Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Ji-Long Ma

Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China

Correspondence e-mail: fuyangqiu_2007@126.com

Received 11 January 2007
Accepted 11 January 2007

The title molecule, $C_{16}H_{13}NO_4$, crystallizes with two molecules in the asymmetric unit. The dihedral angles between the two benzene rings are 5.1 (2) and 6.2 (2)°.

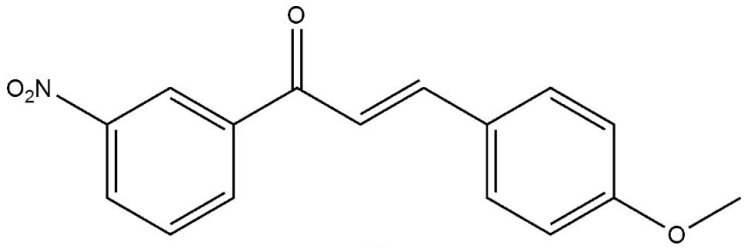
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.088
wR factor = 0.205
Data-to-parameter ratio = 13.7

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

Comment

We have recently reported the synthesis and crystal structure of the chalcone derivative (*E*)-3-(2-methoxyphenyl)-1-(4-nitrophenyl)prop-2-en-1-one (Ma, 2007). We now report similar data for its isomer, the title compound, (I).



(I)

Compound (I) crystallizes with two unique molecules in the asymmetric unit (Fig. 1). Most bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The C8═C9 and C24═C25 bond lengths [1.339 (7) and 1.319 (7) Å, respectively] conform to the value expected for a carbon–carbon double bond. The C7—C8 and C23—C24 bond lengths [1.457 (7) and 1.455 (7) Å, respectively] are shortened somewhat compared to a typical C—C single bond, due to conjugation effects in the molecule. The dihedral angles between the least-squares planes of the two benzene rings are 5.1 (2)° for C1–C6 and C10–C15 and 6.2 (2)° for C17–C22 and C26–C31.

Several weak π–π stacking interactions appear to stabilize the crystal packing of (I). All four benzene rings are involved, and the centroid-centroid separations vary between 3.847 (3) and 4.000 (3) Å.

Experimental

An aqueous solution of potassium hydroxide (10%, 2 ml) was added with stirring overnight to a solution of 4-methoxybenzaldehyde (2 mmol, 0.27 g) and 1-(3-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 the solution to stand in air for 10 d, yellow block-shaped crystals of (I) formed at the bottom of the vessel 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

$C_{16}H_{13}NO_4$
M_r = 283.27
Monoclinic, $P2_1/c$
a = 13.252 (3) Å
b = 15.431 (3) Å
c = 13.974 (3) Å
β = 110.62 (3)°
V = 2674.5 (9) Å^3
Z = 8
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.980, T_{max} = 0.990
5459 measured reflections
5229 independent reflections
1760 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.088
$wR(F^2)$ = 0.205
S = 0.99
5229 reflections
381 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and 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*.

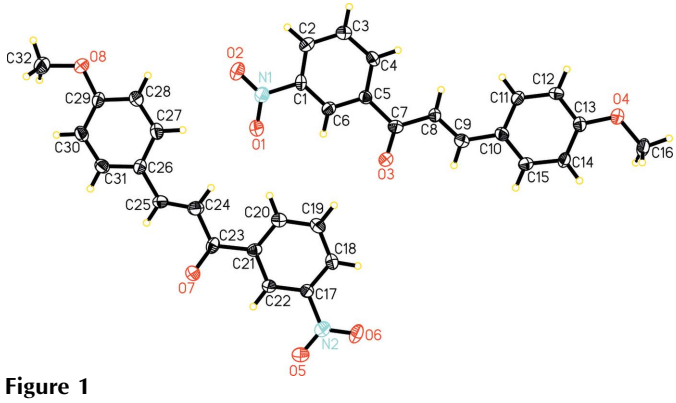


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

The author thanks the Education Office of Anhui Province, China, for a 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 (2001). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Ma, J.-L. (2007). *Acta Cryst.* E**63**, o806–o807.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.