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2-Bromo-1-(4-methylphenyl)-3-[4-(methyl-sulfanyl)phenyl]prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 366 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.054
Data-to-parameter ratio = 22.0

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

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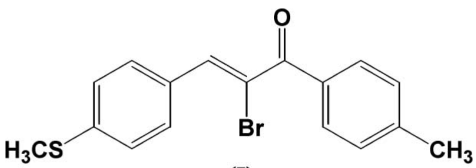
The title compound, $C_{17}H_{15}BrOS$, crystallizes in a non-centrosymmetric space group and shows significant nonlinear optical activity.

Comment

The present-day demand is for large and high quality ferroelectric, piezoelectric single crystals with minimum defects and inhomogenities. The important goal of crystal growth is the improvement of microscopic and macroscopic homogeneity, which is a necessity for any application. Different types of crystals being used are semiconductor crystals, oxide crystals, alkali halide crystals, and nonlinear optical (NLO) crystals. The NLO effect in organic molecules originates from a strong donor–acceptor intermolecular interaction, a delocalized π-electron system, and also the ability to crystallize in non-centrosymmetric space groups. Among several organic compounds reported for NLO properties, chalcone derivatives are notable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show an NLO property with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002). Substitution on either of the phenyl rings greatly influences the non-centrosymmetric crystal packing (Butcher *et al.*, 2006). It is speculated that, in order to improve activity, more bulky substituents should be introduced to increase the spontaneous polarization of a non-centrosymmetric crystal (Fichou *et al.*, 1988). The molecular hyperpolarizability, β, is strongly influenced not only by the electronic effect, but also by the steric effect of the substituent (Cho *et al.*, 1996). Bromo substituents can obviously improve the molecular first-order hyperpolarizabilities and can effectively reduce the dipole–dipole interactions between the molecules (Zhao *et al.*, 2002). α-Bromochalcones are used to synthesize triazolothiadiazines which are found to be anticancer agents (Holla *et al.*, 2001). Prompted by this, and in a continuation of our quest to synthesize newer materials which can find use in the photonics industry (Butcher *et al.*, 2006), we have synthesized a new α-bromochalcone and have found it to possess SHG efficiency. Its quantitative estimation is yet to be done. In view of the importance of the title compound, (I), the crystal structure is reported here.

The metrical parameters of (I) are similar to those observed in other chalcone derivatives (Butcher *et al.*, 2006). The title compound crystallizes in the polar space group $P2_1$ but contains no chiral centers. The source of the chirality of this compound lies in the fact that the two dissimilar rings are not coplanar. The two rings are significantly twisted with respect to each other [dihedral angle between ring planes is

68.15 (6)°]. There are also two weak intermolecular C—H⋯O hydrogen bonds (Table 2) which contribute to the packing.



(I)

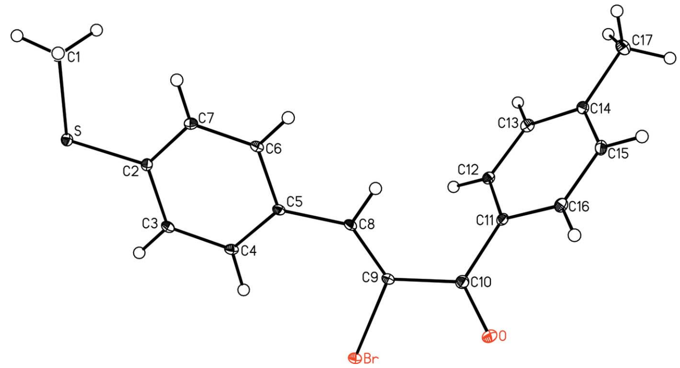


Figure 1
View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

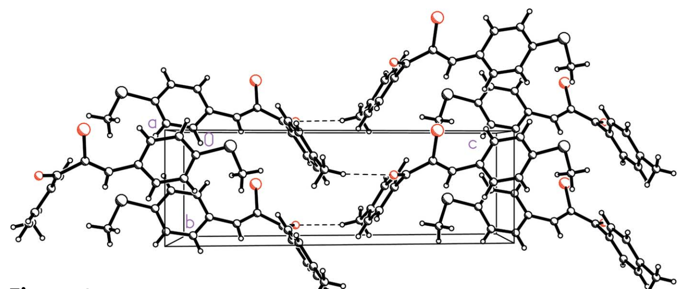


Figure 2
The molecular packing, viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

Experimental

A mixture of 2,3-dibromo-1-(4-methylphenyl)-3-[4-(methylsulfanyl)phenyl]propan-1-one (0.42 g, 0.001 mol) and triethylamine (0.5 g, 0.005 mol) in dry benzene (50 ml) was stirred for 24 h. The precipitated triethylamine hydrochloride was removed by filtration. The filtrate was concentrated under reduced pressure and allowed to cool. The precipitated solid was filtered, dried and recrystallized from an acetone-toluene mixture (9:1) (yield: 85%, m.p. 406 K). Calculated for $C_{17}H_{15}BrOS$; C 58.93, H 4.35%; found C, 58.90, H, 4.35%.

Crystal data

$C_{17}H_{15}BrOS$
M_r = 347.26
Monoclinic, $P2_1$
a = 7.9708 (9) Å
b = 5.5031 (6) Å
c = 16.9923 (18) Å
β = 98.291 (2)°
V = 737.56 (14) Å^3
Z = 2
D_x = 1.564 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6302 reflections
θ = 2.4–30.5°
μ = 2.92 mm^{-1}
T = 366 (2) K
Chunk, colorless
0.65 × 0.30 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.230, T_{max} = 0.482
8184 measured reflections
4028 independent reflections
3821 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 30.8°
$h = -9 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.055
S = 0.95
4028 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 1516 Friedel pairs
Flack parameter: 0.029 (6)

Table 1
Selected geometric parameters (Å, °).

Br—C9	1.889 (2)	C5—C8	1.463 (2)
S—C2	1.7613 (18)	C8—C9	1.344 (2)
S—C1	1.803 (2)	C9—C10	1.502 (3)
O—C10	1.220 (2)	C10—C11	1.489 (3)
C2—S—C1	102.45 (9)	O—C10—C11	121.15 (17)
C8—C9—Br	124.68 (15)	O—C10—C9	120.26 (19)
C10—C9—Br	113.62 (13)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C13—H13A⋯O^{i}	0.93	2.51	3.392 (2)	159
C17—H17B⋯O^{ii}	0.96	2.51	3.420 (3)	158

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

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 distances of 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C or C—S bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and with U_{iso}(H) = 1.2U_{eq}(C). The highest electron-density peak is located 0.81 Å from the Br atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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