

## 1-(4-Chlorophenyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

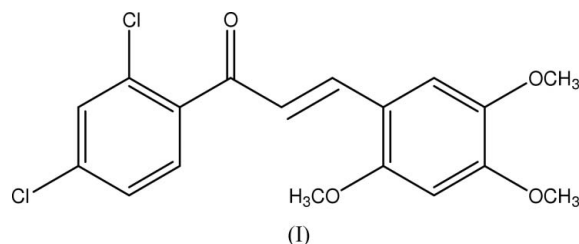
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## Key indicators

Single-crystal X-ray study  
T = 297 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
R factor = 0.054  
wR factor = 0.178  
Data-to-parameter ratio = 34.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.In the title compound,  $\text{C}_{18}\text{H}_{16}\text{Cl}_2\text{O}_4$ , the dihedral angle between the benzene rings is  $65.9 (1)^\circ$ . The crystal packing is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions.Received 14 June 2006  
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## Comment

Chalcones are important biological compounds that exhibit antibacterial, antifungal, antitumor and anti-inflammatory properties. They are also intermediates in the biosynthesis of flavonoids that are found widely in plants and have an array of biological activities. Furthermore, many chalcone derivatives exhibit excellent non-linear optical (NLO) properties (Fichou *et al.*, 1988; Uchida *et al.*, 1998; Patil *et al.*, 2006a,b). We have synthesized a new chalcone derivative, (I) (Fig. 1), which crystallizes in a centrosymmetric space group and therefore does not exhibit second-order non-linear optical properties.Bond distances and angles in (I) have normal values (Allen *et al.*, 1987), comparable with related structures (Teh *et al.*, 2006a,b; Patil *et al.*, 2006a,b). The least-squares plane through the enone group (C7, C8, C9 and O4) makes dihedral angles of  $19.1 (2)$  and  $59.8 (1)^\circ$  with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the benzene rings is  $65.9 (1)^\circ$ . The methoxy group attached at C1 is slightly twisted away from the C1–C6 benzene ring plane, with a C16–O1–C1–C2 torsion angle of  $16.0 (3)^\circ$ . The methoxy groups at C3 and C4 are almost coplanar with the C1–C6 benzene ring, with C17–O2–C3–C2 and C18–O3–C4–C5 torsion angles of  $8.0 (2)$  and  $-2.3 (2)^\circ$ , respectively.An intramolecular C7–H7A $\cdots$ O1 hydrogen bond generates an  $S(5)$  ring motif (Bernstein *et al.*, 1995). C5–H5A $\cdots$ O4<sup>i</sup> and C8–H8A $\cdots$ O4<sup>i</sup> (Table 1) interactions form a pair of bifurcated acceptor bonds, generating a ring of graph-set motif  $R_2^1(5)$  (Bernstein *et al.*, 1995). C15–H15A $\cdots$ O3<sup>ii</sup> (Table 1) interactions further stabilize the crystal packing.

## Experimental

Chalcone derivative (I) was prepared by adding NaOH (10 ml, 30%) to 2,4,5-trimethoxybenzaldehyde (0.01 mol) and 4-chloroacetophenone (0.01 mol) in ethyl alcohol (60 ml). After stirring the reac-

tion mixture for 2 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand for 12 h. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. The purity of the compound was checked by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of an acetone solution at room temperature over a period of 9 d.

