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(2*E*)-1-(2,4-Dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.084
Data-to-parameter ratio = 21.1

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

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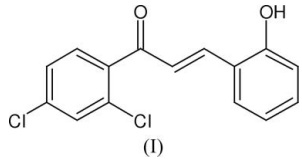
The geometric parameters of the title molecule, $C_{15}H_{10}Cl_2O_2$, are in the ususal ranges. The central double bond is *trans* configured. The dihedral angle between the dichlorophenyl and hydroxyphenyl rings is 71.38 (3)°. The crystal packing is stabilized by O—H···O hydrogen bonds and C—H···O contacts.

Comment

Chalcones are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and foodstuff and recently of great interest for their interesting pharmacological activities (Di Carlo *et al.*, 1999). Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities (Dimmock *et al.*, 1999; Go *et al.*, 2005). Among several organic compounds reported to show nonlinear optical (NLO) properties, chalcone derivatives are suitable materials because of their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO properties having two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Sarojini *et al.*, 2006). To exhibit NLO properties it is a prerequisite that the compound crystallizes in a non-centrosymmetric space group. Substitution of either of the phenyl rings greatly influences non-centrosymmetric crystal packing. It is speculated that in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of a non-centrosymmetric crystal (Fichou *et al.*, 1988). The molecular hyperpolarizability, β, is strongly influenced not only by the electronic effect but also by the steric effect of the substituent (Cho *et al.*, 1996).



(I)

The crystal structures of various dichloro-substituted chalcones have been reported (*e.g.* Teh *et al.*, 2006; Ng *et al.*, 2006). We have reported the crystal structures of 1-(2,4-dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Yathirajan *et al.*, 2006) and (2*E*)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl) phenyl]prop-2-en-1-one (Butcher *et al.*, 2007). In continuation of our work on chalcones, the present paper reports the crystal structure of a newly synthesized chalcone, (I).

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). The central double bond is *trans* configured. The torsion angle between the carbonyl group and the C atoms of the double bond is 1.23 (18)°. The dihedral angle between the dichlorophenyl and hydroxyphenyl rings is 71.38 (3)°. In the crystal structure, O—H···O hydrogen bonds link the molecules into zigzag chains running along the *a* axis. The crystal packing is further stabilized by C—H···O contacts (Table 1).

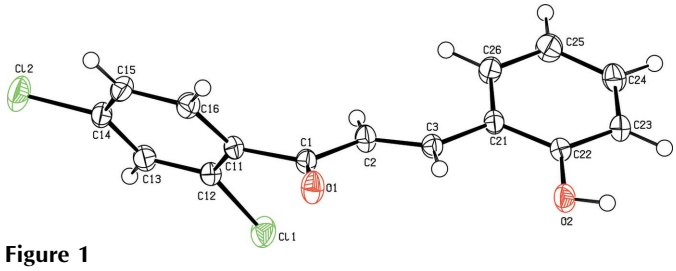


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

Experimental

2,4-Dichloroacetophenone (1.89 g, 0.01 mol) in methanol (20 ml) was mixed with salicylaldehyde (1.22 g, 0.01 mol) and the mixture was treated with 4 ml of a 30% potassium hydroxide solution at 278 K. The reaction mixture was then brought to room temperature, stirred for 3 h and neutralized with dilute acetic acid. The solid that precipitated was filtered off and washed with water, dried and recrystallized from an acetone–toluene (1:1) mixture (m.p. 411–413 K). Analysis for $C_{15}H_{10}Cl_2O_2$ found (calculated): C 61.38 (61.46), H 3.36 (3.44)%.

Crystal data

$C_{15}H_{10}Cl_2O_2$
M_r = 293.13
Orthorhombic, *Pbca*
a = 14.5702 (5) Å
b = 8.8146 (4) Å
c = 20.6699 (7) Å
V = 2654.65 (18) Å^3
Z = 8
D_x = 1.467 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 173 (2) K
Block, orange
0.36 × 0.33 × 0.32 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.846, T_{max} = 0.861
47302 measured reflections
3736 independent reflections
3486 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 29.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.06
3736 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 1.2454P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0073 (7)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.85 (2)	1.89 (2)	2.7408 (12)	176 (2)
C15—H15···O2^{ii}	0.95	2.43	3.3485 (15)	162

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

H atoms were found in a difference map, but those bonded to C were refined using a riding model with C—H = 0.95 Å; U_{iso}(H) was set to 1.2U_{eq}(C). The hydroxyl H atom was freely refined.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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