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(2*E*)-3-(3,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one

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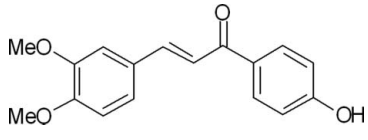
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.132; data-to-parameter ratio = 15.7.

In the title compound, $C_{17}H_{16}O_4$, the dihedral angle between the mean planes of the hydroxyphenyl and dimethoxyphenyl rings is 19.34 (7)°. The mean plane of the prop-2-en-1-one group, the active site in this molecule, makes angles of 7.40 (8) and 13.25 (8)°, respectively, with the hydroxyphenyl and dimethoxyphenyl rings. The crystal packing is stabilized by O—H···O hydrogen bonds, weak intermolecular C—H···O and π–π stacking interactions [centroid–centroid distance = 3.7386 (9) Å].

Related literature

For related chalcone structures, see: Butcher *et al.* (2006); Cao *et al.* (2005); Harrison *et al.* (2007); Jasinski *et al.* (2010, 2011*a*,*b*); Ngaini *et al.* (2009); Radha Krishna *et al.* (2005); Sharma *et al.* (1997); Wu *et al.* (2005)



Experimental

Crystal data

$C_{17}H_{16}O_4$
M_r = 284.30
Orthorhombic, *Pbca*
a = 15.1435 (1) Å
b = 8.4364 (1) Å
c = 22.9454 (2) Å
V = 2931.43 (5) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 295 K
0.57 × 0.28 × 0.19 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.606, T_{max} = 1.000
9187 measured reflections
3022 independent reflections
2545 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.132
S = 1.05
3022 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2^{i}	0.82	1.90	2.7154 (15)	176
C6—H6A···O4^{ii}	0.93	2.46	3.2803 (16)	147

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2725).

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supplementary materials

Acta Cryst. (2011). E**67**, o813 [**doi:10.1107/S1600536811007781**]

(2*E*)-3-(3,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one

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Comment

In continuation to our studies on crystal structures of chalcones (Jasinski *et al.*, 2010, 2011*a*, 2011*b*), we report here the synthesis, Fig. 1, and crystal structure of a new chalcone, (I), Fig. 2. The dihedral angle between the mean planes of the hydroxyphenyl and dimethoxyphenyl rings is 19.34 (7)\ % (Fig. 2). The mean plane of the prop-2-en-1-one group, the active site in this molecule, makes angles of 7.40 (8) ° and 13.25 (8) °, respectively, with the hydroxyphenyl and dimethoxyphenyl rings. Bond lengths and angles are normal and correspond to those observed in related compounds (Butcher *et al.*, 2006; Cao *et al.*, 2005; Harrison *et al.*, 2007; Jasinski *et al.*, 2010, 2011*a*, 2011*b*; Ngaini *et al.*, 2009; Radha Krishna *et al.*, 2005; Sharma *et al.*, 1997; Wu *et al.*, 2005). Crystal packing is stabilized by O—H···O hydrogen bonds, weak C—H···O contacts (Table 2) and π—π stacking interactions (Table 3); see Fig. 3.

Experimental

4-Hydroxyacetophenone (1.36 g, 0.01 mol) was mixed with 3,4-dimethoxybenzaldehyde (1.66 g, 0.01 mol) and dissolved in ethanol (40 ml), Fig.1. To this solution, 5 ml of KOH (50%) was added at 278 K. The reaction mixture stirred overnight at room temperature and poured on to crushed ice. The pH of this mixture was adjusted to 3–4 with 2 *M* HCl aqueous solution. The resulting crude solid was filtered, washed successively with dilute HCl solution and distilled water, and finally recrystallized from ethyl alcohol (95%) to give the pure chalcone. Crystals suitable for X-ray diffraction studies were grown by the slow evaporation of the solution of the compound in ethyl alcohol:DMF (4:1) (*M*.pt.: 438–442 K). Composition: Found (Calculated) for $C_{17}H_{16}O_4$, C 75.22 (75.28); H: 5.95 (5.92) %.

Refinement

The hydroxyl hydrogen was located by a Fourier map, fixed at 0.82 Å and refined using the riding model. All of the remaining H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.93 Å (CH) and 0.96 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.19–1.20 (CH), 1.50 (CH_3) or 1.50 (OH) times U_{eq} of the parent atom.

Figures

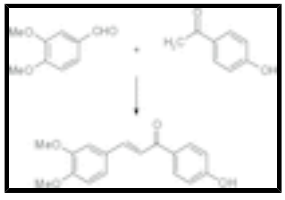

Fig. 1. Reaction scheme for (I).

