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Key indicators

Single-crystal X-ray study
 $T = 296\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in main residue
 R factor = 0.070
 wR factor = 0.195
Data-to-parameter ratio = 17.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2-Chloro-1-(3-mesityl-3-methylcyclobutyl)ethanone

The title compound, $\text{C}_{16}\text{H}_{21}\text{ClO}$, has a non-planar configura-
tion. The crystal packing is mainly stabilized by intramolecular
 $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions.Received 1 December 2005
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Comment

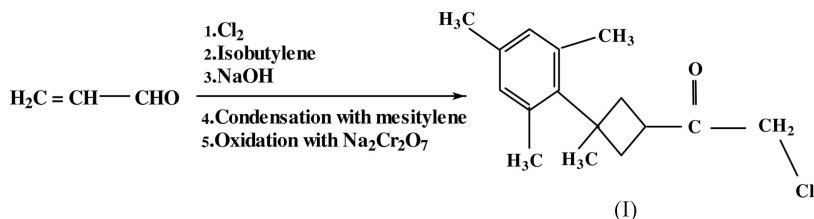
It has been shown that 3-substituted cyclobutane carboxylic
acid derivatives have antidepressant activities and liquid-
crystal properties (Dehmlow & Schmidt, 1990; Escaler *et al.*,
1977). Substituted α -haloketones, like the title compound, (I),
are used for different purposes, especially in the synthesis of
heterocyclic substances (Çukurovalı *et al.*, 2002; Gompper &
Christmann, 1959). The extensive synthetic possibilities of this
compound, due to the presence of various reaction sites, hold
promise for the preparation of new heterocyclic chemicals.

Fig. 1 shows the molecular structure and conformation of (I) with the atomic numbering scheme. Selected bond lengths and angles in (I) are given in Table 1. In cyclobutane ring *A* (C1–C4), the puckering parameter Q_2 is $-0.228(2)\text{ \AA}$ (Cremer & Pople, 1975). In this study, the C4/C1/C2 plane forms a dihedral angle of $23.8(3)^\circ$ with the C2/C3/C4 plane, which deviates from the values reported in previous studies (Swenson *et al.*, 1997; Yüksektepe *et al.*, 2004). The geometry of the cyclobutane ring is influenced by the steric effect of the methyl group. The bond lengths and angles in the four-membered ring

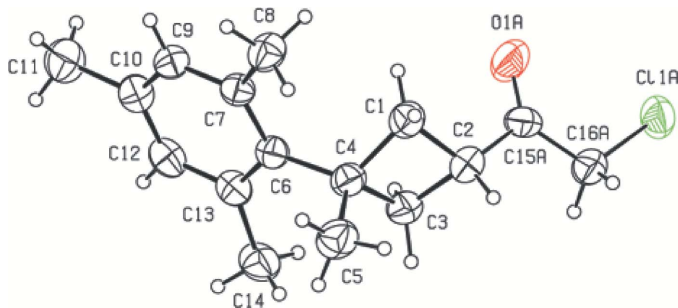


Figure 1
An ORTEP3 (Farrugia, 1997) drawing of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 30% probability level. The minor occupancy disordered atoms have been omitted.

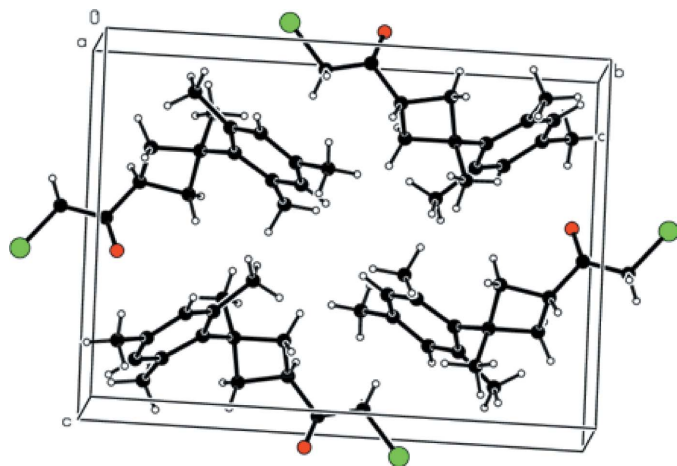


Figure 2
A projection of the molecular packing of (I) approximately along the *a* axis. The minor occupancy disordered atoms have been omitted.

are normal (Allen *et al.*, 1987). The chloroacetaldehyde group shows disorder and atoms C15, C16, O1 and Cl1 were modelled in two different orientations, with occupancy factors of 0.61 (2) for atoms with suffix *A* and 0.39 (2) for those with suffix *B* (Fig. 1).

Experimental

The synthesis of the title compound was realised according to the literature method of Akhmedov *et al.* (1991) with some modification, as given in the reaction scheme. Shiny crystals suitable for X-ray analysis were obtained by crystallization from ethanol (yield: 80%, m.p. 366 K). IR (KBr, ν cm^{-1}): 1724 (C=O), 732 ($-\text{CH}_2-\text{Cl}$). ^1H NMR (CDCl_3): δ 1.63 (*s*, 3H, CH_3 on cyclobutane), 2.22 (*s*, 3H, *p*- CH_3 on mesitylene), 2.25 (*s*, 6H, *o*- CH_3 on mesitylene), 2.42–2.78 (*m*, 4H, $-\text{CH}_2-$), 6.80 (*s*, 2H, aromatics on mesitylene). ^{13}C NMR (CDCl_3): δ 48.88 (C₁), 205.47 (C₂), 41.89 (C₃), 42.59 (C₄), 26.95 (C₅), 40.19 (C₆), 145.09 (C₇), 132.48 (C₈), 132.44 (C₉), 136.96 (C₁₀), 22.46 (C₁₁), 23.37 (C₁₂).

Crystal data

$\text{C}_{16}\text{H}_{21}\text{ClO}$	$D_x = 1.192 \text{ Mg m}^{-3}$
$M_r = 264.78$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 26744 reflections
$a = 8.3808$ (17) Å	$\theta = 2.2\text{--}27.9^\circ$
$b = 15.236$ (4) Å	$\mu = 0.25 \text{ mm}^{-1}$
$c = 12.472$ (3) Å	$T = 296 \text{ K}$
$\beta = 112.173$ (15)°	Prism, colourless
$V = 1474.8$ (6) Å ³	$0.73 \times 0.57 \times 0.37 \text{ mm}$
$Z = 4$	

Data collection

Stoe IPDS-2 diffractometer	1993 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.069$
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	$\theta_{\text{max}} = 27.8^\circ$
$T_{\text{min}} = 0.841$, $T_{\text{max}} = 0.914$	$h = -10 \rightarrow 10$
23037 measured reflections	$k = -19 \rightarrow 20$
3378 independent reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.070$	$w = 1/[\sigma^2(F_o^2) + (0.1242P)^2]$
$wR(F^2) = 0.195$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3378 reflections	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
197 parameters	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C11A—C16A	1.807 (12)	O1A—C15A	1.187 (16)
C11B—C16B	1.68 (2)	O1B—C15B	1.22 (2)
O1A—C15A—C2	121.2 (11)	O1B—C15B—C2	125.8 (18)
O1A—C15A—C16A	126.3 (12)	C11A—C16A—C15A	113.5 (8)
O1B—C15B—C16B	115.3 (18)	C11B—C16B—C15B	113.8 (13)

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.93, 0.96, 0.97 and 0.98 Å for aromatic, methyl, methylene and methine H atoms, respectively. The displacement parameters of the H atoms were constrained to be $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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