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3-(3-Bromophenyl)-1-phenylprop-2-en-1-one

Shea-Lin Ng,[a] P. S. Patil,[b] Ibrahim Abdul Razak,[a] Hoong-Kun Fun[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) = 0.002 Å
R factor = 0.030
wR factor = 0.090
Data-to-parameter ratio = 47.7

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

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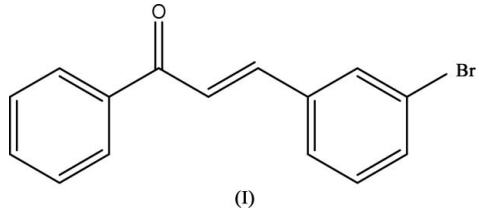
The enone group and the benzene rings of the title compound, $C_{15}H_{11}BrO$, are each planar. The molecules are linked *via* C—H···O interactions into wave-like chains along the *c* axis and the chains are stacked along the *b* axis.

Comment

Chalcones show an impressive array of pharmacological activities, such as antiprotozoal (Nielsen *et al.*, 1998; Li *et al.*, 1995; Liu *et al.*, 2001), anti-inflammatory (Hsieh *et al.*, 1998), nitric oxide inhibition (Rojas *et al.*, 2002) and anticancer properties. Recently it has been noted that bromo-substituted derivatives of chalcones exhibit extremely high and fast non-linearity (Fichou *et al.*, 1988; Zhang *et al.*, 1990; Zhao *et al.*, 2000), and show preferences to crystallize as non-centrosymmetric structures. For this reason, they have been the objective of several experimental and theoretical studies, aimed mainly at the determination of their crystal structures (Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Radha Krishna *et al.*, 2005; Uchida *et al.*, 1995). We report here the synthesis and crystal structure of the title compound, (I).



(I)

The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and similar to those observed in other comparable structures (Jeyabharathi *et al.*, 2002; Patil *et al.*, 2006; Ravishankar *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Teh *et al.*, 2006). The short H5···H8 (2.28 Å) contact causes the bond angle C9—C10—C11 [123.08 (9)°] to deviate significantly from 120°. In addition, the short H8···H11 (2.14 Å) contact results in a slight widening of the C5—C6—C7 angle to 122.58 (9)°.

The molecule of (I) (Fig. 1) is approximately planar. The enone group (O1/C7–C9) and the two benzene rings, C1–C6 and C10–C15, are each planar with largest deviations of 0.023 (1), 0.008 (1) and 0.008 (1) Å for atoms C9, C4 and C10,

respectively. The enone group makes dihedral angles of 13.59 (6) and 12.22 (6)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the two benzene rings is 3.95 (4)°.

In the crystal structure, atom O1 is involved in both intra- and intermolecular hydrogen bonds. Intermolecular C5—H5···O1^{i} (symmetry code as in Table 1) interactions link the molecules into wave-like chains along the *c* axis. The chains are stacked along the *b* axis. The intramolecular C7—H7···O1 interaction generates an *S*(5) ring motif (Bernstein *et al.*, 1995).

Experimental

Compound (I) was obtained by the condensation of 3-bromobenzaldehyde (0.01 mol) and acetophenone (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 and allowed to stand for 24 h. The resulting crude solid compound was collected by filtration, dried and recrystallized twice from acetone. Crystals suitable for X-ray diffraction study were grown by slow evaporation of an acetone solution over a period of 10 d.

Crystal data

$C_{15}H_{11}BrO$
M_r = 287.15
Monoclinic, $P2_1/c$
a = 14.3238 (2) Å
b = 7.4913 (1) Å
c = 11.2786 (2) Å
β = 100.325 (1)°
V = 1190.64 (3) Å^3
Z = 4
D_x = 1.602 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6943 reflections
θ = 1.5–40.0°
μ = 3.43 mm^{-1}
T = 100.0 (1) K
Block, colourless
0.75 × 0.33 × 0.30 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.065, T_{max} = 0.357
48289 measured reflections
7339 independent reflections
5499 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 40.0°
$h = -25 \rightarrow 25$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.090
S = 1.10
7339 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.2439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1	0.93	2.45	2.7909 (15)	102
C5—H5···O1^{i}	0.93	2.50	3.4106 (15)	166

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

H atoms were placed in calculated positions, with a C—H distance of 0.93 Å. The U_{iso}(H) values were constrained to be 1.2U_{eq}(C).

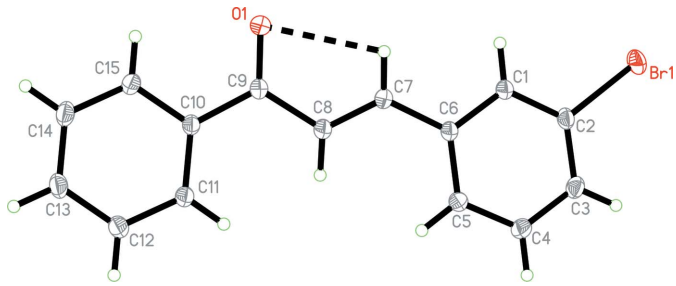


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates a hydrogen bond.

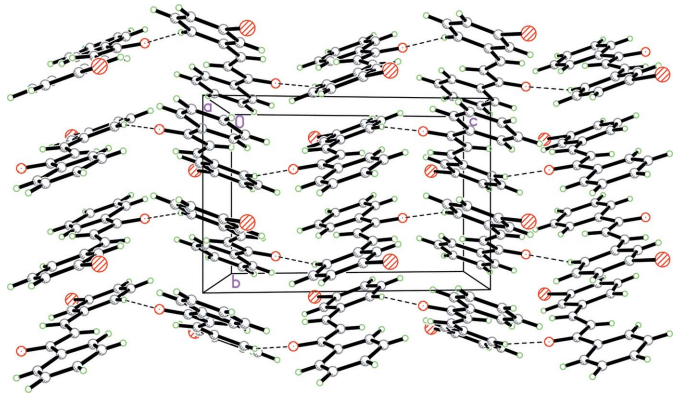


Figure 2
The crystal packing of (I), viewed approximately down the *a* axis. Hydrogen bonds are shown as dashed lines.

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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