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Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.032
wR factor = 0.074
Data-to-parameter ratio = 14.7

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

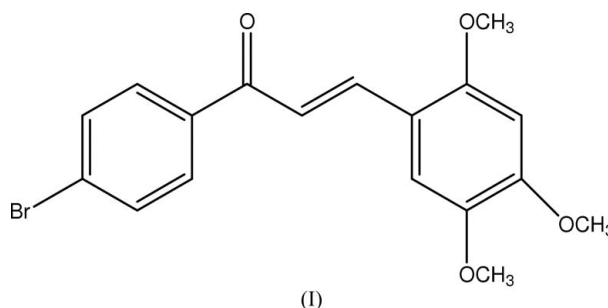
1-(4-Bromophenyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one

In the title compound, $\text{C}_{18}\text{H}_{17}\text{BrO}_4$, the dihedral angle between the benzene rings is $9.60(16)^\circ$. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions and $\text{Br}\cdots\text{O}$ short contacts.

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Comment

Our long-standing interest in optical second harmonic generation (SHG) in organic materials, particularly in chalcone derivatives (Patil *et al.*, 2006*a,b,c*), has led us to synthesize the title compound, (I) (Fig. 1). Crystals of (I) exhibit second-order non-linear optical properties as they crystallize in a non-centrosymmetric space group. A quantitative estimation is yet to be performed. In view of the importance of (I), its synthesis and crystal structure are reported here.



All bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Patil *et al.*, 2006*a,b,c*). The enone unit makes dihedral angles of $4.87(15)$ and $9.77(12)^\circ$, respectively, with the C1–C6 and C10–C15 benzene rings. The dihedral angle between the benzene rings is $9.60(16)^\circ$. The three methoxy groups attached at C11, C13 and C14 are almost coplanar with the C10–C15 benzene ring, with C16–O2–C11–C12, C17–O3–C13–C12 and C18–O4–C14–C15 torsion angles of $-13.7(5)$, $6.4(5)$ and $-5.7(5)^\circ$, respectively.

Intramolecular $\text{C9}-\text{H9A}\cdots\text{O1}$ and $\text{C9}-\text{H9A}\cdots\text{O2}$ interactions are observed (Table 1); both interactions generate an $S(5)$ ring motif (Bernstein *et al.*, 1995). The crystal structure is stabilized by intermolecular $\text{C12}-\text{H12A}\cdots\text{O1}^i$ and $\text{C16}-\text{H16B}\cdots\text{O1}^i$ interactions (symmetry code as given in Table 1) and these interactions generate a ring of graph-set motif $R_2^1(7)$. The short $\text{Br1}\cdots\text{O4}(-\frac{3}{2}+x, \frac{3}{2}-y, 1-z)$ contact [$3.264(2) \text{ \AA}$] also contributes to the stabilization of the crystal structure.

Experimental

4-Bromoacetophenone (0.01 mol) in ethanol (30 ml) was mixed with 2,4,5-trimethoxybenzaldehyde (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 12 h, after which time the solid product was collected by filtration and dried. Crystals of (I) were recrystallized from an acetone solution.

Crystal data

$C_{18}H_{17}BrO_4$	$Z = 4$
$M_r = 377.23$	$D_x = 1.555 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.3031 (3) \text{ \AA}$	$\mu = 2.57 \text{ mm}^{-1}$
$b = 10.3422 (4) \text{ \AA}$	$T = 100.0 (1) \text{ K}$
$c = 21.3355 (9) \text{ \AA}$	Block, yellow
$V = 1611.47 (11) \text{ \AA}^3$	$0.27 \times 0.15 \times 0.11 \text{ mm}$

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	31612 measured reflections
ω scans	3101 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2005)	2434 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.577$, $T_{\max} = 0.754$	$R_{\text{int}} = 0.089$
	$\theta_{\text{max}} = 25.9^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.5972P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.074$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$
3101 reflections	$\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$
211 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1295 Friedel pairs
	Flack parameter: 0.006 (13)

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C9-H9A\cdots O1$	0.93	2.45	2.799 (5)	102
$C9-H9A\cdots O2$	0.93	2.36	2.720 (5)	103
$C12-H12A\cdots O1^i$	0.93	2.57	3.470 (4)	164
$C16-H16B\cdots O1^i$	0.96	2.57	3.303 (5)	133

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

H atoms were placed in calculated positions ($C-H = 0.93-0.96 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

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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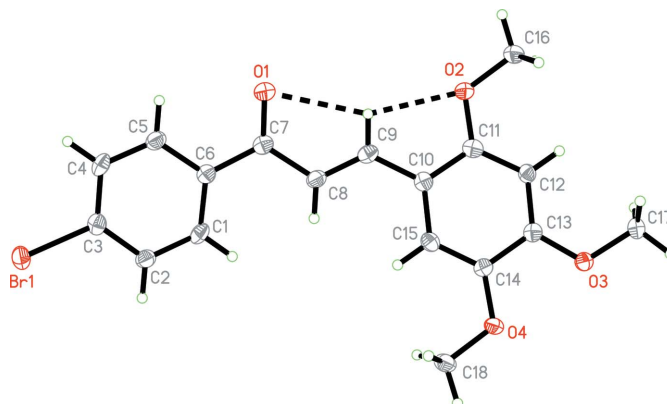


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Dashed lines indicate intra-molecular $C-H\cdots O$ hydrogen bonds.

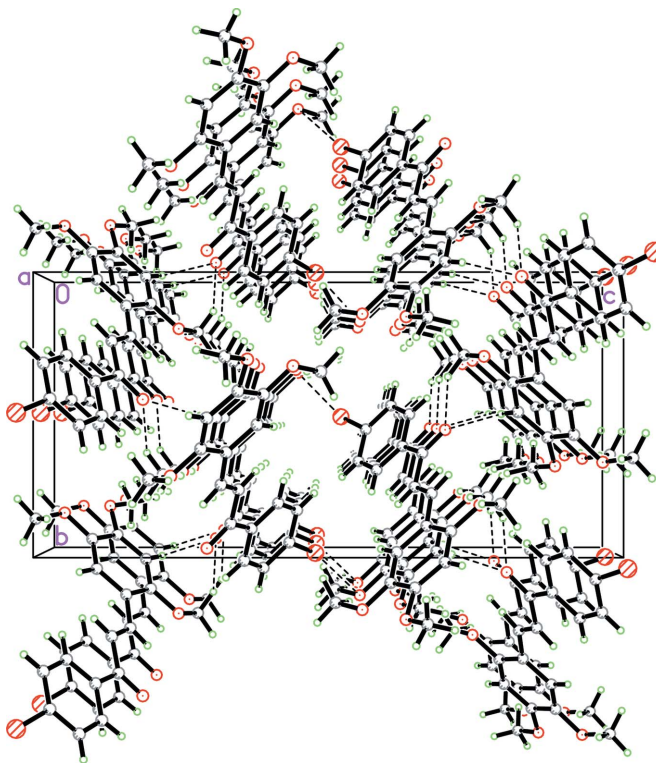


Figure 2

The crystal packing of (I), viewed down the a axis. Dashed lines indicate $C-H\cdots O$ hydrogen bonds and $Br\cdots O$ short contacts.

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