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

**Xiangshan Wang,* Daqing Shi and Shujiang Tu**

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China

Correspondence e-mail: xswang@xznu.edu.cn

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**Key indicators**

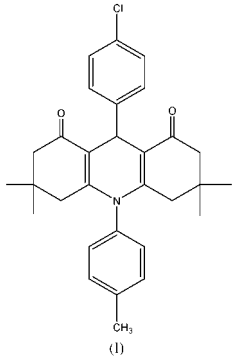
Single-crystal X-ray study
$T$ = 296 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.040
$wR$ factor = 0.103
Data-to-parameter ratio = 15.4

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

The title compound, $C_{30}H_{32}ClNO_2$, has been synthesized by the reaction of 4-chlorobenzaldehyde, 5,5-dimethyl-1,3-cyclohexanedione and *p*-toluidine in ethylene glycol under microwave irradiation. X-ray analysis reveals that the 1,4-dihydropyridine ring adopts a boat conformation, and the other two partially saturated six-membered rings adopt half-chair conformations.

## Comment

1,4–Dihydropyridines (DHP) are well known compounds, as a consequence of their pharmacological profile as calcium channel modulators (Janis *et al.*, 1987). Chemical modifications of the DHP ring, such as the presence of different substituents (Eisner & Kuthan, 1972) or heteroatoms (Chorvat & Rorig, 1988), have extended the structure–activity relationships and afforded some insight into the molecular interactions at the receptor level. We report here the crystal structure of the title compound, (I).




(I)

The 1,4-dihydropyridine ring adopts a boat conformation (Fig. 1); atoms C7, C12, C14 and C19 are coplanar, while atoms C13 and N deviate from the plane by 0.192 (3) and 0.091 (3) Å, respectively. The dihedral angle between the two phenyl rings is 15.26 (6)°. The C7═C12 and C14═C19 bond distances are 1.349 (2) and 1.347 (2) Å (Table 1), close to that of a typical C═C double bond (1.34 Å). The values of the corresponding C═C bond distances in the 1,4-dihydropyridine moiety are 1.341 (3)–1.356 (3) Å for diether 4-(3,4-methylenedioxylphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (Tu *et al.*, 2002) and 1.336 (2)–1.365 (2) Å for 7,7-dimethyl-2,4-diphenyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline (Wang, Shi & Tu, 2002).

In the other two partially saturated six-membered rings, atom C9 deviates from the C7—C8/C10—C12 plane by 0.644 (3) Å, and atom C17 deviates from the C14—C16/C18—C19 plane by 0.628 (3) Å, suggesting that these rings adopt half-chair confirmations; this structure is similar to that of 7,7-

dimethyl-2-amino-3-cyano-4-(3,4-methylenedioxylphenyl)-5-oxo-5,6,7,8-tetrahydro-4*H*-benzo[*b*]pyran (Wang, Shi, Tu *et al.*, 2002).

## Experimental

The title compound, (I), was prepared by the reaction of 4-chlorobenzaldehyde, 5,5-dimethyl-1,3-cyclohexanedione and *p*-toluidine in ethylene glycol under microwave irradiation (m.p. 546–548 K). Single crystals of (I), suitable for X-ray diffraction, were obtained by slow evaporation from an ethanol solution.

*Crystal data*

$C_{30}H_{32}ClNO_2$
$M_r$ = 474.02
Monoclinic, $P2_1/n$
$a$ = 15.246 (2) Å
$b$ = 11.007 (2) Å
$c$ = 16.244 (2) Å
$\beta$ = 102.31 (1)°
$V$ = 2663.0 (7) Å$^3$
$Z$ = 4
$D_x$ = 1.182 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 29 reflections
$\theta$ = 2.8–12.9°
$\mu$ = 0.17 mm$^{-1}$
$T$ = 296 (2) K
Block, colorless
0.44 × 0.36 × 0.36 mm

*Data collection*

Siemens *P*4 diffractometer
$\omega$ scans
Absorption correction: empirical (*SHELXS*86; Sheldrick, 1990)
$T_{min}$ = 0.948, $T_{max}$ = 0.965
5509 measured reflections
4826 independent reflections
2812 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.012
$\theta_{max}$ = 25.3°
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 13$
$l = -19 \rightarrow 19$
3 standard reflections
every 97 reflections
intensity decay: 3.0%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.103
$S$ = 0.91
4826 reflections
313 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0113 (7)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl—C1 | 1.744 (2) | N—C7 | 1.400 (2) |
| O1—C11 | 1.230 (2) | N—C20 | 1.448 (2) |
| O2—C15 | 1.227 (2) | C7—C12 | 1.349 (2) |
| N—C19 | 1.399 (2) | C14—C19 | 1.347 (2) |
| | | | |
| C19—N—C7 | 119.69 (15) | C19—C14—C15 | 120.24 (17) |
| C12—C7—N | 120.81 (16) | C19—C14—C13 | 122.85 (17) |
| C12—C7—C8 | 122.42 (16) | C15—C14—C13 | 116.86 (16) |
| N—C7—C8 | 116.76 (15) | C14—C19—N | 121.22 (16) |
| C7—C12—C11 | 119.93 (17) | C14—C19—C18 | 122.55 (17) |
| C7—C12—C13 | 123.05 (16) | N—C19—C18 | 116.19 (16) |
| C11—C12—C13 | 117.02 (15) | | |
| | | | |
| C19—N—C7—C12 | 7.7 (3) | C13—C14—C19—N | −2.4 (3) |
| N—C7—C12—C13 | 6.3 (3) | C7—N—C19—C14 | −9.7 (3) |
| C7—C12—C13—C14 | −16.3 (2) | | |

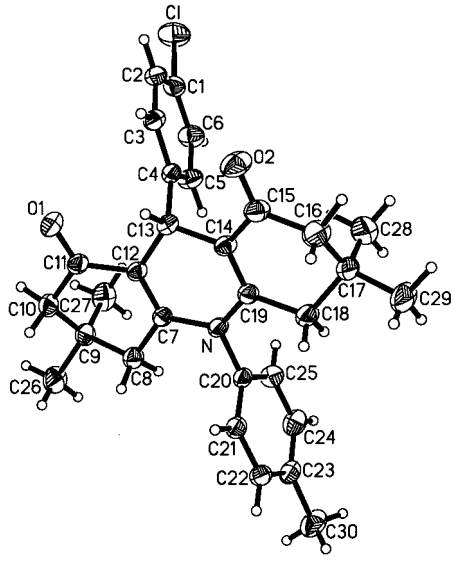



**Figure 1**
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

All H atoms were positioned geometrically and refined as riding [C—H = 0.93–0.98 Å]. There are solvent accessible voids of 43 Å$^3$ in the crystal structure. However, solvent molecules were not detected, which agrees with the elemental analysis.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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