(2*E*)-3-(Biphenyl-4-yl)-1-(4-bromophenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.016 Å
R factor = 0.064
wR factor = 0.158
Data-to-parameter ratio = 11.7

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

The title compound, $C_{21}H_{15}BrO$, was obtained from 4-bromoacetophenone and biphenyl-4-carbaldehyde. The geometry of the molecule is unexceptional. The compound crystallizes isostructurally with the corresponding chloro compound.

Comment

For an introduction, see Fischer *et al.* (2007*a*).

(I)
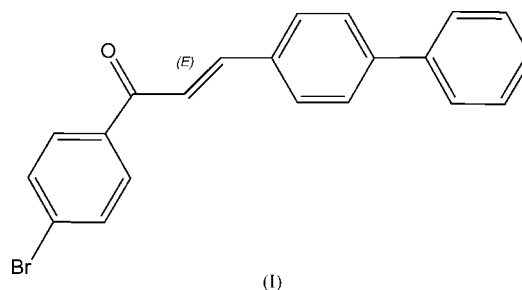
The title chalcone, (I), was prepared by treating 4-bromo-acetophenone with biphenyl-4-carbaldehyde in the presence of KOH.

Fig. 1 shows the molecular structure. The geometry of the molecule is unexceptional. The molecule deviates significantly from planarity [dihedral angles of 5.4 (3)° within the biphenyl group and 48.4 (3)° between the C10–C15 ring and the bromophenyl ring]. The compound is isostructural with the corresponding chloro compound (Fischer *et al.*, 2007*b*).

Experimental

4-Bromoacetophenone (1.99 g, 0.01 mol) in methanol (20 ml) was mixed with biphenyl-4-carbaldehyde (1.82 g, 0.01 mol) and the mixture was treated with a 30% potassium hydroxide solution (3 ml) at 278 K. The reaction mixture was then brought to room tempera-
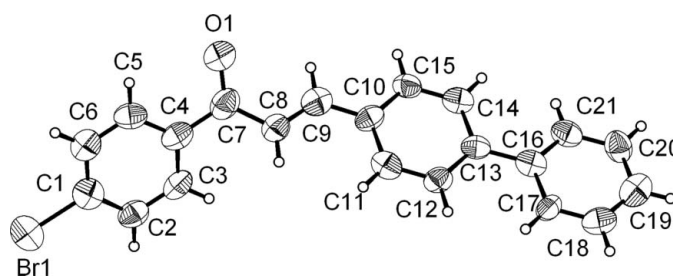
Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

ture and stirred for 3 h. The precipitated solid was filtered off, washed with water, dried and recrystallized from acetone (m.p. 449–451 K). Analysis (%) for $C_{21}H_{15}BrO$ found (Calculated): C 69.32 (69.44), H 4.10 (4.16).

Crystal data

$C_{21}H_{15}BrO$	$V = 1675.9\ (15)\ \text{Å}^3$
$M_r = 363.26$	$Z = 4$
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 37.35\ (3)\ \text{Å}$	$\mu = 2.45\ \text{mm}^{-1}$
$b = 7.3663\ (15)\ \text{Å}$	$T = 296\ \text{K}$
$c = 6.0978\ (17)\ \text{Å}$	$0.44 \times 0.23 \times 0.05\ \text{mm}$
$\beta = 92.63\ (4)°$	

Data collection

Bruker–Nonius KappaCCD diffractometer	4893 measured reflections
	2434 independent reflections
Absorption correction: numerical (Herrendorf & Bärnighausen, 1997)	1640 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.075$
$T_{min} = 0.530$, $T_{max} = 0.864$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$	$\Delta\rho_{max} = 0.24\ \text{e}\ \text{Å}^{-3}$
$wR(F^2) = 0.158$	$\Delta\rho_{min} = -0.34\ \text{e}\ \text{Å}^{-3}$
$S = 1.17$	Absolute structure: Flack (1983),
2434 reflections	924 Friedel pairs
208 parameters	Flack parameter: $-0.01\ (3)$
H-atom parameters constrained	

H atoms were placed at calculated positions and refined as riding on the respective carrier atom, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The structure appears to exhibit turbostratic disorder, which could be detected in precession photographs that were simu-

lated from the CCD data. The disorder was accounted for in the data processing with *EVALCCD* (Duisenberg *et al.*, 2003).

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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