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

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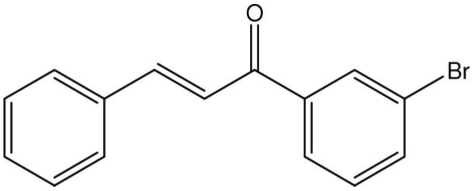
Key indicators: single-crystal X-ray study; *T* = 100 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.026; *wR* factor = 0.079; data-to-parameter ratio = 22.1.

In the title compound, $C_{15}H_{11}BrO$, the dihedral angle between the two benzene rings is 49.93 (8)°. The molecules are arranged into infinite chains along the *c* axis through weak C—H···Br interactions. The chains are stacked along the *a* axis, forming layers.

Related literature

For related literature on hydrogen-bond motifs, see Bernstein *et al.* (1995). For related literature on values of bond lengths and angles, see Allen *et al.* (1987). For related structures see, for example, Patil, Dharmaprakash, Fun *et al.*, (2006); Patil, Dharmaprakash, Ramakrishna *et al.*, (2007); Patil, Ng, *et al.*, (2007); Patil, Rosli *et al.*, (2007); Patil, Teh *et al.*, (2006); Shettigar *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{11}BrO$
M_r = 287.15
Triclinic, $P\overline{1}$
a = 5.8253 (2) Å
b = 7.6325 (3) Å
c = 13.3374 (4) Å
α = 83.051 (2)°
β = 89.919 (2)°
γ = 87.378 (2)°
V = 588.02 (4) Å^3
Z = 2
Mo *K*α radiation
μ = 3.47 mm^{-1}
T = 100.0 (1) K
0.63 × 0.52 × 0.36 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min}$ = 0.129, $T_{\max}$ = 0.297
11699 measured reflections
3398 independent reflections
3157 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.079
S = 1.17
3398 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.81 e Å^{-3}
$\Delta\rho_{\min}$ = −0.35 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O1	0.93	2.52	2.836 (2)	100
C3—H3*A*···Br1$^{\rm i}$	0.93	2.97	3.533 (2)	120

Symmetry code: (i) $x - 1, y, z - 1$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2290).

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supplementary materials

Acta Cryst. (2007). E**63**, o2501 [**doi:10.1107/S1600536807018168**]

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

M. M. Rosli, P. S. Patil, H.-K. Fun, I. A. Razak and S. M. Dharmaprakash

Comment

Among several organic compounds reported for their NLO properties, chalcone derivatives are prominent materials for their excellent blue light transmittance and good crystallizability (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007). The title compound, (I), was prepared as part of our ongoing studies on nonlinear optical (NLO) materials (Patil *et al.*, 2007). Crystal of the title compound , (I) (Fig. 1), do not exhibit second-order nonlinear optical properties as they crystallize in a centrosymmeric space group.

In (I), bond lengths and angles have normal values (Allen *et al.*, 1987) and comparable to those in related structures (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007). The least-squares plane through the O1/C7/C8/C9 enone group makes dihedral angles of 24.04 (7)° and 27.55 (7)° with the C1—C6 and C10—C15 benzene rings, respectively. The dihedral angle between the two benzene rings is 49.93 (8)°.

In the crystal structure of (I), the intramolecular C7—H7A···O1 interaction generates an S(5) ring motif (Bernstein *et al.*, 1995). The molecules are arranged into infinite chains along the c-axis through weak C3—H3A···Br1^{i} interactions. These chain are stacked along the a-axis to form layers.

Experimental

Benzaldehyde (0.01 mol) and 3-bromoacetophenone (0.01 mol)were stirred in 60 ml of methanol at room temperature. 5 ml of 10% of NaOH aqueous solution was added and the mixture was stirred for 2 h. The precipitate was filtered, washed with water, dried and the crude product recrystallized from acetone. Crystal suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

All H atoms were refined using a riding model, with C—H=0.9Å and $U_{iso}(H)=1.2U_{eq}(C)$.

Figures

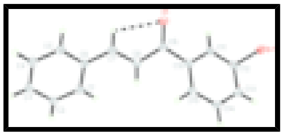

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The intramolecular hydrogen bond is shown as a dashed line.

