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2-Benzyloxy-2-hydroxy-1-phenylethanone

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.126
Data-to-parameter ratio = 15.8

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

The stable title hemiacetal, $C_{15}H_{14}O_3$, has been prepared. One attractive feature in the structure is the *gauche* conformation determined by stereoelectronic factors. A hydrogen bond is formed between two neighbouring molecules, in which the hydroxyl group acts as both donor and acceptor.

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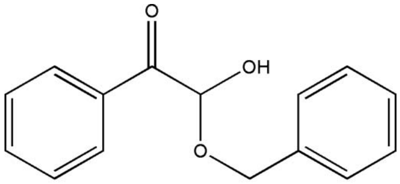
Comment

Most acyclic hemiacetals are unstable and not isolable, except chloral alcoholate (Hashimoto *et al.*, 1994). Surprisingly, the title compound, (I), a hemiacetal prepared from the reaction of phenyl glyoxal hydrate with benzyl alcohol, is stable. An X-ray crystal structure determination of (I) was carried out in order to elucidate the structure, and the result is presented here.



(I)

The structure of (I) resembles chloral alcoholate, in which the carbonyl group is attached to an electron-deficient C atom. As shown in Fig. 1, the carbonyl group is approximately coplanar with the hydroxyl group with an O1—C7—C8—O2 torsion angle of 11.1 (2)°. The C9—O3—C8—O2 and H2—O2—C8—O3 torsion angles of (I) are 80.2 (2) and 90.0 (2)°, respectively, and indicate a *gauche* conformation (Fig. 1 and Table 1). As shown in Fig. 2, the hydroxyl group forms hydrogen bonds with both O1 and O2 from another molecule of (I).

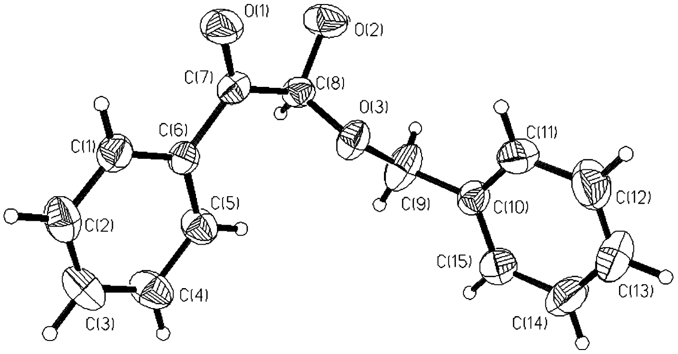


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

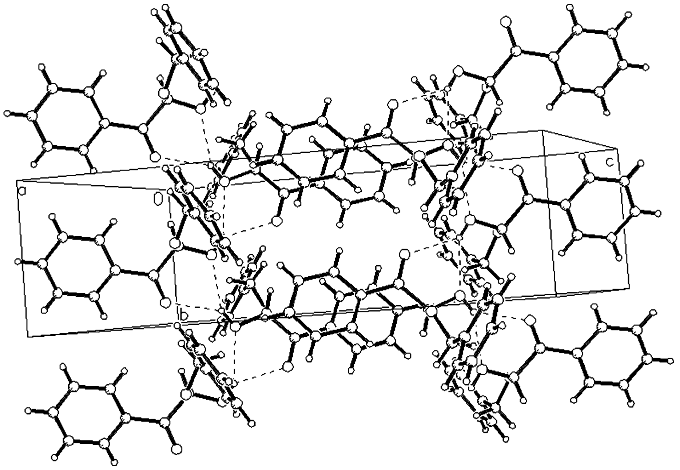


Figure 2
The hydrogen-bonding scheme in (I). O—H···O hydrogen bonds are shown as dashed lines.

Experimental

To a solution of phenyl glyoxal hydrate (15.2 g, 0.1 mol) and benzyl alcohol (10.8 g, 0.1 mol) in anhydrous dichloromethane (100 ml) was added 25 g 4 Å molecular sieves. The mixture was gently stirred with a magnetic stirrer for 24 h at room temperature. The reaction mixture was filtered from the molecular sieves which were rinsed with 20 ml dicholoromethane, then the filtrate and washings were concentrated under a vacuum to give an oily yellow–orange liquid. The crude product was purified by vacuum distillation to afford 2-benzyloxy-2-hydroxy-1-phenylethanone (14.8 g, yield 61%) and single crystals suitable for crystallographic analysis were obtained by slow evaporation of a toluene solution. Spectroscopic analysis: IR (KBr, ν, cm^{-1}): 3412, 3364, 1693, 1599, 1579, 1495, 1450, 1341, 1227, 1056; ^{1}H NMR (CDCl$_3$, δ, p.p.m.): 7.95 (*d*, 2H), 7.59–7.68 (*m*, 1H), 7.40–7.49 (*m*, 2H), 7.29–7.38 (*m*, 5H), 5.74 (*s*, 1H), 4.85 (*q*, 2H); ^{13}C NMR (CDCl$_3$, δ, p.p.m.): 193.8, 136.7, 134.3, 134.0, 132.6, 129.7, 129.3, 128.6, 128.3, 90.8, 73.6. MS (ESI): 242 (100%). Analysis calculated for $C_{15}H_{14}O_3$: C 74.36, H 5.82%; found: C 73.98, H 5.56%.

Crystal data

$C_{15}H_{14}O_3$
M_r = 242.26
Monoclinic, $P2_1/c$
a = 12.019 (3) Å
b = 5.6824 (13) Å
c = 19.049 (4) Å
β = 99.439 (4)°
V = 1283.4 (5) Å^3
Z = 4
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1709 reflections
θ = 3.0–23.9°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, white
0.26 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.983
6834 measured reflections
2609 independent reflections
1488 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.4°
$h = -11 \rightarrow 15$
$k = -7 \rightarrow 7$
$l = -23 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.126$
S = 1.00
2609 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.1183P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.022 (3)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.215 (2)	O3—C9	1.422 (2)
O2—C8	1.391 (2)	C7—C8	1.520 (2)
O3—C8	1.401 (2)	C8—H8	0.980
C8—O3—C9	113.9 (1)	O2—C8—C7	108.5 (1)
O2—C8—O3	112.1 (2)		
C9—O3—C8—O2	−80.2 (2)	O3—C8—O2—H2	90.0
C6—C7—C8—O2	169.5 (1)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	2.19	2.864 (2)	140 (1)
O2—H2···O2^{i}	0.82	2.25	2.986 (2)	149 (1)

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

All H atoms were initially located in a difference Fourier map; they were then placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and O—H = 0.82 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,O)$.

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*.

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