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Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.051
wR factor = 0.153
Data-to-parameter ratio = 16.8

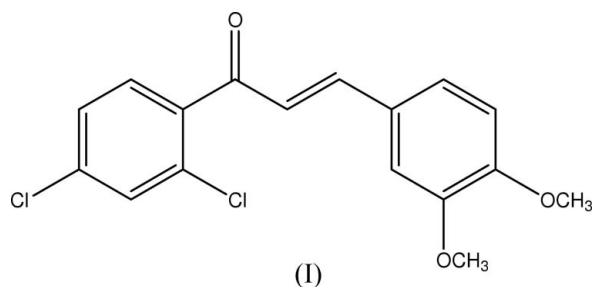
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1-(2,4-Dichlorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one

In the title compound, $\text{C}_{17}\text{H}_{14}\text{Cl}_2\text{O}_3$, the dihedral angle between the benzene rings is $45.42(15)^\circ$. In the crystal structure, molecules form layers parallel to the *bc* plane, and these are stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and by $\pi-\pi$ interactions between the benzene rings with a centroid-centroid distance of 3.848 \AA .

Comment

Chalcones show an impressive array of pharmacological properties, such as antiprotozoal (Nielsen *et al.*, 1998; Li *et al.*, 1995; Liu *et al.*, 2001), anti-inflammatory (Hsieh *et al.*, 1998) and nitric oxide inhibition activities (Rojas *et al.*, 2002). Recently, it has been noted that derivatives of chalcones exhibit extremely high and fast non-linearity (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006a,b; Zhang *et al.*, 1990; Zhao *et al.*, 2000). We and others have undertaken a number of theoretical and structural studies of such compounds (Ng *et al.*, 2006; Patil *et al.*, 2006a,b; Teh *et al.*, 2006; Radha Krishna *et al.*, 2005; Sathiyamoorthi *et al.*, 2005; Uchida *et al.*, 1995), and we report here the structure of the title compound (I) (Fig. 1). Crystals of (I) do not exhibit second-order non-linear optical properties as they crystallize in a centrosymmetric space group.



Bond lengths and angles for (I) are within normal ranges (Allen *et al.*, 1987) and are comparable with those in related structures (Ng *et al.*, 2006; Patil *et al.*, 2006a,b; Teh *et al.*, 2006; Radha Krishna *et al.*, 2005; Sathiyamoorthi *et al.*, 2005). The dihedral angle between the benzene rings is $45.42(15)^\circ$. The enone group makes dihedral angles of $46.15(8)^\circ$ and $1.22(14)^\circ$ with the C1-C6 and C10-C15 rings, respectively. The two methoxy groups attached at C13 and C14 are almost coplanar with the C10-C15 benzene ring, with C16-O1-C13-C12 and C17-O2-C14-C15 torsion angles of $-1.1(4)^\circ$ and $0.5(4)^\circ$, respectively.

Two intramolecular hydrogen bonds, $\text{C9}-\text{H9A}\cdots\text{O3}$ and $\text{C8}-\text{H8A}\cdots\text{Cl1}$ (Table 1), generate *S*(5) and *S*(6) ring motifs, respectively, in the molecule (Bernstein *et al.*, 1995). The

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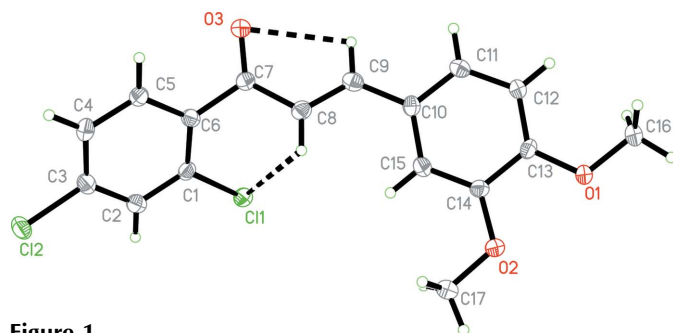


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown as dashed lines.

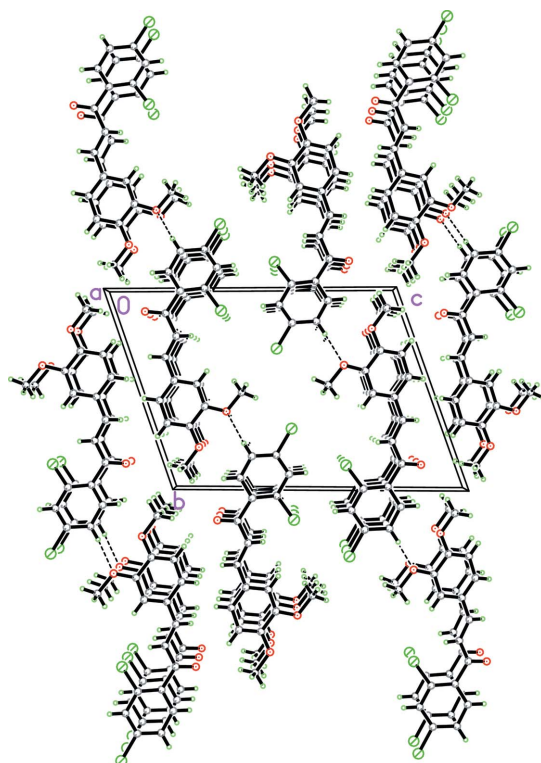


Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

crystal structure consists of layers of molecules parallel to the *bc* plane and stabilized by intermolecular C4—H4A...O2ⁱ hydrogen bonds along the *b* axis (Table 1). The crystal structure is also stabilized by π — π interactions between the benzene rings along the *a* axis, with a centroid-centroid distance of 3.848 Å.

Experimental

Compound (I) was obtained by the condensation of 3,4-dimethoxybenzaldehyde (0.01 mol) with 2,4-dichloroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (5 ml, 20%). After stirring for 4 h, the contents of the flask were poured into ice-cold water (250 ml), and the resulting crude solid was collected by filtration. The compound was dried and purified by repeated recrystallization from

acetone. Crystals of (I), suitable for a single-crystal diffraction study, were grown by slow evaporation of an acetone solution.

Crystal data

C₁₇H₁₄Cl₂O₃
M_r = 337.18
 Triclinic, *P* $\bar{1}$
a = 3.8479 (2) Å
b = 12.2341 (6) Å
c = 16.8454 (7) Å
 α = 70.487 (3)°
 β = 84.170 (4)°
 γ = 86.707 (3)°

V = 743.36 (6) Å³
Z = 2
D_x = 1.506 Mg m⁻³
 Mo *K* α radiation
 μ = 0.45 mm⁻¹
T = 100.0 (1) K
 Plate, yellow
 0.35 × 0.15 × 0.04 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.814, *T_{max}* = 0.981

12829 measured reflections
 3372 independent reflections
 2434 reflections with *I* > 2 σ (*I*)
R_{int} = 0.082
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.051
wR (*F*²) = 0.153
S = 1.05
 3372 reflections
 201 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + 0.6876P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.39 \text{ e } \text{Å}^{-3}$

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>
C4—H4A...O2 ⁱ	0.93	2.57	3.475 (4)	165
C8—H8A...Cl1	0.93	2.78	3.139 (3)	103
C9—H9A...O3	0.93	2.55	2.866 (4)	100

Symmetry code: (i) *x*, *y* − 1, *z*.

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. *U*_{iso}(H) values were set equal to 1.5*U*_{eq} of the carrier atom for methyl H atoms and 1.2*U*_{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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