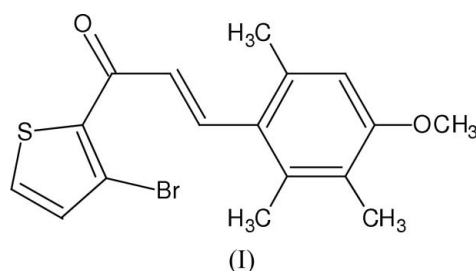


(2E)-1-(3-Bromo-2-thienyl)-3-(4-methoxy-2,3,6-trimethylphenyl)prop-2-en-1-one**H. S. Yathirajan,^a B. Narayana,^b
B. V. Ashalatha,^b B. K. Sarojini^c
and Michael Bolte^{d*}**^aDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^bDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, GermanyCorrespondence e-mail:
bolte@chemie.uni-frankfurt.de**Key indicators**Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C})$ = 0.005 Å
R factor = 0.054
wR factor = 0.141
Data-to-parameter ratio = 18.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title molecule, $\text{C}_{17}\text{H}_{17}\text{BrO}_2\text{S}$, the central $\text{C}=\text{C}$ double bond is *trans* configured and geometric parameters are in the normal ranges.

Comment

Chalcones and the corresponding heterocyclic analogues are valuable intermediates in organic synthesis (Dhar, 1981) and show numerous biological effects (Opletalova & Sedivy, 1999; Dimmock *et al.*, 1999). In addition, with appropriate substituents, chalcones are a class of non-linear optical (NLO) materials (Fichou *et al.*, 1988; Butcher *et al.*, 2006; Harrison, Yathirajan, Sarojini *et al.*, 2006). Among several organic compounds reported to have NLO properties, chalcone derivatives are important materials because of their excellent blue-light transmittance and good crystallization ability. They provide a configuration necessary to show NLO properties, 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). Thiophene analogues of antiviral chalcones have been studied (Binder *et al.*, 1985) and the crystal structures of 3-hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one (Baxter *et al.*, 1990) and 1-(4-chlorophenyl)-3-(2-thienyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. We have recently reported the crystal structures of (2E)-1-(3-bromo-2-thienyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one (Yathirajan *et al.*, 2006) and (2E)-1-(3-bromo-2-thienyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one (Yathirajan *et al.*, 2006a). The crystal structure of (2E)-1-(3-bromo-2-thienyl)-3-(4-methoxyphenyl)prop-2-en-1-one has been reported by Harrison, Yathirajan, Ashalatha *et al.* (2006). In continuation of our work on the crystal structures of chalcones (Yathirajan *et al.*, 2006b,c), the present paper reports the crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). The central double bond is *trans* configured. The carbonyl group is almost coplanar with the thienyl ring, but

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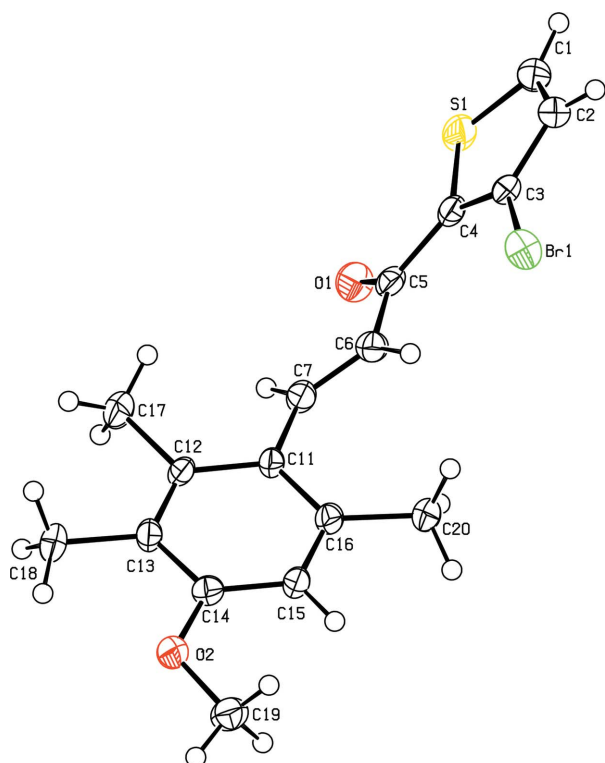


Figure 1

The molecular structure of (I), with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

the mean plane composed of the double bond and atoms attached to it is slightly twisted out of the thienyl ring plane (Table 1). The angle between the ring planes is 51.11 (11)°.

Experimental

2-Acetyl-3-bromothiophene (10 g, 0.048 mol) in methanol (50 ml) was mixed with 4-methoxy-2,3,6-trimethylbenzaldehyde (8.6 g, 0.048 mol) and the mixture was treated with 30% potassium hydroxide solution (10 ml) at 278 K. The reaction mixture was then brought to room temperature and stirred for 4 h. The solid which precipitated was filtered off and washed with water, dried and recrystallized from acetone (yield 81%; m.p. 402–404 K). Analysis for $C_{17}H_{17}BrO_2S$, found (calculated): C:55.82 (55.90%), H: 4.58 (4.69%).

Crystal data

$C_{17}H_{17}BrO_2S$	$Z = 4$
$M_r = 365.28$	$D_x = 1.540 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.1973 (7) \text{ \AA}$	$\mu = 2.74 \text{ mm}^{-1}$
$b = 12.3023 (11) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 16.0999 (13) \text{ \AA}$	Block, yellow
$\beta = 103.953 (6)^\circ$	$0.29 \times 0.26 \times 0.22 \text{ mm}$
$V = 1575.7 (2) \text{ \AA}^3$	

Data collection

Stoe IPDS II two-circle diffractometer	11689 measured reflections
ω scans	3630 independent reflections
Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)]	3007 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.474$, $T_{\max} = 0.548$	$R_{\text{int}} = 0.093$
	$\theta_{\text{max}} = 27.6^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 1.4331P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.80 \text{ e \AA}^{-3}$
3630 reflections	$\Delta\rho_{\text{min}} = -1.24 \text{ e \AA}^{-3}$
195 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.0095 (16)

Table 1

Selected torsion angles (°).

S1—C4—C5—O1	−3.7 (4)	C4—C5—C6—C7	−161.8 (3)
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H atoms were found in a difference map but they were refined using a riding model, with C—H = 0.95 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, or C—H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl groups were allowed to rotate but not to tip. The deepest hole is located 0.80 Å from atom Br1.

Data collection: X-Area (Stoe & Cie, 2001); cell refinement: X-Area; data reduction: X-Area; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PLATON.

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