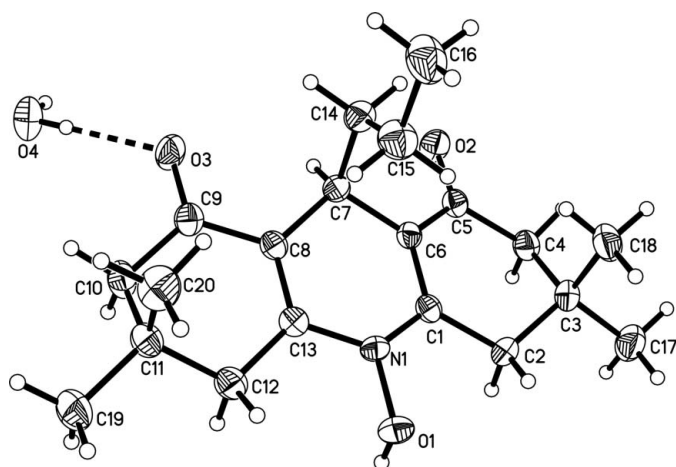
Water H atoms were located in a difference map and refined with an O–H distance restraint of 0.82 (1) Å. The remaining H atoms were placed in calculated positions, with O–H = 0.82 Å and C–H = 0.96–0.98 Å. The  $U_{\text{iso}}(\text{H})$  values were constrained to  $1.5U_{\text{eq}}$  of the carrier atom for the methyl and hydroxyl H atoms and  $1.2U_{\text{eq}}$  for the remaining H atoms. In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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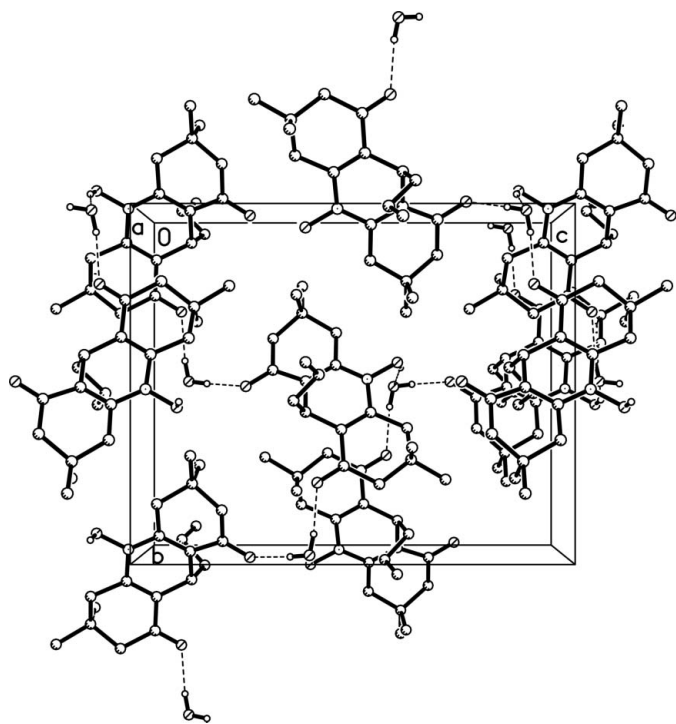
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**Figure 1**

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates an O–H...O hydrogen bond.



**Figure 2**

A packing diagram of (I), projected along the  $a$  axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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