

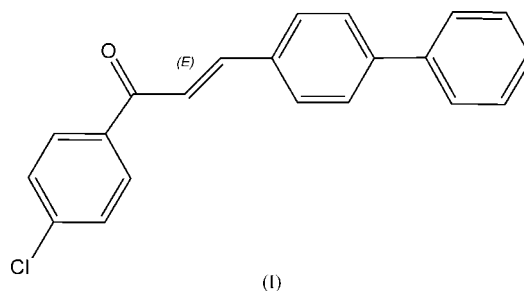
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Key indicatorsSingle-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.067
 wR factor = 0.160
Data-to-parameter ratio = 13.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(2E)-3-(Biphenyl-4-yl)-1-(4-chlorophenyl)-prop-2-en-1-one**The title compound, $\text{C}_{21}\text{H}_{15}\text{ClO}$, 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.

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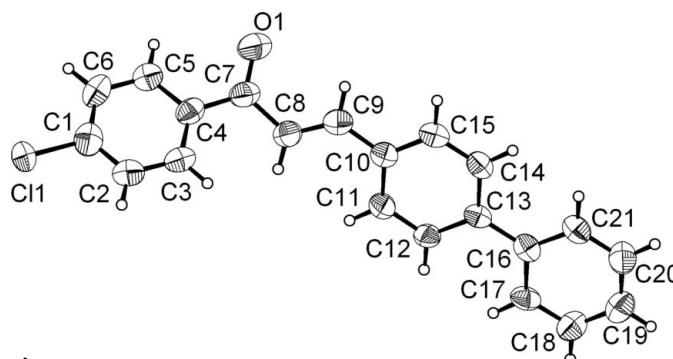
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CommentFor an introduction, see Fischer *et al.* (2007a).

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.*, 2007b).**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 recrystallized from acetone (m.p. 439–441 K). Analysis (%) for C₂₁H₁₅ClO found (calculated): C 76.83 (76.94), H 4.86 (4.92).

Crystal data

C ₂₁ H ₁₅ ClO	V = 1611.4 (10) Å ³
M _r = 318.78	Z = 4
Monoclinic, Cc	Mo Kα radiation
a = 36.723 (14) Å	μ = 0.24 mm ⁻¹
b = 7.303 (3) Å	T = 296 K
c = 6.0172 (16) Å	0.58 × 0.48 × 0.04 mm
β = 93.06 (3)°	

Data collection

Bruker–Nonius KappaCCD diffractometer	7961 measured reflections
Absorption correction: numerical (Herrendorf & Bärnighausen, 1997)	2757 independent reflections
T _{min} = 0.716, T _{max} = 0.940	1756 reflections with I > 2σ(I)
	R _{int} = 0.095

Refinement

R[F ² > 2σ(F ²)] = 0.067	Δρ _{max} = 0.20 e Å ⁻³
wR(F ²) = 0.160	Δρ _{min} = -0.16 e Å ⁻³
S = 1.12	Absolute structure: Flack (1983),
2757 reflections	1263 Friedel pairs
208 parameters	Flack parameter: 0.02 (15)
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: *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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References

Altomare, A., Cascarano, C., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Burla, M. C., Polidori, G., Camalli, M. & Spagna, R. (1997). *SIR97*. University of Bari, Italy.

Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.

Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.

Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.

Fischer, A., Yathirajan, H. S., Ashalatha, B. V., Narayana, B. & Sarojini, B. K. (2007a). *Acta Cryst.* **E63**, o1349–o1350.

Fischer, A., Yathirajan, H. S., Ashalatha, B. V., Narayana, B. & Sarojini, B. K. (2007b). *Acta Cryst.* **E63**, o1355–o1356.

Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.

Herrendorf, W. & Bärnighausen, H. (1997). *HABITUS*. University of Karlsruhe, Germany.

Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Westrip, S. P. (2007). *publCIF*. In preparation.