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

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.126
Data-to-parameter ratio = 22.7

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

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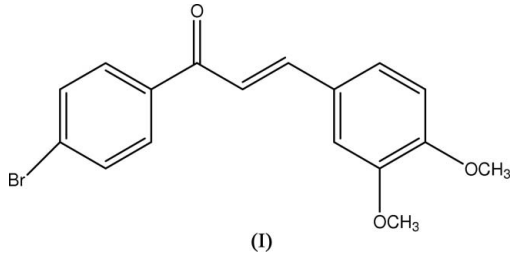
Each of the two unique molecules of the title compound, $C_{17}H_{15}BrO_3$ is essentially planar. The crystal structure is stabilized by intramolecular and intermolecular C—H···O hydrogen bonds. These interactions link the symmetry-related molecules into infinite chains along the *c* axis. These chains are then stacked parallel to the *b* axis.

Comment

Chalcone is an important chemical compound and is studied extensively because of its significant applications in various fields. In biology and biochemistry, chalcone is claimed as one of the compounds that plays a vital role in anti-inflammatory, antimalarial, antifertility and antitumor activities (De Vincenzo *et al.*, 1995; Kumar *et al.*, 2003). Furthermore, chalcone derivatives have attracted much interest as they exhibit extremely high and fast nonlinearity (Fichou *et al.*, 1988; Patil, Teh *et al.*, 2006; Uchida *et al.*, 1998; Zhang *et al.*, 1990). Crystals of the title compound, (I), do not exhibit second-order nonlinear optical properties as they crystallize in a centrosymmetric space group. In view of the interest in the behavior of chalcone and its derivatives, a systematic study of their synthesis and single-crystal structure determinations has been carried out (Ng, Patil *et al.*, 2006; Ng, Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2006; Patil, Teh *et al.*, 2006; Radha Krishna *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi & Fun, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Teh *et al.*, 2006; Uchida *et al.*, 1995). We report here the synthesis and crystal stucture of (I) (Fig. 1).



(I)

The asymmetric unit of (I) contains two molecules, *A* and *B*. The bond lengths and angles in both molecules are similar, show normal values (Allen *et al.*, 1987) and are comparable to the corresponding values in related structures (Jeyabharathi *et al.*, 2002; Ng, Patil *et al.*, 2006; Ng, Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2006; Patil, Teh *et al.*, 2006; Ravishankar *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi & Fun, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005;

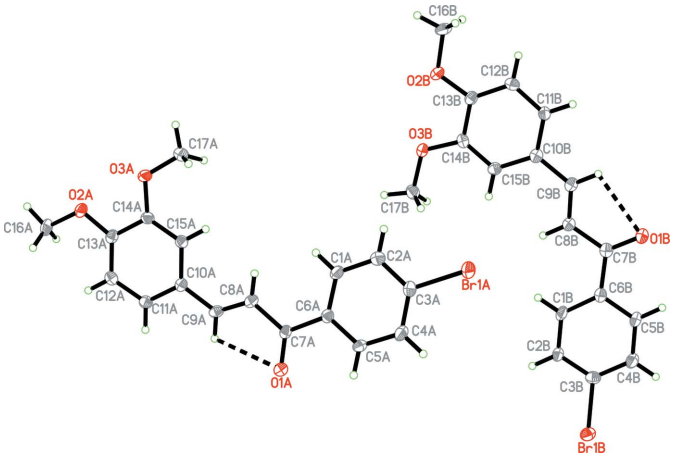


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atom numbering. The dashed lines indicate intramolecular hydrogen bonds.

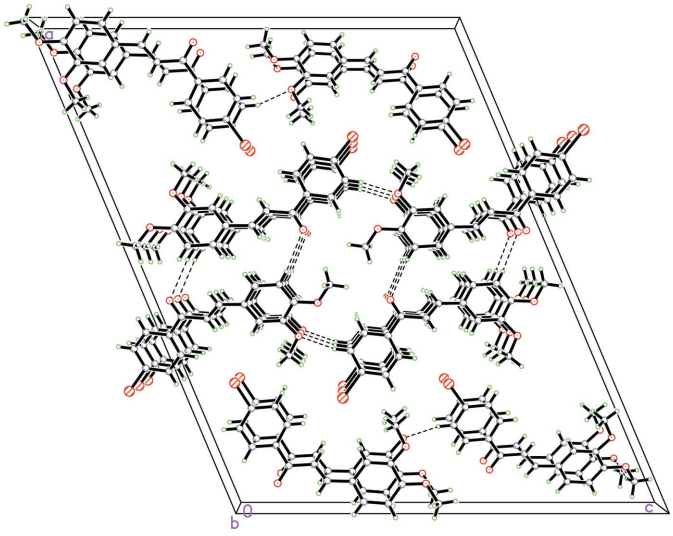


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Teh *et al.*, 2006). Each chalcone molecule is essentially planar with dihedral angles between the two benzene rings of 9.30 (15)° in molecule *A* and 4.85 (16)° in molecule *B*. In both molecules, the methoxy groups are coplanar with the attached ring. The torsion angles C16—O2—C13—C12 and C17—O3—C14—C15 are −3.9 (5)°, 2.0 (5)° in *A* and −4.1 (5)°, −0.1 (5)° in *B*, respectively.

