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

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In the title molecule, $C_{16}H_{13}ClO_2$, all bond lengths and angles show normal values. The two benzene rings make a dihedral angle of 21.0 (4)°. The crystal packing is stabilized by van der Waals forces.

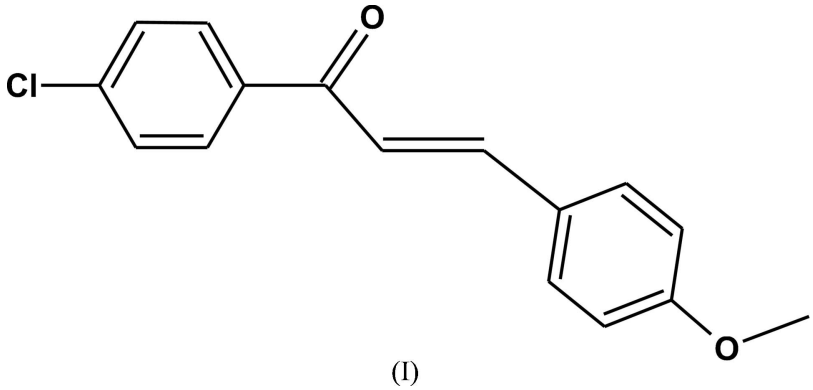
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.099
wR factor = 0.188
Data-to-parameter ratio = 13.6

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

Comment

Chalcone derivatives play an important role in organic chemistry (Song *et al.*, 2002; Christophe *et al.*, 1998; Xu *et al.*, 1996). In a continuation of our work on the structural characterization of chalcone derivatives, we report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987). The C8═C9 bond length of 1.334 (8) Å reveals its double-bond character. The two benzene rings make a dihedral angle of 21.0 (4)°. The crystal packing is stabilized by van der Waals forces.

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide

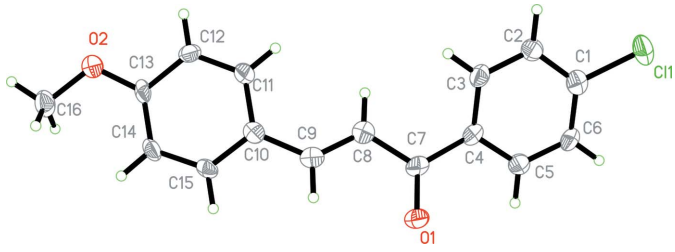


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

(10%, 2 ml) was added with stirring overnight to a solution of 4-methoxybenzaldehyde (2 mmol, 0.27 g) and 1-(4-chlorophenyl)ethanone (2 mmol, 0.31 g) in ethanol (95%, 15 ml) at room temperature. The reaction mixture was then poured into water (10 ml) and neutralized with hydrochloric acid (5%). A yellow solid precipitated from the solution. The solid was dissolved in ethanol (15 ml) and stirred for about 10 min to give a clear solution. After keeping the solution in air for 8 d, yellow block-shaped crystals were formed at the bottom of the vesssl on slow evaporation of the solvent. They were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$. The compound was isolated in 76% yield.

Crystal data

$C_{16}H_{13}ClO_2$
M_r = 272.71
Orthorhombic, $Pna2_1$
a = 12.810 (3) Å
b = 25.693 (5) Å
c = 3.9920 (8) Å
V = 1313.9 (5) Å^3
Z = 4
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2268 reflections
θ = 2.9–26.4°
μ = 0.28 mm^{-1}
T = 298 (2) K
Block, yellow
0.40 × 0.40 × 0.30 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.895, T_{max} = 0.920
5311 measured reflections
2349 independent reflections
2011 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.5°
$h = -15 \rightarrow 13$
$k = -31 \rightarrow 24$
$l = -4 \rightarrow 4$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.099
$wR(F^2)$ = 0.188
S = 1.34
2349 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 1.5662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 940 Friedel pairs
Flack parameter: 0.2 (2)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.205 (7)	C7—C8	1.473 (8)
O2—C13	1.350 (7)	C8—C9	1.334 (8)
O2—C16	1.417 (8)	C9—C10	1.460 (8)
C4—C7	1.488 (8)		
O1—C7—C8	121.2 (6)	C9—C8—C7	121.2 (6)
O1—C7—C4	120.5 (6)	C8—C9—C10	129.8 (6)
C8—C7—C4	118.3 (5)		

All H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and C—H = 0.96 Å for the aliphatic H atoms) and were refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The Cl atom has only moderate anomalous scattering, leading to a low precision for the Flack (1983) parameter.

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

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