

1-(4-Hydroxyphenyl)-3-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å

R factor = 0.044

wR factor = 0.129

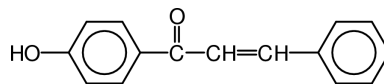
Data-to-parameter ratio = 13.5

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

In the title molecule, $\text{C}_{15}\text{H}_{12}\text{O}_2$, the carbonyl group is in an *s-cis* conformation. The dihedral angle between the planes of the 4-hydroxyphenyl group and the phenyl ring is 34.96 (10)°. Electron conjugation is observed between the central $-\text{CH}=\text{CH}-\text{C}(=\text{O})-$ group and the attached rings. The crystal structure is stabilized by $\text{O}-\text{H}\cdots\text{O}$ -type intermolecular hydrogen bonds.

Comment

It is well known that, in ketones, the carbonyl group plays an important role in the antibacterial activity of chalcones. Earlier crystal structure studies of some of the α,β -unsaturated ketone derivatives (Shanmuga Sundara Raj *et al.*, 1996, 1998) have shown that there are two possible conformational isomers of ketones, one corresponding to the *s-cis* and the other to the *s-trans* form.



(I)

The title compound, (I), assumes an *s-cis* conformation, as can be seen from the torsion angle $\text{C}7-\text{C}8-\text{C}9-\text{O}1$ of -11.4 (3)°. The dihedral angle between the 4-hydroxyphenyl and phenyl rings is 34.96 (10)°. The central $-\text{CH}=\text{CH}-\text{C}(=\text{O})-$ group is oriented at angles of 13.04 (19) and 25.19 (14)° with respect to the phenyl and 4-hydroxyphenyl rings, respectively. The lengths of the $\text{C}6-\text{C}7$ [1.468 (3) Å], $\text{C}7-\text{C}8$ [1.324 (3) Å], $\text{C}8-\text{C}9$ [1.475 (3) Å], $\text{C}9-\text{O}1$ [1.241 (2) Å] and $\text{C}9-\text{C}10$ [1.468 (3) Å] bonds indicate conjugation. The widening of the bond angle $\text{C}6-\text{C}7-\text{C}8$ to 126.6 (2)° may be due to the close approach (2.20 Å) of atoms $\text{H}8$ and $\text{H}5$. A slight increase in the bond angle $\text{C}7-\text{C}8-\text{C}9$ to 122.4 (2)° may be attributed to the short intramolecular non-bonded interaction between $\text{O}1$ and $\text{H}7$ (2.49 Å). The unsaturated ketone group is not strictly planar, as is evident from the torsion angles $\text{C}15-\text{C}10-\text{C}9-\text{C}8$ [155.73 (19)°], $\text{C}10-\text{C}9-\text{C}8-\text{C}7$ [168.50 (2)°], $\text{C}9-\text{C}8-\text{C}7-\text{C}6$ [-177.17 (19)°] and $\text{C}8-\text{C}7-\text{C}6-\text{C}1$ [170.50 (2)°]. Atoms $\text{H}7$ and $\text{H}8$ are *trans* to each other. The crystal structure is stabilized by $\text{O}-\text{H}\cdots\text{O}$ -type intermolecular hydrogen bonds (Table 1).

Experimental

NaOH (0.22 g) in alcohol solution (100 ml) was treated with 0.5 M 4-hydroxyacetophenone (6.8 g) and stirred well. 0.5 M of benzaldehyde (5.3 g) was added to the solution. Stirring was continued for 2 h. A

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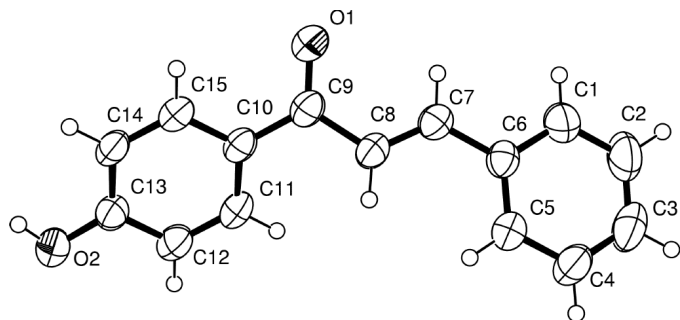


Figure 1

The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

viscous liquid was obtained when stirring was no longer effective. It was kept in a refrigerator overnight. A yellow crude product was obtained; yield (5.9 g). Compound (I) was recrystallized from rectified spirit.

Crystal data

$C_{15}H_{12}O_2$
 $M_r = 224.25$
 Orthorhombic, $Pbca$
 $a = 8.4663$ (10) Å
 $b = 22.384$ (2) Å
 $c = 12.216$ (3) Å
 $V = 2315.2$ (6) Å³
 $Z = 8$
 $D_x = 1.287$ Mg m⁻³

Data collection

Enraf-Nonius CAD-4
 diffractometer
 ω - 2θ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.822$, $T_{\max} = 0.905$
 2107 measured reflections
 2107 independent reflections

Cu $K\alpha$ radiation
 Cell parameters from 25
 reflections
 $\theta = 20$ – 30°
 $\mu = 0.68$ mm⁻¹
 $T = 293$ (2) K
 Rectangular, yellow
 $0.30 \times 0.22 \times 0.15$ mm

1518 reflections with $I > 2\sigma(I)$
 $\theta_{\max} = 67.9^\circ$
 $h = 0 \rightarrow 10$
 $k = 0 \rightarrow 26$
 $l = -14 \rightarrow 0$
 2 standard reflections
 frequency: 120 min
 intensity decay: negligible

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.129$
 $S = 1.09$
 2107 reflections
 156 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.8408P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.15$ e Å⁻³
 $\Delta\rho_{\min} = -0.14$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0018 (3)

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2A \cdots O1^i$	0.82	1.90	2.704 (2)	168
$C7-H7 \cdots O1$	0.93	2.49	2.816 (3)	101

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

Data collection: *CAD-4 EXPRESS* (Enraf-Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL97*.

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