Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Methyl 3-(4-methoxyphenyl)prop-2-enoate

Maciej Bujak,[a] Jacek Zaleski,[a]* Victor Prezhdo[b] and Boris Uspenskiy[c]

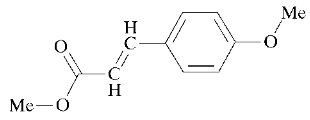
[a]Institute of Chemistry, University of Opole, Oleska 48, 45-052 Opole, Poland, [b]Institute of Chemistry, Jan Kochanowski University, Chęcińska 5, 25-020 Kielce, Poland, and [c]Department of Chemistry, Kharkov Politechnic University, Frunze 21, 61-002 Kharkov, Ukraine
Correspondence e-mail: zaleski@uni.opole.pl

Received 2 July 2001
Accepted 14 November 2001
Online 16 January 2002

The title molecule, $C_{11}H_{12}O_3$, is almost planar, with an average deviation of the C and O atoms from the least-squares plane of 0.146 (4) Å. The geometry about the C═C bond is *trans*. The phenyl ring and –$COOCH_3$ group are twisted with respect to the double bond by 9.3 (3) and 5.6 (5)°, respectively. The endocyclic angle at the junction of the propenoate group and the phenyl ring is decreased from 120° by 2.6 (2)°, whereas two neighbouring angles around the ring are increased by 2.3 (2) and 0.9 (2)°. This is probably associated with the charge-transfer interaction of the phenyl ring and –$COOCH_3$ group through the C═C double bond. The molecules are joined together through C—H···O hydrogen bonds between the methoxy and ester groups to form characteristic zigzag chains extended along the *c* axis.

Comment

The properties and structure of cinnamic acid and its derivatives, together with their donor–acceptor complexes with other organic compounds, have been reported by a number of workers. One of the major reasons for investigations of these compounds is to analyse their intermolecular hydrogen-bonding interactions from the point of view of crystal engineering, *i.e.* the design of new materials with particular chemical and physical properties (Nakanishi & Sasada, 1978; Bryan & White, 1982; Desiraju & Sarma, 1983; Desiraju *et al.*, 1984; Desiraju & Sharma, 1991). It was found that intermolecular interactions, even weak hydrogen bonds, may play a major role in the self-assembly of molecules in crystals, in their specific molecular architecture and in their properties. The analysis of intermolecular interactions, their strengths and their specific geometries may reveal structural features which govern the self-assembly of those molecules, which seems to be very important for the design of new materials. It was found that C—H···O hydrogen bonds may organize molecules into different patterns. Five different C—H···O hydrogen-bond patterns in the structures of organic nitro compounds have been studied by Sharma & Desiraju (1994). Recently, zero-, one-, two- and three-dimensional schemes of the same type of hydrogen bonds have been reported for diaryl sulfones (Glidewell *et al.*, 2001). In the light of this work, we have established the structure of the title compound, (I).



(I)

The molecule of (I) (Fig. 1) is nearly planar. The largest deviations from the least-squares plane are observed for C2 [0.208 (2) Å], C10 [0.252 (4) Å], C11 [0.266 (3) Å] and O2 [0.181 (3) Å], and the average deviation of non-H atoms from the least-squares plane is 0.146 (4) Å. The torsion angles which most significantly deviate from 0 or 180° are C6—C1—C7—C8 and C2—C1—C7—C8 [8.7 (3)°], and C7—C8—C9—O2 and C7—C8—C9—O1 [5.2 (5)°] (Table 1). This corresponds with the twists of the phenyl ring and –$COOCH_3$ group with respect to the C8═C7 double bond of 9.3 (3) and 5.6 (5)°, respectively (Fig. 1).

