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

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The geometric parameters of the title molecule, $C_{16}H_{12}Cl_2O_3$, are in the normal ranges. The central double bond is *trans* configured. In the crystal structure, molecules are linked into centrosymmetric O—H···O hydrogen-bonded dimers. In addition, there is a single π–π stacking interaction between benzene rings of the dichlorophenyl groups.

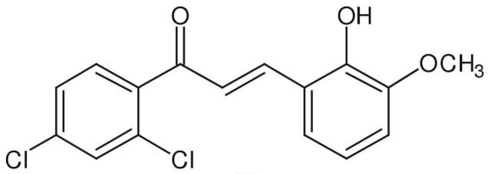
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.081
Data-to-parameter ratio = 16.7

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

Comment

The background to this study is set out in the preceding paper (Yathirajan *et al.*, 2006). 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 carbonyl group is twisted by −42.28 (17)° from the the plane of the dichlorophenyl ring. The torsion angle between the carbonyl group and the C atoms of the C═C double bond is −6.3 (2)°. The torsion angle between the C atoms of the double bond and the adjacent aromatic ring (C2═C3—C21—C26) is −11.92 (19)°. The two benzene rings are not coplanar [dihedral angle = 61.59 (4)°]. The crystal packing (Fig. 2) is characterized by O—H···O hydrogen bonds (Table 1) linking the molecules into centrosymmetric dimers. In addition, a π–π stacking interaction between two dichlorophenyl rings can be observed (centroid–centroid distance = 3.727 Å; symmetry operator to generate the second molecule: $-\frac{1}{2} + x, y, -\frac{1}{2} - z$).

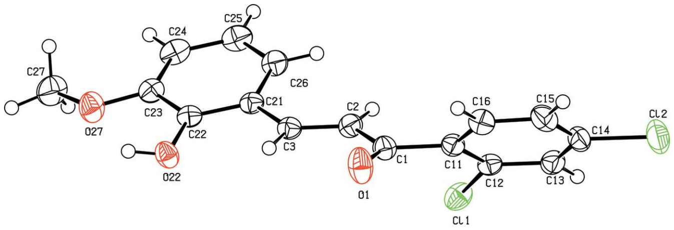


Figure 1
The molecular structure of (I) showing displacement ellipsoids drawn at the 50% probability level.

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Experimental

To a stirred solution of 2,4-dichloroacetophenone (1.89 g, 0.01 mol) and 2-hydroxy-3-methoxybenzaldehyde (1.52 g, 0.01 mol) in methanol (25 ml), 40% KOH solution (5 ml) was added. The mixture was stirred overnight, quenched in ice, acidified and filtered. The solid that precipitated was filtered off and washed with water, dried and recrystallized from acetone–toluene (1:1) mixture (m.p. 385–387 K). Analysis for $C_{16}H_{12}Cl_2O_3$ found (calculated): C 59.38 (59.46), H 3.63 (3.74)%.

Crystal data

$C_{16}H_{12}Cl_2O_3$
$M_r = 323.16$
Orthorhombic, *Pbca*
$a = 7.1477$ (3) Å
$b = 16.9604$ (11) Å
$c = 24.2071$ (13) Å
$V = 2934.6$ (3) Å^3
$Z = 8$
$D_x = 1.463$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.45$ mm^{-1}
$T = 173$ (2) K
Block, brown–yellow
0.35 × 0.34 × 0.33 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{min} = 0.859$, $T_{max} = 0.866$
21745 measured reflections
3277 independent reflections
2843 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.081$
$S = 1.06$
3277 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.5024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0047 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O22—H22···O1^{i}	0.86 (2)	1.99 (2)	2.7898 (14)	155 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

H atoms were found in a difference map, but those bonded to C atoms were refined using a riding model with C—H = 0.95 Å for $C_{aromatic}$ and C—H = 0.98 Å for C_{methyl}. U_{iso}(H) was set to $1.2U_{eq}$(C) or $1.5U_{eq}(C_{methyl})$. The methyl group was allowed to rotate but not to tip. 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: *XP* in *SHELXTL-Plus* (Sheldrick, 1991) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

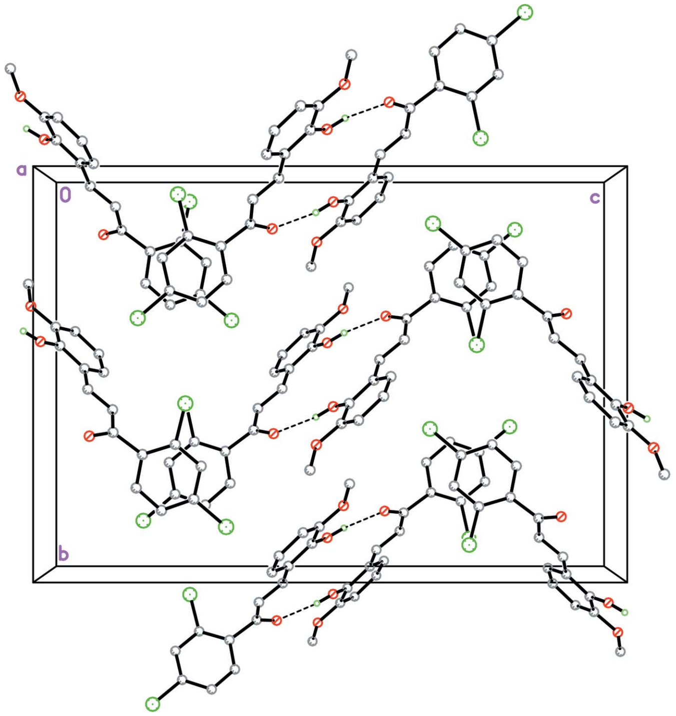

Figure 2
Partial packing diagram with H atoms not involved in hydrogen bonding omitted for clarity. Hydrogen bonds are shown as dashed lines.

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