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

Yu-xia Zhou

Shandong Vocational College of Science and Technology, Weifang 261061, People's Republic of China
Correspondence e-mail: zhouyuxiajidian@163.com

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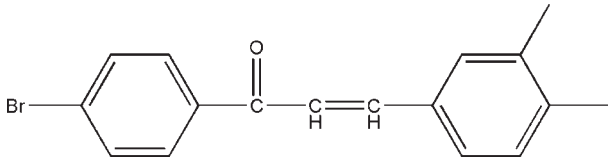
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.095; data-to-parameter ratio = 15.1.

In the title chalcone derivative, $C_{17}H_{15}BrO$, the dihedral angle between the two benzene rings is 48.13 (4)°. In the crystal, a short Br···Br contact of 3.5052 (10) Å occurs.

Related literature

For a related structure and background to chalcones, see: Fun *et al.* (2008).



Experimental

Crystal data

$C_{17}H_{15}BrO$
M_r = 315.20
Triclinic, $P\overline{1}$
a = 5.9786 (14) Å
b = 7.8437 (19) Å
c = 15.744 (4) Å
α = 99.054 (4)°
β = 99.602 (4)°
γ = 95.659 (4)°
V = 713.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.87 mm^{-1}
T = 298 K
0.25 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
3911 measured reflections
2620 independent reflections
2198 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.095
S = 1.09
2620 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5445).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Fun, H.-K., Chantrapromma, S., Patil, P. S., D'Silva, E. D. & Dharmaprakash, S. M. (2008). *Acta Cryst.* E**64**, o954–o955.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o1412 [https://doi.org/10.1107/S1600536810018106]

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

Yu-xia Zhou

S1. Comment

As part of our search for new biologically active compounds we synthesized the title compound(I) and report its crystal structure herein.

In the crystal structure of compound(I)(fig.1),the dihedral angle between the two benzene rings(C1—C6) and (C7—C12) is 48.13 (4)°. All of the bond lengths and bond angles are in normal ranges and comparable to those in related structure (Fun *et al.*, 2008).

S2. Experimental

A mixture of 4-bromohypnone (0.02 mol) and 3,4-dimethylbenzaldehyde (0.02 mol) and 10%NaOH (5 ml) was stirred in ethanol (30 ml) for 1.5 h to afford the title compound (yield 73%). Yellow blocks of (I) were obtailed by recrystallization from ethyl acetate at room temperature.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93-0.96 Å, and with U_{iso}(H) = 1.2U_{eq} of the parent atoms.

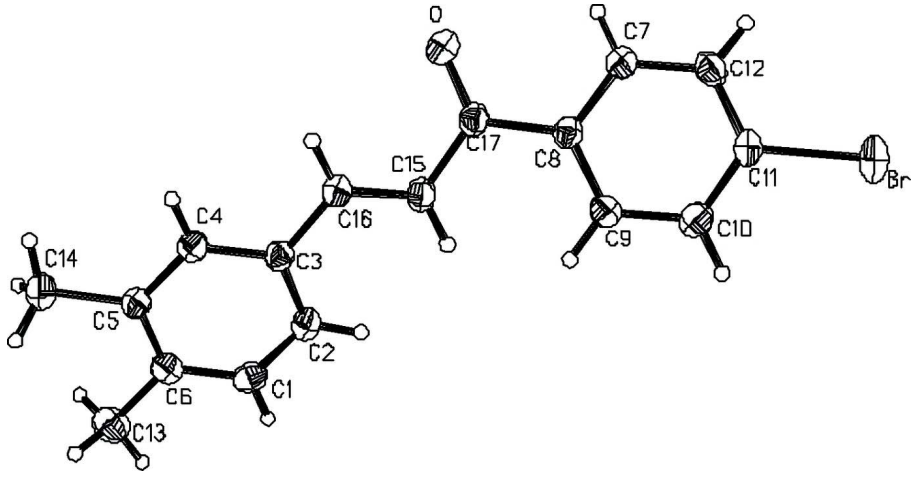


Figure 1

The molecular structure of (I) with displacement ellipsoids are drawn at the 30% probability level.

