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

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.008 Å
R factor = 0.067
wR factor = 0.160
Data-to-parameter ratio = 13.3

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

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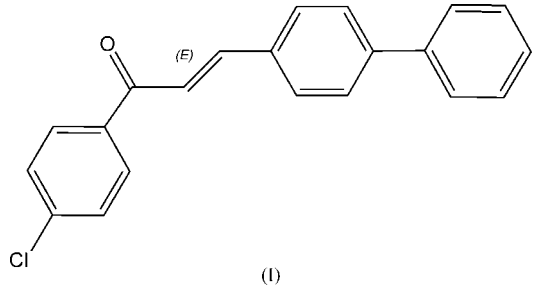
The title compound, $C_{21}H_{15}ClO$, was prepared from biphenyl-4-carbaldehyde and 4-chloroacetophenone. Single crystals were obtained from acetone. The compound is isostructural with the corresponding Br compound. The molecule deviates significantly from planarity.

Comment

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



(I)

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

Fig. 1 shows the molecular structure. The geometry of the molecule is unexceptional; its geometry deviates significantly from planarity [dihedral angles 4.42 (16)° within the biphenyl group and 48.85 (16)° between the C10–C15 ring and the chlorophenyl ring].

The compound is isostructural with the corresponding bromo compound (Fischer *et al.*, 2007*b*).

Experimental

4-Chloroacetophenone (1.54 g, 0.01 mol) in methanol (20 ml) was mixed with biphenyl-4-carbaldehyde (1.82 g, 0.01 mol) and the

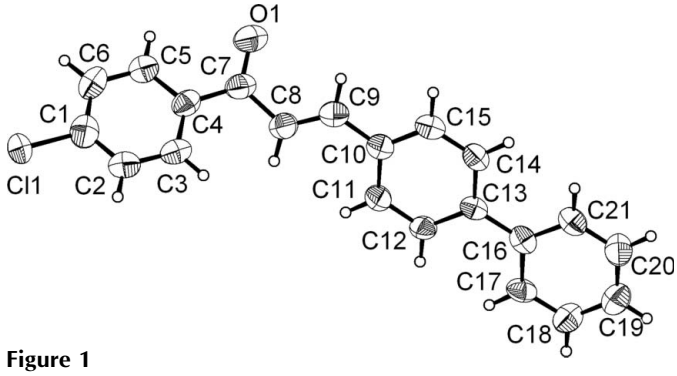


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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, dried and recrytallized from acetone (m.p. 439–441 K). Analysis (%) for $C_{21}H_{15}ClO$ found (calculated): C 76.83 (76.94), H 4.86 (4.92).

Crystal data

$C_{21}H_{15}ClO$
M_r = 318.78
Monoclinic, *Cc*
a = 36.723 (14) Å
b = 7.303 (3) Å
c = 6.0172 (16) Å
β = 93.06 (3)°
V = 1611.4 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.58 × 0.48 × 0.04 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: numerical (Herrendorf & Bärnighausen, 1997)
T_{min} = 0.716, T_{max} = 0.940
7961 measured reflections
2757 independent reflections
1756 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.160
S = 1.12
2757 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983), 1263 Friedel pairs
Flack parameter: 0.02 (15)

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 simulated 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: *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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