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10-(4-Bromophenyl)-9-(4-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

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The crystal structure of the title compound, $C_{30}H_{32}BrNO_3$, is stabilized by two C—H···O intermolecular hydrogen bonds and one weak C—H···π interaction. C—H···O hydrogen bonds generate $C(10)$ chains and an $R_2^2(16)$ ring motif. In the title compound, the central pyridine ring in the acridinedione system is approximately planar while the outer two rings adopt half-chair conformations. The buckling angle between the two halves [at the N···C(PhOMe) line] of 6.94 (2)° shows the degree of planarity of the acridinedione system. The dihedral angle between the planes of the two aromatic rings is 9.66 (2)°.

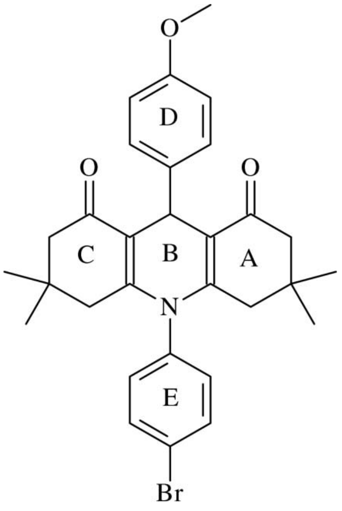
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.121
Data-to-parameter ratio = 16.3

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

Comment

The present work is part of a structural study of tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione compounds (Odabaşoğlu *et al.*, 2007) and we report here the structure of the title compound, (I).



(I)

Bond distances and angles in (I) are in good agreement with the corresponding values obtained for related 3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione derivatives (Odabaşoğlu *et al.*, 2007; Sivaraman *et al.*, 1996). The molecular structure of (I), with the atom-labelling scheme, is shown in Fig. 1, and selected geometric parameters are given in Table 1.

Rings *A* to *E* are as defined in the scheme. Benzene rings *D* and *E* are orthogonal to the central ring *B*, forming dihedral angles of 80.38 (2) and 89.60 (2)°, respectively. The valence angles around the N atom sum to 359.8° (Table 1), and these values are indicative of sp^2 hybridization of the N atom. Due to electron delocalization, the C7—N1 and N1—C28 bond

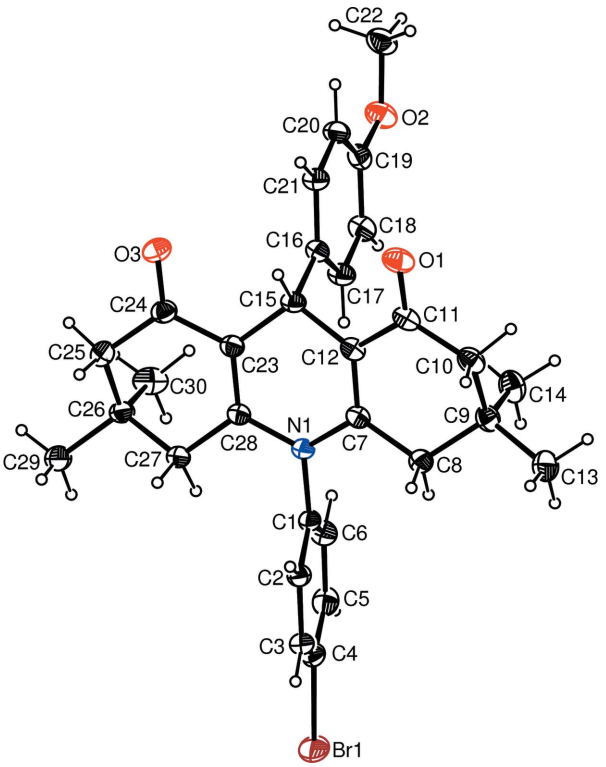


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

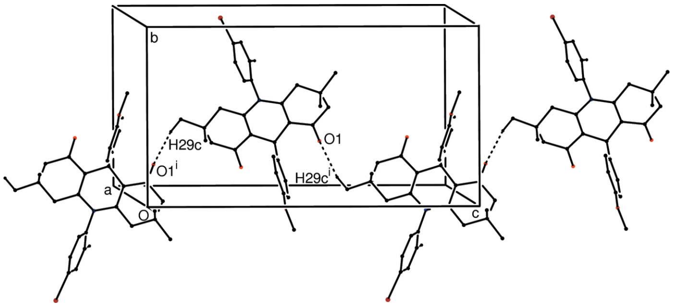


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded (dashed lines) chain. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$.]

lengths are shorter than the C—N single-bond value [N—C = 1.468 (2)–1.474 (2) Å (Odabaşoğlu *et al.*, 2003); 1.47 Å (Loudon, 2002)].

