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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 17.2

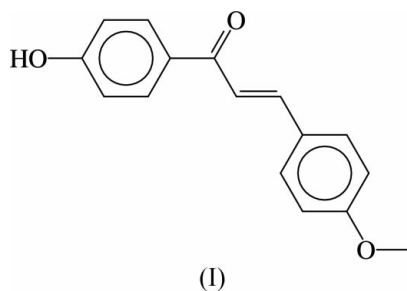
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

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

The title molecule, $\text{C}_{16}\text{H}_{14}\text{O}_3$, is slightly distorted from planarity, the dihedral angle between the two benzene rings being $9.51(7)^\circ$. The configuration of the keto group with respect to the olefinic double bond is *s-cis*. $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, and $\text{C}-\text{H}\cdots\text{O}$ and $\pi-\pi$ interactions, link the molecules to form a three-dimensional network. The $\text{C}-\text{H}\cdots\text{O}$ interactions form rings of graph-set motifs $S(5)$, $R_2^1(6)$ and $R_2^1(7)$.

Comment

Chalcones and their heterocyclic analogues exhibit anti-inflammatory, antitumour (Shibata, 1994; Xia *et al.*, 2000), antibacterial, antifungal (Gafner *et al.*, 1996; Popova *et al.*, 2001), antitubercular, antiviral, antiprotozoal and gastro-protective (Opletalova & Sedivy, 1999) activities. The different bioactivities of a variety of chalcones have been reviewed by Dimmock *et al.* (1999). Hydroxychalcones can be readily reacted with acryloyl and methacryloyl chloride to obtain acrylate and methacrylate monomers, which are useful for the preparation of photo-cross-linkable polymers (Subramanian *et al.*, 2001; Balaji & Nanjundan, 2002). The structure determination of the title compound, (I), was undertaken as part of our study of chalcones.



In the title molecule, the keto group is in the *s-cis* configuration with respect to the olefinic double bond [$\text{C}7-\text{C}8-\text{C}9-\text{O}1 = -5.4(2)^\circ$; Fig. 1]. The methoxy group is coplanar with the attached ring, the $\text{C}16-\text{O}2-\text{C}3-\text{C}4$ torsion angle being $-4.7(2)^\circ$. The molecule is slightly twisted, the dihedral angle between the two aromatic rings being $9.51(7)^\circ$. The bond lengths and angles are comparable with those reported for related structures (Raj *et al.*, 1996; Shanmuga Sundara Raj *et al.*, 1997; Jeyabharathi *et al.*, 2002; Ravishankar *et al.*, 2003; Thamarai Selvi *et al.*, 2003).

The short $\text{H}5\cdots\text{H}8$ (2.15 \AA) and $\text{H}8\cdots\text{H}11$ (2.00 \AA) contacts result in the widening of the $\text{C}6-\text{C}7-\text{C}8$ [$126.11(12)^\circ$] and $\text{C}9-\text{C}10-\text{C}11$ [$122.68(11)^\circ$] angles from 120° . The narrowing of the $\text{O}2-\text{C}3-\text{C}2$ [$116.13(11)^\circ$] angle

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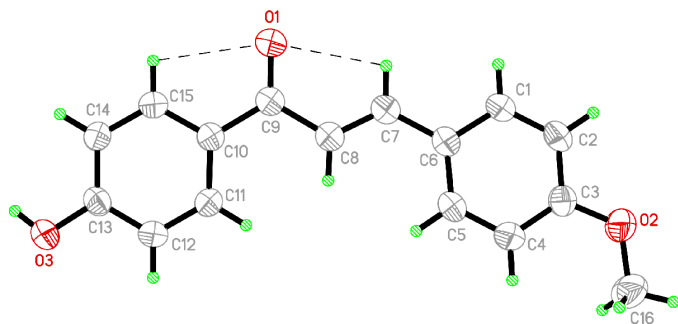


Figure 1

A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

and the resultant widening of the O2—C3—C4 [124.08 (12)°] angle from normal values are a result of the close H4···H16B (2.33 Å) and H4···H16C (2.30 Å) contacts. Similar features have been reported previously for related structures (Ravishankar *et al.*, 2003; Thamarai Selvi *et al.*, 2003).

In the molecular structure of (I), each of the C7—H7···O1 and C15—H15···O1 interactions generates an *S*(5) ring motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995).

In the crystal structure of (I), the keto and hydroxy O atoms are involved in intermolecular O—H···O hydrogen bonds. The crystal structure is further stabilized by C—H···O interactions (Table 1), the geometries of which agree with those reported by Jeffrey (1997) and Desiraju & Steiner (1999). The O3—H3···O1ⁱ and C14—H14···O1ⁱ interactions together form a pair of bifurcated acceptor bonds which generate a ring of graph-set motif $R_2^1(6)$ (Etter *et al.*, 1990). Also, the C4—H4···O3ⁱⁱⁱ and C16—H16C···O3ⁱⁱⁱ interactions constitute a pair of bifurcated acceptor bonds generating a ring of graph-set motif $R_2^1(7)$ (Fig. 2). An $R_2^1(6)$ motif is formed by the C1—H1···O2ⁱⁱ and C7—H7···O2ⁱⁱ interactions. All symmetry codes are given in Table 1.

