Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (2*E*)-1-(3-Hydroxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one

**Ray J. Butcher,[a] Jerry P. Jasinski,[b]* B. Narayana,[c] K. Lakshmana[c] and H. S. Yathirajan[d]**

[a]Department of Chemistry, Howard University, 525 College Street NW, Washington DC 20059, USA, [b]Department of Chemistry, Keene State College, 229 Main Street, Keene NH 03435-2001, USA, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India
Correspondence e-mail: jjasinski@keene.edu

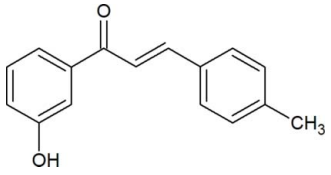
Received 16 July 2007; accepted 25 July 2007

Key indicators: single-crystal X-ray study; $T$ = 203 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.044; $wR$ factor = 0.116; data-to-parameter ratio = 25.6.

Two new chalcones of general type (2*E*)-1-(3-hydroxyphenyl)-3-(4-*R*-phenyl)prop-2-en-1-one are reported, one where $R$ = methyl, $C_{16}H_{14}O_2$, in the present paper, and one where $R$ = chloro, $C_{15}H_{11}ClO_2$, in the following paper [Butcher, Jasinski, Narayana, Lakshmana & Yathirajan (2007). *Acta Cryst.* E**63**, o3661]. In both structures, the 3-hydroxyphenyl and 4-(methyl/chloro)phenyl groups are coplanar with each other and also with the propyl-2-ketone oxygen. Crystal packing is stabilized by intermolecular O—H···O hydrogen bonding between the hydroxyl H atom and the propyl-2-ketone O atom.

## Related literature

For related structures, see: Yathirajan *et al.* (2007); Fischer *et al.* (2007); Harrison *et al.* (2006). For related literature, see: Carlo *et al.* (1999); Fichou *et al.* (1988); Goto *et al.* (1991); Uchida *et al.* (1998); Zhao *et al.* (2000); Sarojini *et al.* (2006).




## Experimental

### *Crystal data*

$C_{16}H_{14}O_2$
$M_r$ = 238.27
Monoclinic, $P2_1/n$
$a$ = 7.6363 (5) Å
$b$ = 11.0786 (5) Å
$c$ = 15.2355 (8) Å
$\beta$ = 104.038 (6)°
$V$ = 1250.42 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 203 K
0.51 × 0.47 × 0.32 mm

### *Data collection*

Oxford Diffraction Gemini R diffractometer
Absorption correction: none
17875 measured reflections
4225 independent reflections
1758 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
$S$ = 0.85
4225 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.83 | 1.91 | 2.7083 (12) | 161.2 |

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

KL thanks Mangalore University for use of their research facilities. RJB acknowledges the NSF MRI program (CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2079).

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  doi:10.1107/S1600536807036641 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o3660 [ **doi:10.1107/S1600536807036641** ]

# (2*E*)-1-(3-Hydroxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one

**R. J. Butcher, J. P. Jasinski, B. Narayana, K. Lakshmana and H. S. Yathirajan**

## Comment

Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities. Among several organic compounds reported for non-linear optical (NLO) property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. We have synthesized two new chalcones, of general formula (2E)-1-(3-Hydroxyphenyl)-3-(4-*R*-phenyl)prop-2-en-1-one, with *R*=methyl ($C_{16}H_{14}O_2$) (I), reported in the present paper, and *R*=Chloro ($C_{15}H_{11}ClO_2$) (II), reported in the following one (Butcher *et al.*, 2007).

Fig. 1 presents a molecular diagram for (I).

The 3-hydroxyphenyl and 4-methylphenyl groups are coplanar with each other and with the propyl 2 ketone group forming torsion angles of 179.28 (11)°, C7—C1—C2—C3, and 177.38 (11)°, C9—C10—C15—C14, respectively.

Intermolecular O—H···O hydrogen bonding interactions involving the H1 hydroxyl atom and prop-2-en O2 atom (Table 1) link the molecules (almost perpendicular to each other) into a planar array (Fig. 2). In spite of crystallizing in different space groups ((I) in P21/n, (II) in P21/c) both compounds are very nealy isostructural.

