Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,5-Bis(phthalimidomethyl)acridine

Sophia Tapper,[a] Fiona H. Fry,[a] Stephen J. Simpson[a]* and James H. R. Tucker[b]

[a]School of Biosciences, Geoffrey Pope Building, University of Exeter, Stocker Road, Exeter EX4 4QD, England, and [b]School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, England

Correspondence e-mail: s.j.simpson@exeter.ac.uk

Key indicators

Single-crystal synchrotron study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.110
Data-to-parameter ratio = 10.2

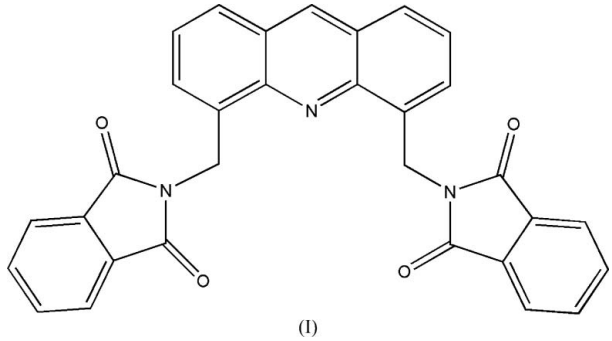
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 January 2007
Accepted 12 January 2007

The structure of the title symmetrically disubstituted acridine derivative [systematic name: *N*,*N*′-(acridine-4,5-diyldimethylene)bisphthalimide], $C_{31}H_{19}N_3O_4$, has been determined at 120 K using synchrotron radiation. The molecule contains a planar acridine and two planar phthalimide fragments. The pseudo-torsion angle N—C···C—N between the phthalimidomethyl groups, where C···C is an intramolecular contact between the methylene C atoms, is 95.9 (2)°; the phthalimide rings are almost parallel to each other.

Comment

Certain acridine derivatives have been shown to have immunosuppresive properties (Farr *et al.*, 1965; Hess & Stewart, 1975; Hess *et al.*, 1971). Recently, acridine derivatives have been shown to exert toxicity towards *Plasmodium*, *Trypanosoma*, and *Leishmania* parasites (Di Giorgio *et al.*, 2005). Many of the compounds of interest are either 4-substituted or 4,5-disubstituted acridines. The title compound, (I), is a key starting material in the elaboration of the 4- and 5-positions of the acridine nucleus for the synthesis of novel hydrogen-bonding receptors. The single-crystal structure of 4-(phthalimidomethyl)acridine has been reported (Chiron & Galy, 2003) and a comparison of the relative arrangement of the planar systems in both this molecule and (I) was deemed to be of interest.



(I)

The structure of (I), is shown in Fig. 1. The two planar phthalimido groups are almost parallel to each other, the dihedral angle between the mean planes being 5.1 (2)°; these planes are inclined at 80.6 (2) and 81.5 (2)° with respect to the mean plane of the acridine system. The latter angle is 85.6 (2)° for the monosubstituted 4-(phthalimidomethyl)acridine. The pseudo-torsion angle N2—C14···C23—N3 is large [95.9 (2)°], resulting in one phthalimidomethyl group being approximately bisected by the plane of the acridine system and the other being nearly perpendicular to it.

Experimental

The title compound was prepared by a modification of the published method (Chiron & Galy, 2003) and spectroscopic data were in agreement with previous reports (Hess & Stewart, 1975). Crystals suitable for diffraction analysis were grown by slow cooling of a dimethylsulfoxide solution. Data were collected at the Daresbury SRS station 9.8 using a silicon 111 monochromator.

Crystal data

$C_{31}H_{19}N_3O_4$
$M_r = 497.49$
Orthorhombic, $Pna2_1$
$a = 40.462$ (12) Å
$b = 4.7732$ (14) Å
$c = 11.719$ (4) Å
$V = 2263.3$ (12) Å^3
$Z = 4$
$D_x = 1.460$ Mg m^{-3}
Synchrotron radiation
$\lambda = 0.6905$ Å
$\mu = 0.10$ mm^{-1}
$T = 120$ (2) K
Block, colourless
0.17 × 0.07 × 0.03 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
fine–slice ω scans
Absorption correction: none
15033 measured reflections
3485 independent reflections
3261 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 29.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.110$
$S = 1.11$
3485 reflections
343 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.0792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected torsion angles (°).

C4—C5—C14—N2	−114.29 (19)	C9—C8—C23—N3	−14.1 (3)
C6—C5—C14—N2	68.9 (2)	C7—C8—C23—N3	165.48 (16)

H atoms were included in calculated positions, C—H = 0.95–0.99 Å, and refined as riding on their respective C atoms, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$. In the absence of any significant anomalous scattering, Friedel equivalents were merged prior to the final refinements.

Data collection: *APEX2* (Bruker 2005); cell refinement: *SAINT* (Bruker 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

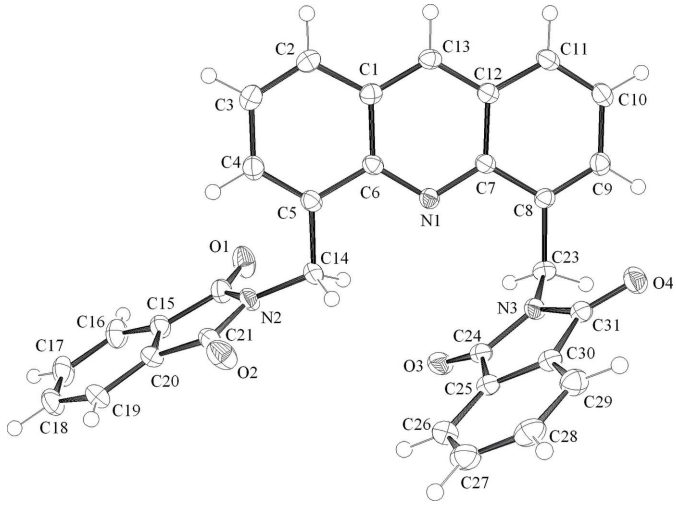


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

We acknowledge the use of the EPSRC's Chemical Database Service at Daresbury. The EPSRC National Crystallography Service is thanked for performing the data collection at Daresbury.

References

Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Chiron, J. & Galy, J.-P. (2003). *Heterocycles*, **16**, 1653–1672.
Di Giorgio, C., De Méo, M., Chiron, J., Delmas, F., Nikoyan, A., Severine, J., Dumenil, G., Timon-David, P. & Galy, J.-P. (2005). *Bioorg. Med. Chem.* **13**, 5560–5568.
Farr, R. S., Samuelson, J. S. & Stewart, P. B. (1965). *J. Immunol.* **94**, 682–686.
Farrugia, L. J. (1999). J. *Appl. Cryst.* **32**, 837–838.
Hess, F., Cullen, E. & Grozinger, K. (1971). *Tetrahedron Lett.* **12**, 2591–2594.
Hess, F. R. & Stewart, P. B. (1975). *J. Med. Chem.* **18**, 320–321.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. Release 97.2. University of Göttingen, Germany.