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Key indicators

Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.048
 wR factor = 0.125
Data-to-parameter ratio = 39.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

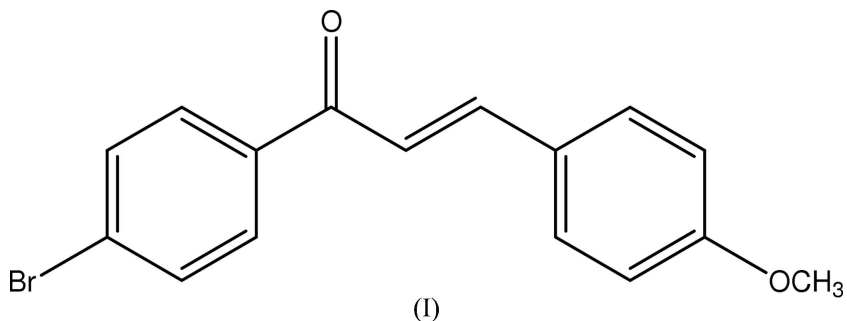
1-(4-Bromophenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one

Each of the two unique molecules of the title compound, $\text{C}_{16}\text{H}_{13}\text{BrO}_2$, is non-planar, the dihedral angle between the two benzene rings being $55.04(7)^\circ$ in one molecule and $51.45(6)^\circ$ in the other. In the crystal structure, the molecules are stabilized by short $\text{Br}\cdots\text{O}$ interactions which link the molecules into chains along the a axis. These chains are stacked down the b axis.

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Comment

The title compound, (I), was prepared as part of our ongoing studies (Patil *et al.*, 2006*a,b*) of non-linear optical (NLO) properties of chalcone derivatives (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Zhang *et al.*, 1990; Zhao *et al.*, 2000). Crystals of (I) do not exhibit second-order non-linear optical properties as they crystallize in a centrosymmetric space group.



The asymmetric unit of (I) contains two molecules, *A* and *B* (Fig. 1). The bond lengths and angles in both molecules are similar, showing normal values (Allen *et al.*, 1987), and are comparable to those in related structures (Patil *et al.*, 2006*a,b*). The dihedral angle between the two benzene rings is $55.04(7)^\circ$ in molecule *A* and $51.45(6)^\circ$ in molecule *B*. The least-squares plane through the enone unit (O1/C7–C9) makes dihedral angles of $24.03(13)$ and $31.22(13)^\circ$ with the planes of the C1–C6 and C10–C15 benzene rings, respectively, in molecule *A* and $25.56(9)$ and $25.90(10)^\circ$, respectively, in molecule *B*. The methoxy group attached at C13 is almost coplanar with the C10–C15 benzene ring, with C16–O2–C13–C12 torsion angles of $-170.33(19)$ and $171.05(19)^\circ$, respectively, for *A* and *B*.

In each independent molecule, an intramolecular C–H \cdots O interaction (Table 1) generates an $S(5)$ ring motif (Bernstein *et al.*, 1995). The short $\text{Br1A}\cdots\text{O2A}^i$ [$3.056(2)$ Å] and $\text{Br1B}\cdots\text{O2B}^i$ [$3.022(2)$ Å] [symmetry code: (i) $1+x, y, z$] contacts form chains of molecules along the a axis. The chains are stacked down the b axis (Fig. 2).

Experimental

4-Bromoacetophenone (0.01 mol) in ethanol (25 ml) was mixed with 4-methoxybenzaldehyde (0.01 mol) in ethanol (25 ml) and the mixture was treated with an aqueous solution of sodium hydroxide (5 ml, 20%). This mixture was stirred well and left to stand for 12 h. The resulting crude solid mass was collected by filtration and recrystallized from acetone.

Crystal data

$C_{16}H_{13}BrO_2$	$Z = 8$
$M_r = 317.17$	$D_x = 1.612 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 15.7797 (3) \text{ \AA}$	$\mu = 3.14 \text{ mm}^{-1}$
$b = 5.8463 (1) \text{ \AA}$	$T = 100.0 (1) \text{ K}$
$c = 32.4291 (6) \text{ \AA}$	Block, yellow
$\beta = 119.088 (1)^\circ$	$0.42 \times 0.28 \times 0.24 \text{ mm}$
$V = 2614.35 (9) \text{ \AA}^3$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	92812 measured reflections
ω scans	13630 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	10641 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.241$, $T_{\max} = 0.522$ (expected range = 0.217–0.471)	$R_{\text{int}} = 0.056$
	$\theta_{\text{max}} = 37.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 4.617P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.125$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.17$	$\Delta\rho_{\text{max}} = 1.13 \text{ e \AA}^{-3}$
13630 reflections	$\Delta\rho_{\text{min}} = -2.11 \text{ e \AA}^{-3}$
345 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C9A-H9A\cdots O1A$	0.95	2.45	2.800 (3)	102
$C9B-H9B\cdots O1B$	0.95	2.48	2.808 (3)	100

H atoms were placed in calculated positions, with C–H distances in the range 0.95–0.98 \AA , and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. The highest peak is located 0.65 \AA from atom C9B and the deepest hole is 1.77 \AA from Br1A.

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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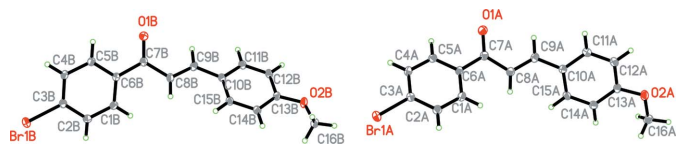


Figure 1

The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

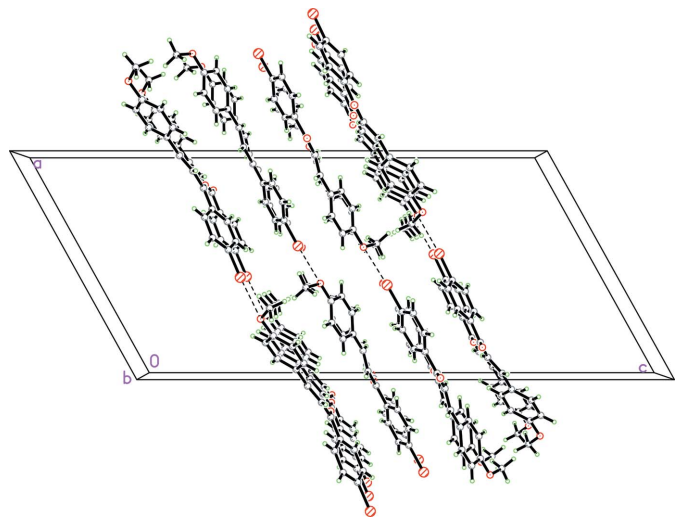


Figure 2

Part of the crystal packing of (I), viewed down the b axis. Dashed lines represent $\text{Br}\cdots\text{O}$ short contacts.

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