Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Furyl)-1-(4-methoxyphenyl)prop-2-en-1-one

Jeannie Bee-Jan Teh,[a] P. S. Patil,[b] Hoong-Kun Fun,[a]* Ibrahim Abdul Razak,[a] Venkataraya Shettigar[b] and S. M. Dharmaprakash[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.065
wR factor = 0.180
Data-to-parameter ratio = 20.8

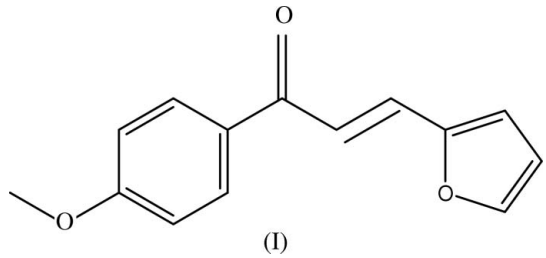
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 March 2006
Accepted 16 March 2006

In the title molecule, $C_{14}H_{12}O_3$, the dihedral angle between the benzene and furan rings is 9.22 (7)°. The crystal structure is stabilized by $\pi\cdots\pi$ and by C–H$\cdots\pi$ interations.

Comment

Chalcone and its derivatives are an important class of chemical compounds which are being studied extensively because of their significant use or applications in various sectors. The interest in these substances, for several disciplines, lies in their biological activities, including antifungal (Boeck *et al.*, 2005) and anticoagulant properties (Shuib *et al.*, 1999). The compounds are also used as depigmenting agents (Khatib *et al.*, 2005). In the field of organic non-linear optics (NLO), chalcone derivatives are significant materials for their excellent blue light transmittance (Fichou *et al.*, 1988; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*), much better than that observed in inorganic crystals. In view of these features associated with chalcones, the structure determination of the title compound, (I), was undertaken. The crystal does not exhibit second-order NLO properties as it crystallizes in a centrosymmetric space group.



(I)

A molecular view of (I) is shown in Fig. 1. Bond lengths and angles display normal values (Allen *et al.*, 1987), comparable with related structures (Sathiya Moorthi, Chinnakali, Nanjundan, Santhi *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Ravishankar *et al.*, 2005; Teh *et al.*, 2006; Patil *et al.*, 2006*a*,*b*; Ng *et al.*, 2006; Rosli *et al.*, 2006). The least-squares plane through the enone fragment makes dihedral angles of 12.60 (9) and 15.45 (7)° with the C1–C4/O1 and C8–C13 rings, respectively. The dihedral angle between the rings is 9.22 (7)°. The methoxy group attached at C11 is essentially coplanar with the C8–C13 benzene ring.

The crystal structure is stabilized by π–π interactions involving the C1–C4/O1 ring at (x, y, z) and the C8–C13 ring at ($-1+x$, y, z); the centroid–centroid distance is 3.6535 (10) Å. The crystal structure is further stabilized by C—H$\cdots\pi$ interations (Table 1) involving the C1–C4/O1 and C8–C13 rings.

Experimental

Compound (I) was synthesized by the Claisen–Schmidt condensation of 2-furfuraldehyde (0.01 mol) with 4-methoxyacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (2 ml, 30%). After stirring for 3 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand for 24 h. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. The purity of the compound was checked by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction experiments were grown by slow evaporation of an acetone solution.

Crystal data

$C_{14}H_{12}O_3$
$M_r = 228.24$
Monoclinic, $P2_1/c$
$a = 7.3872\ (4)$ Å
$b = 18.8794\ (10)$ Å
$c = 10.3992\ (4)$ Å
$\beta = 130.156\ (3)^\circ$
$V = 1108.48\ (9)$ Å^3
$Z = 4$
$D_x = 1.368$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5995 reflections
$\theta = 2.2$–30.0°
$\mu = 0.10$ mm^{-1}
$T = 100.0\ (1)$ K
Block, orange
0.49 × 0.34 × 0.33 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.759$, $T_{max} = 0.969$
21915 measured reflections
3231 independent reflections
2663 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 30.0^\circ$
$h = -10 \rightarrow 10$
$k = -26 \rightarrow 26$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.180$
$S = 1.10$
3231 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 0.6622P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···$Cg1^{i}$	0.93	2.65	3.477 (2)	148
C14—H14B···$Cg2^{ii}$	0.96	2.83	3.587 (2)	136

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$. $Cg1$ and $Cg2$ are the centroids of the C1–C4/O1 and C8–C13 rings, respectively.

