

1-(4-Chlorophenyl)-3-(4-hydroxyphenyl)-
prop-2-en-1-oneT. Ravishankar,^a K. Chinnakali,^{a*}
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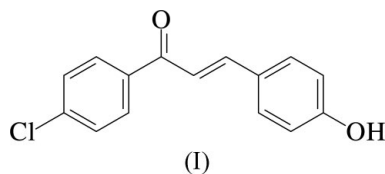
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.045
 wR factor = 0.108
Data-to-parameter ratio = 17.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title molecule, $\text{C}_{15}\text{H}_{11}\text{ClO}_2$, the ketone group is in the *s-cis* conformation with respect to the olefinic double bond. The two aromatic rings form a dihedral angle of $26.07(8)^\circ$. Screw-related molecules are linked *via* $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a chain along the *c* axis. Weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ interactions interconnect the chains into a three-dimensional network.

Comment

Chalcones, which are α,β -unsaturated ketones, possess multi-protecting biochemical activities, including antibacterial, antifungal, sedative, germicidal, cardiovascular and anti-fertility. The cytotoxic, anticancer, chemopreventative, mutagenic, antiviral, antiprotozoal and insecticidal activities of a variety of chalcones have been reviewed by Dimmock *et al.* (1999). It has been proven that halogen substitution at the benzene nucleus enhances greatly the activity of chalcones. In recent years, the synthesis of polymers having a photosensitive functional group has been an active field of research in polymer science. Monomers having structures similar to the title compound, (I), have been polymerized in solution using free radical initiators (Balaji & Nanjundan, 2001; Subramanian *et al.*, 2001). These polymers undergo cross-linking upon irradiation with UV light or an electron beam and are in use as photoresistors (Hyder Ali & Srinivasan, 1997; Rehab & Salahuddin, 1999). These photosensitive polymers find application in the fields of integrated circuit technology and photocurable coatings (Nagamatzu & Inui, 1977). The structure determination of (I) was undertaken as part of our study of chalcones.



In the title compound, the spatial arrangement of the keto group with respect to the olefinic double bond is *s-cis*, as seen from the $\text{C}7-\text{C}8-\text{C}9-\text{O}1$ torsion angle of $8.6(4)^\circ$ (Fig. 1). A similar conformation has been reported previously for related structures (Ravishankar, Chinnakali, Nanjundan, Jone Selvamalar *et al.*, 2003; Ravishankar, Chinnakali, Nanjundan, Radhakrishnan *et al.*, 2003). The unsaturated ketone system is not strictly planar. The two benzene rings and the unsaturated ketone system together form a curved structure, with a dihedral angle of $26.07(8)^\circ$ between the two benzene rings. This deviation from planarity affects the π -electron conjugation.

Received 10 January 2005

Accepted 18 January 2005

Online 22 January 2005

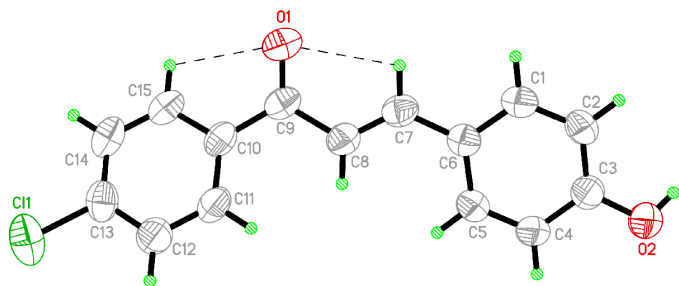


Figure 1

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

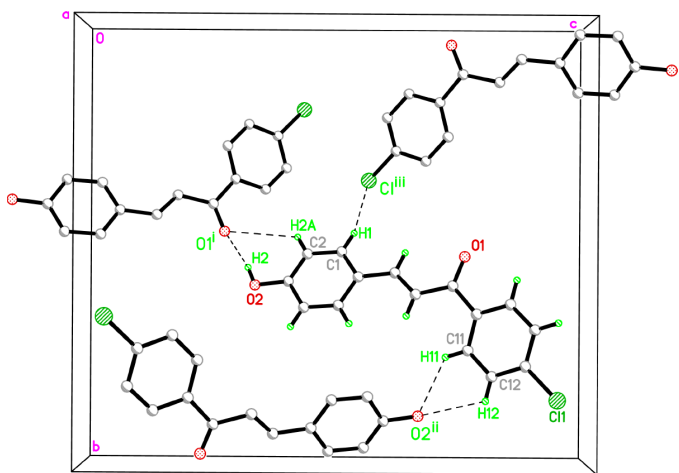


Figure 2

Part of the network structure of (I), showing O—H...O, C—H...Cl and C—H...O hydrogen-bonding interactions as dashed lines. Atoms involved in the interactions are labelled. Other H atoms have been omitted.