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

Crystal data

$C_{17}H_{15}BrO$
$M_r = 315.20$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.9786\ (14)$ Å
$b = 7.8437\ (19)$ Å
$c = 15.744\ (4)$ Å
$\alpha = 99.054\ (4)°$
$\beta = 99.602\ (4)°$
$\gamma = 95.659\ (4)°$
$V = 713.0\ (3)$ Å^3
$Z = 2$
$F(000) = 320$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2198 reflections
$\theta = 1.3–25.5°$
$\mu = 2.87$ mm^{-1}
$T = 298$ K
Bar, yellow
0.25 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
3911 measured reflections
2620 independent reflections
2198 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.3°$
$h = -7\rightarrow7$
$k = -9\rightarrow6$
$l = -18\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.095$
$S = 1.09$
2620 reflections
173 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.2458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.048 (4)

Special details

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 $F^2 > \sigma(F^2)$ 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_{iso}*/U_{eq}
Br	0.57731 (6)	0.43242 (4)	0.100602 (19)	0.06655 (18)
C11	0.5449 (5)	0.3857 (3)	0.21288 (17)	0.0440 (6)
O	0.2750 (3)	0.2761 (3)	0.48223 (13)	0.0628 (6)

C10	0.7328 (5)	0.4220 (4)	0.27985 (18)	0.0482 (6)
H10A	0.8724	0.4717	0.2706	0.058*
C17	0.4645 (5)	0.2760 (4)	0.46327 (17)	0.0455 (6)
C12	0.3349 (5)	0.3142 (4)	0.22550 (18)	0.0506 (7)
H12A	0.2100	0.2898	0.1796	0.061*
C9	0.7107 (4)	0.3834 (3)	0.36099 (17)	0.0448 (6)
H9A	0.8374	0.4048	0.4061	0.054*
C8	0.5010 (4)	0.3129 (3)	0.37593 (16)	0.0395 (5)
C6	1.1464 (4)	0.0981 (3)	0.80706 (18)	0.0453 (6)
C5	0.9589 (4)	0.1781 (4)	0.82839 (17)	0.0448 (6)
C3	0.8289 (4)	0.1904 (3)	0.67426 (17)	0.0408 (6)
C4	0.8024 (4)	0.2208 (3)	0.76150 (17)	0.0437 (6)
H4A	0.6759	0.2714	0.7755	0.052*
C16	0.6528 (5)	0.2356 (3)	0.60745 (17)	0.0437 (6)
H16A	0.5194	0.2656	0.6256	0.052*
C2	1.0206 (5)	0.1157 (3)	0.65442 (18)	0.0459 (6)
H2A	1.0448	0.0967	0.5970	0.055*
C7	0.3131 (5)	0.2796 (4)	0.30725 (17)	0.0464 (6)
H7A	0.1717	0.2335	0.3167	0.056*
C15	0.6631 (5)	0.2384 (4)	0.52402 (18)	0.0477 (6)
H15A	0.7966	0.2164	0.5036	0.057*
C1	1.1749 (5)	0.0697 (3)	0.72054 (19)	0.0474 (6)
H1A	1.3008	0.0184	0.7064	0.057*
C14	0.9249 (6)	0.2180 (5)	0.9221 (2)	0.0674 (9)
H14A	0.7885	0.2726	0.9242	0.101*
H14B	1.0541	0.2950	0.9567	0.101*
H14C	0.9103	0.1119	0.9450	0.101*
C13	1.3147 (6)	0.0413 (4)	0.8765 (2)	0.0635 (8)
H13A	1.4312	−0.0106	0.8501	0.095*
H13B	1.2362	−0.0421	0.9034	0.095*
H13C	1.3838	0.1406	0.9201	0.095*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0949 (3)	0.0686 (3)	0.0421 (2)	0.01006 (17)	0.01910 (16)	0.02128 (15)
C11	0.0583 (16)	0.0408 (13)	0.0358 (13)	0.0098 (12)	0.0132 (12)	0.0091 (11)
O	0.0507 (12)	0.0955 (16)	0.0468 (11)	0.0114 (11)	0.0174 (9)	0.0161 (11)
C10	0.0477 (15)	0.0507 (15)	0.0470 (15)	0.0019 (12)	0.0133 (12)	0.0092 (12)
C17	0.0508 (16)	0.0485 (15)	0.0367 (13)	0.0058 (12)	0.0101 (11)	0.0043 (11)
C12	0.0514 (16)	0.0571 (17)	0.0394 (14)	0.0025 (13)	−0.0017 (12)	0.0104 (12)
C9	0.0420 (14)	0.0502 (15)	0.0387 (14)	0.0038 (11)	0.0027 (11)	0.0042 (11)
C8	0.0449 (14)	0.0387 (13)	0.0361 (13)	0.0085 (10)	0.0108 (10)	0.0052 (10)
C6	0.0446 (14)	0.0401 (13)	0.0501 (15)	0.0030 (11)	0.0045 (12)	0.0112 (12)
C5	0.0434 (14)	0.0507 (15)	0.0403 (14)	0.0011 (11)	0.0081 (11)	0.0106 (12)
C3	0.0434 (14)	0.0406 (13)	0.0395 (13)	0.0027 (10)	0.0096 (11)	0.0104 (11)
C4	0.0417 (14)	0.0500 (15)	0.0421 (14)	0.0088 (11)	0.0120 (11)	0.0098 (12)
C16	0.0459 (14)	0.0452 (14)	0.0413 (14)	0.0061 (11)	0.0113 (11)	0.0086 (11)