In addition to the above interactions, the crystal packing is further stabilized by a face-to-face π — π interaction between the C10—C15 benzene ring at (*x*, *y*, *z*) and the inversion-related ring at (−*x*, 1 − *y*, −*z*). These rings are stacked 3.378 (1) Å apart, with a centroid···centroid distance of 3.692 (1) Å.

Experimental

The title compound was prepared by the Claisen–Schmidt condensation of equimolar quantities of 4-hydroxyacetophenone (4.08 g, 0.03 mol) and 4-methoxybenzaldehyde (4.03 g, 0.03 mol) in aqueous ethanol, in the presence of sodium hydroxide. The product was recrystallized from ethanol by slow evaporation.

Crystal data

C ₁₆ H ₁₄ O ₃	Mo K α radiation
<i>M_r</i> = 254.27	Cell parameters from 6162 reflections
Orthorhombic, <i>Pbca</i>	θ = 4.9–54.7°
<i>a</i> = 13.4346 (8) Å	μ = 0.09 mm ^{−1}
<i>b</i> = 11.4998 (7) Å	<i>T</i> = 293 (2) K
<i>c</i> = 16.6055 (10) Å	Block, colourless
<i>V</i> = 2565.5 (3) Å ³	0.59 × 0.41 × 0.28 mm
<i>Z</i> = 8	
<i>D_x</i> = 1.317 Mg m ^{−3}	

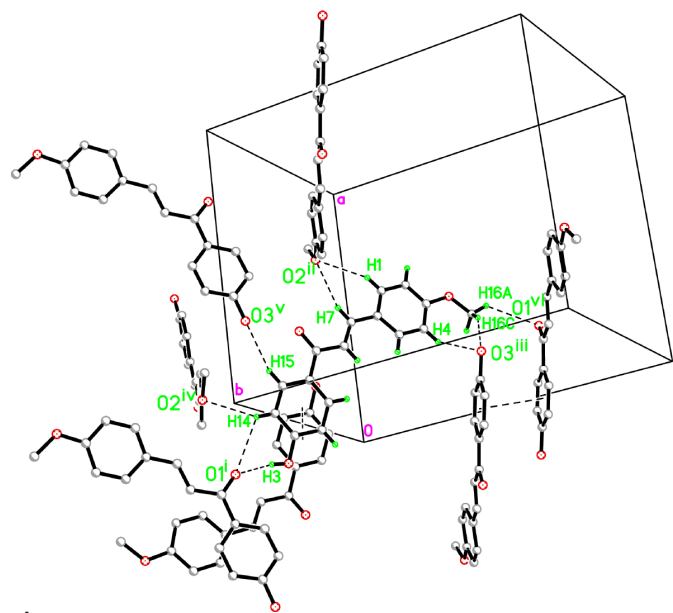


Figure 2

Part of the crystal packing of (I), showing O—H···O and C—H···O hydrogen bonds as dashed lines. Only the H atoms involved in the interactions are labelled. Other H atoms have been omitted. Symmetry codes are given in Table 1. The π — π interaction is also shown as a dashed line.

Data collection

Siemens SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: none
 15 000 measured reflections
 3015 independent reflections

2513 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 28.3^\circ$
 $h = -16 \rightarrow 17$
 $k = -10 \rightarrow 15$
 $l = -21 \rightarrow 22$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.126$
 $S = 1.07$
 3015 reflections
 175 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.4382P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXTL* (Sheldrick, 1997)
 Extinction coefficient: 0.0097 (13)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O3—H3···O1 ⁱ	0.82	1.88	2.688 (2)	169
C1—H1···O2 ⁱⁱ	0.93	2.86	3.674 (2)	147
C4—H4···O3 ⁱⁱⁱ	0.93	2.72	3.393 (2)	130
C7—H7···O1 ^{iv}	0.93	2.50	2.808 (2)	100
C7—H7···O2 ⁱⁱ	0.93	2.53	3.425 (2)	162
C14—H14···O1 ⁱ	0.93	2.93	3.547 (2)	125
C14—H14···O2 ^v	0.93	2.63	3.455 (2)	149
C15—H15···O1 ^{iv}	0.93	2.54	2.828 (2)	99
C15—H15···O3 ^{vi}	0.93	2.60	3.490 (2)	162
C16—H16A···O1 ^{vii}	0.96	2.82	3.344 (2)	116
C16—H16C···O3 ⁱⁱⁱ	0.96	2.68	3.548 (2)	151

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) x, y, z ; (v) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (vi) $x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (vii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

H atoms were positioned geometrically and refined with a riding model, with O—H = 0.82 Å, C—H = 0.93–0.96 Å and $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times U_{eq} of the carrier atom. The rotational orientations of the methyl and hydroxyl groups were determined by circular difference electron-density syntheses.

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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