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

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Key indicators

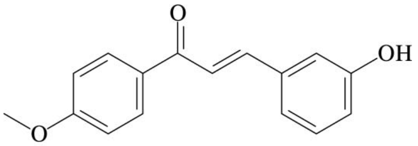
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.055
wR factor = 0.169
Data-to-parameter ratio = 12.6

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

The title compound, $C_{16}H_{14}O_3$, crystallizes in the triclinic system, with two independent molecules in the asymmetric unit; these are related by a non-crystallographic twofold rotation axis. The two molecules differ slightly in the relative orientation of the two aromatic rings. They are linked by C—H···π interactions to form a dimer and O—H···O hydrogen bonds link the dimers into chains along the *c* axis. C—H···π interactions interlink the chains into a three-dimensional network.

Comment

Chalcones and their analogues are relatively easily available, not only by isolation from natural products but also by the methods of classical and combinatorial synthesis. Chalcones are being considered as anticancer agents, since they are natural compounds that are particularly cytotoxic towards K562 leukemia or melanoma cells (Sabzevari *et al.*, 2004). The cytotoxic, anticancer, chemopreventative and mutagenic properties of a number of chalcones have been reviewed by Dimmock *et al.* (1999). The antibacterial, fungistatic and fungicidal properties of these compounds have been reviewed by Opletalova (2000) and Opletalova & Sedivy (1999). Chalcones and their analogues are used as potential therapeutic agents in diseases of the cardiovascular system (Opletalova *et al.*, 2003). Photo-cross-linkable polymers having the chalcone moiety act as negative photoresist materials used in a wide variety of applications (Balaji *et al.*, 2003). Chalcones are also used in designing effective second-order non-linear optical materials (Zhao *et al.*, 2000). The structure determination of the title compound, (I), was undertaken as part of our study of chalcones.



(I)

The asymmetric unit of (I) consists of two independent molecules which are related by a non-crystallographic twofold rotation axis. A displacement ellipsoid plot of the two independent molecules, *A* and *B*, is shown in Fig. 1. In both molecules, the methyl group is disordered over two different orientations, related by an approximately 180° rotation around the O3—C13 bond. The corresponding bond lengths and angles of the two molecules agree with each other and are comparable with those reported for the related structures 1-(4-chlorophenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one (Ravi-

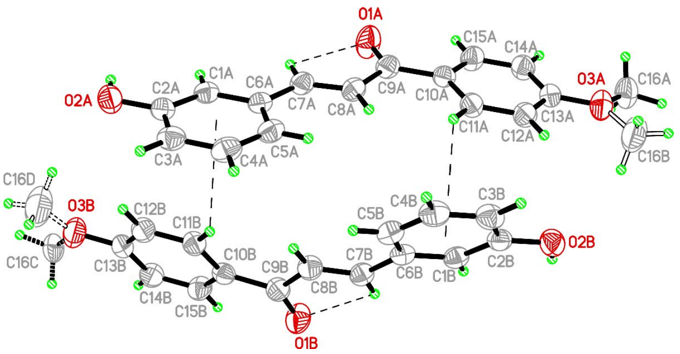


Figure 1
The structures of the two independent molecules of (I), showing the atomic numbering scheme and 30% probability displacement ellipsoids. Methyl groups are disordered with half-occupancy. Intramolecular hydrogen bonds and C—H···π interactions are shown as dashed lines.

