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10-Benzyl-3,3,6,6,9-pentamethyl-3,4,6,7,9,10-hexahydroacridine-1,8(2*H*,5*H*)-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.065
wR factor = 0.197
Data-to-parameter ratio = 13.0

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

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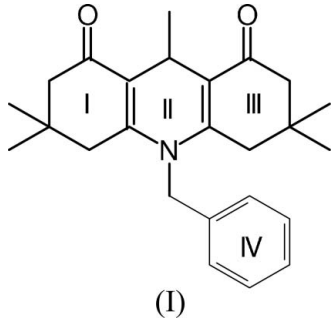
The title compound, $C_{25}H_{31}NO_2$, crystallizes with two molecules in the asymmetric unit. In both molecules, the central dihydropyridine ring adopts a flattened boat conformation. In molecule *A*, the outer rings adopt sofa conformations, whereas in molecule *B*, one of the outer rings is disordered and the other ring adopts a sofa conformation. In the crystal structure, C—H···O interactions link the molecules to form a tape that runs along the *b* axis.

Comment

Acridine and its derivatives exhibit a wide spectrum of biological activities, such as mutagenic, antitumour (Talacki *et al.*, 1974), anti-amoebic (Prasad Krishna *et al.*, 1984), hypertensive and anti-inflammatory (Asthana *et al.*, 1991). Acridine-containing drugs have been found to possess antiprotozoal activity (Karolak-Wojciechowska *et al.*, 1996) and are used for the treatment of Alzheimer's disease (Bandoli *et al.*, 1994). Substituted hexahydroacridine-1,8-diones resemble K-channel openers, which relax KCl-preconcentrated urinary-bladder muscle *in vitro* (Trivedi *et al.*, 1995; Li *et al.*, 1996). Acridine-1,8-diones exhibit fluorescence and laser activities (Selladurai *et al.*, 1990). Decahydroacridine-1,8-diones act as photosensitizers (Timpe *et al.*, 1993) and also possess other important photophysical and electrochemical properties (Mohan *et al.*, 1996). Acridinediones were found to have laser activity around 475–495 nm (Murugan *et al.*, 1998). The present study of the title compound, (I), is part of a series of investigations on the crystal structures of acridinedione derivatives.



(I)

There are two molecules in the asymmetric unit. As reported in related acridinedione derivatives (Ganesh, Velmurugan *et al.*, 1998; Ganesh, Banumathi *et al.*, 1998; Ganesh *et al.*, 1999; Sankaranarayanan *et al.*, 1998, 1999; Jeyakanthan *et al.*, 2000, 2002; Aravindan *et al.*, 2003), the acridine system is folded about the line passing through atoms C9 and N10, with a dihedral angle of 18.9 (1) and 18.1 (1)° for

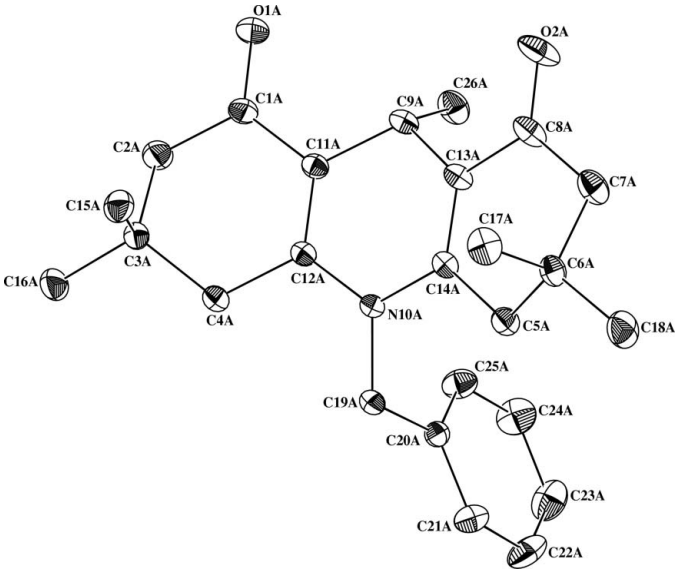


Figure 1
One of the two independent molecules of the title compound, showing 35% probability displacement ellipsoids. H atoms have been omitted.

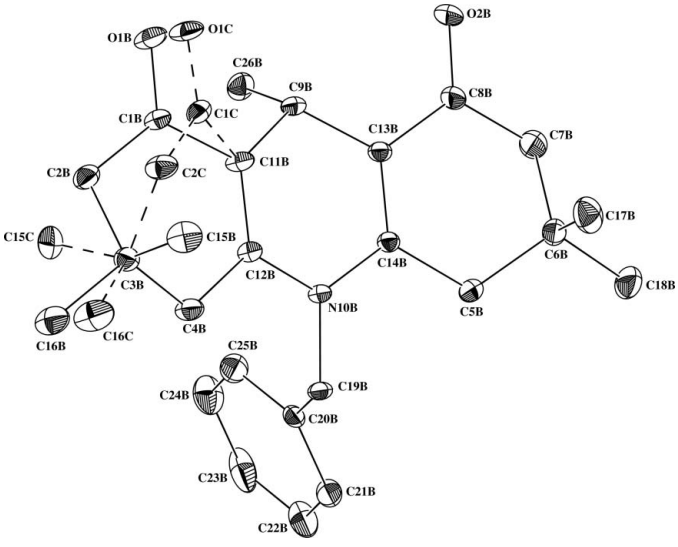


Figure 2
The other independent molecule of the title compound, showing 35% probability displacement ellipsoids. H atoms have been omitted. Both disorder components are shown.

molecules *A* and *B*, respectively, between the two halves of the molecule (C9/C11/C1/C2/C4/C12/N10 and C9/C13/C8/C7/C5/C14/N10 for molecule *A*, and C9/C11/C3/C4/C12/N10 and C9/C13/C8/C7/C5/C14/N10 for molecule *B*). The dihedral angles between the least-squares plane through the central dihydropyridine (C11/C12/C13/C14) and phenyl rings (C20–C25) are 81.8 (1) and 84.2 (1)° for molecule *A* and *B*, respectively. The methyl groups attached to the dihydropyridine rings are in a pseudo-axial position.