#### Crystal data

$C_{18}H_{16}Cl_2O_4$	$V = 868.29 (3) \text{ \AA}^3$
$M_r = 367.21$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.405 \text{ Mg m}^{-3}$
$a = 8.4985 (1) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.3394 (2) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$c = 11.4856 (2) \text{ \AA}$	$T = 297 (2) \text{ K}$
$\alpha = 83.199 (1)^\circ$	Block, yellow
$\beta = 74.701 (1)^\circ$	$0.41 \times 0.38 \times 0.29 \text{ mm}$
$\gamma = 82.419 (1)^\circ$	

#### Data collection

Brucker SMART APEX2 CCD area-detector diffractometer	18803 measured reflections
$\omega$ scans	7577 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	4710 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.816$ , $T_{\max} = 0.895$	$R_{\text{int}} = 0.022$
	$\theta_{\text{max}} = 35.0^\circ$

#### Refinement

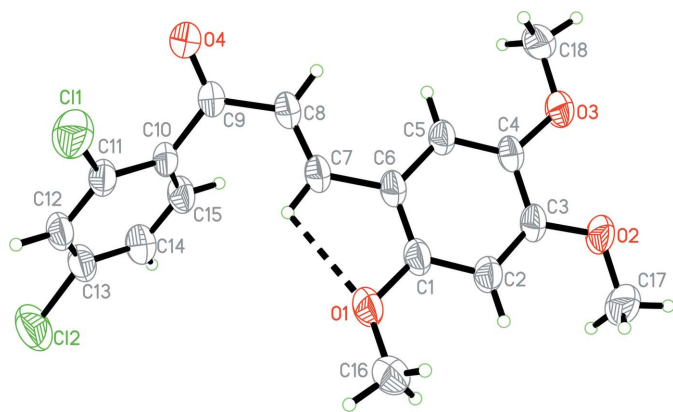
Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0838P)^2 + 0.1675P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.178$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.65 \text{ e \AA}^{-3}$
7577 reflections	$\Delta\rho_{\text{min}} = -0.47 \text{ e \AA}^{-3}$
221 parameters	Extinction correction: <i>SHELXTL</i>
H-atom parameters constrained	Extinction coefficient: 0.045 (5)

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

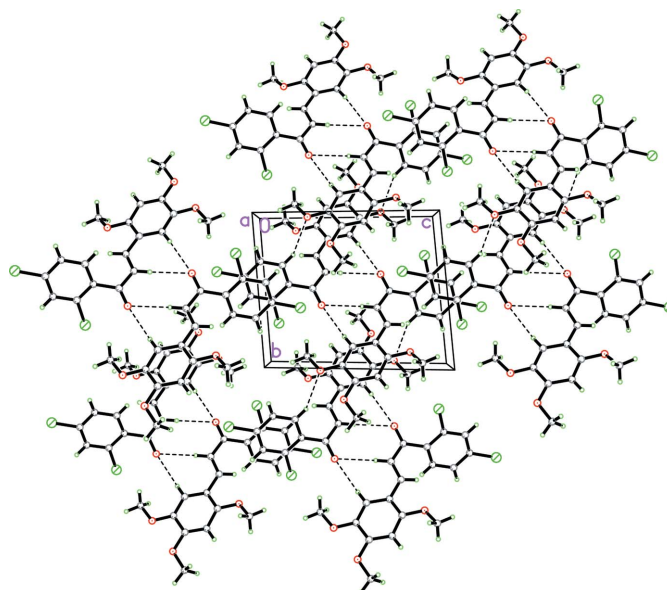
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5A\cdots O4^i$	0.93	2.51	3.420 (2)	165
$C7-H7A\cdots O1$	0.93	2.38	2.727 (2)	102
$C8-H8A\cdots O4^i$	0.93	2.48	3.410 (2)	174
$C15-H15A\cdots O3^{ii}$	0.93	2.46	3.295 (2)	149

Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x + 1, -y, -z + 1$ .



**Figure 1**

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



**Figure 2**

The crystal packing of (I), viewed down the  $a$  axis. Hydrogen bonds are shown as dashed lines.

H atoms were placed in calculated positions, with C—H distances of 0.93 or 0.96  $\text{\AA}$ . The  $U_{\text{iso}}$  values set equal to  $1.5U_{\text{eq}}$  of the carrier atom for methyl H atoms and  $1.2U_{\text{eq}}$  for the remaining H atoms.

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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