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

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Crystal data

$C_{15}H_{11}BrO$

$M_r = 287.15$

Triclinic, $P\overline{1}$

Hall symbol: -P 1

$a = 5.8253$ (2) Å

$b = 7.6325$ (3) Å

$c = 13.3374$ (4) Å

$\alpha = 83.051$ (2)°

$\beta = 89.919$ (2)°

$\gamma = 87.378$ (2)°

$V = 588.02$ (4) Å^3

$Z = 2$

$F_{000} = 288$

$D_x = 1.622$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 7148 reflections

$\theta = 1.5$–30.0°

$\mu = 3.47$ mm^{-1}

$T = 100.0$ (1) K

Block, colourless

0.63 × 0.52 × 0.36 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels mm^{-1}

$T = 297(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{min} = 0.129$, $T_{max} = 0.297$

11699 measured reflections

3398 independent reflections

3157 reflections with $I > 2\sigma(I)$

$R_{int} = 0.023$

$\theta_{max} = 30.0$°

$\theta_{min} = 1.5$°

$h = -8 \rightarrow 8$

$k = -10 \rightarrow 10$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.079$

$S = 1.17$

3398 reflections

154 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.1299P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.81$ e Å^{-3}

$\Delta\rho_{min} = -0.35$ e Å^{-3}

Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\mathrm{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Br1	0.18482 (3)	0.30834 (2)	0.437256 (12)	0.02195 (7)
O1	0.2233 (2)	0.27315 (18)	0.03021 (10)	0.0235 (3)
C1	−0.4563 (3)	0.0879 (2)	−0.17687 (13)	0.0191 (3)
H1A	−0.5041	0.0685	−0.1101	0.023*
C2	−0.5930 (3)	0.0399 (2)	−0.25316 (14)	0.0204 (3)
H2A	−0.7314	−0.0126	−0.2371	0.024*
C3	−0.5245 (3)	0.0696 (2)	−0.35343 (14)	0.0220 (3)
H3A	−0.6167	0.0369	−0.4043	0.026*
C4	−0.3181 (3)	0.1483 (2)	−0.37739 (14)	0.0227 (3)
H4A	−0.2729	0.1698	−0.4445	0.027*
C5	−0.1788 (3)	0.1951 (2)	−0.30139 (13)	0.0195 (3)
H5A	−0.0398	0.2462	−0.3179	0.023*
C6	−0.2459 (3)	0.1658 (2)	−0.20008 (13)	0.0170 (3)
C7	−0.0958 (3)	0.2175 (2)	−0.12186 (13)	0.0185 (3)
H7A	0.0542	0.2425	−0.1404	0.022*
C8	−0.1547 (3)	0.2320 (2)	−0.02598 (13)	0.0202 (3)
H8A	−0.3049	0.2128	−0.0052	0.024*
C9	0.0163 (3)	0.2781 (2)	0.04731 (13)	0.0185 (3)
C10	−0.0722 (3)	0.3293 (2)	0.14550 (13)	0.0176 (3)
C11	0.0729 (3)	0.3005 (2)	0.22996 (13)	0.0173 (3)
H11A	0.2204	0.2502	0.2250	0.021*
C12	−0.0070 (3)	0.3483 (2)	0.32109 (13)	0.0176 (3)
C13	−0.2258 (3)	0.4256 (2)	0.33028 (14)	0.0200 (3)
H13A	−0.2764	0.4568	0.3921	0.024*
C14	−0.3671 (3)	0.4554 (2)	0.24598 (14)	0.0206 (3)
H14A	−0.5128	0.5087	0.2509	0.025*
C15	−0.2924 (3)	0.4060 (2)	0.15401 (14)	0.0193 (3)
H15A	−0.3893	0.4242	0.0980	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02079 (10)	0.02853 (11)	0.01666 (10)	0.00418 (7)	−0.00231 (6)	−0.00519 (6)
O1	0.0172 (6)	0.0335 (7)	0.0200 (6)	−0.0009 (5)	0.0001 (5)	−0.0036 (5)
C1	0.0168 (7)	0.0195 (7)	0.0201 (8)	0.0008 (6)	0.0000 (6)	−0.0004 (6)
C2	0.0175 (7)	0.0176 (7)	0.0256 (8)	0.0004 (6)	−0.0024 (6)	−0.0018 (6)
C3	0.0234 (8)	0.0216 (7)	0.0209 (8)	0.0018 (6)	−0.0050 (6)	−0.0034 (6)
C4	0.0253 (9)	0.0247 (8)	0.0181 (8)	0.0006 (7)	−0.0008 (6)	−0.0026 (6)
C5	0.0189 (7)	0.0195 (7)	0.0198 (8)	0.0005 (6)	0.0008 (6)	−0.0020 (6)
C6	0.0152 (7)	0.0158 (6)	0.0200 (8)	0.0020 (6)	−0.0009 (6)	−0.0027 (5)
C7	0.0163 (7)	0.0185 (7)	0.0205 (8)	0.0009 (6)	−0.0011 (6)	−0.0025 (6)
C8	0.0168 (7)	0.0234 (7)	0.0200 (8)	−0.0015 (6)	−0.0007 (6)	−0.0013 (6)
C9	0.0182 (7)	0.0194 (7)	0.0174 (7)	−0.0001 (6)	−0.0011 (6)	−0.0006 (6)
C10	0.0178 (7)	0.0176 (7)	0.0173 (7)	−0.0018 (6)	−0.0004 (6)	−0.0014 (5)
C11	0.0152 (7)	0.0173 (7)	0.0192 (8)	0.0003 (6)	−0.0006 (6)	−0.0026 (5)
C12	0.0173 (7)	0.0179 (7)	0.0176 (7)	0.0006 (6)	−0.0024 (6)	−0.0021 (5)
C13	0.0186 (8)	0.0197 (7)	0.0222 (8)	−0.0002 (6)	0.0023 (6)	−0.0048 (6)
C14	0.0163 (7)	0.0184 (7)	0.0267 (9)	0.0025 (6)	−0.0001 (6)	−0.0027 (6)
C15	0.0171 (7)	0.0189 (7)	0.0213 (8)	0.0003 (6)	−0.0027 (6)	−0.0006 (6)