## Experimental

To a mixture of 1-(3-hydroxyphenyl)ethanone,1.36 g (0.01 mol) and 4-methylbenzaldehyde 1.2 g (0.01 mol) in ethanol (20 ml), a solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring. The mixture was stirred at room temperature for 6 h. The precipitated solid was filtered, washed with cold ethanol, dried and the crystals were obtained from ethanol (yield: 83%; m.p.:395–396 K). Elemental analysis found: C: 80.51; H: 5.85%. $C_{16}H_{14}O_2$ requires C, 80.65, H, 5.92%.

## Refinement

All of the H atoms, except H1 which was located from difference Fourier map, were inferred from neighbouring sites. All H atoms were included in the riding model approximation with C—H = 0.94 or 0.97 Å, and with $U_{iso}$(H) = 1.18–1.50$U_{eq}$(C,*O*).

## Figures

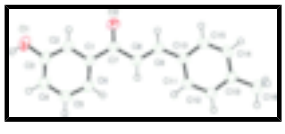

Fig. 1. Molecular structure of (I), showing atom labelling and 50% probability displacement ellipsoids.

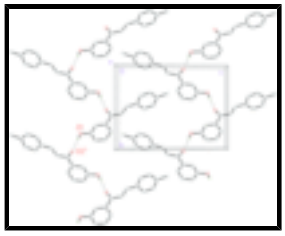

Fig. 2. Packing diagram of (I) viewed down the *a* axis. Dashed lines indicate O–H···O hydrogen bonds. Symmetry code: as in Table 1

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

*Crystal data*

| | |
|---|---|
| $C_{16}H_{14}O_2$ | $F_{000}$ = 504 |
| $M_r$ = 238.27 | $D_x$ = 1.266 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 4283 reflections |
| $a$ = 7.6363 (5) Å | θ = 4.6–32.5º |
| $b$ = 11.0786 (5) Å | μ = 0.08 mm$^{-1}$ |
| $c$ = 15.2355 (8) Å | $T$ = 203 K |
| β = 104.038 (6)º | Prism, colorless |
| $V$ = 1250.42 (12) Å$^3$ | 0.51 × 0.47 × 0.32 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini R diffractometer | 1758 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.041 |
| Monochromator: graphite | $\theta_{max}$ = 32.5º |
| $T$ = 203 K | $\theta_{min}$ = 4.6º |
| φ and ω scans | $h$ = −11→11 |
| Absorption correction: none | $k$ = −15→16 |
| 17875 measured reflections | $l$ = −22→22 |
| 4225 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | H-atom parameters constrained |
| $wR(F^2)$ = 0.116 | $w = 1/[\sigma^2(F_o^2) + (0.0599P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.85 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4225 reflections | $\Delta\rho_{max}$ = 0.17 e Å$^{-3}$ |
| 165 parameters | $\Delta\rho_{min}$ = −0.25 e Å$^{-3}$ |

