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

Xiao-Yang Qiu,[a,b] Sen-Lin Yang,[a] Wei-Sheng Liu[b]* and Hai-Liang Zhu[c]*

[a]Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and [c]Institute of Functional Biomolecules, State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: liuws@lzu.edu.cn, hailiang_zhu@163.com

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In the title compound, $C_{16}H_{14}O_3$, the dihedral angle between the two benzene rings is 25.8 (2)°. Molecules are linked into ribbons through O—H···O=C hydrogen bonds.

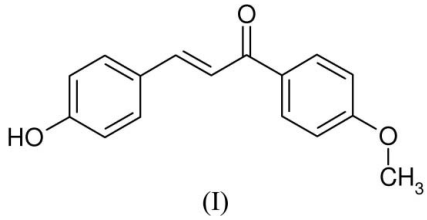
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.139
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.

Comment

Recently, we have reported the structures of a few chalcone derivatives (Qiu *et al.*, 2006, 2006*a*), including the analogous chloro derivative (Qiu *et al.*, 2006*b*). As an extension of our work on the structural characterization of chalcone derivatives, the title compound, (I), is reported here.



(I)

In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C8=C9 bond length of 1.328 (3) Å conforms to the value for a C=C double bond. The dihedral angle between the two benzene rings is 25.8 (2)°. In the crystal structure, molecules are linked through intermolecular O—H···O=C hydrogen bonds, forming ribbons along the *a*-axis direction (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide (5%, 1 ml) was added with stirring overnight to a solution of 4-hydroxybenzaldehyde (1 mmol, 0.12 g) and 4-methoxyacetophenone (1 mmol, 0.15 g) in ethanol (15 ml) at room temperature. The reaction mixture was then poured on to ice and neutralized with aqueous hydrochloric acid (5%). A white solid was prepared after neutralization and obtained from an ethanol solution. The solid (0.05 mmol,

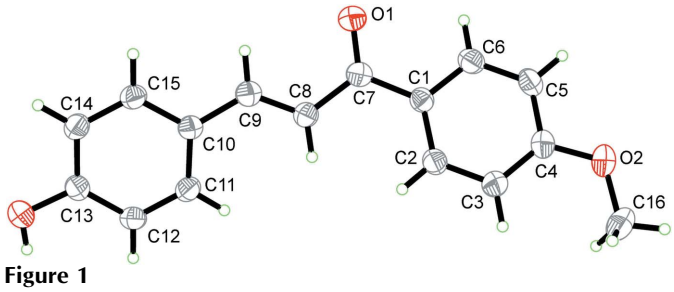


Figure 1
The structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms and the atom-numbering scheme.

0.013 g) was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear colourless solution. After keeping the solution in air for 9 d, colourless plate-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. These were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$ (yield 53%).

Crystal data

$C_{16}H_{14}O_3$
M_r = 254.27
Orthorhombic, *Pbca*
a = 13.3482 (9) Å
b = 7.6922 (5) Å
c = 25.3822 (17) Å
V = 2606.2 (3) Å^3
Z = 8
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Plate, colourless
0.34 × 0.17 × 0.07 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.986
14929 measured reflections
2978 independent reflections
1485 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.139
S = 1.00
2978 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.0775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H13···O1^{i}	0.82	1.89	2.651 (2)	154

Symmetry code: (i) $x+\frac{1}{2}, y, -z+\frac{3}{2}$.

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H and O—H distances of 0.93–0.96 and 0.82 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

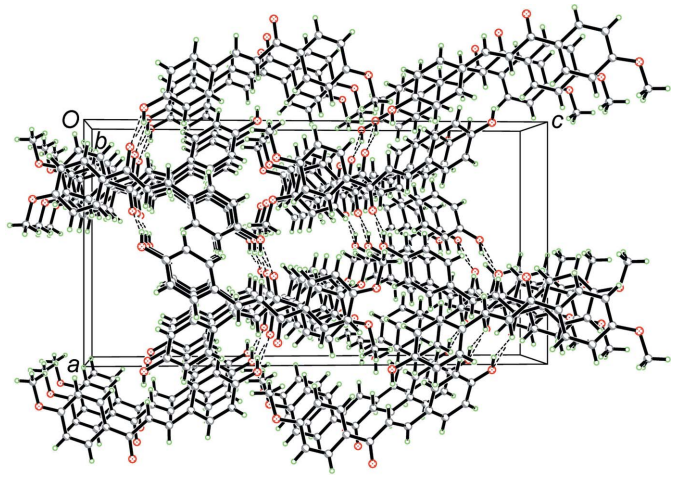


Figure 2
The crystal packing viewed along the *b* axis, showing the intermolecular O—H···O hydrogen bonds (dashed lines) linking the molecules into ribbons running along *a*.

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