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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.078
 wR factor = 0.170
Data-to-parameter ratio = 13.1

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

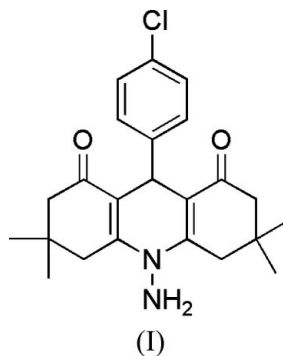
10-Amino-9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,9,10-hexahydroacridine-1,8(2H,7H)-dione

The title compound, $\text{C}_{23}\text{H}_{27}\text{ClN}_2\text{O}_2$, has been synthesized by the reaction of 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7-hexahydroanthene-1,8-dione with hydrazine in ethanol under microwave irradiation. The dihydropyridine ring adopts a boat conformation.

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Comment

Acridine belongs to a class of compounds which are special not only because of their interesting chemical and physical properties, but also due to their immense utility in the pharmaceutical and dye industries. The discovery of acridines as antimalarial and antitumor agents has attracted the attention of organic chemists and thus led to intensive interest in the synthesis of several drugs based on acridine (Khurana *et al.*, 1990; Matsumoto *et al.*, 1983; Nakano *et al.*, 1982). Chemical modifications of the acridine ring system, such as the introduction of an aryl group on the N atom, causes laser activity (Murugan *et al.*, 1998). In this paper, we report the crystal structure of the title compound, (I).



In (I), the dihydropyridine ring adopts a boat conformation, with atoms N1 and C7 deviating from the C6/C1/C8/C13 plane by 0.093 (3) and 0.263 (3) Å, respectively (Fig. 1). Both cyclohexene rings adopt an envelope conformation: atom C3 deviates from the C1, C2, C4/C6 plane by 0.668 (3) Å and atom C11 deviates from the C8–C10/C12/C13 plane by 0.653 (3) Å. The dihedral angle between the C6/C1/C8/C13 plane and the C18–C23 benzene ring is 101.13 (7)°. The molecules are connected *via* N–H...O hydrogen bonds (Table 2), forming a three-dimensional network (Fig. 2).

Experimental

The title compound, (I), was prepared by the reaction of 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-2,3,4,5,6,7-hexahydroanthene-1,8-dione (1 mmol) with hydrazine (5 mmol) in ethanol under microwave irradiation. Single crystals of (I) suitable for X-ray

diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 85%; m.p. 550–551 K). IR (cm^{-1}): 3337 (NH_2), 1632 (CO); ^1H NMR ($\text{DMSO}-d_6$): δ 0.86 (6H, s, 2CH_3), 1.02 (6H, s, 2CH_3), 1.99–2.91 (8H, m, 4CH_2), 4.94 (H, s, CH), 5.30 (2H, s, NH_2), 7.14 (2H, d, $J = 8.0$ Hz, ArH), 7.26 (2H, d, $J = 8.0$ Hz, ArH).

Crystal data

$\text{C}_{23}\text{H}_{27}\text{ClN}_2\text{O}_2$	$Z = 2$
$M_r = 398.92$	$D_x = 1.222$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.8057$ (18) Å	Cell parameters from 1226 reflections
$b = 11.211$ (2) Å	$\theta = 2.7$ – 27.5°
$c = 12.097$ (3) Å	$\mu = 0.20$ mm^{-1}
$\alpha = 70.148$ (3) $^\circ$	$T = 298$ (2) K
$\beta = 84.255$ (4) $^\circ$	Chunk, yellow
$\gamma = 74.874$ (4) $^\circ$	$0.28 \times 0.21 \times 0.08$ mm
$V = 1084.2$ (4) Å 3	

Data collection

Bruker SMART CCD area-detector diffractometer	3322 independent reflections
φ and ω scans	2330 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.057$
$T_{\text{min}} = 0.947$, $T_{\text{max}} = 0.985$	$\theta_{\text{max}} = 25.0^\circ$
4387 measured reflections	$h = -10 \rightarrow 7$
	$k = -13 \rightarrow 10$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.078$	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2]$
$wR(F^2) = 0.170$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3322 reflections	$\Delta\rho_{\text{max}} = 0.31$ e Å $^{-3}$
253 parameters	$\Delta\rho_{\text{min}} = -0.31$ e Å $^{-3}$

Table 1

Selected geometric parameters (Å, $^\circ$).