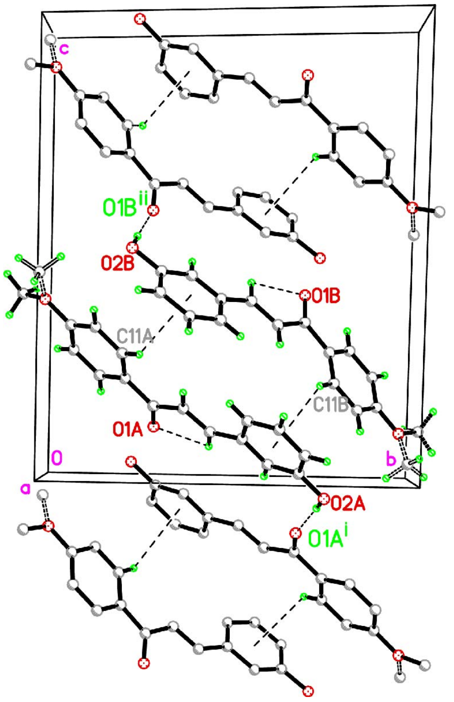


Figure 2
A view of the C—H···π hydrogen-bonded dimers and O—H···O hydrogen-bonded chain formation. All the intra- and intermolecular interactions are shown as dashed lines.

shankar *et al.*, 2005) and 1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (Sathiya Moorthi *et al.*, 2005). The short H···H contacts which cause the narrowing or widening of neighbouring C—C—C angles from the normal value of 120° are H5*A*···H8*A* (2.27 Å), H5*B*···H8*B* (2.33 Å), H8*A*···H11*A* (2.11 Å) and H8*B*···H11*B* (2.14 Å). A significant conformational difference is observed between molecules *A* and *B*, in that the dihedral angle between the two aromatic rings is 6.3 (1)° in molecule *A*, whereas in molecule *B* the angle is 20.8 (1)°. The non-H atoms of the methoxy groups are almost coplanar with the attached rings.

In the molecular structure, each of the C7*A*—H7*A*···O1*A* and C7*B*—H7*B*···O1*B* interactions generates an *S*(5) ring motif. In the asymmetric unit, the *A*/*B* pair is linked by C—H···π intermolecular interactions (C11*A*—H11*A*···*Cg*2 and C11*B*—H11*B*···*Cg*1, where *Cg*1 and *Cg*2 are the centroids of rings C1*A*–6*A* and C1*B*–C6*B*, respectively), forming a dimer. In the crystal structure, the inversion-related dimers are linked by O2*A*—H2*A*···O1*A*$^{\rm i}$ and O2*B*—H2*B*···O1*B*$^{\rm ii}$ (symmetry codes are as given in Table 2) hydrogen bonds, forming a chain along the *c* axis (Fig. 2). The chain structure is further stabilized by weak C—H···O interactions (Table 2), whose geometry agrees with those reported by Jeffrey (1997) and Desiraju & Steiner (1999). Adjacent chains are interlinked by weak C—H···π interactions, forming a three-dimensional network (Table 2). Part of the network is shown in Fig. 3.

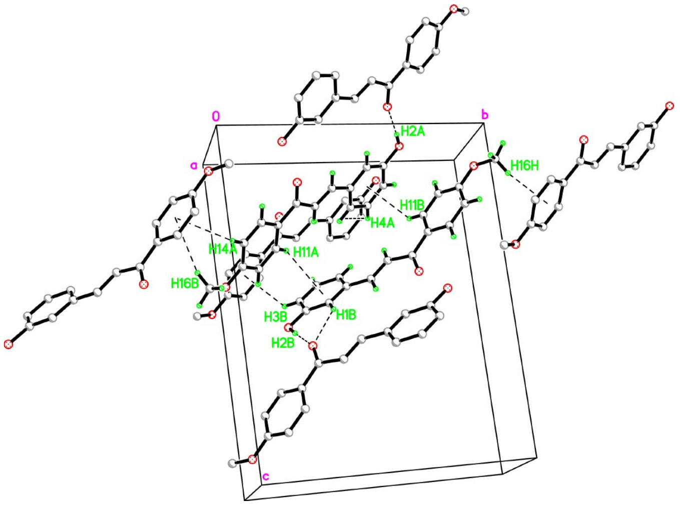


Figure 3
Part of the crystal packing of (I), showing O—H···O, C—H···O and C—H···π interactions as dashed lines. Only the H atoms involved in the interactions are labelled.