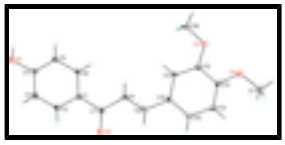

Fig. 2. Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

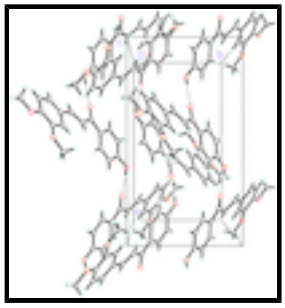

Fig. 3. Packing diagram of the title compound viewed down the *c* axis. Dashed lines indicate O—H···O hydrogen bonds.

(2*E*)-3-(3,4-Dimethoxyphenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{16}O_4$	$F(000) = 1200$
$M_r = 284.30$	$D_x = 1.288$ Mg m^{-3}
Orthorhombic, *Pbca*	Cu *Kα* radiation, λ = 1.54184 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5957 reflections
$a = 15.1435$ (1) Å	θ = 4.8–77.2°
$b = 8.4364$ (1) Å	μ = 0.75 mm^{-1}
$c = 22.9454$ (2) Å	$T = 295$ K
$V = 2931.43$ (5) Å^3	Thick needle, pale yellow
$Z = 8$	0.57 × 0.28 × 0.19 mm

Data collection

Oxford Diffraction Gemini R diffractometer	3022 independent reflections
Radiation source: fine-focus sealed tube	2545 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.019$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 77.4°$, $\theta_{min} = 4.8°$
φ and ω scans	$h = -19 \rightarrow 16$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)	$k = -10 \rightarrow 8$
$T_{min} = 0.606$, $T_{max} = 1.000$	$l = -29 \rightarrow 27$
9187 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.132$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0854P)^2 + 0.2601P]$ where $P = (F_o^2 + 2F_c^2)/3$
3022 reflections	$(\Delta/\sigma)_{max} < 0.001$
193 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.35344 (7)	0.04833 (15)	0.56975 (5)	0.0633 (3)
H1A	0.3054	0.0598	0.5538	0.095*
O2	0.69247 (6)	0.40373 (15)	0.47932 (5)	0.0632 (3)
O3	0.52144 (7)	0.68821 (14)	0.18477 (4)	0.0623 (3)
O4	0.64891 (8)	0.87474 (16)	0.15770 (5)	0.0709 (4)
C1	0.54831 (8)	0.30167 (16)	0.48339 (5)	0.0446 (3)
C2	0.56558 (9)	0.21781 (19)	0.53484 (6)	0.0531 (3)
H2A	0.6224	0.2190	0.5503	0.064*
C3	0.50099 (9)	0.1343 (2)	0.56289 (6)	0.0565 (4)
H3A	0.5142	0.0786	0.5968	0.068*
C4	0.41531 (9)	0.13271 (17)	0.54069 (6)	0.0488 (3)
C5	0.39652 (9)	0.21501 (18)	0.48989 (6)	0.0514 (3)
H5A	0.3395	0.2144	0.4749	0.062*
C6	0.46232 (9)	0.29769 (17)	0.46166 (6)	0.0486 (3)
H6A	0.4491	0.3519	0.4275	0.058*
C7	0.61991 (8)	0.39056 (17)	0.45507 (6)	0.0467 (3)
C8	0.60426 (8)	0.46360 (16)	0.39746 (5)	0.0468 (3)
H8A	0.5557	0.4317	0.3756	0.056*
C9	0.65801 (8)	0.57388 (16)	0.37626 (6)	0.0470 (3)
H9A	0.7045	0.6039	0.4004	0.056*
C10	0.65336 (8)	0.65384 (15)	0.31995 (5)	0.0432 (3)
C11	0.58497 (8)	0.62733 (15)	0.27941 (5)	0.0444 (3)
H11A	0.5393	0.5580	0.2886	0.053*
C12	0.58516 (8)	0.70317 (16)	0.22628 (5)	0.0457 (3)
C13	0.65482 (9)	0.80698 (17)	0.21138 (6)	0.0481 (3)

