Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(3,5-Dimethoxyphenyl)-1-(3-nitrophenyl)-prop-2-enone

Xiao-Yang Qiu* and Sen-Lin Yang

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

Correspondence e-mail: xiaoyang_qiu@126.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.142
Data-to-parameter ratio = 14.0

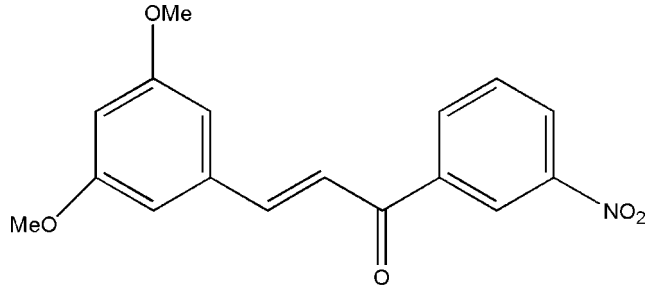
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 2 October 2006
Accepted 20 November 2006

In the title molecule, $C_{17}H_{15}NO_5$, all bond lengths and angles show normal values. There are two molecules in the asymmetric unit. The dihedral angles between the benzene rings are 9.0 (2) and 11.7 (2)° in the two molecules. The crystal packing is stabilized by van der Waals forces.

Comment

Recently, we have reported a few chalcone derivatives (Qiu & Yang *et al.*, 2006; Qiu & Liu *et al.*, 2006). As an extension of our work on the structural characterization of chalcone derivatives, the title compound, (I), is reported here (Fig. 1).



(I)

The asymmetric unit of (I) consists of two independent molecules. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angles between the benzene rings are 9.0 (2) and 11.7 (2)° in the two molecules. The crystal structure is stabilized by van der Waals forces.

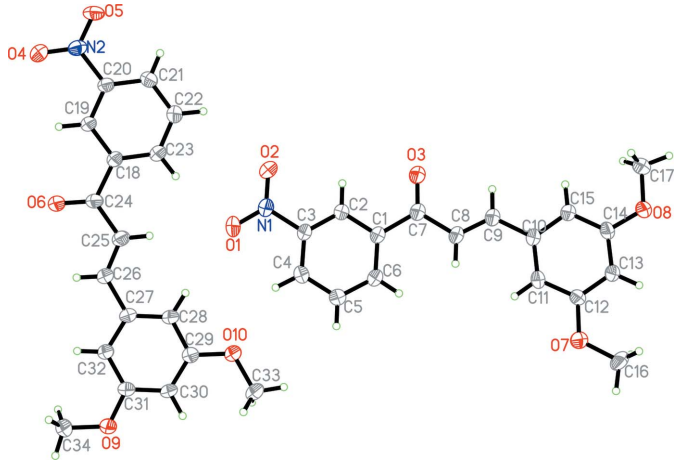


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide (10%, 1 ml) was added with stirring overnight to a solution of 3,5-dimethoxybenzaldehyde (1 mmol, 0.17 g) and 1-(3-nitrophenyl)-ethanone (1 mmol, 0.17 g) in ethanol (15 ml) at room temperature. The reaction mixture was then poured on to ice and neutralized with hydrochloric acid (5%). A yellow solid precipitated from the solution. The solid was dissolved in acetone (14 ml) and stirred for about 10 min to give a clear yellow solution. After allowing the solution to stand in air for 10 d, yellow block-shaped crystals formed at the bottom of the vessel by slow evaporation of the solvent. These were collected, washed three times with acetone and dried in a vacuum desiccator with anhydrous $CaCl_2$. The compound was isolated in 72% yield.

Crystal data

$C_{17}H_{15}NO_5$	$Z = 8$
$M_r = 313.30$	$D_x = 1.388$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 8.2658$ (3) Å	$\mu = 0.10$ mm^{-1}
$b = 15.8334$ (4) Å	$T = 298$ (2) K
$c = 22.9084$ (7) Å	Block, yellow
$\beta = 90.747$ (2)°	0.28 × 0.17 × 0.06 mm
$V = 2997.90$ (16) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	16559 measured reflections
	5873 independent reflections
ω scans	2540 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.054$
	$\theta_{max} = 26.0°$
$T_{min} = 0.975$, $T_{max} = 0.991$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.052$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.142$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 0.86$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
5873 reflections	Extinction correction: *SHELXL97*
420 parameters	Extinction coefficient: 0.00053 (17)
H-atom parameters constrained	

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 and 0.96 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$.

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* (Bruker, 1997); 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 (1997). *SHELXTL*, Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
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.