The C1—C2 bond is elongated, whereas the C2—C3 bond is shortened. The C6—C1—C2 angle is significantly diminished from 120°, whereas two neighbouring angles, C5—C6—C1 and C3—C2—C1, are increased by 2.3 (2) and 0.9 (2)°, respectively, from 120°. This is probably associated with the charge-transfer interaction of the phenyl ring and –$COOCH_3$ group through the C7═C8 double bond (Domenicano *et al.*, 1975*a*,*b*). The asymmetry of the exocyclic angles at atoms C1 and C4 agrees quite well with the values found in similar structures (Domiano *et al.*, 1979).

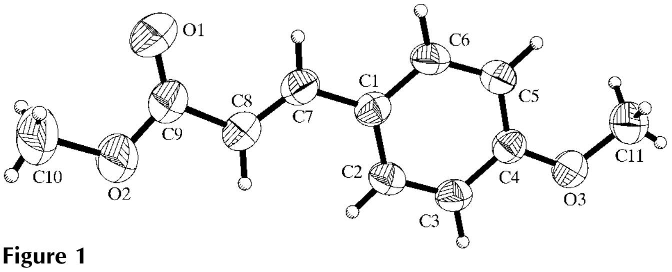


Figure 1
A view of the molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

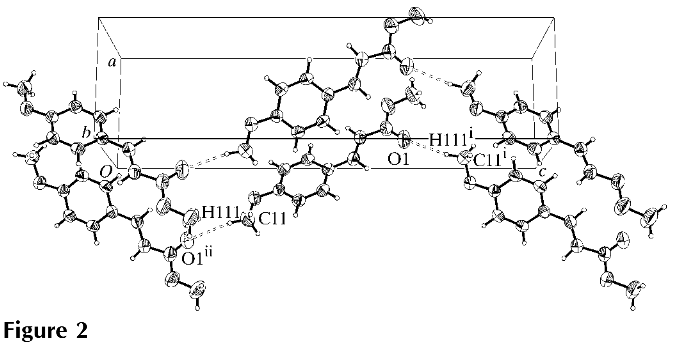


Figure 2
The crystal structure of (I) showing the formation of the zigzag chains [symmetry codes: (i) $-x-\frac{1}{2}, y, z+\frac{1}{2}$; (ii) $-x-\frac{1}{2}, y, z-\frac{1}{2}$].

DOI: 10.1107/S0108270101019539

The geometry of the methoxy group is governed by the repulsion between the C11 methyl group and the aromatic ring, leading to an enlargement of the O3—C4—C5 angle and a reduction of O3—C4—C3. Similar repulsion between the C10 methyl group and O1, and between O1 and C7—H7, leads to enlargements of the O1—C9—O2 and O1—C9—C8 angles, respectively. At the same time, the O2—C9—C8 angle decreases to 111.1 (2)°. Like the methoxy group, the C9—O2—C10 angle is smaller than 120°, resulting in repulsion between two lone pairs on O2 and the neighbouring atoms.

The repulsion between C8—H8 and C2—H2 leads to enlargement of the C8—C7—C1 and C2—C1—C7 angles. The length of C7═C8 is typical for complexes of cinnamic acid (Iwamoto *et al.*, 1989; Iwamoto & Kashino, 1990).

The molecules of (I) are joined head-to-tail through a C—H···O hydrogen bond between the methoxy and ester groups (Table 2), forming characteristic zigzag chains along the *c* axis (Fig. 2). The molecules are piled up along the *a* axis to form two parallel plane-to-plane stacks, overlapping to form columns. The angle between molecules from neighbouring stacks is 50.4 (1)°.

Experimental

The title compound was obtained from the *para*-methoxy derivative of cinnamic acid (chemically pure, NPO Bohimreaktiv, Russia) according to the literature procedure of Fischer & Speier (1895). Crystals of (I) were grown from a methanol solution by slow evaporation.

