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3-(4-Chlorophenyl)-3-hydroxy-1-phenylpropan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.167
Data-to-parameter ratio = 13.8

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

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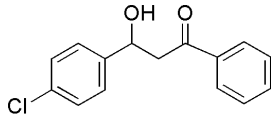
The title compound, $C_{15}H_{13}ClO_2$, was synthesized by a Reformatsky reaction in an aqueous medium. The two benzene rings are approximately parallel. Molecules are connected by intermolecular O—H···O hydrogen bonds, forming extended chains in the a axis direction.

Comment

We have recently investigated the Reformatsky reaction (Bieber *et al.*, 1997) in aqueous media (Chan *et al.*, 1994; Shen *et al.*, 1997). A new compound, namely 3-(4-chlorophenyl)-3-hydroxy-1-phenylpropan-1-one, (I), has been synthesized by the reaction of 4-chlorobenzaldehyde and 2-bromoacetophenone in the presence of zinc in an aqueous medium. An X-ray crystal structure determination of (I) was carried out in order to elucidate the structure and the results are presented here.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The two benzene rings are approximately parallel, forming a dihedral angle of 5.3 (2)°, different from what is found in 3-(2,4-dichlorophenyl)-3-hydroxy-1-phenylpropan-1-one (Yu *et al.*, 2003), where the two benzene rings are orthogonal. The angle C10—C9—C8 is 121.0 (2)°, indicating that C9 is sp^2 hybridized. Molecules related by unit-cell translations are connected by intermolecular O—H···O hydrogen bonds (Table 2), forming extended chains in the a-axis direction.

Experimental

The title compound was synthesized by adding a mixture of 4-chlorobenzaldehyde (0.421 g, 3 mmol) and 2-bromoacetophenone (0.892 g, 4.5 mmol) to a mixture of a saturated solution of calcium chloride (12 ml), zinc (0.781 g, 12 mmol), ammonium chloride (1.5 g), a trace amount of iodine, cetyltrimethylammonium bromide (0.005 g) and THF (1 ml). The mixture was stirred at room temperature for 2 h. and extracted with diethyl ether, evaporated and separated by flash chromatography (eluent ethyl acetate–petroleum ether). A colourless powder was obtained (yield 82%) and single crystals suitable for crystallographic analysis were obtained by slow evaporation of an ethyl acetate–petroleum ether solution (m.p. 370–371 K). Spectroscopic analysis: IR (KBr, ν, cm^{-1}): 3468, 1668; ^1H NMR ($CDCl_3$, δ, p.p.m.): 7.95–7.24 (*m*, 9H), 5.30 (*t*, 1H), 3.32 (*m*, 2H). Analysis required for $C_{15}H_{13}ClO_2$: C 69.10, H 4.99%; found: C 69.21, H 4.91%.

Crystal data

$C_{15}H_{13}ClO_2$
$M_r = 260.70$
Monoclinic, $P2_1/c$
$a = 5.360\ (9)$ Å
$b = 8.697\ (14)$ Å
$c = 27.46\ (5)$ Å
$\beta = 90.17\ (3)^\circ$
$V = 1280\ (4)$ Å^3
$Z = 4$
$D_x = 1.353$ Mg m^{-3}
Mo Kα radiation
Cell parameters from 1001 reflections
$\theta = 3.0$–25.1°
$\mu = 0.29$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
$0.30 \times 0.20 \times 0.06$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.933$, $T_{max} = 0.983$
6347 measured reflections
2270 independent reflections
1511 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 25.0^\circ$
$h = -4 \rightarrow 6$
$k = -10 \rightarrow 10$
$l = -29 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.167$
$S = 1.07$
2270 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.428 (3)	O2—C9	1.223 (3)
O2—C9—C10	120.0 (2)	C13—C14—C15	119.9 (3)
C10—C9—C8	121.0 (2)		
O1—C7—C8—C9	66.4 (3)	O2—C9—C10—C15	177.7 (2)
C6—C7—C8—C9	−167.9 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	2.032	2.847 (4)	172.35

Symmetry code: (i) $1 + x, y, z$.

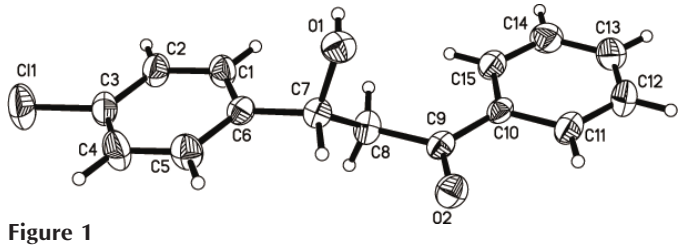


Figure 1
View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

All H atoms were positioned geometrically and refined as riding (O—H = 0.82 Å and C—H = 0.93–0.98 Å), with U_{iso}(H) values of 1.2 (CH and CH_2) or 1.5 (OH) times U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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