Primary atom site location: structure-invariant direct methods

Extinction correction: none

*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 $F^2 > 2\text{sigma}(F^2)$ 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 | 0.27826 (12) | 0.81623 (8) | −0.32669 (5) | 0.0513 (3) |
| H1 | 0.3198 | 0.8765 | −0.3469 | 0.062* |
| O2 | 0.16473 (12) | 0.53175 (8) | −0.10106 (5) | 0.0468 (3) |
| C1 | 0.34731 (15) | 0.70371 (9) | −0.09667 (7) | 0.0334 (3) |
| C2 | 0.28544 (16) | 0.71691 (10) | −0.19000 (7) | 0.0364 (3) |
| H2A | 0.2020 | 0.6612 | −0.2229 | 0.044* |
| C3 | 0.34501 (17) | 0.81074 (11) | −0.23490 (8) | 0.0398 (3) |
| C4 | 0.46574 (17) | 0.89442 (11) | −0.18716 (8) | 0.0447 (3) |
| H4A | 0.5069 | 0.9582 | −0.2176 | 0.054* |
| C5 | 0.52540 (17) | 0.88334 (11) | −0.09424 (9) | 0.0467 (3) |
| H5A | 0.6055 | 0.9411 | −0.0616 | 0.056* |
| C6 | 0.46886 (17) | 0.78835 (11) | −0.04843 (8) | 0.0418 (3) |
| H6A | 0.5121 | 0.7811 | 0.0146 | 0.050* |
| C7 | 0.27868 (16) | 0.59904 (10) | −0.05359 (7) | 0.0337 (3) |
| C8 | 0.34413 (16) | 0.57549 (10) | 0.04372 (7) | 0.0345 (3) |
| H8A | 0.4405 | 0.6212 | 0.0779 | 0.041* |
| C9 | 0.26887 (16) | 0.49007 (10) | 0.08446 (8) | 0.0356 (3) |
| H9A | 0.1722 | 0.4474 | 0.0475 | 0.043* |
| C10 | 0.31911 (15) | 0.45520 (10) | 0.17970 (7) | 0.0331 (3) |
| C11 | 0.45407 (17) | 0.51396 (10) | 0.24336 (8) | 0.0389 (3) |
| H11A | 0.5124 | 0.5811 | 0.2256 | 0.047* |
| C12 | 0.50356 (17) | 0.47543 (11) | 0.33183 (8) | 0.0427 (3) |
| H12A | 0.5951 | 0.5167 | 0.3734 | 0.051* |
| C13 | 0.42019 (17) | 0.37636 (11) | 0.36085 (8) | 0.0397 (3) |
| C14 | 0.28463 (18) | 0.31886 (11) | 0.29785 (8) | 0.0450 (3) |
| H14A | 0.2252 | 0.2525 | 0.3160 | 0.054* |
| C15 | 0.23477 (17) | 0.35694 (10) | 0.20888 (8) | 0.0410 (3) |
| H15A | 0.1426 | 0.3159 | 0.1675 | 0.049* |
| C16 | 0.4797 (2) | 0.33072 (13) | 0.45672 (8) | 0.0566 (4) |
| H16A | 0.3762 | 0.3262 | 0.4830 | 0.085* |
| H16B | 0.5685 | 0.3855 | 0.4920 | 0.085* |