Atoms C11 and O2 deviate by 0.020 (3) and 0.007 (3) Å, respectively, from the plane of the attached benzene rings. The widening of the C5—C6—C7 angle to 123.05 (18)° and C6—C7—C8 to 128.03 (18)° can be ascribed to the short interatomic contact between atoms H5 and H8 (2.23 Å). In addition, the strain induced by the short H8...H11 (2.14 Å) contact results in a slight opening of the C9—C10—C11 angle to 123.03 (18)°. Intramolecular C7—H7...O1 and C15—H15...O1 interactions generate *S*(5) ring motifs (Etter *et al.*, 1990; Bernstein *et al.*, 1995).

In the crystal structure, O2—H2...O1ⁱ intermolecular hydrogen bonds link screw-related molecules into a chain along the *c* axis. The chains are interlinked via C—H...O and C—H...Cl interactions (Table 1) into a three-dimensional network. In the network, the O2—H2...O1ⁱ and C2—H2A...O1ⁱ interactions together form a pair of bifurcated acceptor bonds, which generate a ring of graph-set motif *R*₂¹(6). In addition, the C11—H11...O2ⁱⁱⁱ and C12—H12...O2ⁱⁱ interactions constitute a pair of bifurcated acceptor bonds, generating a ring of graph-set motif *R*₂¹(5) (Fig. 2). The symmetry codes are given in Table 1. The geometries of the above C—H...O interactions agree with those reported by Jeffrey (1997) and Desiraju & Steiner (1999).

Experimental

The title compound was prepared by the Claisen–Schmidt condensation of 4-chloroacetophenone (3.80 g, 0.025 mol) and 4-hydroxybenzaldehyde (3.05 g, 0.025 mol) in aqueous alcohol in the presence of sodium hydroxide. The crude product was isolated by neutralizing with dilute HCl. The title compound was filtered and washed with water and alcohol. Single crystals suitable for X-ray diffraction were grown from a 1:1 methanol–chloroform mixture.

Crystal data

C₁₅H₁₁ClO₂
M_r = 258.69
 Orthorhombic, *P*2₁2₁2₁
a = 4.0781 (6) Å
b = 16.344 (3) Å
c = 18.664 (3) Å
V = 1244.0 (4) Å³
Z = 4
D_x = 1.381 Mg m^{−3}

Mo *K*α radiation
 Cell parameters from 2214 reflections
 θ = 5.0–45.2°
 μ = 0.30 mm^{−1}
T = 293 (2) K
 Needle, colourless
 0.41 × 0.15 × 0.11 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.889, *T*_{max} = 0.968
 7590 measured reflections

2846 independent reflections
 2294 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.026
 θ _{max} = 28.3°
h = −5 → 4
k = −20 → 21
l = −23 → 23

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.045
wR(*F*²) = 0.108
S = 1.04
 2846 reflections
 163 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.0833P]$
 where $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)_{max} = 0.001
 $\Delta\rho$ _{max} = 0.21 e Å^{−3}
 $\Delta\rho$ _{min} = −0.13 e Å^{−3}
 Extinction correction: none
 Absolute structure: Flack (1983),
 1078 Friedel pairs
 Flack parameter: 0.02 (8)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2...O1 ⁱ	0.82	1.93	2.743 (2)	169
C7—H7...O1 ⁱⁱⁱ	0.93	2.49	2.817 (2)	101
C15—H15...O1 ⁱⁱ	0.93	2.50	2.787 (3)	98
C2—H2A...O1 ⁱ	0.93	2.99	3.598 (3)	125
C11—H11...O2 ⁱⁱⁱ	0.93	2.57	3.288 (3)	135
C12—H12...O2 ⁱⁱⁱ	0.93	2.97	3.480 (3)	116
C1—H1...Cl1 ^{iv}	0.93	2.89	3.753 (2)	154

Symmetry codes: (i) $-x - \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (ii) *x, y, z*; (iii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (iv) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.

H atoms were placed in calculated positions with O—H and C—H distances of 0.82 and 0.93 Å, respectively. The *U*_{iso}(H) values were constrained to be 1.5*U*_{eq} of the carrier atom for hydroxy and 1.2*U*_{eq} for the remaining H atoms.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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