The puckering of the dihydropyridine ring is quite small, owing to the π conjugation in the C11—C12—N10—C14—C13 system. Similar features have also been observed in other related acridinedione derivatives (Gunasekaran *et al.*, 1996; Ganesh, Banumathi *et al.*, 1998; Ganesh *et al.*, 1999; Sankaranarayanan *et al.*, 1998; Aravindan *et al.*, 2003). The sum of the bond angles around N10 (358.7 and 359.9° for molecules *A* and *B*, respectively) indicates sp^2-hybridization.

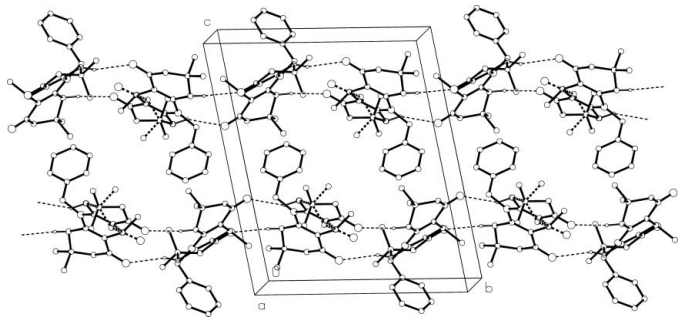


Figure 3
The molecular packing of (I), viewed approximately down the *a* axis, showing the C—H···O-mediated tape motif along the *b* axis. Hydrogen bonds are shown as dashed lines.

In the crystal structure, C—H···O interactions (Table 2) link molecules *A* and *B* to form tapes that run along *b* axis (Fig. 3).

Experimental

A mixture of 2,2′-ethylidenebis(5,5-dimethylcyclohexane-1,3-dione) (1.65 g, 5,3 mmol) and benzylamine (0.5 g, 5.3 mmol) was refluxed in acetic acid (20 ml) for 6 h. The reaction mixture was cooled and poured on to crushed ice. The resulting solid was filtered off and purified by column chromatography over alumina (neutral) and eluted with $CHCl_3$–MeOH (2:1), to give the title compound. Single crystals were grown by slow evaporation of a solution in $CHCl_3$–MeOH (1:1).

Crystal data

$C_{25}H_{31}NO_2$	$Z = 4$
$M_r = 377.51$	$D_x = 1.167$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.3359$ (1) Å	Cell parameters from 4761 reflections
$b = 13.8339$ (3) Å	$\theta = 1.3$–$28.4°$
$c = 16.2254$ (4) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 101.153$ (1)°	$T = 293$ (2) K
$\beta = 90.934$ (1)°	Plate, yellow
$\gamma = 108.687$ (1)°	0.46 × 0.24 × 0.08 mm
$V = 2148.53$ (8) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	7331 independent reflections
	4386 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.031$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -12 \rightarrow 10$
$T_{min} = 0.967$, $T_{max} = 0.994$	$k = -16 \rightarrow 16$
11586 measured reflections	$l = -19 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0876P)^2 + 0.573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.065$	
$wR(F^2) = 0.197$	
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
7331 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
563 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1*A*—C1*A*	1.229 (3)	O1*C*—C1*C*	1.223 (19)
O2*A*—C8*A*	1.232 (4)	O2*B*—C8*B*	1.241 (4)
N10*A*—C14*A*	1.399 (3)	N10*B*—C12*B*	1.399 (3)
N10*A*—C12*A*	1.404 (3)	N10*B*—C14*B*	1.402 (4)
C11*A*—C12*A*	1.349 (4)	C11*B*—C12*B*	1.359 (4)
C13*A*—C14*A*	1.350 (4)	C13*B*—C14*B*	1.359 (4)
O1*B*—C1*B*	1.225 (13)		
C14*A*—N10*A*—C12*A*	119.4 (2)	C12*B*—N10*B*—C14*B*	119.8 (2)
C14*A*—N10*A*—C19*A*	119.6 (2)	C12*B*—N10*B*—C19*B*	121.3 (2)
C12*A*—N10*A*—C19*A*	120.7 (2)	C14*B*—N10*B*—C19*B*	118.8 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4*A*—H4*A*1···O2*B*	0.97	2.47	3.369 (4)	153
C5*A*—H5*A*2···O1*B*	0.97	2.35	3.291 (12)	163
C4*B*—H4*B*1···O2*A*^{i}	0.97	2.48	3.362 (4)	152
C5*B*—H5*B*2···O1*A*^{i}	0.97	2.39	3.324 (4)	163

Symmetry code: (i) $x, y-1, z$.

All H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$. In molecule *B*, atoms C1*B* and C2*B*, as well as the carbonyl atom O1*B* and methyl groups C15*B* and C16*B*, were found to be disordered, and the site-occupancy factors of the major and minor conformations were refined to 0.591 (8):0.409 (8)].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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