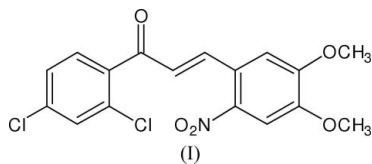


(2E)-1-(2,4-Dichlorophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one**H. S. Yathirajan,^a Anil N. Mayekar,^a B. Narayana,^a B. K. Sarojini^b and Michael Bolte^{c*}**^aDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^bDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^cInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, GermanyCorrespondence e-mail:
bolte@chemie.uni-frankfurt.de**Key indicators**Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.041
 wR factor = 0.092
Data-to-parameter ratio = 14.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The C=C double bond in the title molecule, C₁₇H₁₃Cl₂NO₅, is *trans* configured. The dihedral angle between the two benzene rings is 47.98 (4)°.**Comment**

Chalcones, one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soya-based foodstuffs, have recently been the subject of great interest because of their pharmacological activities (Di Carlo *et al.*, 1999). Chalcones, or 1,3-diaryl-2-propen-1-ones, belong to the flavonoid family. Chemically, they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β -unsaturated carbonyl system. A vast number of naturally occurring chalcones are polyhydroxylated on the aryl rings. The radical-quenching properties of the phenolic groups present in many chalcones have raised interest in using these compounds or chalcone-rich plant extracts as drugs or food preservatives (Dhar, 1981). Reviews on the bioactivities of various chalcones are given by Dimmock *et al.* (1999) and Go *et al.* (2005). Recently, it has been noted that, among many organic compounds reported for their second-harmonic generation, chalcone derivatives have excellent blue-light transmittance and good crystallizability (Fichou *et al.*, 1988; Goto *et al.*, 1991; Uchida *et al.*, 1998; Sarojini *et al.*, 2006). In a continuation of our broad programme on chalcones (Yathirajan *et al.*, 2007), the present paper reports the crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database Database, Version 5.28, November 2006; updated January 2007; Allen, 2002; Mogul, Version 1.1; Bruno *et al.*, 2004). The C=C double bond is *trans* configured and twisted considerably from the plane of the adjacent aromatic ring (see Table 1 for key torsion angles). The dihedral angle between the two benzene rings is 47.98 (4)°. The nitro group and the two methoxy groups are twisted slightly from the plane of the benzene ring to which they are attached (Table 1).

Experimental

40% KOH solution (5 ml) was added to a thoroughly stirred solution of 2,4-dichloroacetophenone (1.89 g, 0.01 mol) and 4,5-dimethoxy-2-

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nitrobenzaldehyde (2.11 g, 0.01 mol) in methanol (25 ml). The resulting mixture was stirred overnight and then filtered. The product was crystallized from an acetone/toluene mixture (1:1) (m.p. 464–466 K). Analysis for $C_{17}H_{13}Cl_2NO_5$ found (calculated) (%): C 53.31 (53.42), H 3.39 (3.43), N 3.57 (3.66).

Crystal data

$C_{17}H_{13}Cl_2NO_5$

$M_r = 382.18$

Monoclinic, $C2/c$

$a = 7.6843$ (7) Å

$b = 15.9464$ (11) Å

$c = 26.851$ (3) Å

$\beta = 96.946$ (8)°

$V = 3266.1$ (5) Å³

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 0.43$ mm⁻¹

$T = 173$ (2) K

$0.42 \times 0.40 \times 0.39$ mm

Data collection

Stoe IPDSII two-circle diffractometer

Absorption correction: multi-scan

(*MULABS*; Spek, 2003;

Blessing, 1995)

$T_{\min} = 0.841$, $T_{\max} = 0.851$

13923 measured reflections

3298 independent reflections

2852 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.092$

$S = 1.02$

3298 reflections

229 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.31$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Selected torsion angles (°).

C2–C3–C21–C26	29.8 (2)	C27–O4–C24–C23	–7.4 (2)
O2–N1–C22–C21	15.1 (2)	C28–O5–C25–C26	0.9 (2)
O3–N1–C22–C23	13.8 (2)		

H atoms were found in a difference map, but were refined using a riding model with aromatic C–H = 0.95 Å or methyl C–H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl C})$. The methyl groups were allowed to rotate but not to tip.

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*.

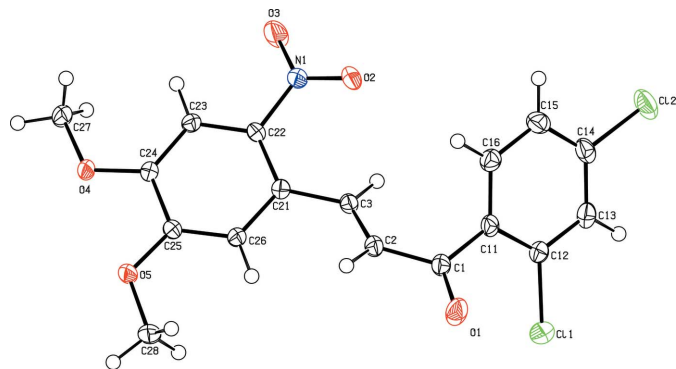


Figure 1

The molecular structure of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

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