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4-*tert*-Butyl-γ-chlorobutyrophenone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.065
wR factor = 0.140
Data-to-parameter ratio = 9.7

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

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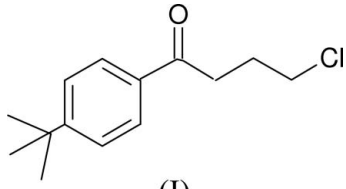
The title compound, $C_{14}H_{19}ClO$, possesses C_s symmetry with all but two C atoms of the *tert*-butyl group lying in the mirror plane. In the crystal structure, the molecules stack along the *b* axis and are connected by weak C—H$\cdots\pi$ interactions.

Comment

The title compound, 4-*tert*-butyl-γ-chlorobutyrophenone (or 4′-*tert*-butyl-4-chlorobutyrophenone), (I), belongs to the chemical class of butyrophenones, which are used as tranquilizers and act as antipsychotics through their action as dopamine antagonists (Brea *et al.*, 2003). As part of our continuing interest in the solid state studies on molecules of pharmaceutical interest, in this report we discuss the structure and crystal packing of compound (I).



(I)

The molecular structure of compound (I) is illustrated in Fig. 1. The molecule possesses C_s symmetry, with atoms Cl1, O1 and C1–C12 lying in the mirror plane.

In the crystal structure, symmetry-related molecules stack along the *b* axis and this arrangement is stabilized by C—H$\cdots\pi$ interactions (Fig. 2 and Table 1) with typical dimensions (Nishio *et al.*, 1998). The rest of the packing is governed by van der Waals forces.

Experimental

Crystals of compound (I) (obtained from Arvee Pharma, Mysore, India) were grown by evaporation of a hexane solution.

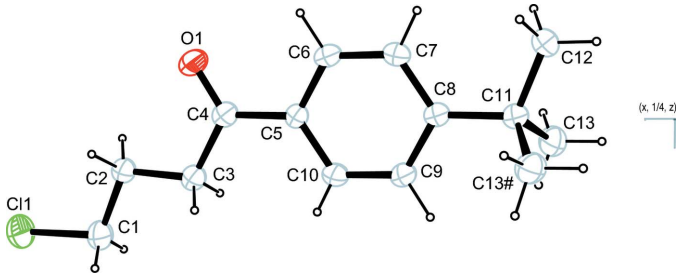


Figure 1
The molecular structure of compound (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (#) x, $-y+\frac{1}{2}$, z.]

Crystal data

$C_{14}H_{19}ClO$
M_r = 238.76
Monoclinic, $P2_1/m$
a = 8.247 (1) Å
b = 7.242 (1) Å
c = 11.414 (2) Å
β = 99.548 (3)°
V = 672.3 (2) Å^3
Z = 2
D_x = 1.179 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1047 reflections
θ = 5–26°
μ = 0.26 mm^{-1}
T = 293 (2) K
Block, colorless
0.33 × 0.31 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.90, T_{max} = 0.94
3612 measured reflections
1333 independent reflections
948 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.4°
$h = -9 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.140
S = 1.16
1333 reflections
137 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.014P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···$Cg1^{i}$	1.00 (2)	2.92 (2)	3.837 (1)	154 (2)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+1$. *Cg*1 is the centroid of the C5–C10 ring.

H atoms were located in difference electron-density maps and were refined isotropically. The distance C12—H12*B* and the angle C11—C12—H12*B* were restrained to 0.95 (1) Å and 112 (1)°. respectively. The refined distances are in the ranges: C_{ar}—H = 0.87 (3)–0.99 (3) Å, methyl C—H = 0.95 (3)–1.00 (3) Å, and methylene C—H = 0.95 (3)–1.00 (3) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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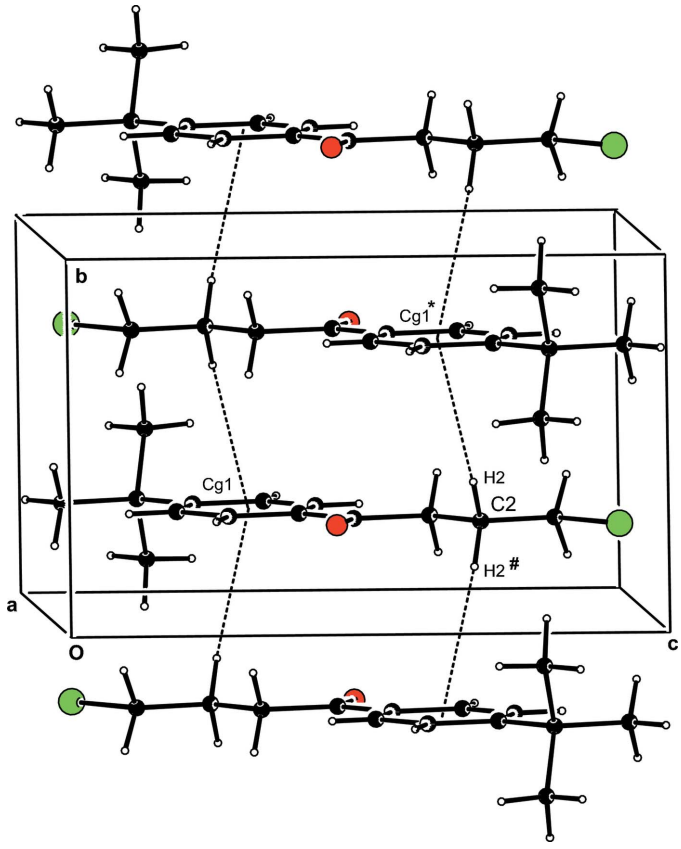

Figure 2
The crystal packing in (I), viewed approximately along the *a* axis, showing the co-operative association of the molecules, forming chains *via* C—H···π interactions (dashed lines). *Cg*1 is the centroid of the C5–C10 ring. The atoms labeled with an asterisk (*) or a hash (#) are at the symmetry positions $(1-x, -\frac{1}{2}+y, 1-z)$ and $(x, -y+\frac{1}{2}, z)$, respectively. Color key: C, black, H white, Cl green, O red.

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