C14	0.72135 (9)	0.83476 (17)	0.25115 (6)	0.0517 (3)
H14A	0.7671	0.9040	0.2420	0.062*
C15	0.71971 (9)	0.75892 (18)	0.30489 (6)	0.0506 (3)
H15A	0.7645	0.7794	0.3315	0.061*
C16	0.44645 (10)	0.5955 (2)	0.19866 (7)	0.0639 (4)
H16A	0.4646	0.4889	0.2071	0.096*
H16B	0.4065	0.5949	0.1662	0.096*
H16C	0.4174	0.6397	0.2321	0.096*
C17	0.71898 (15)	0.9741 (3)	0.13898 (8)	0.0870 (6)
H17A	0.7210	1.0672	0.1630	0.130*
H17B	0.7095	1.0044	0.0991	0.130*
H17C	0.7739	0.9179	0.1421	0.130*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0503 (5)	0.0816 (8)	0.0582 (6)	0.0019 (5)	0.0053 (4)	0.0155 (5)
O2	0.0424 (5)	0.0845 (8)	0.0628 (6)	−0.0018 (5)	−0.0107 (4)	0.0177 (6)
O3	0.0555 (6)	0.0791 (7)	0.0522 (5)	−0.0210 (5)	−0.0170 (4)	0.0141 (5)
O4	0.0766 (7)	0.0823 (8)	0.0539 (6)	−0.0329 (6)	−0.0121 (5)	0.0175 (6)
C1	0.0423 (6)	0.0489 (7)	0.0426 (6)	0.0079 (5)	−0.0023 (5)	−0.0020 (5)
C2	0.0424 (6)	0.0675 (9)	0.0495 (7)	0.0072 (6)	−0.0075 (5)	0.0054 (6)
C3	0.0520 (7)	0.0708 (9)	0.0469 (7)	0.0090 (7)	−0.0031 (5)	0.0115 (7)
C4	0.0457 (7)	0.0551 (8)	0.0455 (6)	0.0066 (6)	0.0049 (5)	−0.0012 (6)
C5	0.0405 (6)	0.0639 (8)	0.0496 (7)	0.0051 (6)	−0.0033 (5)	0.0023 (6)
C6	0.0446 (6)	0.0585 (8)	0.0428 (6)	0.0065 (5)	−0.0040 (5)	0.0048 (5)
C7	0.0414 (6)	0.0523 (7)	0.0464 (6)	0.0083 (5)	−0.0031 (5)	−0.0011 (5)
C8	0.0423 (6)	0.0549 (7)	0.0431 (6)	0.0039 (5)	−0.0028 (5)	−0.0027 (5)
C9	0.0441 (6)	0.0493 (7)	0.0476 (6)	0.0051 (5)	−0.0080 (5)	−0.0035 (5)
C10	0.0408 (6)	0.0442 (6)	0.0447 (6)	0.0039 (5)	−0.0034 (5)	−0.0034 (5)
C11	0.0387 (6)	0.0466 (7)	0.0479 (6)	−0.0022 (5)	−0.0028 (5)	−0.0003 (5)
C12	0.0415 (6)	0.0504 (7)	0.0451 (6)	−0.0033 (5)	−0.0053 (5)	−0.0026 (5)
C13	0.0493 (7)	0.0488 (7)	0.0463 (6)	−0.0054 (5)	−0.0011 (5)	−0.0003 (5)
C14	0.0462 (7)	0.0537 (7)	0.0553 (7)	−0.0111 (6)	−0.0019 (5)	−0.0017 (6)
C15	0.0428 (6)	0.0558 (8)	0.0533 (7)	−0.0036 (6)	−0.0105 (5)	−0.0049 (6)
C16	0.0474 (7)	0.0847 (11)	0.0596 (8)	−0.0175 (7)	−0.0120 (6)	0.0011 (8)
C17	0.0952 (14)	0.0961 (14)	0.0697 (10)	−0.0435 (12)	−0.0063 (9)	0.0232 (10)

Geometric parameters (Å, °)

O1—C4	1.3524 (17)	C8—C9	1.328 (2)
O1—H1A	0.8200	C8—H8A	0.9300
O2—C7	1.2368 (16)	C9—C10	1.4592 (18)
O3—C12	1.3617 (15)	C9—H9A	0.9300
O3—C16	1.4153 (17)	C10—C15	1.3837 (19)
O4—C13	1.3608 (17)	C10—C11	1.4100 (16)
O4—C17	1.419 (2)	C11—C12	1.3768 (18)
C1—C6	1.3947 (18)	C11—H11A	0.9300
C1—C2	1.4009 (18)	C12—C13	1.4131 (18)