Experimental

The title compound was obtained by stirring a mixture of 4-methoxyacetophenone (4.15 g, 0.03 mol), 3-hydroxybenzaldehyde (3.66 g, 0.03 mol), a 20% solution of NaOH and ethanol at 273 K for 24 h, and neutralizing the mixture with dilute hydrochloric acid. The crude product was recrystallized from ethanol.

Crystal data

$C_{16}H_{14}O_3$
$M_r = 254.27$
Triclinic, $P\overline{1}$
$a = 5.6459$ (9) Å
$b = 13.973$ (2) Å
$c = 16.875$ (3) Å
$\alpha = 88.517$ (3)°
$\beta = 85.574$ (3)°
$\gamma = 81.742$ (3)°
$V = 1313.4$ (4) Å^3
$Z = 4$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3262 reflections
$\theta = 2.4$–26.7°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.50 × 0.41 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.957$, $T_{\rm max} = 0.972$
9588 measured reflections
4603 independent reflections
3571 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\rm max} = 25.0$°
$h = -6 \rightarrow 6$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 20$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.169$
$S = 1.04$
4603 reflections
365 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1135P)^2 + 0.018P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected torsion angles (°).

C16*B*—O3*A*—C13*A*—C12*A*	4.3 (5)	C16*D*—O3*B*—C13*B*—C12*B*	−3.8 (6)
C16*A*—O3*A*—C13*A*—C14*A*	−5.0 (4)	C16*C*—O3*B*—C13*B*—C14*B*	3.6 (4)

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C1*A*–C6*A*, C1*B*–C6*B*, C10*A*–C15*A* and C10*B*–C15*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7*A*—H7*A*···O1*A*	0.93	2.40	2.758 (2)	102
C7*B*—H7*B*···O1*B*	0.93	2.39	2.752 (2)	103
C11*A*—H11*A*···*Cg*2	0.93	3.10	3.812 (2)	134
C11*B*—H11*B*···*Cg*1	0.93	2.97	3.666 (2)	133
O2*A*—H2*A*···O1*A*^{i}	0.82	1.92	2.737 (2)	175
O2*B*—H2*B*···O1*B*^{ii}	0.82	1.93	2.747 (2)	176
C1*B*—H1*B*···O1*B*^{ii}	0.93	2.53	3.234 (2)	132
C16*A*—H16*A*···O2*B*^{iii}	0.96	2.56	3.424 (5)	149
C3*B*—H3*B*···*Cg*3^{iv}	0.93	2.96	3.644 (2)	131
C4*A*—H4*A*···*Cg*4^{iv}	0.93	3.10	3.683 (2)	122
C14*A*—H14*A*···*Cg*4^{v}	0.93	3.11	3.917 (2)	146
C16*A*—H16*B*···*Cg*4^{v}	0.96	3.06	3.939 (5)	152
C16*C*—H16*H*···*Cg*3^{vi}	0.96	2.88	3.697 (5)	144

Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $1-x, 1-y, 1-z$; (iii) $2-x, -y, 1-z$; (iv) $1+x, y, z$; (v) $x, y-1, z$; (vi) $x-1, 1+y, z$.

In both molecules, the methyl group was found to be disordered over two orientations related by an approximate 180° rotation around the O3—C13 bond. The site occupancies of the disordered positions C16*A*/C16*B* and C16*C*/C16*D* were initially refined to 0.547 (5)/0.453 (5) and 0.578 (8)/0.422 (5), respectively, and later fixed at 0.5 as the disordered atoms lie close to inversion centres. Corresponding bond lengths in the disordered components were restrained to be equal and the displacement parameters of the disordered atoms were approximated to isotropic behaviour. H atoms were placed in idealized positions and constrained to ride on their parent atoms, with O—H = 0.82 Å, C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2 or 1.5 times U_{eq} of the carrier atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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