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1-(4-Chlorophenyl)-3-(4-ethoxyphenyl)-prop-2-en-1-one

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The title compound, $C_{17}H_{15}ClO_2$, crystallizes in a non-centrosymmetric space group and exhibits non-linear optical properties. The molecule exists in an *E* configuration, with a dihedral angle of 7.44 (9)° between the two benzene rings.

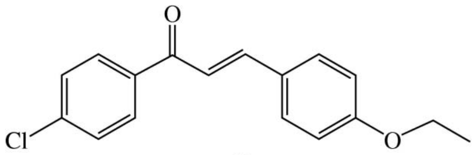
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.104
Data-to-parameter ratio = 20.8

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

Comment

Non-linear optical (NLO) properties of organic molecules and materials have been intensively studied in recent years because of their potential applications in electro-optic modulation, frequency mixing and second-harmonic generation (SHG) (Chemla & Zyss, 1987). During our studies on the second-order NLO properties of crystalline chalcone derivatives (Fun *et al.*, 2007; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007), we have prepared the title compound, (I). Compound (I) crystallizes in a non-centrosymmetric space group and exhibits second-order non-linear optical properties.



(I)

In (I), the molecule exhibits an *E* configuration with respect to the C8=C9 double bond (Fig. 1). The torsion angle C7—C8—C9—C10 is −178.96 (18)° and the dihedral angle between the C1–C6 and C10–C15 benzene rings is 8.73 (9)°. The mean plane through the enone unit (C7–C9/O1) makes dihedral angles of 11.18 (9) and 7.44 (9)° with the planes of the C1–C6 and C10–C15 benzene rings, respectively. The ethoxy group is slightly displaced from the plane of the C10–C15 benzene ring, giving a C13—O2—C16—C17 torsion angle of 173.06 (16)°. The bond distances and angles in (I) lie within normal ranges (Allen *et al.*, 1987) and are comparable with those in related structures (Patil, Dharmaprakash *et al.*, 2006; Fun *et al.*, 2007).

Experimental

4-Ethoxybenzaldehyde (0.01 mol) and 4-chloroacetophenone (0.01 mol) were stirred in 60 ml of methanol at room temperature. 5 ml of 10% NaOH aqueous solution was added and the mixture was stirred for 4 h. The precipitate was filtered off, washed with water and dried, and the crude product was recrystallized from acetone. Single crystals of (I) suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature over several days.

Crystal data

$C_{17}H_{15}ClO_2$
$M_r = 286.74$
Monoclinic, $P2_1$
$a = 3.9479$ (1) Å
$b = 10.1234$ (3) Å
$c = 17.2553$ (6) Å
$\beta = 91.823$ (2)°

$V = 689.28$ (4) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.28$ mm^{-1}
$T = 100$ (2) K
0.44 × 0.32 × 0.10 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005) $T_{\min} = 0.889$, $T_{\max} = 0.973$

11477 measured reflections
3788 independent reflections
3336 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.104$
$S = 1.04$
3788 reflections
182 parameters
1 restraint

H-atom parameters constrained
$\Delta\rho_{\max} = 0.54$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}
Absolute structure: Flack (1983), 1674 Friedel pairs
Flack parameter: 0.00 (6)

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H atoms or $1.2U_{\rm eq}({\rm C})$ for the remaining H atoms. The methyl group was allowed to rotate about its local threefold axis.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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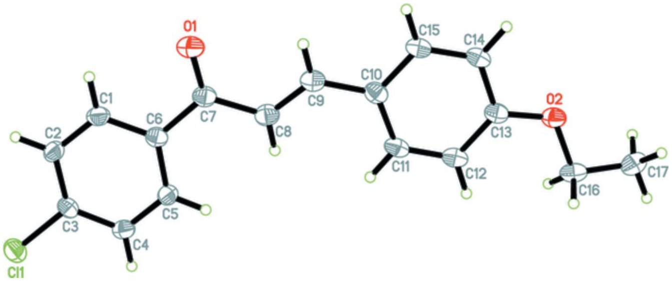

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms.

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