N1–C1	1.399 (5)	C6–C7	1.540 (6)
N1–C13	1.426 (5)	C7–C8	1.520 (6)
N1–N2	1.438 (5)	C7–C18	1.564 (7)
C1–N1–C13	120.0 (3)	N1–C1–C2	116.9 (4)
C1–N1–N2	120.0 (4)	C8–C7–C6	110.2 (4)
C13–N1–N2	116.9 (4)	C13–C8–C7	121.8 (4)
C6–C1–N1	120.7 (4)	C8–C13–N1	121.4 (4)

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2A}\cdots\text{O2}^i$	0.86	2.58	3.123 (5)	122

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

All H atoms were positioned geometrically and treated as riding, with $\text{C}-\text{H} = 0.93$ – 0.98 Å and $\text{N}-\text{H} = 0.86$ Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C}, \text{N})$ for others.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

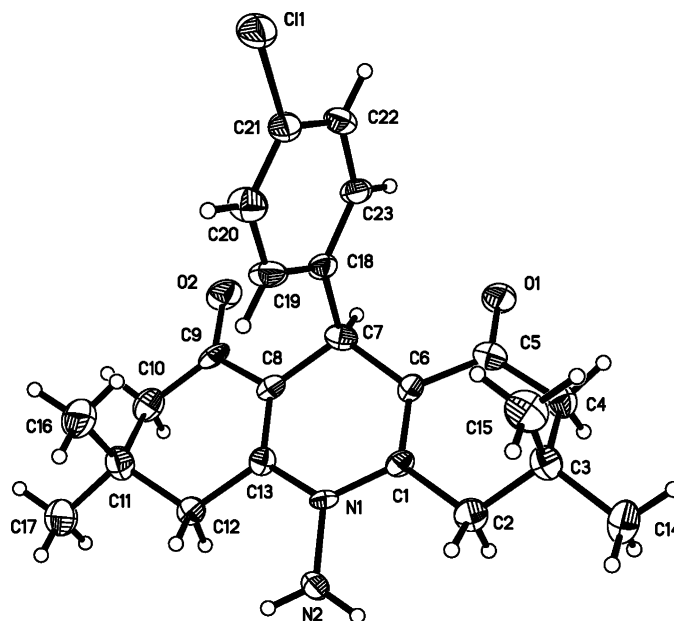


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids.

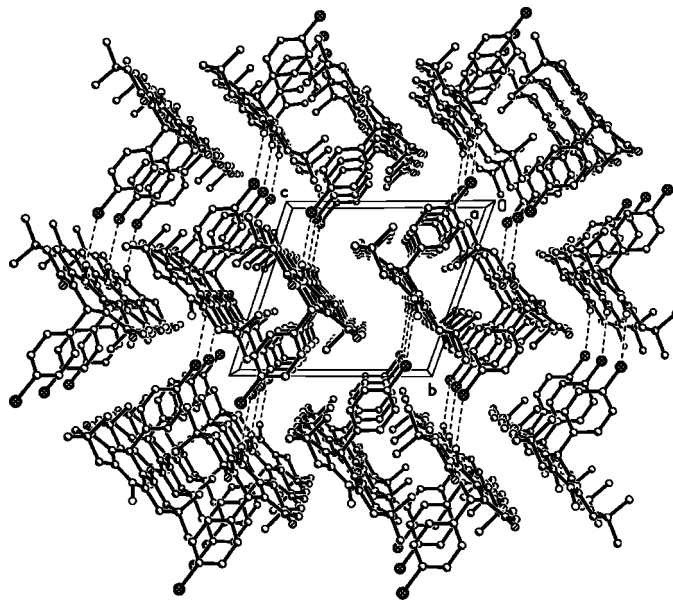


Figure 2

A packing diagram of (I) projected along the a axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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