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10-(2-Fluorophenyl)-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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In the title compound, $C_{30}H_{32}FNO_3$, the central heterocyclic ring of the tetrahydroacridinedione system is planar while the two outer rings adopt envelope conformations. The buckling angle between the two halves of the acridinedione system is 10.61 (2)°, which shows the relative planarity of the system. The dihedral angle between the planes of the aromatic rings is 6.13 (2)°. The crystal structure is stabilized by three intermolecular C—H···O hydrogen bonds that generate $C(10)$ chains together with $R_2^2(16)$ and $R_3^2(15)$ ring motifs. A weak C—H···π interaction further stabilizes the crystal structure.

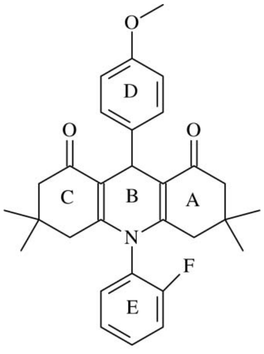
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.101
Data-to-parameter ratio = 15.7

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, Kaya, Büyükgüngör *et al.*, 2007; Odabaşoğlu, Kaya, Büyükgüngör & Yıldırır, 2007) and we report here the structure of the title compound, (I) (Fig. 1).



(I)

Bond distances and angles in compound (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, Kaya, Büyükgüngör *et al.*, 2007; Odabaşoğlu, Kaya, Büyükgüngör & Yıldırır, 2007; Sivaraman *et al.*, 1996) and in comparison with similar systems (Loudon, 2002; Odabaşoğlu *et al.*, 2003). The C1—N1 bond length [1.4381 (15) Å] indicates that there is little, if any, electron delocalization between N1 and the C1–C6 ring. The C7–C12 and C23–C28 rings (*A* and *C*, respectively, in the scheme) adopt envelope conformations, with C9 and C26 as the flap atoms, respectively; puckering parameters (Cremer & Pople, 1975) are $Q(A)$ = 0.4211 (5) Å, $Q(C)$ = 0.4174 (5) Å, $\theta(A)$ = 60.79 (5)°, $\theta(C)$ = 123.55 (5)°, $\varphi(A)$ = 119.1431 (5)° and $\varphi(C)$ = 347.9643 (5)°. (Cremer & Pople, 1975).

In compound (I), the crystal packing is stabilized by intermolecular C—H···O hydrogen bonds (Table 2) and weak C—

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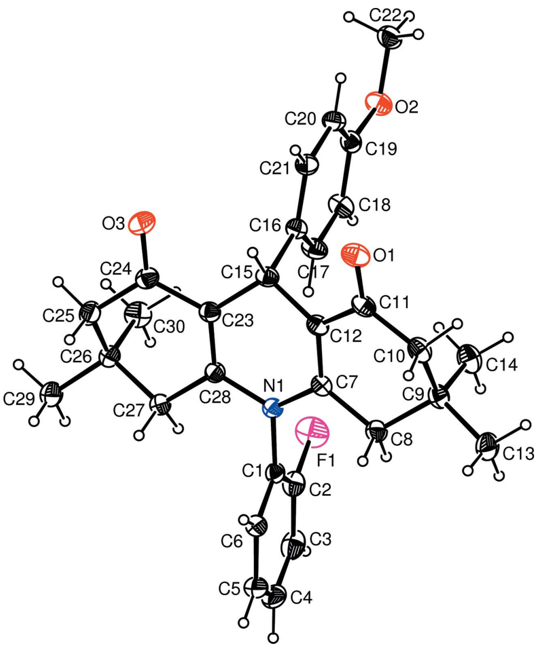

Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

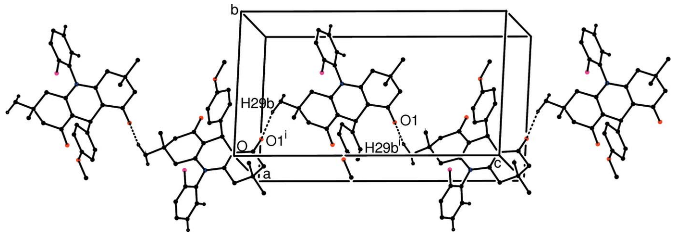

Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded (dashed lines) *C*(10) chain. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$].