H atoms were placed in calculated positions, with C—H distances of 0.93 or 0.96 Å. The U_{iso}(H) values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for Scientific Advancement Grant Allocation (SAGA) No. 304/PFIZIK/653003/A118 and USM short-term grant No. 304/PFIZIK/635028.

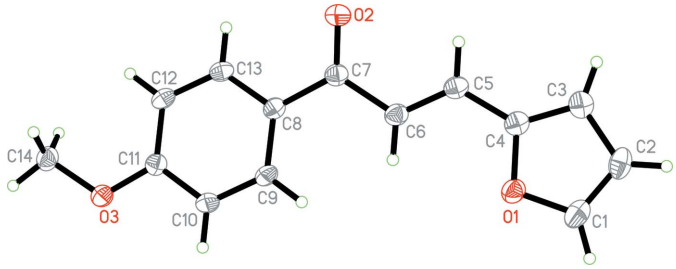


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii.

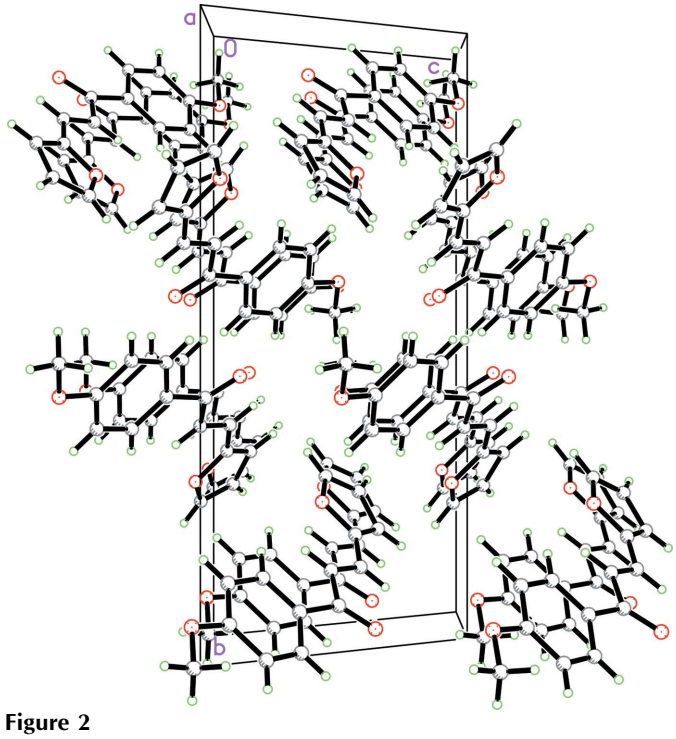


Figure 2
The crystal packing of (I), viewed along the *a* axis.

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.
Boeck, P., Leal, P. C., Yunes, R. A., Filho, V. C., Lopez, S., Sortino, M., Escalante, A., Furlan, R. L. E. & Zacchino, S. (2005). *Arch. Pharm. Chem. Life Sci.* **338**, 87–95.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn. J. Appl. Phys.* **27**, L429–L430.
Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Khatib, S., Nerya, O., Musa, R., Shmuel, M., Tamir, S. & Vaya, J. (2005). *Bioorg. Med. Chem.* **13**, 433–441.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Ng, S. L., Patil, P. S., Razak, I. A., Fun, H.-K. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o893–o895.
Patil, P. S., Teh, J. B. J., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006*a*). *Acta Cryst.* E**62**, o896–o898.
Patil, P. S., Teh, J. B. J., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006*b*). *Acta Cryst.* E**62**. Submitted.

Ravishankar, T., Chinnakali, K., Nanjundan, S., Selvam, P., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o405–o407.
Rosli, M. M., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o1466–o1468.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Radhika, R., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o480–o482.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Santhi, R. & Fun, H.-K. (2005). *Acta Cryst.* E**61**, o3514–o3516.
Sathiya Moorthi, S., Chinnakali, K., Nanjundan, S., Unnithan, C. S., Fun, H.-K. & Yu, X.-L. (2005). *Acta Cryst.* E**61**, o483–o485.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Shuib, N. S., Sam, T. W., Wong, K. C., Chinnakali, K. & Fun, H.-K. (1999). *Acta Cryst.* C**55**, 576–578.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Teh, J. B. J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o890–o892.
Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abdureyim, A. & Watanebe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **314**, 135–140.