Crystal data

$C_{11}H_{12}O_3$
$M_r = 192.21$
Orthorhombic, $Pca2_1$
$a = 6.203\ (1)$ Å
$b = 7.259\ (1)$ Å
$c = 22.657\ (5)$ Å
$V = 1020.2\ (3)$ Å^3
$Z = 4$
$D_x = 1.251$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 44 reflections
$\theta = 6$–$17°$
$\mu = 0.09$ mm^{-1}
$T = 295\ (2)$ K
Pillar, colourless
0.6 × 0.6 × 0.5 mm

Data collection

Kuma KM-4 diffractometer
ω/θ scans
2911 measured reflections
1521 independent reflections
1142 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\rm max} = 30.1°$

$h = -8 \rightarrow 8$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 31$
2 standard reflections every 50 reflections intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.119$
$S = 1.03$
1521 reflections
127 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.0319P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.16$ e Å^{-3}

H atoms were treated as riding, with C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *Kuma Diffraction Software* (Kuma, 1996); cell refinement: *Kuma Diffraction Software* (Kuma, 1996); data reduction: *Kuma Diffraction Software* (Kuma, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990).

Table 1
Selected geometric parameters (Å, °).

C4—O3	1.357 (2)	C10—O2	1.452 (4)
C9—O1	1.194 (3)	C11—O3	1.418 (3)
C9—O2	1.324 (3)		
C4—O3—C11	118.1 (2)	O2—C9—C8	111.1 (2)
C9—O2—C10	116.2 (2)	O3—C4—C3	115.6 (2)
O1—C9—C8	125.7 (2)	O3—C4—C5	125.0 (2)
O1—C9—O2	123.2 (3)		
C6—C1—C7—C8	−170.1 (2)	C7—C8—C9—O2	−174.0 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H111···O1$^{\rm i}$	0.96	2.39	3.336 (4)	170

Symmetry code: (i) $-\frac{1}{2} - x, y, z - \frac{1}{2}$.

MB is a holder of the scholarship 'The Annual Stipend for Young Scientists' of The Foundation for Polish Science in 2001.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1531). Services for accessing these data are described at the back of the journal.

References

Bryan, R. F. & White, D. H. (1982). *Acta Cryst.* B**38**, 1332–1334.

Desiraju, G. R., Kamala, R., Kumari, B. H. & Sarma, J. A. R. P. (1984). *J. Chem. Soc. Perkin Trans.* 2, pp. 181–189.

Desiraju, G. R. & Sarma, J. A. R. P. (1983). *J. Chem. Soc. Chem. Commun.* pp. 45–46.

Desiraju, G. R. & Sharma, C. V. K. M. (1991). *J. Chem. Soc. Chem. Commun.* pp. 1239–1241.

Domenicano, A., Vaciago, A. & Coulson, C. A. (1975*a*). *Acta Cryst.* B**31**, 221–234.

Domenicano, A., Vaciago, A. & Coulson, C. A. (1975*b*). *Acta Cryst.* B**31**, 1630–1641.

Domiano, P., Nardelli, M., Balsamo, A., Macchia, B. & Macchia, F. (1979). *Acta Cryst.* B**35**, 1363–1372.

Fischer, E. & Speier, A. (1895). *Ber. Dtsch Chem. Ges.* **28**, 3252–3257.

Glidewell, C., Harrison, W. T. A., Low, J. N., Sime, J. G. & Wardell, J. L. (2001). *Acta Cryst.* B**57**, 190–200.

Iwamoto, T. & Kashino, S. (1990). *Acta Cryst.* C**46**, 686–688.

Iwamoto, T., Kashino, S. & Haisa, M. (1989). *Acta Cryst.* C**45**, 1753–1758.

Kuma (1995). *Kuma Diffraction Software*. Version 9.0. Kuma Diffraction, Wrocław, Poland.

Kuma (1996). *Kuma Diffraction Software*. Version 8.1.0. Kuma Diffraction, Wrocław, Poland.

Nakanishi, H. & Sasada, Y. (1978). *Acta Cryst.* B**34**, 332–335.

Sharma, C. V. K. & Desiraju, G. R. (1994). *J. Chem. Soc. Perkin Trans.* 2, pp. 2345–2352.

Sheldrick, G. M. (1992). *SHELXTL*. Version 4.3. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.