Geometric parameters (Å, °)

Br1—C12	1.8976 (17)	C7—H7A	0.9300
O1—C9	1.226 (2)	C8—C9	1.480 (2)
C1—C2	1.387 (2)	C8—H8A	0.9300
C1—C6	1.404 (2)	C9—C10	1.496 (2)
C1—H1A	0.9300	C10—C15	1.396 (2)
C2—C3	1.390 (3)	C10—C11	1.399 (2)
C2—H2A	0.9300	C11—C12	1.385 (2)
C3—C4	1.388 (3)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.392 (2)
C4—C5	1.389 (2)	C13—C14	1.385 (3)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.401 (2)	C14—C15	1.390 (3)
C5—H5A	0.9300	C14—H14A	0.9300
C6—C7	1.463 (2)	C15—H15A	0.9300
C7—C8	1.340 (2)		
C2—C1—C6	120.28 (16)	C9—C8—H8A	119.6
C2—C1—H1A	119.9	O1—C9—C8	122.29 (16)
C6—C1—H1A	119.9	O1—C9—C10	120.37 (15)
C1—C2—C3	120.47 (16)	C8—C9—C10	117.33 (15)
C1—C2—H2A	119.8	C15—C10—C11	119.95 (16)
C3—C2—H2A	119.8	C15—C10—C9	121.73 (15)
C4—C3—C2	119.77 (17)	C11—C10—C9	118.31 (15)
C4—C3—H3A	120.1	C12—C11—C10	118.76 (15)
C2—C3—H3A	120.1	C12—C11—H11A	120.6

