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1-(4-Bromophenyl)-3-(2,4-dichlorophenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.007 Å
R factor = 0.050
wR factor = 0.131
Data-to-parameter ratio = 22.8

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

In the title compound, $C_{15}H_9BrCl_2O$, the molecules form chains along the b axis through short Br···Cl contacts. These chains form layers through C—H···O intermolecular interactions and these layers stack parallel to the c axis.

Comment

In recent years, excellent second-order nonlinear optical (NLO) materials capable of efficient frequency conversion of infrared laser radiation into visible and ultraviolet wavelengths have been developed. Among them, materials that can generate highly efficient second-harmonic blue–violet light by using laser diodes are of great interest for various applications, including optical disk data storage, laser remote sensing, laser-driven fusion, color displays, medical diagnostics *etc*. Materials with large second-order optical nonlinearities, short transparency cutoff wavelengths and stable physicochemical performance are needed in order to realize many of these applications.

(I)
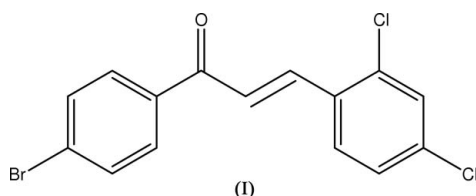
Recently, chalcone derivatives have attracted much interest as they exhibit extremely high and fast nonlinearity (Fichou *et al.*, 1988; Uchida *et al.*, 1998). The title compound, (I), crystallizes in a non-centrosymmetric crystal structure and exhibits a second harmonic generation (SHG) effect. Powder SHG measurement of (I) showed a conversion efficiency 1.5 times that of a urea standard.

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Sathiya Moorthi, Chinnakali, Nanjundan, Santhi *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Ravishankar *et al.*, 2005; Teh *et al.*, 2006; Patil *et al.*, 2006; Ng *et al.*, 2006; Rosli *et al.*, 2006). The least-squares plane through the enone group makes dihedral angles of 13.88 (24) and 9.78 (24)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the benzene rings is 23.58 (16)°.

Intramolecular C9–H9*A*···O1 and C9–H9*A*···Cl2 interactions are observed in the molecular structure of (I); both interactions generate an *S*(5) ring motif (Bernstein *et al.*, 1995). In the crystal structure, the C5—H5*A*···O1[i] and C6—
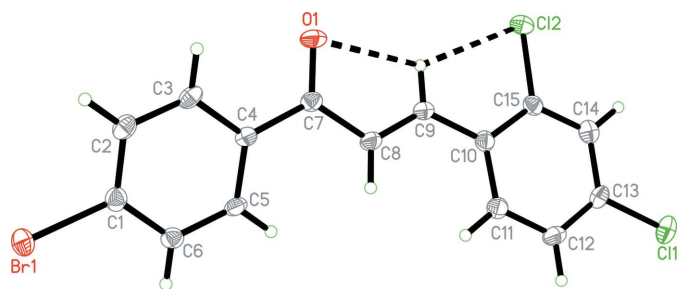
Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are shown as dashed lines.
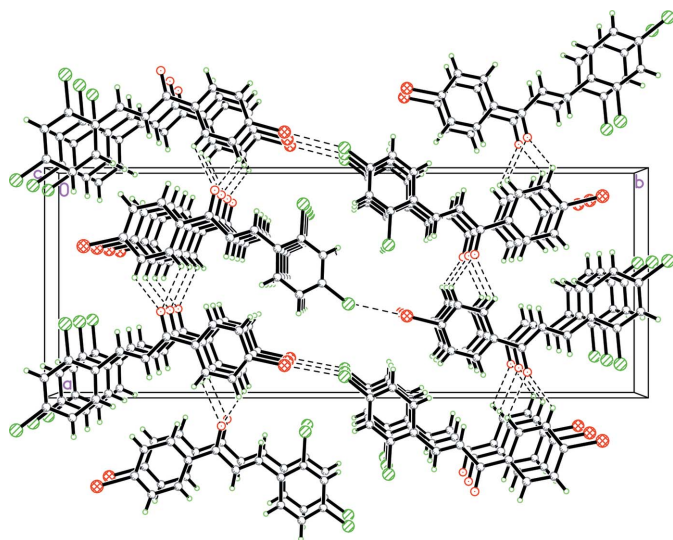

Figure 2
The crystal packing of (I), viewed down the c axis. Hydrogen bonds and Br···Cl interactions are shown as dashed lines.

H6A···O1^i (Table 1) interactions form a pair of bifurcated acceptor bonds, which generates a ring of graph-set motif $R_2^1(5)$ (Bernstein *et al.*, 1995). A short Br1···Cl1($2 - x, \frac{1}{2} + y, -\frac{1}{2} - z$) contact of 3.419 (1) Å is also observed in the structure linking the molecules into infinite chains along the b axis. These infinite chains form layers through the C—H···O intermolecular interactions (Table 1). These layers are stacked parallel to the c axis.

Experimental

Chalcone derivative (I) was obtained by the condensation of 2,4-dichlorobenzaldehyde (0.01 mol) with 4-bromoacetophenone (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. Purity of the compound was checked by thin layer chromatography. Crystals of (I) suitable for single-crystal X-ray diffraction study were grown in 10 d by the slow evaporation technique at room temperature, using acetone as the solvent. The second harmonic generation (SHG) efficiency of (I) was measured with the standard powder technique (Kurtz & Perry, 1968). An incident beam of an Nd:YAG laser (fundamental wavelength 1064 nm, pulse width 8 ns, power 8 mJ per pulse) was applied to the sample, and the generated second harmonic (SH) wave 532 nm was detected with a photomultiplier with reference to that of urea.

Crystal data

$C_{15}H_9BrCl_2O$	$Z = 4$
$M_r = 356.03$	$D_x = 1.756$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 11.4642$ (4) Å	$\mu = 3.44$ mm^{-1}
$b = 30.0972$ (10) Å	$T = 100.0$ (1) K
$c = 3.9020$ (1) Å	Block, yellow
$V = 1346.35$ (7) Å^3	$0.51 \times 0.29 \times 0.22$ mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	30878 measured reflections
ω scans	3923 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	3809 reflections with $I > 2\sigma(I)$
$T_{min} = 0.284$, $T_{max} = 0.515$	$R_{int} = 0.054$
(expected range = 0.259–0.470)	$\theta_{max} = 30.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 5.363P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.20$	$\Delta\rho_{max} = 1.74$ e Å^{-3}
3923 reflections	$\Delta\rho_{min} = -1.16$ e Å^{-3}
172 parameters	Absolute structure: Flack (1983), 1579 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.068 (14)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O1^i	0.93	2.57	3.148 (5)	121
C6—H6A···O1^i	0.93	2.58	3.147 (6)	120
C9—H9A···Cl2	0.93	2.63	3.068 (5)	110
C9—H9A···O1	0.93	2.42	2.765 (6)	102

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

H atoms were placed in calculated positions, with C—H distances of 0.93 Å. The U_{iso}(H) values were constrained to be 1.2U_{eq}(C). The highest peak is located 0.73 Å from atom Br1 and the deepest hole is 1.90 Å from C15.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Bruker, 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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