

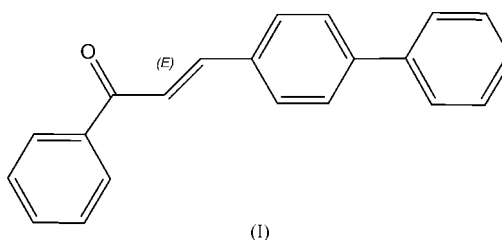
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Key indicatorsSingle-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.059
 wR factor = 0.149
Data-to-parameter ratio = 14.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(2E)-3-(Biphenyl-4-yl)-1-phenylprop-2-en-1-one**The title compound, $C_{21}H_{16}O$, was prepared from biphenyl-4-carbaldehyde and acetophenone. The molecule is essentially planar.

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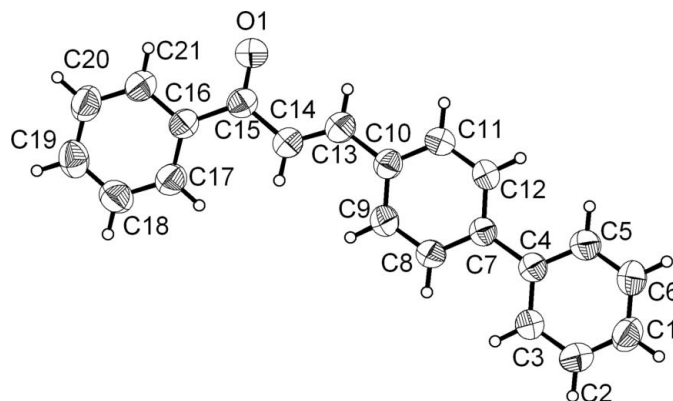
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CommentFor an introduction, see Fischer *et al.* (2007).

The title chalcone, (I), was prepared by treating 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 is essentially planar with dihedral angles of 3.02 (7°) between the phenyl rings of the biphenyl group and 9.89 (8°) between the C7–C12 ring and the phenyl ring.**Experimental**

Acetophenone (1.2 g, 0.01 mol) in methanol (15 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 temperature and stirred for 3 h. The precipitated solid was filtered off, washed with water,

**Figure 1**
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

dried and recrystallized from acetone (m.p. 389–391 K). Analysis (%) for C₂₁H₁₆O found (calculated): C 88.64 (88.70), H 5.60 (5.67).

Crystal data

C ₂₁ H ₁₆ O	$V = 1513.2 (2) \text{ \AA}^3$
$M_r = 284.34$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 11.7645 (10) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 5.8118 (3) \text{ \AA}$	$T = 296 \text{ K}$
$c = 22.426 (2) \text{ \AA}$	$0.38 \times 0.25 \times 0.18 \text{ mm}$
$\beta = 99.304 (8)^\circ$	

Data collection

Bruker-Nonius KappaCCD diffractometer	2933 independent reflections
Absorption correction: none	1893 reflections with $I > 2\sigma(I)$
25186 measured reflections	$R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$	199 parameters
$wR(F^2) = 0.149$	H-atom parameters constrained
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
2933 reflections	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$

H atoms were placed at calculated positions and refined as riding on the respective carrier atom, with C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD*

(Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 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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