In (I), the conformations of the six-membered rings *A* and *C* are envelopes, with C9 and C26 as flap atoms, respectively. The acridine moiety is folded about the line passing through atoms N1 and C15, and the dihedral angle between the two halves (C7–C12/C15/N1 and C23–C28/C15/N1) is 6.94 (2)°, bigger than that [3.3 (2)°] of a similar structure (Subbiah Pandi *et al.*, 2002). Puckering parameters (Cremer & Pople, 1975) are $Q(A)$ = 0.4135 (5) Å, $Q(C)$ = 0.3948 (5) Å, $\theta(A)$ = 60.02 (5)°, $\theta(C)$ = 125.23 (5)°, $\varphi(A)$ = 116.6916 (5)° and $\varphi(C)$ = 356.2389 (5)°.

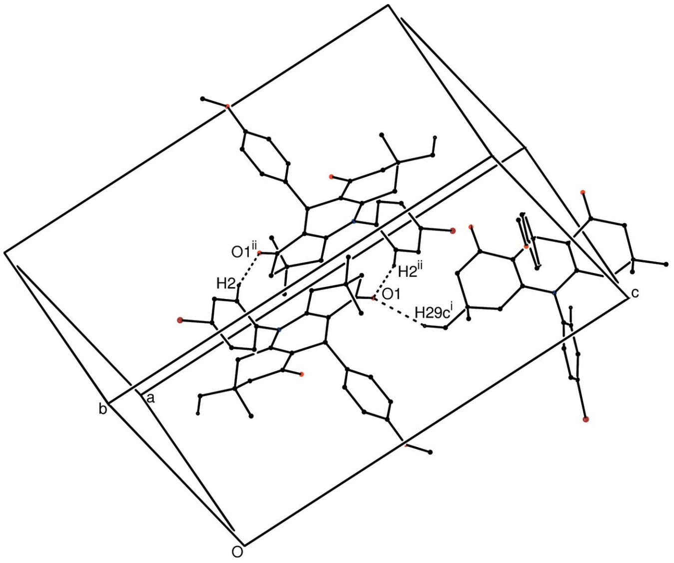


Figure 3
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded (dashed lines) $R^2_2(16)$ ring. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$; (ii) $1 - x, 1 - y, 1 - z$.]

In (I), the crystal packing is stabilized by intermolecular C—H···O hydrogen bonds (Table 2) and weak C—H···π interactions. The C29—H29*C*···O1^{ii} intermolecular hydrogen bonds generate a *C*(10) chain along the *c* axis (Fig. 2 and Table 2). These chains are further connected to other molecules by C2—H2···O1^{i} hydrogen-bonds (Table 2), forming $R^2_2(16)$ motifs (Etter, 1990) (Fig. 3) and a three-dimensional network.

In addition to these intermolecular C—H···O hydrogen bonds, C—H···π interactions also play a role in the packing of (I). For the C22—H22···*Cg*^{iii} contact (*Cg* is the centroid of ring *E*), the distance between atom H22 and the aromatic ring centroid is 3.199 (1) Å [symmetry code: (iii) $x, -1 + y, z$], with a C—H···*Cg* angle of 158°.

Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2007), using 2,2′-[(4-methoxyphenyl)methylene]bis(5,5-dimethylcyclohexane-1,3-dione) and 2-bromobenzenamine as starting materials (yield 81%; m.p. 509 K). Crystals of (I) suitable for X-ray crystallographic analysis were obtained by slow evaporation of an EtOH–H$_2$O (9:1 *v*/*v*) solution at room temperature.

Crystal data

$C_{30}H_{32}BrNO_3$
M_r = 534.48
Monoclinic, $P2_1/c$
a = 12.2412 (5) Å
b = 10.9837 (4) Å
c = 20.1373 (9) Å
β = 101.011 (4)°
V = 2657.69 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 296 K
0.61 × 0.43 × 0.33 mm

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Data collection

Stoe IPDS II diffractometer	37558 measured reflections
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) $T_{\min} = 0.441$, $T_{\max} = 0.671$	5231 independent reflections
	3902 reflections with $I > 2\sigma(I)$
	$R_{\rm int} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$	321 parameters
$wR(F^2) = 0.121$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\max} = 0.63$ e Å^{-3}
5231 reflections	$\Delta\rho_{\min} = -1.00$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.447 (3)	C11—C12	1.455 (4)
C4—Br1	1.897 (3)	C23—C28	1.349 (4)
C7—C12	1.353 (4)	C23—C24	1.459 (4)
C7—N1	1.396 (3)	C24—O3	1.223 (3)
C11—O1	1.227 (3)	C28—N1	1.400 (3)
C7—N1—C28	120.7 (2)	C28—N1—C1	118.9 (2)
C7—N1—C1	120.2 (2)		
C7—C8—C9—C13	170.5 (3)	C30—C26—C27—C28	68.2 (3)
C7—C8—C9—C14	−69.2 (3)	C29—C26—C27—C28	−171.6 (3)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$O1$^{\rm i}$	0.93	2.45	3.342 (4)	161
C29—H29*C*$\cdots$O1$^{\rm ii}$	0.96	2.55	3.440 (4)	154

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

All H atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic H, 0.98 Å for methine H and 0.97 Å for methylene H, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), or with C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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