C1—C7	1.4698 (19)	C13—C14	1.3794 (19)
C2—C3	1.367 (2)	C14—C15	1.389 (2)
C2—H2A	0.9300	C14—H14A	0.9300
C3—C4	1.3940 (19)	C15—H15A	0.9300
C3—H3A	0.9300	C16—H16A	0.9600
C4—C5	1.3863 (19)	C16—H16B	0.9600
C5—C6	1.378 (2)	C16—H16C	0.9600
C5—H5A	0.9300	C17—H17A	0.9600
C6—H6A	0.9300	C17—H17B	0.9600
C7—C8	1.4775 (17)	C17—H17C	0.9600
C4—O1—H1A	109.5	C15—C10—C11	118.05 (12)
C12—O3—C16	117.54 (11)	C15—C10—C9	118.83 (11)
C13—O4—C17	118.23 (12)	C11—C10—C9	123.11 (12)
C6—C1—C2	117.60 (12)	C12—C11—C10	120.59 (12)
C6—C1—C7	122.88 (12)	C12—C11—H11A	119.7
C2—C1—C7	119.51 (12)	C10—C11—H11A	119.7
C3—C2—C1	121.58 (13)	O3—C12—C11	125.08 (12)
C3—C2—H2A	119.2	O3—C12—C13	114.66 (12)
C1—C2—H2A	119.2	C11—C12—C13	120.25 (11)
C2—C3—C4	119.93 (13)	O4—C13—C14	125.14 (12)
C2—C3—H3A	120.0	O4—C13—C12	115.48 (12)
C4—C3—H3A	120.0	C14—C13—C12	119.37 (13)
O1—C4—C5	122.41 (12)	C13—C14—C15	119.73 (13)
O1—C4—C3	118.02 (12)	C13—C14—H14A	120.1
C5—C4—C3	119.57 (13)	C15—C14—H14A	120.1
C6—C5—C4	120.02 (12)	C10—C15—C14	121.98 (12)
C6—C5—H5A	120.0	C10—C15—H15A	119.0
C4—C5—H5A	120.0	C14—C15—H15A	119.0
C5—C6—C1	121.28 (12)	O3—C16—H16A	109.5
C5—C6—H6A	119.4	O3—C16—H16B	109.5
C1—C6—H6A	119.4	H16A—C16—H16B	109.5
O2—C7—C1	120.15 (12)	O3—C16—H16C	109.5
O2—C7—C8	120.51 (12)	H16A—C16—H16C	109.5
C1—C7—C8	119.34 (11)	H16B—C16—H16C	109.5
C9—C8—C7	121.42 (12)	O4—C17—H17A	109.5
C9—C8—H8A	119.3	O4—C17—H17B	109.5
C7—C8—H8A	119.3	H17A—C17—H17B	109.5
C8—C9—C10	128.19 (12)	O4—C17—H17C	109.5
C8—C9—H9A	115.9	H17A—C17—H17C	109.5
C10—C9—H9A	115.9	H17B—C17—H17C	109.5
C6—C1—C2—C3	0.2 (2)	C8—C9—C10—C11	2.9 (2)
C7—C1—C2—C3	179.60 (14)	C15—C10—C11—C12	0.59 (19)
C1—C2—C3—C4	−0.7 (2)	C9—C10—C11—C12	−178.34 (12)
C2—C3—C4—O1	179.88 (14)	C16—O3—C12—C11	4.2 (2)
C2—C3—C4—C5	0.6 (2)	C16—O3—C12—C13	−175.33 (14)
O1—C4—C5—C6	−179.27 (13)	C10—C11—C12—O3	−178.55 (13)
C3—C4—C5—C6	0.0 (2)	C10—C11—C12—C13	1.0 (2)
C4—C5—C6—C1	−0.5 (2)	C17—O4—C13—C14	4.3 (3)

C2—C1—C6—C5	0.3 (2)	C17—O4—C13—C12	−176.96 (16)
C7—C1—C6—C5	−178.98 (13)	O3—C12—C13—O4	−0.94 (19)
C6—C1—C7—O2	172.43 (13)	C11—C12—C13—O4	179.51 (13)
C2—C1—C7—O2	−6.9 (2)	O3—C12—C13—C14	177.85 (13)
C6—C1—C7—C8	−7.6 (2)	C11—C12—C13—C14	−1.7 (2)
C2—C1—C7—C8	173.06 (12)	O4—C13—C14—C15	179.55 (14)
O2—C7—C8—C9	−15.9 (2)	C12—C13—C14—C15	0.9 (2)
C1—C7—C8—C9	164.20 (13)	C11—C10—C15—C14	−1.4 (2)
C7—C8—C9—C10	178.09 (12)	C9—C10—C15—C14	177.55 (13)
C8—C9—C10—C15	−176.03 (14)	C13—C14—C15—C10	0.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2^{i}	0.82	1.90	2.7154 (15)	176
C6—H6A···O4^{ii}	0.93	2.46	3.2803 (16)	147

