organic papers

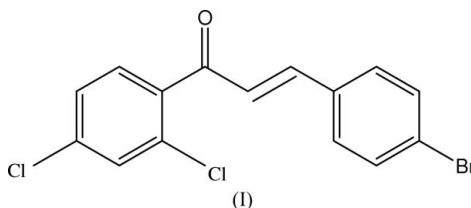# 3-(4-Bromophenyl)-1-(2,4-dichlorophenyl)-prop-2-en-1-one

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Key indicators

In the title compound, $C_{15}H_9BrCl_2$, the dihedral angle between the two benzene rings is 42.39 (4)°. The crystal structure is stabilized by short intermolecular Br···Br contacts.

Comment

Our continuing research on NLO materials (Patil *et al.*, 2006*a*,*b*,*c*; Chantrapromma *et al.*, 2006) has led us to synthesize the title compound, (I). We report here the crystal structure of (I) (Fig. 1). Crystals of (I) do not exhibit second-order non-linear optical properties as this compound crystallizes in a centrosymmetric space group.

Bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Teh *et al.*, 2006*a*,*b*; Patil *et al.*, 2006*a*,*b*,*c*). The least-squares plane through the enone unit (C7–C9/O1) makes dihedral angles of 45.42 (6) and 5.98 (11)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the two benzene rings is 42.39 (4)°. The relatively short distance [3.5923 (2) Å] between the Br1 and Br1^i [symmetry code: (i) $1 - x$, $-y$, $1 - z$] atoms indicates the presence of intermolecular Br···Br interactions, which contribute to the stabilization of the molecular packing (Fig. 2).

Experimental

2,4-Dichloroacetophenone (0.01 mol) in ethanol (30 ml) was mixed with 4-bromobenzaldehyde (0.01 mol) in ethanol (30 ml) and the mixture was treated with an aqueous solution of sodium hydroxide (5 ml, 20%). This mixture was stirred well and left for 24 h. The resulting crude solid mass was collected by filtration and recrystallized from acetone.

Crystal data

$C_{15}H_9BrCl_2O$	$Z = 4$
$M_r = 356.03$	$D_x = 1.781$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 24.9039$ (3) Å	$\mu = 3.49$ mm^{-1}
$b = 3.8474$ (1) Å	$T = 100.0$ (1) K
$c = 13.9069$ (2) Å	Plate, yellow
$\beta = 94.923$ (1)°	$0.21 \times 0.21 \times 0.09$ mm
$V = 1327.58$ (4) Å^3	

Data collection

Brucker SMART APEX2 CCD area-detector diffractometer	42784 measured reflections
ω scans	7604 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	5633 reflections with $I > 2\sigma(I)$
$T_{min} = 0.552$, $T_{max} = 0.738$	$R_{int} = 0.039$
	$\theta_{max} = 38.8°$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2]$
$wR(F^2) = 0.098$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
7604 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
172 parameters	$\Delta\rho_{min} = -0.57$ e Å^{-3}

H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C).

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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Teh, J. B.-J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006a). *Acta Cryst.* E**62**, o2991–o2992.
Teh, J. B.-J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006b). *Acta Cryst.* E**62**, o2399–o2400.
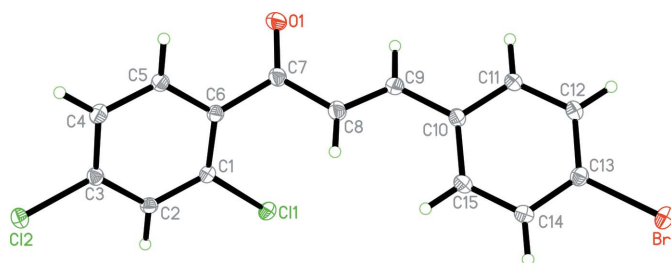
Figure 1
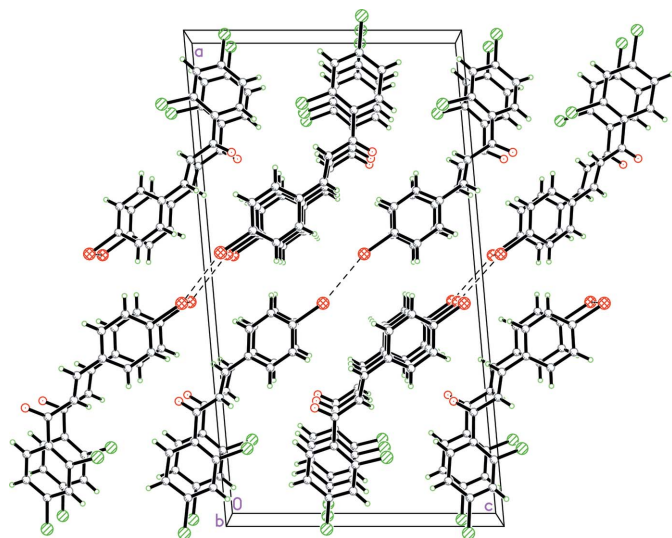The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

Figure 2
The crystal packing of (I), viewed down the *b* axis. Dashed lines indicate Br···Br interactions.