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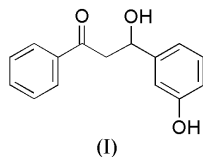
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
Disorder in main residue
 R factor = 0.048
 wR factor = 0.145
Data-to-parameter ratio = 12.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-Hydroxy-3-(3-hydroxyphenyl)-1-phenyl-
propan-1-one

The title compound, $\text{C}_{15}\text{H}_{14}\text{O}_3$, was synthesized by a Reformatsky reaction in an aqueous medium. The two aromatic rings are approximately orthogonal. Intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds are formed between the carbonyl and hydroxyl groups. The hydroxyl group in the central chain is disordered over two sites.

Comment

We have researched the Reformatsky reaction (Bieber *et al.*, 1997) of α -haloketones in an aqueous medium (Chan *et al.*, 1994; Shen *et al.*, 1997). A new compound has been synthesized by the reaction of 2-bromoacetophenone with 3-hydroxybenzaldehyde in the presence of zinc in an aqueous system (Yu *et al.*, 2003).



The molecular structure of the title compound, (I), is illustrated in Fig. 1. The two aromatic rings are approximately orthogonal, forming a dihedral angle of $80.7(1)^\circ$. The angle $\text{C}6-\text{C}7-\text{C}8$ is $119.1(2)^\circ$, indicating that atom $\text{C}7$ is sp^2 -hybridized. The torsion angle $\text{C}6-\text{C}7-\text{C}8-\text{C}9$ is $-165.5(2)^\circ$, indicating these atoms are almost coplanar.

Experimental

3-Hydroxybenzaldehyde (3 mmol) and 2-bromoacetophenone (4.5 mmol) were added to a mixture of zinc (12 mmol), ammonium chloride (1.5 g), a trace amount of iodine, cetyltrimethylammonium bromide (0.005 g) and tetrahydrofuran (1 ml) in a saturated solution of calcium chloride (12 ml). The mixture was stirred at room temperature for 8 h and extracted with diethyl ether, evaporated and separated by flash chromatography (ethyl acetate–petroleum ether). A yellow powder was obtained (yield 53%) and single crystals (m.p. 377–378 K) suitable for crystallographic analysis were obtained by slow evaporation of an ethyl acetate–petroleum ether solution. Spectroscopic analyses, IR [KBr, ν (cm^{-1})]: 3333, 1676; ^1H NMR (CDCl_3): δ 7.95–6.93 (*m*, 9H), 5.28 (*t*, 1H), 3.35 (*d*, 2H), 2.02(*s*, 1H). Elemental analysis, required for $\text{C}_{15}\text{H}_{14}\text{O}_3$: C 74.38, H 5.79%; found: C 74.35, H 5.74%.

Crystal data

$\text{C}_{15}\text{H}_{14}\text{O}_3$
 $M_r = 242.26$
Monoclinic, $P2_1/c$
 $a = 14.251(5)$ Å
 $b = 9.984(3)$ Å
 $c = 8.994(3)$ Å
 $\beta = 105.305(5)^\circ$
 $V = 1234.3(7)$ Å³
 $Z = 4$

$D_x = 1.304$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 877
reflections
 $\theta = 3.2$ – 23.4°
 $\mu = 0.09$ mm⁻¹
 $T = 293(2)$ K
Block, colourless
 $0.34 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: none
 6168 measured reflections
 2173 independent reflections

1313 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -16 \rightarrow 11$
 $k = -11 \rightarrow 11$
 $l = -9 \rightarrow 10$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.145$
 $S = 0.99$
 2173 reflections
 176 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.3761P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C7	1.216 (3)	C9—O2	1.477 (3)
O3—C14	1.374 (3)	C7—C8	1.506 (4)
O2—C9—C10	108.9 (2)	C15—C14—C13	120.4 (2)
O1—C7—C8	120.6 (2)	O3—C14—C15—C10	179.9 (2)
C6—C7—C8—C9	−165.5 (2)	O2—C9—C8—C7	63.0 (3)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H2 \cdots O1 ¹	0.82	2.15	2.960 (3)	171
O3—H3 \cdots O2 ¹	0.82	2.03	2.818 (3)	161

Symmetry code: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$.

All H atoms were located in a difference Fourier map and were refined as riding [O—H = 0.82 \AA and C—H = 0.93–0.98 \AA ; $U_{\text{iso}} = 1.0$ (disordered atoms) or $1.5U_{\text{eq}}(\text{O})$ and $1.2U_{\text{eq}}(\text{C})$]. The torsion angles about the C—O bond of the hydroxyl groups were refined. The hydroxyl group attached to atom C9 is disordered over two sites [occupancies 0.72 (4) and 0.28 (4)].

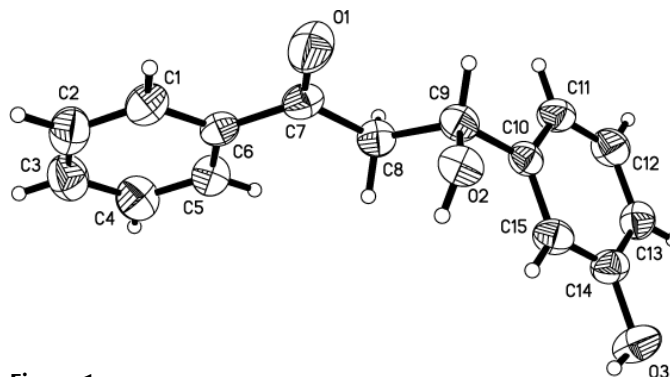


Figure 1

View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. Only the major occupied site of the disordered hydroxyl group is shown.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); 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*.

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