Symmetry codes: (i) *x*−1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

Table 2

Selected geometric parmeters (Å): Cg···Cg π stacking interactions, Cg1 is the centroid of ring C1—C6 [Symmetry codes: (i) 1-x, -y, 1-z]

*Cg*I···*Cg*J	Cg···Cg (Å)	CgI Perp (Å)	Cgj Perp (Å)	Slippage (Å)
Cg1···Cg1^{i}	3.7386 (9)	-3.3959 (6)	-3.3958 (6)	1.56 (4)

Fig. 1

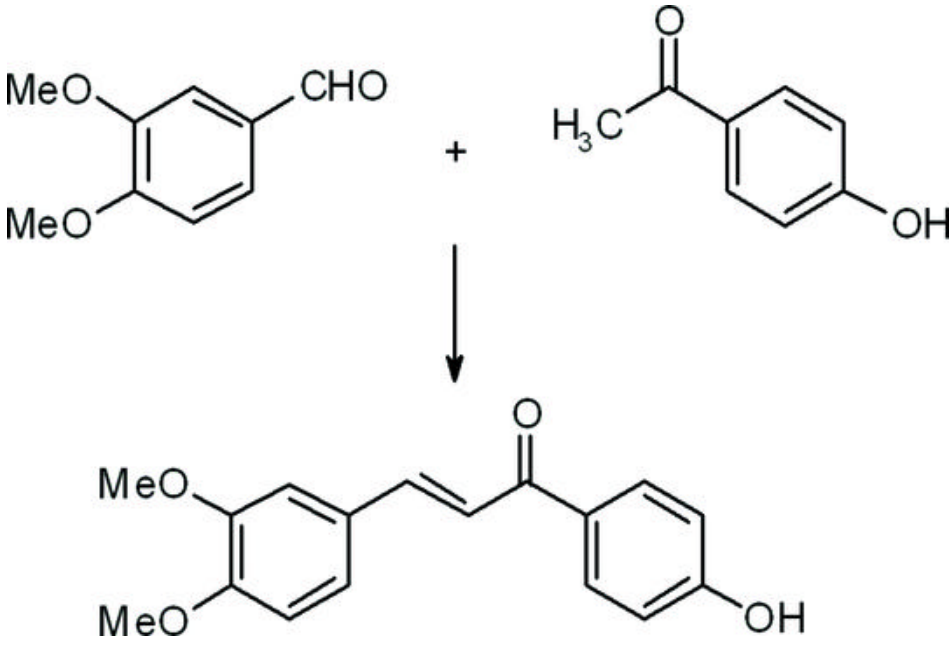

Fig. 2

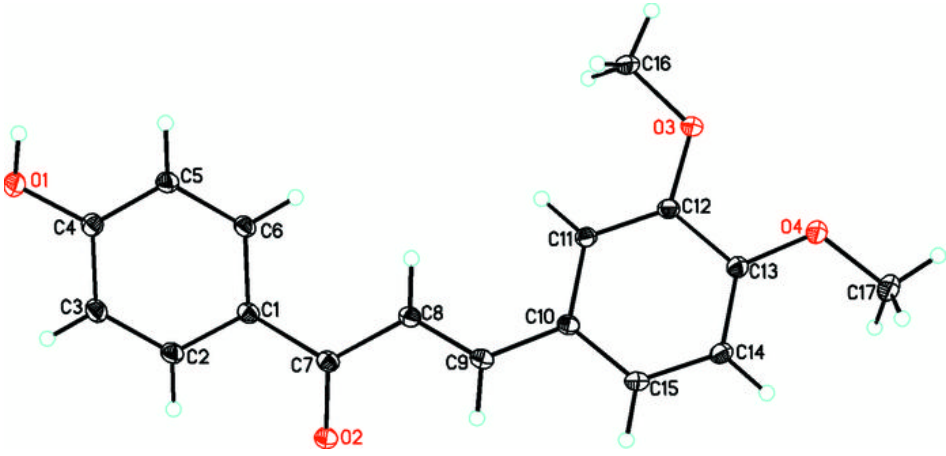
C16
O3
O1
C5
C12
O4
C4
C6
C11
C13
C17
C3
C1
C8
C10
C2
C7
C9
C14
C15
O2

Fig. 3