Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3-Bis(4-bromophenyl)prop-2-en-1-one

Shea-Lin Ng,[a] Venkataraya Shettigar,[b] Ibrahim Abdul Razak,[a] Hoong-Kun Fun,[a]* P. S. Patil[b] 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) = 0.004 Å
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 28.3

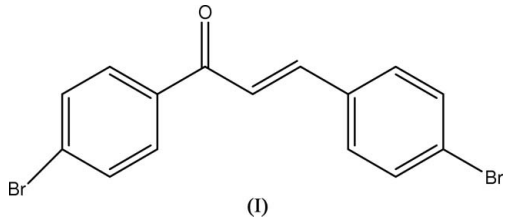
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 March 2006
Accepted 9 March 2006

The enone group and the benzene rings of the title compound, $C_{15}H_{10}Br_2O$, are each planar. The crystal packing is stabillized by weak intermolecular C—H···π interactions involving both aromatic rings; the molecules are stacked along the *b* axis.

Comment

Chalcones present interesting biological properties, such as cytotoxicity (Lawrence *et al.*, 2001), antiherpes activity (Phrutivorapongkul *et al.*, 2003) and antitumour activity (Xia *et al.*, 2000) and may be useful for the chemotherapy of Leishmaniasis (Pandey *et al.*, 2005), among others. In addition, with appropriate subsitutuents, chalcones are a class of non-linear optical (NLO) materials (Fichou *et al.*, 1988; Goto *et al.*, 1991; Patil *et al.*, 2006; Zhao *et al.*, 2000). We present here an X-ray crystallographic structure determination of the title compound, (I). These crystals do not exhibit second-order NLO properties as they crystallized in a centrosymmetric space group.



(I)

The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable to those of related structures (Jeyabharathi *et al.*, 2002; Ng *et al.*, 2006*a,b*; Patil *et al.*, 2006; Ravishankar *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi & Fun, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Teh *et al.*, 2006). The difference in the C1—C6—C7 [122.7 (3)°] and C6—C7—C8 [118.4 (2)°] angles is due to the short H1*A*···H8*A* (2.29 Å) contact. The short H8*A*···H15*A* (2.26 Å) contact causes a slight widening of the bond angle C9—C10—C15 to 122.6 (3)°.

The enone group (O1/C7–C9) and the two benzene rings (C1–C6 and C10–C15) of the chalcone are each planar, with largest deviations of 0.0677 (3), −0.010 (3), 0.010 (3) and 0.009 (2) Å for atoms C7, C2, C3 and C15, respectively.

The molecule is slightly twisted about the C6—C7 bond in (I), with a dihedral angle of 45.55 (9)° between the two benzene rings. The mean plane through the enone group makes dihedral angles of 24.16 (1) and 21.40 (1)°, respectively, with the C1–C6 and C10–C15 benzene rings. In the molecule, an intramolecular C—H···O interaction generates an *S*(5) ring motif (Bernstein *et al.*, 1995).

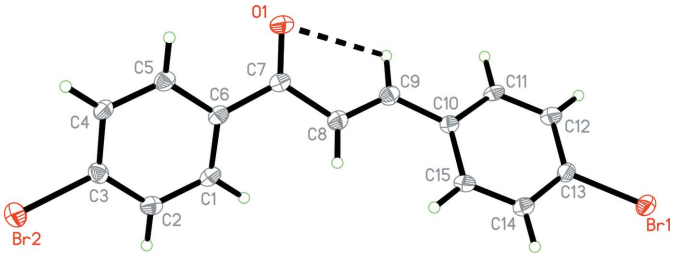


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates an intramolecular hydrogen bond.

