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3-(4-Bromophenyl)-1-(4-chlorophenyl)prop-2-en-1-one

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Key indicators

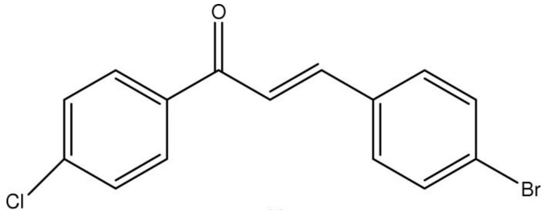
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.118
Data-to-parameter ratio = 37.3

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

The enone group and the benzene rings of the title compound, $C_{15}H_{10}BrClO$, are each planar. The mean plane through the enone group makes dihedral angles of 24.54 (1) and 20.66 (1)° with the chloro- and bromo-substituted benzene rings, respectively. The crystal packing is stabilized by weak intermolecular C—H..π interactions involving both aromatic rings and the molecules are stacked along the *b* axis.

Comment

Chalcones exhibit extremely high and fast non-linearity (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000), and are easy to crystallize as non-centrosymmetric structures. Another importance of this type of compound is their high photosensitivity and thermal stability, which are used in developing various crystalline electro-optical devices (Williams, 1983; Chemla & Zyss, 1987). Furthermore, in biology and biochemistry, chalcone is claimed as one of the compounds that plays a vital role in anti-inflammatory, anti-malarial, antifertility and antitumor activities (De Vincenzo *et al.*, 1995; Kumar *et al.*, 2003). In this work, we report the synthesis and crystal structure of 3-(4-bromophenyl)-1-(4-chlorophenyl)prop-2-en-1-one, (I). Crystals of the title compound do not exhibit second-order non-linear optical properties as they crystallized in a centrosymmetric space group.



(I)

The bond lengths and angles in (I) are normal (Allen *et al.*, 1987) and similar to those observed in other comparable structures (Ng, Patil *et al.*, 2006; Ng, Shettigar *et al.*, 2006; Patil *et al.*, 2006*a*,*b*).

The enone group and the two benzene rings of the chalcone are each planar, with a maximum deviation of 0.008 (2) Å, from the C1–C6 plane, 0.009 (2) Å from C10–C15 and 0.067 (2) Å from O1/C7–C9 for atoms C2, C15 and C7, respectively. The molecule is twisted about the C6—C7 bond, with a dihedral angle of 45.20 (9)° between the two benzene rings. The mean plane through the enone group makes dihedral angles of 24.54 (1)° with the C1–C6 benzene ring and

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20.66 (1)° with the C10–C15 benzene ring. The difference in the C1—C6—C7 [122.1 (2)°] and C6—C7—C8 [118.4 (2)°] angles is caused by the short H1*A*···H8*A* (2.28 Å) contact. Similarly, the short H8*A*···H15*A* (2.24 Å) contact results in a slight widening of the C9—C10—C15 angle to 122.5 (2)°.

Aromatic rings C1–C6 and C10–C15 are involved in weak intermolecular C—H···π interactions (Table 1) which stabilize the crystal structure. The molecules are stacked along the *b* axis (Fig. 2).

Experimental

The title chalcone derivative, (I), was obtained by the condensation of 4-bromobenzaldehyde (0.01 mol) with 4-chloroacetophenone (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 left to stand for 24 h. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. Crystals suitable for single-crystal X-ray diffraction experiments were grown in 7 d by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{15}H_{10}BrClO$
M_r = 321.59
Monoclinic, $P2_1/c$
a = 15.4427 (2) Å
b = 13.9304 (2) Å
c = 5.8527 (1) Å
β = 91.962 (1)°
V = 1258.31 (3) Å^3
Z = 4
D_x = 1.698 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.46 mm^{-1}
T = 100.0 (1) K
Block, yellow
0.46 × 0.12 × 0.05 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min}$ = 0.582, $T_{\max}$ = 0.854
34215 measured reflections
6074 independent reflections
3987 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.076
$\theta_{\max}$ = 36.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
S = 1.05
6074 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.93 e Å^{-3}
$\Delta\rho_{\min}$ = −0.66 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···*Cg*2$^{\rm i}$	0.93	3.00	3.632 (2)	126
C5—H5*A*···*Cg*1$^{\rm ii}$	0.93	2.96	3.503 (2)	119
C9—H9*A*···*Cg*1$^{\rm iii}$	0.93	2.97	3.550 (2)	122
C14—H14*A*···*Cg*2$^{\rm iv}$	0.93	2.78	3.468 (2)	132

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$. *Cg*1 is the centroid of the C1–C6 ring and *Cg*2 is the centroid of the C10–C15 ring.

H atoms were placed in calculated positions and constrained to ride on their carrier atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

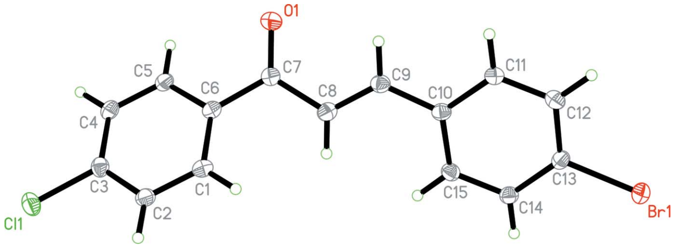

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

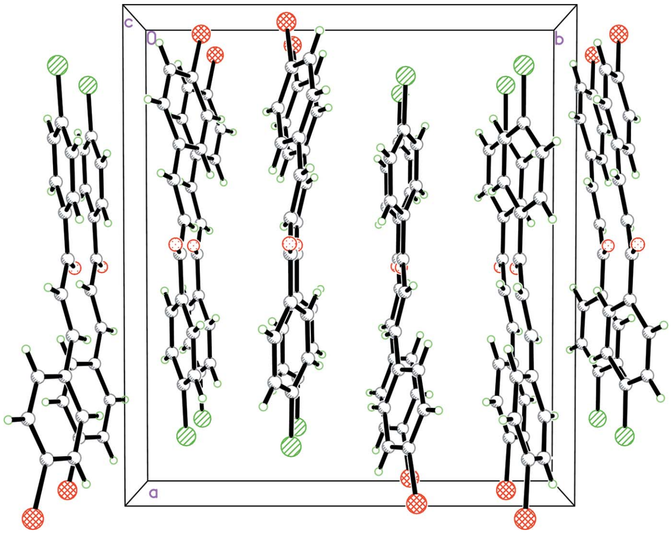

Figure 2
The crystal packing of (I), viewed down the *c* axis.

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).

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