

2,3-Dibromo-3-(4-methoxyphenyl)-1-phenylpropan-1-one

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Key indicators

Single-crystal X-ray study
 $T = 293$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.048
 wR factor = 0.137
 Data-to-parameter ratio = 20.4

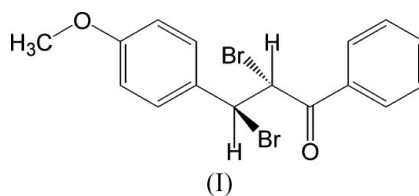
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $\text{C}_{16}\text{H}_{14}\text{Br}_2\text{O}_2$, the C—Br bond lengths are dsignificantly different. One of the Br atoms participates in weak hydrogen-bonding interactions with C—H groups from adjoining molecules.

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Comment

The non-linear optical (NLO) effect in organic molecules originates from a strong donor–acceptor intermolecular interaction, a delocalized π -electron system, helicity due to a twisted backbone (Butcher, Yathirajan, Sarojini, Narayana & Vijaya Raj, 2006), and also the ability to crystallize as a non-centrosymmetric structure. Among several organic compounds reported for their NLO properties, chalcone derivatives are notable for their excellent blue light transmittance and good crystallizability. It has been observed that the substitution of a bromo substituent on either of the phenyl rings greatly influences the non-centrosymmetric crystal packing (Indira *et al.*, 2002). Bromo substituents can obviously improve the molecular first-order hyperpolarizabilities and can effectively reduce dipole–dipole interactions between the molecules (Zhao *et al.*, 2000; Butcher, Yathirajan, Mithun *et al.*, 2006; Butcher, Yathirajan, Anilkumar *et al.*, 2006; Butcher, Yathirajan, Sarojini, Narayana & Mithun, 2006).



A dibromo chalcone derivative, 2,3-dibromo-1-phenyl-3-(4-methoxyphenyl)propan-1-one, (I), was prepared by the bromination of 3-(4-methoxyphenyl)-1-phenyl-2-propen-1-one (chalcone). The molecule of (I) contains two atoms, C8 and C9, which are potentially chiral. However, this compound has crystallized in the space group $P\bar{1}$ with inversion symmetry and does not show any second-harmonic generation (SHG). A similar result was obtained for a related dibromo derivative of a chalcone (Butcher, Yathirajan, Anilkumar *et al.*, 2006), whereas a monobromo derivative did crystallize in a non-centrosymmetric space group (Butcher, Yathirajan, Sarojini, Narayana & Mithun, 2006). Nonetheless, even though the title compound does not possess SHG, it can be exploited for other applications such as optical fiber communications (Aggarwal *et al.*, 2001) as good quality bulk crystals of this compound can be grown. In view of the importance of the title compound, its crystal structure is reported here.

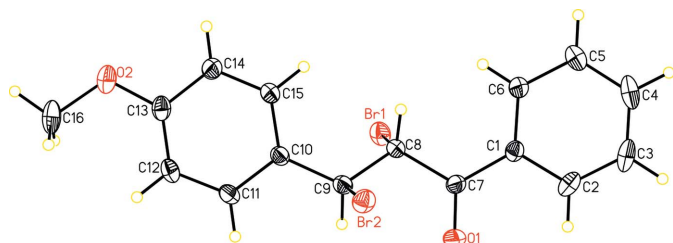


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

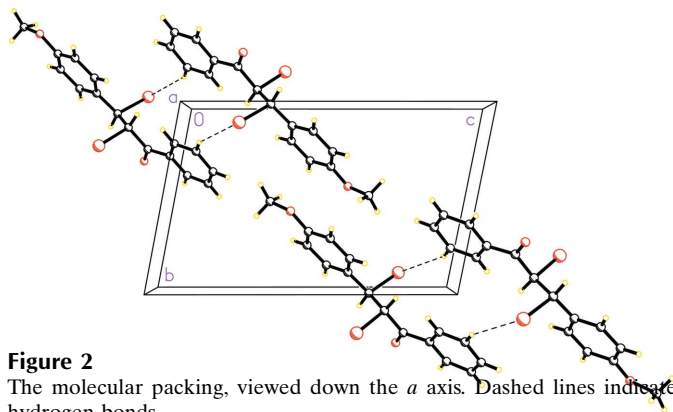


Figure 2
The molecular packing, viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

While, in general, the metrical parameters observed in both dibromo derivatives are very similar (Butcher, Yathirajan, Anilkumar *et al.*, 2006), in (I) the two C—Br bond lengths are significantly different (Table 1). There is weak hydrogen bonding between Br2 and neighboring H atoms of adjoining molecules (Table 2).

Experimental

For the preparation of the title compound, (I), 3-(4-methoxyphenyl)-1-phenyl-2-propen-1-one (chalcone) (23.8 g, 0.1 mol) was treated with bromine in acetic acid (30%) until the orange colour of the solution persisted. After stirring for 30 min, the contents were poured on to crushed ice (200 g). The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol (yield: 85%, m.p. 393 K).

Crystal data

$C_{16}H_{14}Br_2O_2$	$V = 769.8 (4) \text{ \AA}^3$
$M_r = 398.09$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.717 \text{ Mg m}^{-3}$
$a = 5.9055 (19) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.133 (3) \text{ \AA}$	$\mu = 5.26 \text{ mm}^{-1}$
$c = 14.584 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 101.028 (4)^\circ$	Block, colorless
$\beta = 90.411 (4)^\circ$	$0.33 \times 0.26 \times 0.16 \text{ mm}$
$\gamma = 94.264 (5)^\circ$	

Data collection

Bruker APEX-II CCD area-detector diffractometer	7685 measured reflections
φ and ω scans	3711 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2452 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.227$, $T_{\max} = 0.451$	$R_{\text{int}} = 0.031$
	$\theta_{\text{max}} = 28.2^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.137$
 $S = 1.01$
 3711 reflections
 182 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0804P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.12 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.00 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Br1—C8	1.973 (4)	C7—C8	1.534 (5)
Br2—C9	2.012 (4)	C8—C9	1.505 (6)
O1—C7	1.210 (5)	C9—C10	1.507 (5)
C1—C7	1.473 (6)		
O1—C7—C1	121.5 (4)	C7—C8—Br1	104.5 (3)
O1—C7—C8	119.2 (4)	C8—C9—C10	117.4 (3)
C1—C7—C8	119.3 (3)	C8—C9—Br2	104.7 (3)
C9—C8—C7	112.8 (3)	C10—C9—Br2	108.7 (3)
C9—C8—Br1	108.8 (3)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5A \cdots Br2 ⁱ	0.93	3.03	3.867 (5)	151
C6—H6A \cdots Br2 ⁱⁱ	0.93	3.02	3.911 (5)	160

Symmetry codes: (i) $-x, -y + 2, -z$; (ii) $x - 1, y, z$.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H = 0.98 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.95–1.00 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest peak is located 0.86 \AA from atom Br1 and the deepest hole 0.75 \AA also from atom Br1.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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