Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9-(3-Fluorophenyl)-3,3,6,6-tetramethyl-1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione

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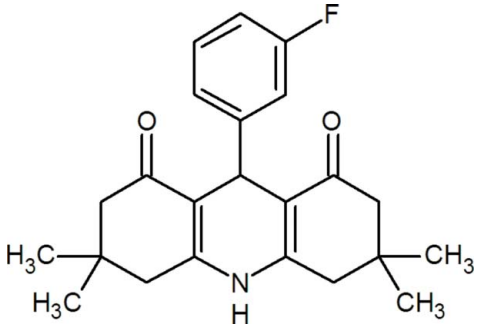
Received 7 December 2012; accepted 12 December 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.118; data-to-parameter ratio = 15.3.

In the title molecule, $C_{23}H_{26}FNO_2$, the central ring of the acridinedione system adopts a slight boat conformation and the four essentially planar atoms of this ring [maximum deviation = 0.019 (1) Å] form a dihedral angle of 89.98 (6)° with the benzene ring. The two outer rings of the acridinedione system adopt sofa conformations. In the crystal, N—H···O hydrogen bonds link the molecules, forming chains along [001].

Related literature

For applications of acridines, see: Murugan *et al.* (1998); Leon *et al.* (2008). Josephrajan *et al.* (2005); Srividya *et al.* (1998, 1996). For related structures, see: Balamurugan *et al.* (2009); Zhao & Teng (2008); Kant *et al.* (2013). For ring conformations, see: Duax & Norton (1975).



Experimental

Crystal data

$C_{23}H_{26}FNO_2$
M_r = 367.45
Monoclinic, $P2_1/c$
a = 11.0505 (3) Å
b = 12.8264 (3) Å
c = 13.8548 (3) Å
β = 100.215 (2)°
V = 1932.63 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.2 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.897, T_{max} = 1.000
30330 measured reflections
3789 independent reflections
2922 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.03
3789 reflections
248 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10···O1^{i}	0.86	2.14	2.990 (2)	168

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

RK acknowledges the Department of Science & Technology for access to the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5569).

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