Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-1-(4-Chlorophenyl)-3-(4-fluorophenyl)-prop-2-en-1-one

Xiao-Yang Qiu,[a]* Zhi-Gang Luo,[b] Sen-Lin Yang[a] and Wei-Sheng Liu[c]

[a]Department of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, People's Republic of China, [b]College of Chemistry and Chemical Engineering, JingGangShan College, Ji'an, JiangXi 343009, People's Republic of China, and [c]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

Correspondence e-mail: xiaoyang_qiu@126.com

Received 11 July 2006
Accepted 20 July 2006

In the title compound, $C_{15}H_{10}ClFO$, the two benzene rings form a dihedral angle of 0.8 (4)°.

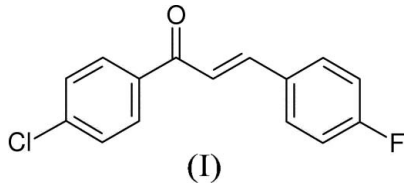
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.087
wR factor = 0.283
Data-to-parameter ratio = 16.8

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

Comment

As an extension of our work on the structural characterization of chalcone derivatives (Qiu, Liu & Zhu, 2006; Qiu, Yang *et al.*, 2006), we report here the structure of the title compound, (I) (Fig. 1). All bond lengths and angles are within normal ranges (Allen *et al.*, 1987), and the dihedral angle between the two benzene rings is 0.8 (4)°.



(I)

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide (10%, 1 ml) was added with overnight stirring to a solution of 4-fluorobenzaldehyde (0.13 g, 1 mmol) and 1-(4-chlorophenyl)-ethanone (0.16 g, 1 mmol) in ethanol (15 ml) at room temperature. The reaction mixture was then poured on to ice and neutralized with hydrochloric acid (5%), causing precipitation of a yellow solid. The solid was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear yellow solution. After keeping the solution in air for 9 d, yellow crystals of (I) were formed at the bottom of the vessel on slow evaporation of the solvent. These were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$. The compound was isolated in 66% yield.

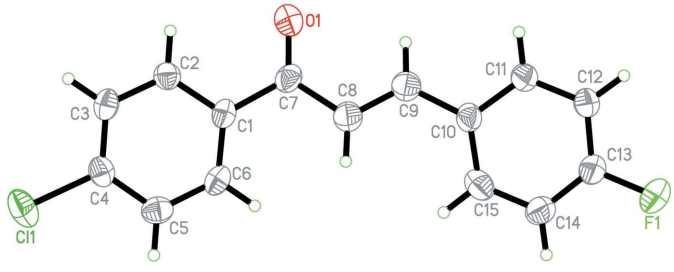


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{15}H_{10}ClFO$	$Z = 4$
$M_r = 260.68$	$D_x = 1.416$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 3.9494$ (8) Å	$\mu = 0.31$ mm^{-1}
$b = 23.305$ (5) Å	$T = 298$ (2) K
$c = 13.388$ (3) Å	Lath, yellow
$\beta = 96.96$ (3)°	0.34 × 0.12 × 0.06 mm
$V = 1223.2$ (5) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7269 measured reflections
ω scans	2742 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1530 reflections with $I > 2\sigma(I)$
$T_{min} = 0.955$, $T_{max} = 0.980$	$R_{int} = 0.041$
	$\theta_{max} = 27.4°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1419P)^2 + 0.7952P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.087$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.283$	$\Delta\rho_{max} = 0.53$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.39$ e Å^{-3}
2742 reflections	
163 parameters	
H-atom parameters constrained	

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2006kj158B.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker. (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Qiu, X.-Y., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o1304–o1305.
Qiu, X.-Y., Yang, S.-L., Liu, W.-S. & Zhu, H. (2006). *Acta Cryst.* E**62**, o1627–o1628.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.