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3-(4-Chlorophenyl)-1-(2-hydroxyphenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.103
Data-to-parameter ratio = 20.6

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

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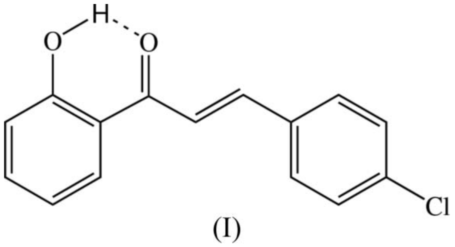
The title compound, $C_{15}H_{11}ClO_2$, is almost planar and adopts an E configuration. The dihedral angle between the two benzene rings is 10.76 (6)°. An intramolecular O—H⋯O hydrogen bond generates an S(6) ring motif. Molecules are arranged in layers approximately parallel to the (204) plane and weak π–π interactions are observed between the layers.

Comment

New nonlinear optical (NLO) materials showing large macrosocpic susceptibilities have attracted considerable attention, since they may be of interest for many applications (Prasad & Williams, 1991; Chemla & Zyss, 1987). The most important requirement for single-crystal NLO materials to exhibit second-order NLO properties is that the molecules should be in a non-centrosymmetric environment (Williams, 1984). We have recently reported the crystal structures of a range of chalcone derivatives, which exhibit NLO properties (Patil, Teh *et al.*, 2006*a*,*b*,*c*; Patil, Dharmaprakash *et al.*, 2006; Patil, Rosli *et al.*, 2006; Shettigar *et al.*, 2006). In our continuing systematic study of chalcone derivatives, we report here the crystal structure of the title compound, (I). However, compound (I) crystallizes in the centrosymmetric space group $P2_1/c$ and does not exhibit second-order NLO properties.



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule is almost planar and displays an E configuration with respect to the C8=C9 double bond [1.3365 (17) Å], the C7—C8—C9—C10 torsion angle being −178.70 (11)°. The dihedral angle between the C1–C6 and C10–C15 benzene rings is 10.76 (6)°. The mean plane through the enone unit (C7–C9/O2) makes dihedral angles of 11.85 (10) and 2.26 (9)° with the planes of the C1–C6 and C10–C15 benzene rings, respectively. An intramolecular O1—H1*O*1⋯O2 (Fig. 1) hydrogen bond generates an S(6) ring motif (Bernstein *et al.*, 1995). Bond distances and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable with those in related structures (Patil, Dharmaprakash *et al.*, 2006; Patil, Teh *et al.*, 2006*a*,*b*,*c*).

In the crystal structure of (I), the molecules are arranged in a head-to-tail fashion to form a layered structure approximately parallel to the (204) plane. A weak π–π interaction is observed between the C10–C15 benzene rings (centroid $Cg1$) of molecules in adjacent layers, with a $Cg1\cdots Cg1^{i}$ distance of 3.8149 (7) Å [symmetry code: (i) $-x, 1-y, 1-z$] (Fig. 2).

Experimental

4-Chlorobenzaldehyde (0.02 mol) and 2-hydroxyacetophenone (0.02 mol) were stirred in methanol (80 ml) at room temperature. An aqueous NaOH solution (20%, 10 ml) was added and the mixture was stirred for 6 h. The precipitate that formed was filtered off, washed with water and dried. The resulting crude product was recrystallized twice from acetone. Single crystals suitable for X-ray structure determination were grown by slow evaporation of an acetone solution of (I) at room temperature.

Crystal data

$C_{15}H_{11}ClO_2$
$M_r = 258.69$
Monoclinic, $P2_1/c$
$a = 8.4442$ (2) Å
$b = 6.8130$ (2) Å
$c = 20.5332$ (5) Å
$\beta = 91.497$ (1)°
$V = 1180.88$ (5) Å^3

$Z = 4$
$D_x = 1.455$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.31$ mm^{-1}
$T = 100.0$ (1) K
Block, yellow
0.55 × 0.50 × 0.38 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.846$, $T_{\max} = 0.890$

16059 measured reflections
3435 independent reflections
3090 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 30.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.103$
$S = 1.10$
3435 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.6768P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1

Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1*O*1$\cdots$O2	0.84 (2)	1.76 (2)	2.5345 (15)	152 (2)
C9—H9*A*$\cdots$O2	0.93	2.42	2.7700 (16)	102

The hydroxyl H atom was located in a difference map and refined isotropically. C-bound H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined using a riding model, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

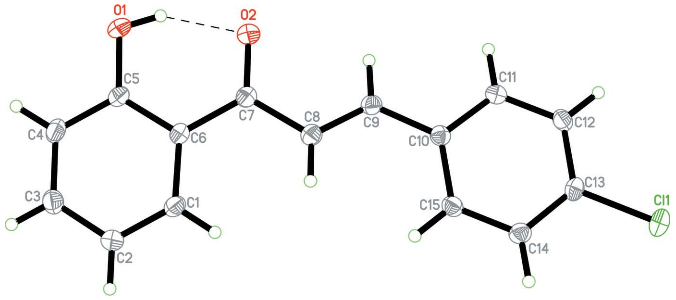


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

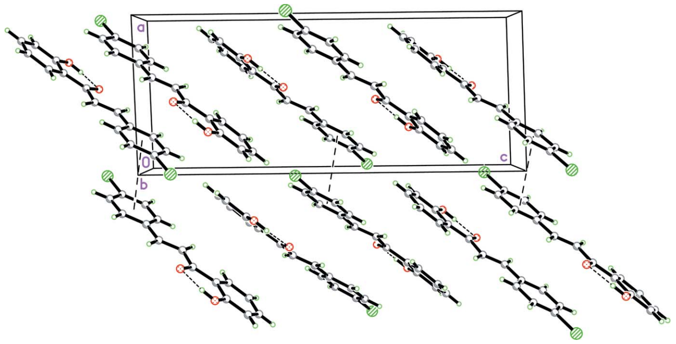


Figure 2
A packing diagram for (I), viewed down the *b* axis. Hydrogen bonds and π–π interactions are shown as dashed lines.

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