

Pengying Zhao,^a Qiyun Shao,^a
Weiyi Zhou,^b Jie Li,^a Ming Lu^c
and Chunbao Li^{a*}^aDepartment of Chemistry, Tianjin University,
Tianjin 300072, People's Republic of China,
^bAnalytical Center, Tianjin University, Tianjin
300072, People's Republic of China, and
^cSchool of Electronic Information Engineering,
Tianjin University, Tianjin 300072, People's
Republic of ChinaCorrespondence e-mail:
lichunbaosyn@sohu.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.036
 wR factor = 0.142
Data-to-parameter ratio = 9.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

2-Hydroxy-1-phenylethanone

The non-hydrogen skeleton of the title compound, $\text{C}_8\text{H}_8\text{O}_2$, is planar. The torsion angles $\text{HO}-\text{C}-\text{C}=\text{O}$ and $\text{O}=\text{C}-\text{C}(\text{Ph})-\text{C}(\text{Ph})$ are -0.9 (4) and 6.0 (4)°, respectively. The hydroxyl group participates in a bifurcated hydrogen bond, giving rise to infinite chains extended along the b axis.

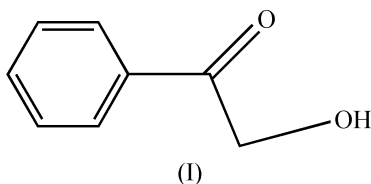
Received 15 November 2004

Accepted 10 January 2005

Online 22 January 2005

Comment

Although the crystal structure of a Ca^{2+} complex of 2-hydroxy-1-phenylethanone, (I), has been reported (Doxsee *et al.*, 1993), the structure of the ligand itself remained unknown. As shown in Fig. 1, the molecule of (I), excluding H atoms, is planar; the torsion angles $\text{HO}-\text{C}-\text{C}=\text{O}$ and $\text{O}=\text{C}-\text{C}(\text{Ph})-\text{C}(\text{Ph})$ are -0.9 (4) and 6.0 (4)°, respectively. The hydroxyl group participates in a bifurcated hydrogen bond involving both hydroxyl and carbonyl O atoms of the neighbouring molecule as acceptors (Table 2). These hydrogen bonds give rise to infinite chains extended along the b axis of the crystal structure (Fig. 2).



Experimental

The title compound was prepared according to known procedures (Yadav *et al.*, 2003; Muthusamy *et al.*, 2002) and crystallized from ethyl acetate and petroleum ether (m.p.: 361 K). IR (KBr, ν , cm^{-1}): 3430, 3391, 1690, 1683; ^1H NMR (CDCl_3): δ 7.94–7.49 (*m*, 5H), 4.88 (*d*, 2H), 3.50 (*t*, 1H).

Crystal data

 $\text{C}_8\text{H}_8\text{O}_2$
 $M_r = 136.14$
Orthorhombic, $P2_12_12_1$
 $a = 4.8223$ (15) Å
 $b = 5.4732$ (16) Å
 $c = 25.484$ (7) Å
 $V = 672.6$ (3) Å³
 $Z = 4$
 $D_x = 1.344$ Mg m⁻³Mo $K\alpha$ radiation
Cell parameters from 1318
reflections
 $\theta = 3.2$ – 23.5°
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
Block, colourless
 $0.20 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer
 φ and ω scans
Absorption correction: none
3890 measured reflections
855 independent reflections650 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\text{max}} = 26.5^\circ$
 $h = -6 \rightarrow 4$
 $k = -6 \rightarrow 5$
 $l = -32 \rightarrow 31$

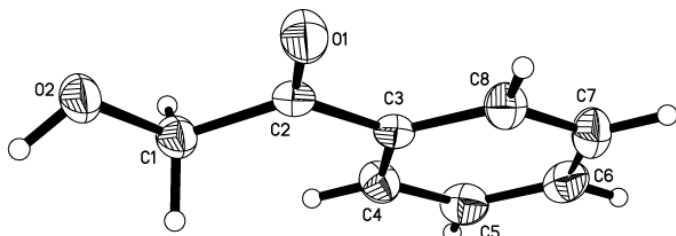


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.142$
 $S = 1.23$
 855 reflections
 95 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0813P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$

Table 1

Selected torsion angles ($^\circ$).

O2—C1—C2—O1	−0.9 (4)	O2—C1—C2—C3	179.9 (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 ⁱ	0.90 (5)	2.16 (5)	2.885 (3)	137 (4)
O2—H2 \cdots O2 ⁱ	0.90 (5)	2.19 (5)	2.960 (2)	143 (3)

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

All H atoms bonded to C atoms were included in the refinement in the riding-model approximation, with $C-H = 0.93\text{--}0.97 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. The hydroxyl H atom was located in a difference Fourier map and refined isotropically [$O2-H2 = 0.90(5) \text{ \AA}$]. In the absence of significant anomalous scattering, Friedel pairs were merged.

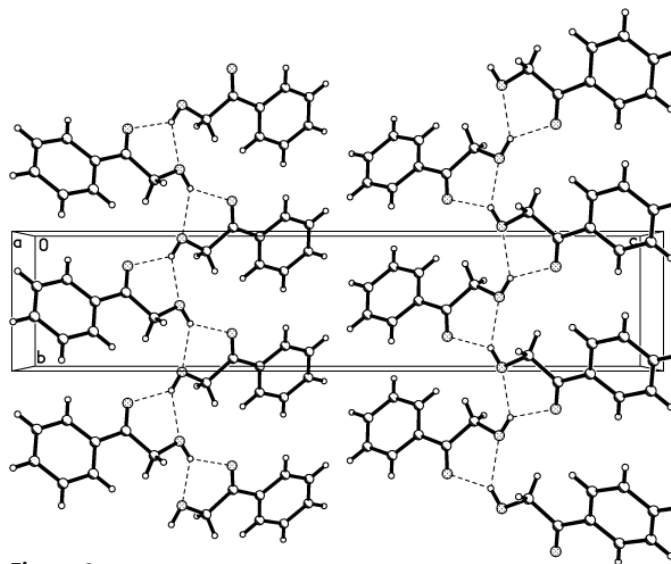


Figure 2
The crystal structure of (I), viewed along the a axis. Dashed lines indicate hydrogen bonds.

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*.

We thank the Tianjin University Young Teacher Foundation for financial support (No. w50501).

References

- Bruker (1997). *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
 Doxsee, K. M., Ferguson, C. M. & Wash, P. L. (1993). *J. Org. Chem.* **58**, 7557–7561.
 Muthusamy, S., Badu, S. A. & Gunanathan, C. (2002). *Synlett*, **3**, 407–410.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Yadav, J. S., Reddy, B. V. S. & Srinivas, M. (2003). *Chem. Lett.* **32**, 1060–1061.