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(*E*)-3-(2-Methoxyphenyl)-1-(4-nitrophenyl)-prop-2-en-1-one

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The molecule of the title compound, $C_{16}H_{13}NO_4$, is almost planar and displays a *trans* configuration with respect to the C=C double bond. The crystal packing is stabilized by weak π–π stacking interactions.

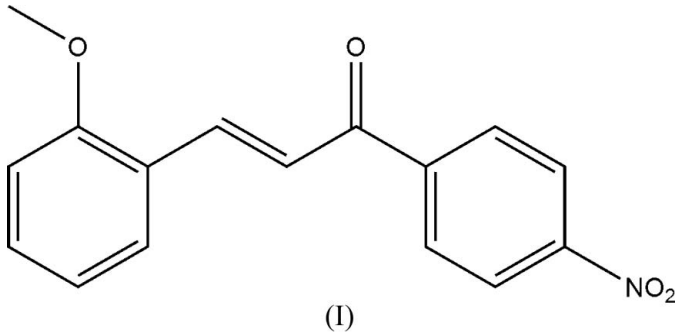
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.078
wR factor = 0.216
Data-to-parameter ratio = 13.9

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). In the title compound, (I) (Fig. 1), most of the bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The C8=C9 bond length of 1.321 (5) Å conforms to that expected for a carbon–carbon double bond. The C7—C8 bond length of 1.460 (6) Å is somewhat shortened compared to the normal value for a C—C single bond, presumably due to conjugation effects in the molecule. The dihedral angle between the least-squares planes of the two benzene rings is 5.64 (19)°.



(I)

In the crystal structure of (I), a weak π–π stacking interaction occurs between the C1- and C10^{i}-containing benzene rings [symmetry code: (i) $1-x, 2-y, 2-z$], with a centroid–centroid separation of 3.816 (3) Å

Experimental

An aqueous solution of potassium hydroxide (10%, 2 ml) was added with stirring overnight to a solution of 2-methoxybenzaldehyde (2 mmol, 0.27 g) and 1-(4-nitrophenyl)ethanone (2 mmol, 0.33 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. This was dissolved in acetone (15 ml) and stirred for about 10 min, giving a clear solution. After allowing this solution to stand in air for 7 d, yellow block-shaped crystals of (I) 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 82% yield.

Crystal data

$C_{16}H_{13}NO_4$
M_r = 283.27
Orthorhombic, *Pbca*
a = 7.4880 (8) Å
b = 12.1608 (11) Å
c = 30.347 (2) Å
V = 2763.4 (4) Å^3
Z = 8
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, yellow
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.962, T_{max} = 0.990
3056 measured reflections
2663 independent reflections
1105 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.216
S = 1.00
2663 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.086P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

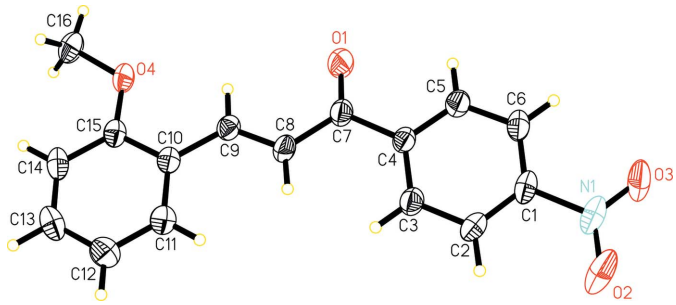


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

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