Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Cyclopropyl-7,7-dimethyl-10-(3-nitrophenyl)-7,8-dihydro-5*H*-indeno[1,2-*b*]quinoline-9,11(6*H*,10*H*)-dione

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.066
wR factor = 0.245
Data-to-parameter ratio = 12.7

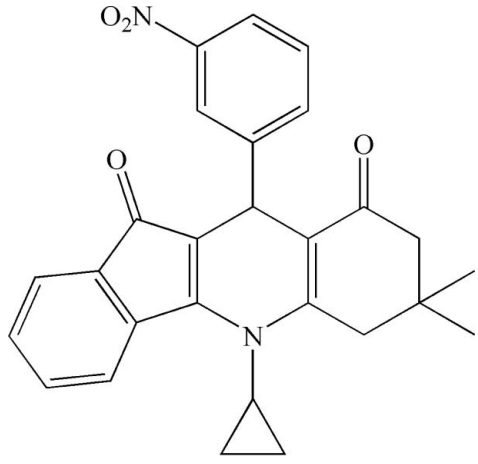
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 19 December 2006
Accepted 26 December 2006

The title compound, $C_{27}H_{24}N_2O_4$, has been synthesized by the reaction of 3-nitrobenzaldehyde and 3-cyclopropylamino-5,5-dimethylcyclohex-2-enone with 1,3-indanedione in a mixed solvent of ethylene glycol and acetic acid under microwave irradiation. The cyclohexenone and fused N-containing rings are not planar and have flattened-boat and boat conformations, respectively.

Comment

1,4-Dihydropyridines (1,4-DHPs) are well known compounds because of their pharmacological profiles as calcium channel modulators (Stout & Meyers, 1982). With a 1,4-DHP parent nucleus, indenoquinoline belongs to a class of compounds which are special not only because of their interesting chemical and physical properties, but also owing to their immense utility in the pharmaceutical industry. The discovery of indenoquinoline as new potent cytotoxic and antitumor agents has attracted the attention of organic chemists (Yamato *et al.*, 1989; Deady *et al.*, 2000; Chen *et al.*, 2002). It is well established that chemical modifications on the indenoquinoline skeletons may bring remarkable changes in biological activity (Deady *et al.*, 1999). We report here the crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

The rings *A* (C1–C6) and *B* (N1/C1/C6–C8/C16) are not planar, having total puckering amplitudes, Q_T, of 0.467 (3) and 0.298 (4) Å, respectively, and flattened-boat and boat conformations [φ = 134.86 (5)°, θ = 52.91 (3)° and φ = −3.86 (6)°, θ = 100.90 (3)°] (Cremer & Pople, 1975). Rings *C* (C8–C10/C15/

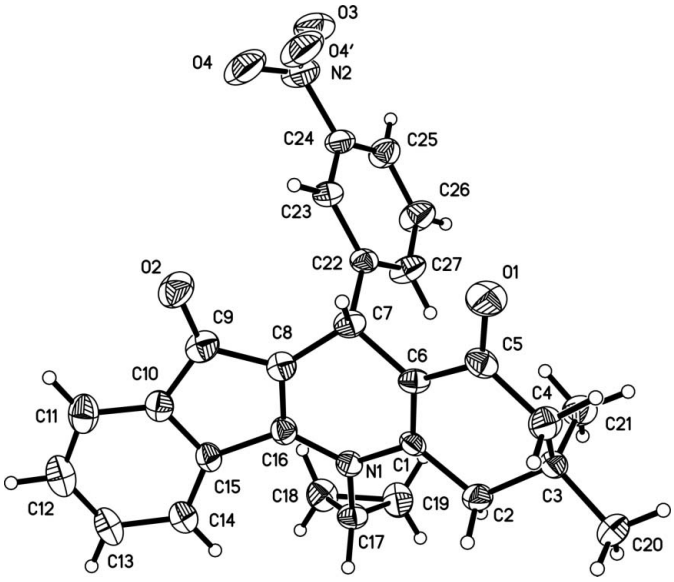


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

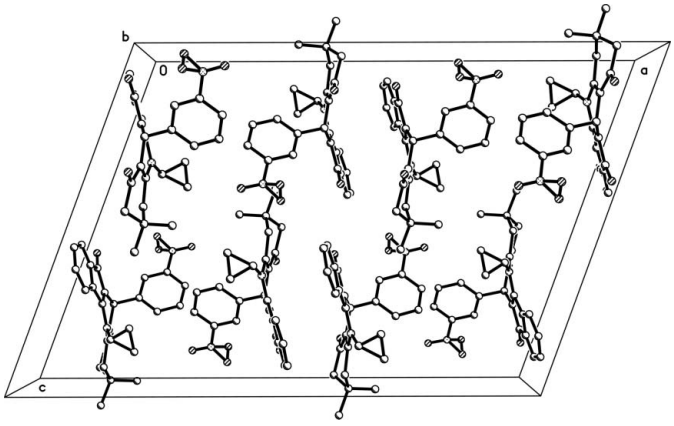


Figure 2
A packing diagram of (I). H atoms have been omitted for clarity.

C16), *D* (C10–C15) and *E* (C22–C27) are, of course, planar and the dihedral angles between them are *C*/*D* = 3.31 (4)°, *C*/*E* = 69.83 (3)° and *D*/*E* = 67.00 (4)°.

As can be seen from the packing diagram (Fig. 2), the molecules are elongated along the *c* axis. Dipole–dipole and van der Waals interactions are effective in the molecular packing.

Experimental

Compound (I) was prepared by the reaction of 3-nitrobenzaldehyde (0.15 g, 1 mmol) and 3-(cyclopropylamino)-5,5-dimethylcyclohex-2-enone (0.18 g, 1 mmol) with 1,3-indanedione (0.15 g, 1 mmol) in a mixed solvent of ethylene glycol (0.5 ml) and acetic acid (1.0 ml) under microwave irradiation for 4 min at 200 W power and 393 K. Upon completion, monitored by TLC, the reaction mixture was cooled to room temperature and then poured into cold water. The solid product was filtered off, washed with water and EtOH (95%), and subsequently dried and recrystallized from EtOH (95%) to give the pure product. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 0.41 g, 94%, m.p. 531–533 K).

Crystal data

$C_{27}H_{24}N_2O_4$	$Z = 8$
$M_r = 440.48$	$D_x = 1.331$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 27.187$ (3) Å	$\mu = 0.09$ mm^{-1}
$b = 9.010$ (2) Å	$T = 298$ (2) K
$c = 19.133$ (3) Å	Block, red
$\beta = 110.250$ (2)°	0.32 × 0.29 × 0.28 mm
$V = 4397.1$ (14) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	10871 measured reflections
φ and ω scans	3871 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1537 reflections with $I > 2\sigma(I)$
$T_{min} = 0.972$, $T_{max} = 0.975$	$R_{int} = 0.094$
	$\theta_{max} = 25.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 5.2279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.066$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.245$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
3871 reflections	
304 parameters	
H-atom parameters constrained	

When the crystal structure was solved, atom O4 of the NO_2 group was found to be disordered. During refinement with anisotropic displacement parameters, the occupancies of the disordered atoms [O4 = 0.822 (11) and O4′ = 0.178 (11)] were refined. H atoms were positioned geometrically, with C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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*.

We are grateful for financial support from the National Science Foundation of China (grant Nos. 20372057 and 20672090), the Natural Science Foundation of Jiangsu Province (grant No. BK 2006033) and the Dean Foundation of Xuzhou Education College (grant No. 2006HX03).

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