C3—C4—C5	120.17 (17)	C10—C11—H11A	120.6
C3—C4—H4A	119.9	C11—C12—C13	121.74 (16)
C5—C4—H4A	119.9	C11—C12—Br1	119.68 (13)
C4—C5—C6	120.59 (16)	C13—C12—Br1	118.58 (13)
C4—C5—H5A	119.7	C14—C13—C12	119.05 (16)
C6—C5—H5A	119.7	C14—C13—H13A	120.5
C5—C6—C1	118.72 (16)	C12—C13—H13A	120.5
C5—C6—C7	119.24 (15)	C13—C14—C15	120.34 (16)
C1—C6—C7	122.04 (15)	C13—C14—H14A	119.8
C8—C7—C6	125.99 (16)	C15—C14—H14A	119.8
C8—C7—H7A	117.0	C14—C15—C10	120.15 (16)
C6—C7—H7A	117.0	C14—C15—H15A	119.9
C7—C8—C9	120.81 (16)	C10—C15—H15A	119.9
C7—C8—H8A	119.6		

C6—C1—C2—C3	−0.6 (3)	C8—C9—C10—C15	−27.8 (2)
C1—C2—C3—C4	−0.1 (3)	O1—C9—C10—C11	−26.0 (2)
C2—C3—C4—C5	0.9 (3)	C8—C9—C10—C11	153.04 (15)
C3—C4—C5—C6	−0.9 (3)	C15—C10—C11—C12	0.5 (2)
C4—C5—C6—C1	0.2 (3)	C9—C10—C11—C12	179.65 (14)
C4—C5—C6—C7	−179.67 (16)	C10—C11—C12—C13	−0.7 (2)
C2—C1—C6—C5	0.5 (2)	C10—C11—C12—Br1	179.27 (12)
C2—C1—C6—C7	−179.61 (16)	C11—C12—C13—C14	0.0 (2)
C5—C6—C7—C8	165.45 (17)	Br1—C12—C13—C14	179.98 (12)
C1—C6—C7—C8	−14.4 (3)	C12—C13—C14—C15	1.1 (3)
C6—C7—C8—C9	177.36 (15)	C13—C14—C15—C10	−1.3 (3)
C7—C8—C9—O1	−13.7 (3)	C11—C10—C15—C14	0.6 (2)
C7—C8—C9—C10	167.28 (16)	C9—C10—C15—C14	−178.60 (15)
O1—C9—C10—C15	153.17 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···O1	0.93	2.52	2.836 (2)	100
C3—H3A···Br1^{i}	0.93	2.97	3.533 (2)	120

Symmetry codes: (i) *x*−1, *y*, *z*−1.

Fig. 1

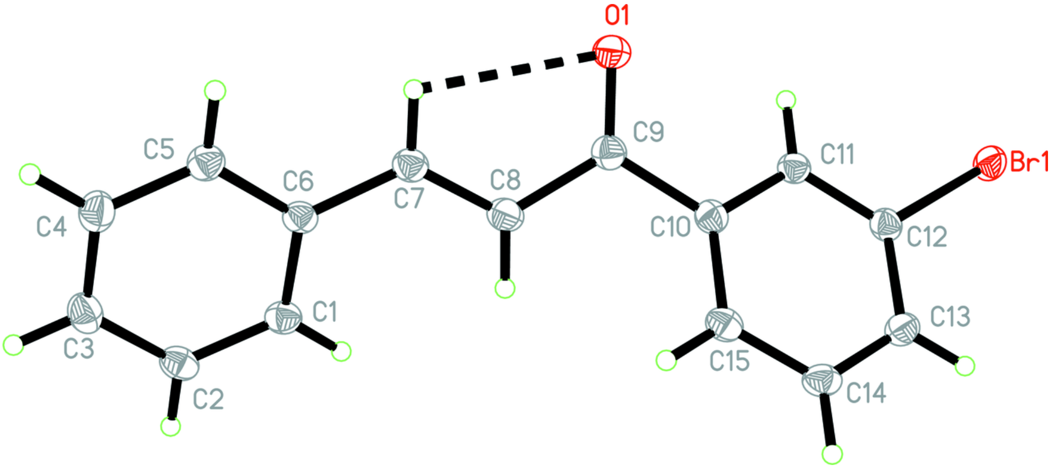

Fig. 2