| | | | | |
|---|---|---|---|---|
| H16C | 0.5325 | 0.2511 | 0.4568 | 0.085* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0618 (7) | 0.0561 (6) | 0.0350 (5) | 0.0106 (5) | 0.0100 (4) | 0.0120 (4) |
| O2 | 0.0501 (6) | 0.0488 (5) | 0.0373 (5) | −0.0068 (4) | 0.0022 (4) | −0.0025 (4) |
| C1 | 0.0333 (7) | 0.0357 (6) | 0.0312 (6) | 0.0072 (5) | 0.0078 (5) | −0.0015 (5) |
| C2 | 0.0354 (7) | 0.0402 (7) | 0.0327 (6) | 0.0078 (5) | 0.0065 (5) | −0.0015 (5) |
| C3 | 0.0432 (8) | 0.0448 (7) | 0.0315 (7) | 0.0141 (6) | 0.0092 (6) | 0.0052 (5) |
| C4 | 0.0449 (8) | 0.0439 (7) | 0.0460 (8) | 0.0055 (6) | 0.0126 (6) | 0.0110 (6) |
| C5 | 0.0443 (8) | 0.0454 (7) | 0.0477 (8) | −0.0058 (6) | 0.0057 (6) | 0.0008 (6) |
| C6 | 0.0440 (8) | 0.0458 (7) | 0.0334 (7) | 0.0005 (6) | 0.0052 (6) | 0.0008 (5) |
| C7 | 0.0320 (7) | 0.0362 (6) | 0.0326 (6) | 0.0067 (5) | 0.0075 (5) | −0.0028 (5) |
| C8 | 0.0338 (7) | 0.0385 (6) | 0.0305 (6) | 0.0017 (5) | 0.0061 (5) | −0.0035 (5) |
| C9 | 0.0341 (7) | 0.0367 (6) | 0.0348 (7) | 0.0019 (5) | 0.0063 (5) | −0.0023 (5) |
| C10 | 0.0317 (6) | 0.0342 (6) | 0.0341 (6) | 0.0039 (5) | 0.0094 (5) | −0.0001 (5) |
| C11 | 0.0406 (7) | 0.0398 (6) | 0.0375 (7) | −0.0073 (6) | 0.0117 (6) | −0.0002 (5) |
| C12 | 0.0434 (8) | 0.0512 (7) | 0.0330 (7) | −0.0084 (6) | 0.0080 (6) | −0.0028 (6) |
| C13 | 0.0408 (7) | 0.0452 (7) | 0.0350 (7) | 0.0008 (6) | 0.0129 (6) | 0.0015 (5) |
| C14 | 0.0480 (8) | 0.0423 (7) | 0.0463 (8) | −0.0067 (6) | 0.0144 (6) | 0.0083 (6) |
| C15 | 0.0369 (7) | 0.0407 (7) | 0.0433 (8) | −0.0055 (6) | 0.0058 (6) | −0.0002 (6) |
| C16 | 0.0664 (10) | 0.0646 (9) | 0.0391 (8) | −0.0072 (8) | 0.0130 (7) | 0.0079 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C3 | 1.3687 (14) | C9—C10 | 1.4601 (15) |
| O1—H1 | 0.8300 | C9—H9A | 0.9400 |
| O2—C7 | 1.2372 (13) | C10—C15 | 1.3915 (15) |
| C1—C2 | 1.3931 (15) | C10—C11 | 1.3934 (16) |
| C1—C6 | 1.3963 (16) | C11—C12 | 1.3765 (16) |
| C1—C7 | 1.4890 (15) | C11—H11A | 0.9400 |
| C2—C3 | 1.3808 (16) | C12—C13 | 1.3936 (16) |
| C2—H2A | 0.9400 | C12—H12A | 0.9400 |
| C3—C4 | 1.3831 (17) | C13—C14 | 1.3844 (17) |
| C4—C5 | 1.3835 (16) | C13—C16 | 1.5078 (16) |
| C4—H4A | 0.9400 | C14—C15 | 1.3820 (16) |
| C5—C6 | 1.3883 (17) | C14—H14A | 0.9400 |
| C5—H5A | 0.9400 | C15—H15A | 0.9400 |
| C6—H6A | 0.9400 | C16—H16A | 0.9700 |
| C7—C8 | 1.4685 (16) | C16—H16B | 0.9700 |
| C8—C9 | 1.3356 (15) | C16—H16C | 0.9700 |
| C8—H8A | 0.9400 | | |
| C3—O1—H1 | 109.5 | C8—C9—H9A | 116.2 |
| C2—C1—C6 | 118.97 (10) | C10—C9—H9A | 116.2 |
| C2—C1—C7 | 117.59 (10) | C15—C10—C11 | 117.69 (11) |
| C6—C1—C7 | 123.44 (10) | C15—C10—C9 | 119.61 (11) |
| C3—C2—C1 | 120.92 (11) | C11—C10—C9 | 122.67 (10) |

