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

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.149
Data-to-parameter ratio = 14.7

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

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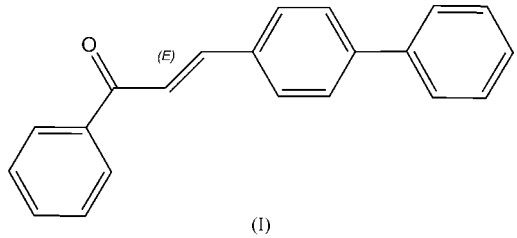
The title compound, $C_{21}H_{16}O$, was prepared from biphenyl-4-carbaldehyde and acetophenone. The molecule is essentially planar.

Comment

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



(I)

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,

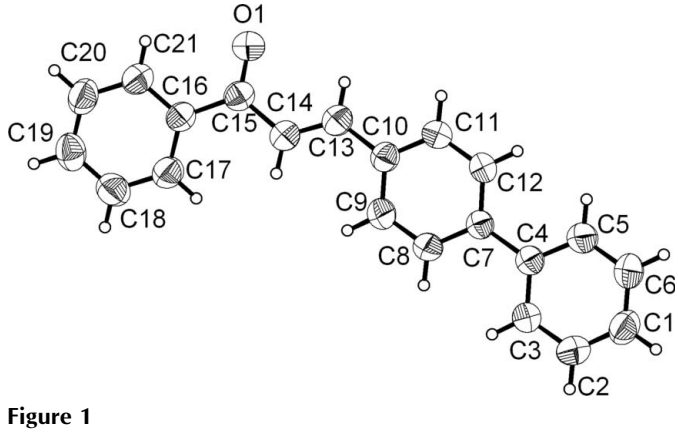


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

dried and recrystallized from acetone (m.p. 389–391 K). Analysis (%) for $C_{21}H_{16}O$ found (calculated): C 88.64 (88.70), H 5.60 (5.67).

Crystal data

$C_{21}H_{16}O$	V = 1513.2 (2) Å^3
M_r = 284.34	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 11.7645 (10) Å	μ = 0.08 mm^{-1}
b = 5.8118 (3) Å	T = 296 K
c = 22.426 (2) Å	0.38 × 0.25 × 0.18 mm
β = 99.304 (8)°	

Data collection

Bruker-Nonius KappaCCD diffractometer	2933 independent reflections
Absorption correction: none	1893 reflections with $I > 2\sigma(I)$
25186 measured reflections	R_{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	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
2933 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-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_{iso}(H) = 1.2U_{eq}(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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