Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Chlorobenzylidene)tetrahydrofuran-2-one

Lan Mo,[a] Wei Wang,[b]* Qiang Li[c] and Xiao-Guang Jia[d]

[a]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China, [b]School of Chemical Engineering, Anshan University of Science and Technology, Anshan 114002, People's Republic of China, [c]Research Institute of Physical & Chemical Engineering of, Nuclear Industry, Tianjin 300180, People's Republic of China, and [d]Huan Nonferrous Metals Geologic Prospecting Institution, Changsha 410015, People's Republic of China

Correspondence e-mail: vivianzhaobing@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.118
Data-to-parameter ratio = 15.7

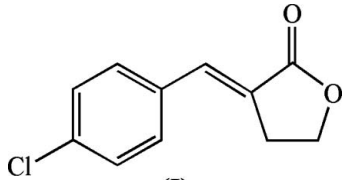
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 January 2006
Accepted 28 April 2006

The title compound, $C_{11}H_9ClO_2$, was synthesized by the reaction of γ-butyrolactone and 4-chlorobenzaldehyde. The whole molecule assumes a planar structure, with an r.m.s. deviation of 0.0543 (3) Å.

Comment

Functionalized γ-lactones have attracted considerable attention because of their importance as building blocks in the synthesis of a number of natural products and biologically relevant compounds (Samarat *et al.*, 2001), for example, precursors of inhibitors of HIV-1 protease(Askin, *et al.*, 1992). We have synthesized the title compound, (I), by the reaction of γ-butyrolactone and 4-chlorobenzaldehyde. An X-ray crystallographic structure determination of (I) was carried out in order to elucidate the structure, and the results are presented here.



(I)

In the molecular structure of (I), the dihedral angle between the benzene and lactone rings is 7.3 (2)°, indicating that the two rings are almost coplanar. The whole molecule assumes a planar structure, with an r. m. s. deviation of 0.0543 (3) Å. Atom C11 has a distorted trigonal geometry, with O2—C11—C8 [129.2 (2)°] and O1—C11—C8 [109.97 (19)°] deviating significantly from the ideal sp^2 value of 120°. Owing to the steric interaction between the lactone ring and benzene ring,

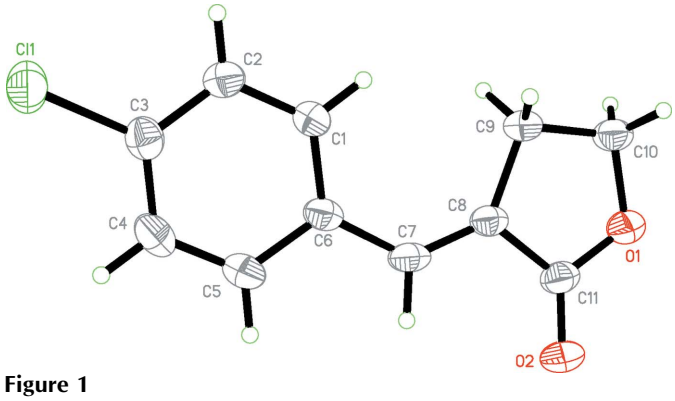


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

the C6—C7—C8 angle [130.6 (2)°] is significantly larger than the the ideal sp^2 value of 120°.

Experimental

The title compound was synthesized by the reaction of 4-chlorobenzaldehyde and γ-butyrolactone in benzene (Zimmer & Rothe, 1959). Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in ethyl acetate–petroleum ether (1:15).

Crystal data

$C_{11}H_9ClO_2$
M_r = 208.63
Monoclinic, $P2_1/c$
a = 15.998 (4) Å
b = 5.2993 (14) Å
c = 12.336 (3) Å
β = 111.215 (4)°
V = 974.9 (4) Å^3
Z = 4
D_x = 1.421 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.917, T_{max} = 0.937
5226 measured reflections
2000 independent reflections
1149 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.00
2000 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å), with $U_{iso}(H) = 1.2U_{eq}$(parent).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

References

Askin, D., Wallace, M. A., Vacca, J. P., Reamer, R. A., Volante, R. P. & Shinkai, I. (1992). *J. Org. Chem.* **57**, 2771–2773.
Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Samarat, A., Fargeas, V., Villieras, J., Lebreton, J. & Amri, H. (2001). *Tetrahedron Lett.* **42**, 1273–1274.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zimmer, H. & Rothe, J. (1959). *J. Org. Chem.* **24**, 28–32.