| | | | |
|---|---|---|---|
| C3—C2—H2A | 119.5 | C12—C11—C10 | 121.18 (11) |
| C1—C2—H2A | 119.5 | C12—C11—H11A | 119.4 |
| O1—C3—C2 | 116.99 (11) | C10—C11—H11A | 119.4 |
| O1—C3—C4 | 122.90 (11) | C11—C12—C13 | 121.12 (12) |
| C2—C3—C4 | 120.11 (11) | C11—C12—H12A | 119.4 |
| C3—C4—C5 | 119.39 (11) | C13—C12—H12A | 119.4 |
| C3—C4—H4A | 120.3 | C14—C13—C12 | 117.69 (11) |
| C5—C4—H4A | 120.3 | C14—C13—C16 | 121.08 (11) |
| C4—C5—C6 | 121.09 (12) | C12—C13—C16 | 121.20 (12) |
| C4—C5—H5A | 119.5 | C15—C14—C13 | 121.42 (11) |
| C6—C5—H5A | 119.5 | C15—C14—H14A | 119.3 |
| C5—C6—C1 | 119.51 (11) | C13—C14—H14A | 119.3 |
| C5—C6—H6A | 120.2 | C14—C15—C10 | 120.89 (12) |
| C1—C6—H6A | 120.2 | C14—C15—H15A | 119.6 |
| O2—C7—C8 | 120.13 (10) | C10—C15—H15A | 119.6 |
| O2—C7—C1 | 118.97 (10) | C13—C16—H16A | 109.5 |
| C8—C7—C1 | 120.89 (10) | C13—C16—H16B | 109.5 |
| C9—C8—C7 | 121.04 (11) | H16A—C16—H16B | 109.5 |
| C9—C8—H8A | 119.5 | C13—C16—H16C | 109.5 |
| C7—C8—H8A | 119.5 | H16A—C16—H16C | 109.5 |
| C8—C9—C10 | 127.61 (11) | H16B—C16—H16C | 109.5 |
| C6—C1—C2—C3 | 1.11 (16) | C1—C7—C8—C9 | 172.51 (10) |
| C7—C1—C2—C3 | −179.07 (10) | C7—C8—C9—C10 | 179.39 (10) |
| C1—C2—C3—O1 | 179.49 (10) | C8—C9—C10—C15 | −174.73 (11) |
| C1—C2—C3—C4 | −0.96 (17) | C8—C9—C10—C11 | 2.99 (18) |
| O1—C3—C4—C5 | 179.28 (11) | C15—C10—C11—C12 | 0.64 (17) |
| C2—C3—C4—C5 | −0.24 (18) | C9—C10—C11—C12 | −177.11 (10) |
| C3—C4—C5—C6 | 1.29 (19) | C10—C11—C12—C13 | −0.08 (18) |
| C4—C5—C6—C1 | −1.14 (18) | C11—C12—C13—C14 | −0.67 (18) |
| C2—C1—C6—C5 | −0.07 (16) | C11—C12—C13—C16 | 177.32 (11) |
| C7—C1—C6—C5 | −179.88 (11) | C12—C13—C14—C15 | 0.86 (18) |
| C2—C1—C7—O2 | −3.16 (15) | C16—C13—C14—C15 | −177.13 (11) |
| C6—C1—C7—O2 | 176.66 (10) | C13—C14—C15—C10 | −0.31 (18) |
| C2—C1—C7—C8 | 176.98 (10) | C11—C10—C15—C14 | −0.45 (17) |
| C6—C1—C7—C8 | −3.20 (16) | C9—C10—C15—C14 | 177.38 (11) |
| O2—C7—C8—C9 | −7.35 (16) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.83 | 1.91 | 2.7083 (12) | 161.2 |

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

**Fig. 1**

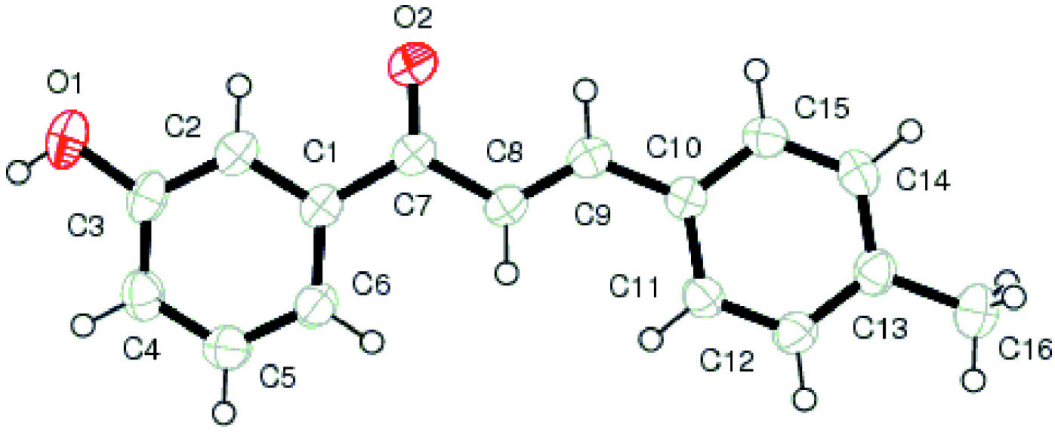

**Fig. 2**