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(2*E*)-3-(4-Butoxyphenyl)-1-(4-chlorophenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.139
Data-to-parameter ratio = 18.7

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

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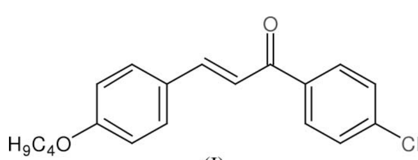
The central double bond in the title molecule, $C_{19}H_{19}ClO_2$, is *trans* configured. Geometric parameters are in normal ranges.

Comment

α,β-Unsaturated ketones, in which the double bond is adjacent to the carbonyl group, have been used as starting materials for the synthesis of various chemicals, including plastics, resins, pesticides, dyes and pharmaceuticals (Opdyke, 1973). Chalcones and the corresponding heterocyclic analogs are valuable intermediates in organic synthesis (Dhar, 1981) and show numerous biological effects (Opletalova & Sedivy, 1999; Dimmock *et al.*, 1999). In addition, with appropriate subsitutuents, chalcones are a class of non-linear optical (NLO) materials (Fichou *et al.*, 1988; Butcher *et al.*, 2006; Harrison *et al.*, 2006; Sarojini *et al.*, 2006). Among several organic compounds reported to have NLO properties, chalcone derivatives are recognized materials because of their excellent blue-light transmittance and good crystallization ability. They provide a necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002). Recently, we have reported the crystal structures of a series of such compounds (Yathirajan *et al.*, 2006*a*,*b*; Yathirajan, Narayana *et al.*, 2006; Yathirajan, Ashalatha *et al.*, 2006). In a continuation of this work, and also considering the importance of flavanoid analogs, we have determined the crystal structure of the title compound, (I). In fact, the title compound crystallizes in a centrosymmetric space group so does not exhibit NLO properties.



(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 central double bond is *trans* configured. The dihedral angle between the two benzene rings is 42.53 (6)°. The central ring (C21–C26) is almost coplanar with the double bond [C2—C3—C21—C26 = 9.9 (2)°] and the chlorophenyl ring is twisted out of the plane of the double bond by 31.8 (2)°.

Experimental

The title compound was synthesized according to a method reported in the literature (Furniss *et al.*, 1989), in a yield of 80%. The compound was purified by recrystallization from ethanol. Crystals were grown by slow evaporation of a solution of (I) in acetone (m.p. 333–335 K). Analysis found (calculated) (%) for $C_{19}H_{19}ClO_2$: C 72.90 (72.49), H 6.05 (6.08).

Crystal data

$C_{19}H_{19}ClO_2$	$V = 811.14$ (14) Å^3
$M_r = 314.79$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.289$ Mg m^{-3}
$a = 5.9580$ (6) Å	Mo $K\alpha$ radiation
$b = 11.6745$ (12) Å	$\mu = 0.24$ mm^{-1}
$c = 12.6433$ (12) Å	$T = 173$ (2) K
$\alpha = 106.346$ (9)°	Plate, light yellow
$\beta = 94.975$ (7)°	0.32 × 0.28 × 0.11 mm
$\gamma = 103.112$ (8)°	

Data collection

Stoe IPDS-II two-circle diffractometer	13618 measured reflections
ω scans	3725 independent reflections
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)	3183 reflections with $I > 2\sigma(I)$
$T_{min} = 0.928$, $T_{max} = 0.977$	$R_{int} = 0.089$
	$\theta_{max} = 27.6°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.1402P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.139$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
3725 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
199 parameters	
H-atom parameters constrained	

H atoms were found in a difference map but they were refined using a riding model, with C—H = 0.95 Å for aromatic and methylene groups and C—H = 0.98 Å for methyl groups. U_{iso}(H) values were set at $1.2U_{eq}$(C) [$1.5U_{eq}$(methyl C)].

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* and *PLATON*.

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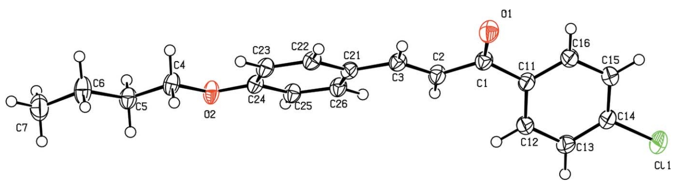

Figure 1
The molecular structure of (I) with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

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