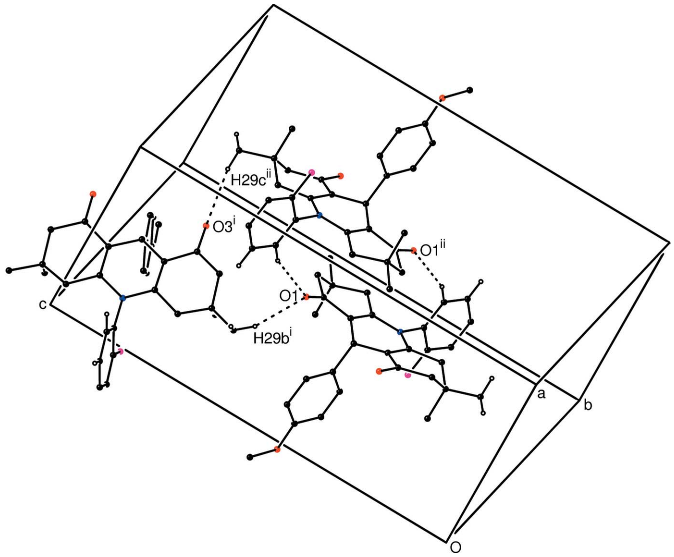

Figure 3
Part of the crystal structure of (II), showing the formation of a hydrogen-bonded (dashed lines) edge-fused $R_2^2(16)R_3^2(15)$ motif. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry codes: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$; (ii) $1 - x, 1 - y, 1 - z$].

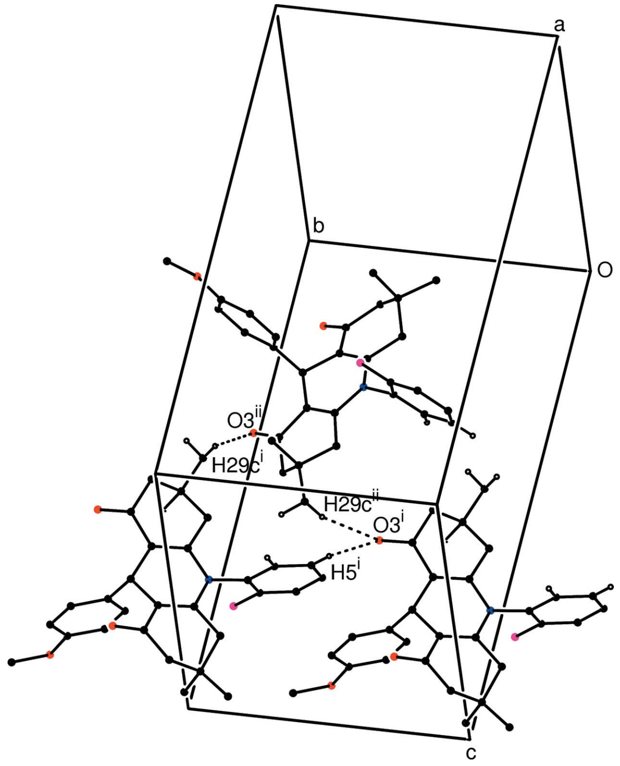

Figure 4
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded (dashed lines) $R_3^2(11)$ ring. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry codes: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$; (ii) $1 - x, 1 - y, 1 - z$].

H$\cdots\pi$ interactions. C29—H29*B*$\cdots$O1^{iii} hydrogen bonds generate a *C*(10) chain along the *c* axis (Fig. 2) and these are further interconnected by C29—H29*C*$\cdots$O3^{iv} hydrogen bonds, to generate edge-fused $R_2^2(16)$ and $R_3^2(15)$ motifs, while C5—H5$\cdots$O3^{i} and C29—H29*C*$\cdots$O3^{iv} hydrogen bonds generate $R_3^2(11)$ motifs (Etter, 1990) (Fig. 4).

C—H$\cdots\pi$ interactions also play a role in the packing of (I). For the C22—H22*C*$\cdots$*Cg*^{v} contact, H22$\cdots$*Cg* = 3.2958 Å and C—H$\cdots$*Cg* = 146° [*Cg* is the centroid of the C1–C6 ring; symmetry code: (v) $x, -1 + y, z$].

Experimental

The title compound was prepared as described by Odabaşoğlu, Kaya, Büyükgüngör *et al.* (2007), using 2,2′-[(4-methoxyphenyl)methylene]bis(5,5-dimethylcyclohexane-1,3-dione) and 2-fluorobenzenamine as starting materials (yield 75%; m.p. 482 K). Crystals of (I) suitable for X-ray crystallographic analysis were obtained by slow evaporation of an EtOH–H$_2$O (8:2 *v*/*v*) solution at room temperature.

Crystal data

$C_{30}H_{32}FNO_3$
$M_r = 473.57$
Monoclinic, $P2_1/c$
$a = 12.2403\ (6)$ Å
$b = 10.4616\ (3)$ Å
$c = 20.2330\ (9)$ Å
$\beta = 100.942\ (4)^\circ$

$V = 2543.80\ (18)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 296$ K
0.77 × 0.65 × 0.50 mm

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Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.952$, $T_{\max} = 0.971$

34276 measured reflections
4984 independent reflections
4015 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.102$
$S = 1.06$
4984 reflections
317 parameters

7 restraints
H-atom parameters constrained
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3$^{\rm i}$	0.93	2.58	3.507 (2)	172
C6—H6···O1$^{\rm ii}$	0.93	2.52	3.3962 (17)	157
C29—H29*B*···O1$^{\rm iii}$	0.96	2.51	3.3902 (18)	153
C29—H29*C*···O3$^{\rm iv}$	0.96	2.57	3.505 (2)	164

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

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 $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$, and with C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ 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, 1997); 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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