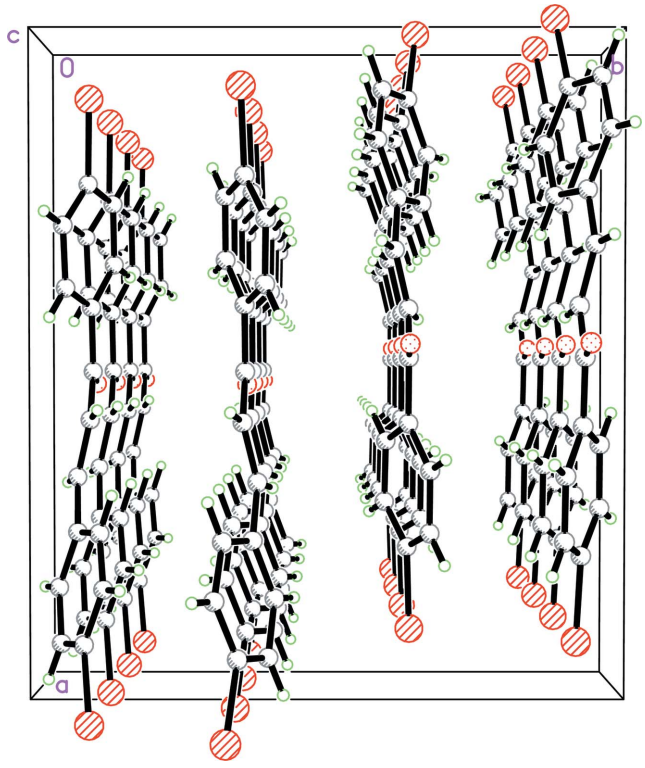


Figure 2
The crystal packing of (I), viewed down the *c* axis.

The crystal packing is stabilized by weak intermolecular C—H···π interactions involving both aromatic rings, C1–C6 ring (centroid *Cg*1) and C10—C15 ring (centroid *Cg*2) (Table 1). The molecules are stacked along the *b* axis.

Experimental

Compound (I) was obtained by the condensation of 4-bromobenzaldehyde (0.01 mol) with 4-bromoacetophenone (0.01 mol) in ethanol (60 ml) in the presence of a catalytic amount of NaOH (2 ml, 20%). After stirring for 2 h, the contents of the flask were poured into ice-cold water, and the resulting crude solid was collected by filtration. The compound was dried and purified by recrystallization. The purity of the compound was checked by thin layer chromatography. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of an acetone solution at room temperature, over a period of 10 d.

Crystal data

$C_{15}H_{10}Br_2O$
M_r = 366.05
Monoclinic, $P2_1/c$
a = 15.7504 (5) Å
b = 13.9442 (5) Å
c = 5.8289 (2) Å
β = 92.034 (2)°
V = 1279.38 (8) Å^3
Z = 4
D_x = 1.900 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4415 reflections
θ = 1.3–32.5°
μ = 6.32 mm^{-1}
T = 100.0 (1) K
Block, yellow
0.49 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*, Bruker 2005)
T_{min} = 0.127, T_{max} = 0.301
14888 measured reflections
4614 independent reflections
3185 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 32.5°
$h = -23 \rightarrow 21$
$k = -21 \rightarrow 18$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.112
S = 1.09
4614 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.51	2.822 (4)	100
C5—H5A···$Cg1^{i}$	0.93	2.96	3.504 (3)	119
C9—H9A···$Cg1^{ii}$	0.93	2.97	3.532 (3)	121
C14—H14A···$Cg2^{iii}$	0.93	2.76	3.459 (3)	132

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+2$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$. *Cg*1 is the centroid of the C1–C6 ring and *Cg*2 is the centroid of the C10—C15 ring.

H atoms were placed in calculated positions and constrained to ride on their carrier atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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 the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118 and the short-term grant No. 304/PFIZIK/635028.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
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* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn J. Appl. Phys.* **27**, L429–L430.

Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Jeyabharathi, A., Ponnuswamy, M. N., Nanjundan, S., Fun, H. K., Chantrapromma, S., Usman, A. & Razak, I. A. (2002). *Acta Cryst.* C**58**, o26–o28.
Lawrence, N. J., Rennison, D., McGown, A. T., Ducki, S., Gul, L. A., Hadfield, J. A. & Khan, N. (2001). *J. Comb. Chem.* **3**, 421–426.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Ng, S. L., Patil, P. S., Razak, I. A., Fun, H. K. & Dharmaprakash, S. M. (2006*a*). *Acta Cryst.* E**62**, o893–o895.
Ng, S. L., Patil, P. S., Razak, I. A., Fun, H. K. & Dharmaprakash, S. M. (2006*b*). *Acta Cryst.* E**62**, o1228–o1230.
Pandey, S., Suryawanshi, S. N., Gupta, S. & Srivastava, V. M. L. (2005). *Eur. J. Med. Chem.* **40**, 751–756.
Patil, P. S., Teh, J. B. J., Fun, H. K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o896–o898.
Phrutivorapongkul, A., Lipipun, V., Ruangrungsi, N., Kirtikara, K., Nishikawa, K., Maruyama, S., Watanabe, T. & Ishikawa, T. (2003). *Chem. Pharm. Bull.* **51**, 187–190.
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.
Xia, Y., Yang, Z. Y., Xia, P., Bastow, K. F., Nakanishi, Y. & Lee, K. H. (2000). *Bioorg. Med. Chem. Lett.* **10**, 699– 701.
Zhao, B., Lu, W.-Q., Zhou, Z.-H. & Wu, Y. (2000). *J. Mater. Chem.* **10**, 1513–1517.