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

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Key indicators

Single-crystal X-ray study
$T = 100$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.057
wR factor = 0.141
Data-to-parameter ratio = 38.8

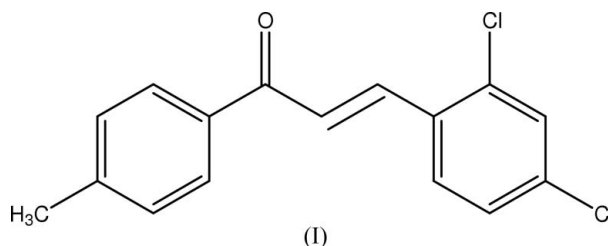For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{16}H_{12}Cl_2O$, exhibits second-order nonlinear optical properties as it crystallizes in a non-centrosymmetric space group. The dihedral angle between the benzene rings is 34.02 (6)°. Intermolecular C—H···O interactions link the molecules to form chains along the *c* axis.

Comment

The title compound, (I) (Fig. 1), was prepared as part of our ongoing studies (Patil, Rosli *et al.*, 2006; Patil, Teh *et al.*, 2006*a,b*) of the nonlinear optical properties of chalcone derivatives (Fichou *et al.*, 1988; Uchida *et al.*, 1998). It crystallizes in non-centrosymmetric space group $Pna2_1$, which is consistent with its significant second harmonic generation response of 1.2 times (Nd:YAG laser, 1.064 μm, 8 ns, 10 Hz, 8 mJ) that of urea (Watson *et al.*, 1993).

(I)

Bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and are comparable to those in related structures (Teh *et al.*, 2006*a,b*; Patil, Rosli *et al.*, 2006; Patil, Teh *et al.*, 2006*a,b*). The least-squares plane through the enone unit (C7–C9/O1) makes dihedral angles of 21.85 (11) and 12.24 (11)° with the planes of the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the two benzene rings is 34.02 (6)°. Intramolecular C9—H9*A*···Cl1 and C9—H9*A*···O1 interactions generate an *S*(5) ring motif (Bernstein *et al.*, 1995). The crystal packing (Fig. 2) is stabilized by intermolecular C—H···O hydrogen bonds (Table 2), which form chains of molecules along the *c* axis.

Experimental

A mixture of 2,4-dichlorobenzaldehyde (0.01 mol) and 4-methyl-acetophenone (0.01 mol) in ethanol (60 ml) was stirred for 2 h in the presence of NaOH (5 ml, 30%). The contents of the flask were then poured into ice–cold water (250 ml), and left to stand for 12 h. The resulting crude solid of (I) was collected by filtration, dried and purified by repeated recrystallization from acetone (yield 84%). The purity of the compound was checked by thin-layer chromatography. Crystals of (I) suitable for X-ray diffraction were grown by slow

evaporation of an acetone solution at room temperature over a period of 7 d.

Crystal data

$C_{16}H_{12}Cl_2O$
$M_r = 291.16$
Orthorhombic, $Pna2_1$
$a = 28.3884 (5)$ Å
$b = 3.9343 (1)$ Å
$c = 12.0092 (2)$ Å
$V = 1341.29 (5)$ Å^3

$Z = 4$
$D_x = 1.442$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.47$ mm^{-1}
$T = 100.0 (1)$ K
Slab, yellow
$0.51 \times 0.43 \times 0.08$ mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2005)
$T_{min} = 0.866$, $T_{max} = 0.962$

35136 measured reflections
6715 independent reflections
6036 reflections with $I > 2\sigma(I)$
$R_{int} = 0.079$
$\theta_{max} = 37.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.141$
$S = 1.18$
6715 reflections
173 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.6516P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}
Absolute structure: Flack (1983), 3071 Friedel pairs
Flack parameter: 0.02 (6)

Table 1
Selected torsion angles (°).

C1—C6—C7—C8	−19.9 (3)	C7—C8—C9—C10	178.71 (18)
C6—C7—C8—C9	166.95 (18)	C8—C9—C10—C15	−5.4 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C9—H9A⋯Cl1	0.93	2.61	3.048 (2)	110
C9—H9A⋯O1	0.93	2.48	2.812 (2)	101
C14—H14A⋯O1^i	0.93	2.42	3.325 (3)	166

Symmetry code: (i) $-x + 2, -y + 1, z + \frac{1}{2}$.

H atoms were placed in calculated positions, with C—H distances of 0.93 or 0.96 Å. The $U_{iso}(H)$ values were set equal to $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ 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).
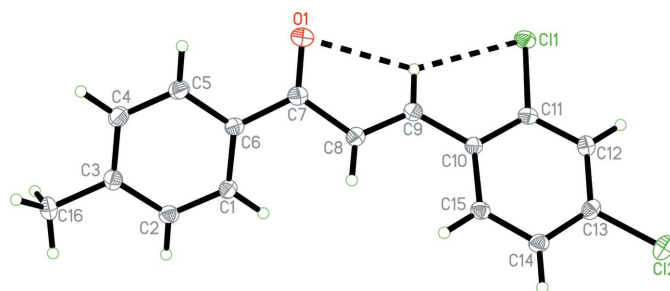
Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are shown as dashed lines.
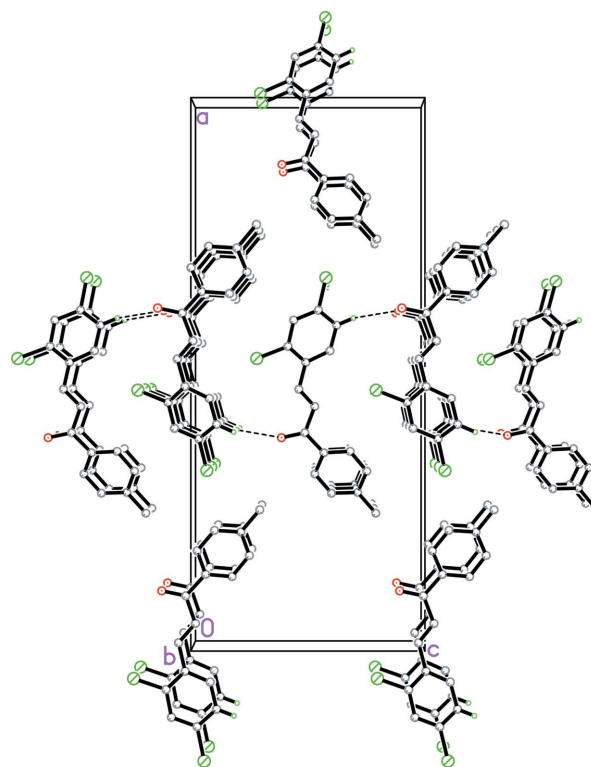

Figure 2
The crystal packing of (I), viewed down the b axis. H atoms have been omitted unless they are involved in hydrogen bonds (dashed lines).

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