In the crystal structure, all O atoms are involved in intramolecular and intermolecular C—H···O interactions (Table 1). The molecules are linked by intermolecular C12—H12···O1 interactions into cyclic centrosymmetric $R_2^2(16)$ dimers (Bernstein *et al.*, 1995). These dimers are interlinked by C4—H4···O3 intermolecular interactions forming infinite chains along the *c* axis. These chains are then stacked parallel to the *b* axis and molecules within the stacks are interlinked by intermolecular C16—H16···O2 interactions.

Experimental

Compound (I) was obtained by the condensation of 3,4-dimethoxybenzaldehyde (0.01 mol) with 4-bromoacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (5 ml, 20%). After stirring for 4 h, the contents of the flask were poured into ice-cold water (250 ml), and the resulting crude solid was collected by filtration. The compound was dried and purified by repeated recrystallization from acetone. Purity of the compound was checked by thin layer chromatography. Crystals of (I) suitable for a single-crystal X-ray diffraction study were grown by slow evaporation of an acetone solution.

Crystal data

$C_{17}H_{15}BrO_3$
M_r = 347.20
Monoclinic, $P2_1/c$
a = 31.3937 (5) Å
b = 4.0139 (1) Å
c = 25.2400 (4) Å
β = 112.885 (1)°
V = 2930.17 (10) Å^3
Z = 8
D_x = 1.574 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8323 reflections
θ = 0.7–30.2°
μ = 2.81 mm^{-1}
T = 100.0 (1) K
Block, colorless
0.34 × 0.22 × 0.17 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.513, T_{max} = 0.640
82050 measured reflections
8691 independent reflections
6361 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 30.2°
$h = -44 \rightarrow 43$
$k = -5 \rightarrow 5$
$l = -35 \rightarrow 35$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.126
S = 1.15
8691 reflections
383 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 4.4325P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9*A*—H9*AA*···O1*A*	0.93	2.51	2.835 (4)	100
C4*A*—H4*AA*···O3*A*^{i}	0.93	2.34	3.180 (4)	151
C12*A*—H12*A*···O1*A*^{ii}	0.93	2.58	3.478 (4)	162
C16*A*—H16*C*···O2*A*^{iii}	0.96	2.59	3.501 (4)	158
C9*B*—H9*BA*···O1*B*	0.93	2.51	2.832 (4)	100
C4*B*—H4*BA*···O3*B*^{i}	0.93	2.44	3.260 (4)	148
C12*B*—H12*B*···O1*B*^{iv}	0.93	2.58	3.467 (4)	159
C16*B*—H16*E*···O2*B*^{v}	0.96	2.57	3.475 (4)	157

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, y-1, z$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x, y+1, z$.

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. The highest peak is located 0.72 Å from atom Br1*A*.

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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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version V7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
De Vincenzo, R., Scambia, G., Benedetti, P. P., Ranelletti, F. O., Bonanno, G., Ercoli, A., Delle, M. F., Ferrari, F., Piantelli, M. & Mancuso, S. (1995). *Anticancer Drug Des.* **10**, 481–490.
Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn J. Appl. Phys.* **27**, L429–L430.
Jeyabharathi, A., Ponnuswamy, M. N., Nanjundan, S., Fun, H.-K., Chantrapromma, S., Usman, A. & Razak, I. A. (2002). *Acta Cryst.* C**58**, o26–o28.
Kumar, S. K., Hager, E., Pettit, C., Gurulingappa, H., Davidson, N. E. & Khan, S. R. (2003). *J. Med. Chem.* **46**, 2813–2815.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Ng, S.-L., Patil, P. S., Razak, I. A., Fun, H.-K. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o1228–o1230.
Ng, S.-L., Shettigar, V., Razak, I. A., Fun, H.-K., Patil, P. S. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o1421–o1423.
Patil, P. S., Ng, S.-L., Razak, I. A., Fun, H.-K. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o1463–o1465.
Patil, P. S., Teh, J. B.-J., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o896–o898.
Radha Krishna, J., Kumar, N. J., Krishnaiah, M., Rao, C. V., Rao, Y. K. & Puranic, V. G. (2005). *Acta Cryst.* E**61**, o1323–o1325.
Ravishankar, T., Chinnakali, K., Nanjundan, S., Selvam, P., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o405–o407.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Radhika, R., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o480–o482.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Santhi, R. & Fun, H.-K. (2005). *Acta Cryst.* E**61**, o3514–o3516.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Selvam, P., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o743–o745.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Unnithan, C. S., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o483–o485.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Teh, J. B.-J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o890–o892.
Uchida, T., Kozawa, K., Kimura, Y. & Goto, Y. (1995). *Synth. Met.* **71**, 1705–1706.
Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abdureyim, A. & Watanebe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **314**, 135–140.
Zhang, G., Kinoshita, T., Sasaki, K., Goto, Y. & Nakayam, M. (1990). *J. Cryst. Growth*, **100**, 411–416.