Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(3-Bromophenyl)-1-(4-bromophenyl)-prop-2-en-1-one

Jeannie Bee-Jan Teh,[a] P. S. Patil,[b] Hoong-Kun Fun,[a]* Ibrahim Abdul Razak[a] and S. M. Dharmaprakash[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.006 Å
R factor = 0.047
wR factor = 0.109
Data-to-parameter ratio = 18.2

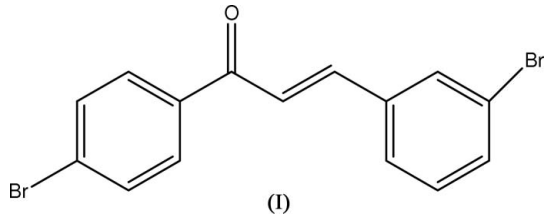
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 May 2006
Accepted 15 May 2006

In the title compound, $C_{15}H_{10}Br_2O$, the dihedral angle between the benzene rings is 48.0 (1)°. The crystal structure is stabilized by weak intermolecular Br···Br contacts and C—H···π interactions.

Comment

Chalcone derivatives are receiving increasing interest in the field of non-linear optics due to their excellent blue light transmittance, good crystal stability, large non-linear optical coefficients and relatively short cut-off wavelengths of transmittance (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000). Here, we present the title compound, (I), crystals of which, however, do not exhibit second-order non-linear optical properties as they crystallize in a centrosymmetric space group.



(I)

Bond lengths and angles in (I) display normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Teh *et al.*, 2006; Patil *et al.*, 2006*a*,*b*; Ng *et al.*, 2006; Rosli *et al.*, 2006). The least-squares plane through the enone fragment makes dihedral angles of 26.6 (2) and 22.7 (2)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the benzene rings is 48.0 (1)°.

The relatively short distances between neighbouring Br atoms [Br1···Br2^{i} 3.7748 (7) Å, Br2···Br1^{ii} 3.7747 (7) Å, Br2···Br2^{iii} 3.7776 (6) Å and Br2···Br2^{iv} 3.7776 (6) Å; symmetry codes: (i) $2-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (ii) $2-x, \frac{1}{2}+y, \frac{3}{2}-z$; (iii) $x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$] indicate the presence of weak intermolecular Br···Br interactions, which contribute to the stabilization of the crystal packing (Fig. 2), along with the C—H···π interations (Table 1).

Experimental

Chalcone derivative (I) was obtained by the condensation of 3-bromobenzaldehyde (0.01 mol) with 4-bromoacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (2 ml, 30%). After stirring for 2 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand for 24 h. The resulting crude solid was collected by filtration, dried and purified by repeated

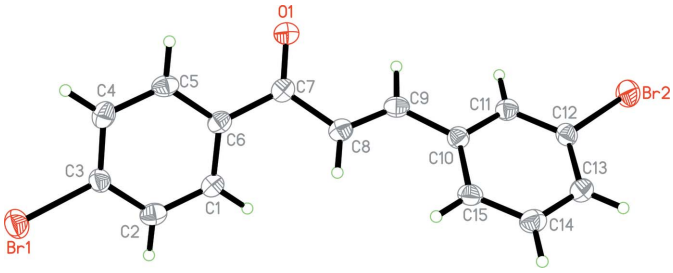


Figure 1
View of (I), with the atomic numbering and 50% probability displacement ellipsoids.

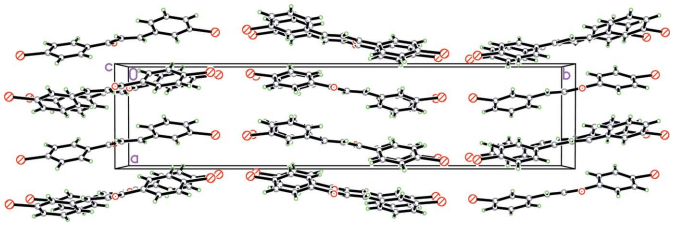


Figure 2
The crystal packing, viewed down the *c* axis.

recrystallization from acetone. The purity of the compound was checked by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction experiments were grown in 7 d by the slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{15}H_{10}Br_2O$
M_r = 366.05
Monoclinic, $P2_1/c$
a = 7.1411 (2) Å
b = 31.4292 (8) Å
c = 5.7876 (2) Å
β = 91.275 (2)°
V = 1298.64 (7) Å^3
Z = 4
D_x = 1.872 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.23 mm^{-1}
T = 100.0 (1) K
Block, yellow
0.40 × 0.20 × 0.12 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.126, T_{max} = 0.530
(expected range = 0.113–0.474)
14661 measured reflections
2962 independent reflections
2448 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.109
S = 1.20
2962 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 4.6217P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···$Cg2^{i}$	0.93	2.75	3.428 (5)	131
C5—H5A···$Cg2^{ii}$	0.93	2.69	3.342 (5)	127
C14—H14A···$Cg1^{iii}$	0.93	2.69	3.373 (5)	131

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1, -y, -z+2$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C10–C15 rings, respectively.

H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The highest peak is located 0.96 Å from atom Br2.

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).

The authors thank the Malaysian Government and Universiti Sains Malaysia for Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118 and USM short-term grant No. 304/PFIZIK/635028. PSP and SMD are grateful to DRDO, Government of India, for financial assistance.

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