C2	0.0528 (15)	0.0460 (14)	0.0401 (14)	0.0052 (12)	0.0147 (12)	0.0052 (11)
C7	0.0423 (14)	0.0534 (16)	0.0428 (15)	0.0010 (12)	0.0067 (11)	0.0107 (12)
C15	0.0525 (16)	0.0562 (16)	0.0389 (14)	0.0138 (13)	0.0139 (12)	0.0120 (12)
C1	0.0432 (14)	0.0430 (14)	0.0580 (17)	0.0092 (11)	0.0149 (12)	0.0071 (12)
C14	0.0606 (19)	0.103 (3)	0.0422 (17)	0.0175 (17)	0.0120 (14)	0.0157 (17)
C13	0.0604 (19)	0.067 (2)	0.064 (2)	0.0181 (15)	0.0032 (15)	0.0181 (16)

Geometric parameters (Å, º)

Br—C11	1.898 (3)	C3—C2	1.396 (4)
C11—C10	1.379 (4)	C3—C4	1.395 (4)
C11—C12	1.382 (4)	C3—C16	1.470 (4)
O—C17	1.219 (3)	C4—H4A	0.9300
C10—C9	1.382 (4)	C16—C15	1.329 (4)
C10—H10A	0.9300	C16—H16A	0.9300
C17—C15	1.480 (4)	C2—C1	1.389 (4)
C17—C8	1.495 (4)	C2—H2A	0.9300
C12—C7	1.381 (4)	C7—H7A	0.9300
C12—H12A	0.9300	C15—H15A	0.9300
C9—C8	1.391 (4)	C1—H1A	0.9300
C9—H9A	0.9300	C14—H14A	0.9600
C8—C7	1.396 (4)	C14—H14B	0.9600
C6—C1	1.387 (4)	C14—H14C	0.9600
C6—C5	1.400 (4)	C13—H13A	0.9600
C6—C13	1.510 (4)	C13—H13B	0.9600
C5—C4	1.393 (4)	C13—H13C	0.9600
C5—C14	1.512 (4)		
C10—C11—C12	121.5 (2)	C3—C4—H4A	118.9
C10—C11—Br	119.1 (2)	C15—C16—C3	127.2 (3)
C12—C11—Br	119.4 (2)	C15—C16—H16A	116.4
C11—C10—C9	119.1 (2)	C3—C16—H16A	116.4
C11—C10—H10A	120.5	C1—C2—C3	119.9 (2)
C9—C10—H10A	120.5	C1—C2—H2A	120.1
O—C17—C15	122.0 (3)	C3—C2—H2A	120.1
O—C17—C8	119.9 (2)	C12—C7—C8	120.7 (2)
C15—C17—C8	118.0 (2)	C12—C7—H7A	119.7
C11—C12—C7	119.1 (2)	C8—C7—H7A	119.7
C11—C12—H12A	120.5	C16—C15—C17	120.7 (3)
C7—C12—H12A	120.5	C16—C15—H15A	119.6
C10—C9—C8	120.8 (2)	C17—C15—H15A	119.6
C10—C9—H9A	119.6	C6—C1—C2	121.8 (2)
C8—C9—H9A	119.6	C6—C1—H1A	119.1
C9—C8—C7	118.9 (2)	C2—C1—H1A	119.1
C9—C8—C17	123.1 (2)	C5—C14—H14A	109.5
C7—C8—C17	117.9 (2)	C5—C14—H14B	109.5
C1—C6—C5	119.0 (2)	H14A—C14—H14B	109.5
C1—C6—C13	120.0 (3)	C5—C14—H14C	109.5

C5—C6—C13	121.0 (3)	H14A—C14—H14C	109.5
C4—C5—C6	118.9 (2)	H14B—C14—H14C	109.5
C4—C5—C14	120.0 (2)	C6—C13—H13A	109.5
C6—C5—C14	121.1 (3)	C6—C13—H13B	109.5
C2—C3—C4	118.2 (2)	H13A—C13—H13B	109.5
C2—C3—C16	123.1 (2)	C6—C13—H13C	109.5
C4—C3—C16	118.8 (2)	H13A—C13—H13C	109.5
C5—C4—C3	122.3 (2)	H13B—C13—H13C	109.5
C5—C4—H4A	118.9		