

(2E)-3-(4-Chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one

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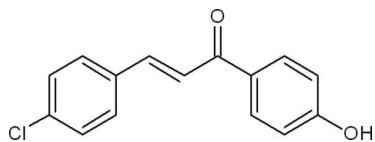
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 24.5.

In the title compound, $C_{15}H_{11}ClO_2$, the dihedral angle between the mean planes of the chlorobenzene and hydroxybenzene rings is $6.5(6)^\circ$. The mean plane of the prop-2-en-1-one group makes an angle of $18.0(1)^\circ$ with the hydroxyphenyl ring and $11.5(1)^\circ$ with the chlorophenyl ring. The crystal packing is stabilized by intermolecular $O-H\cdots O$ hydrogen bonds, weak $C-H\cdots O$, $C-H\cdots\pi$ and $\pi-\pi$ stacking interactions [centroid-centroid distances = $3.7771(7)$ and $3.6917(7)$ Å].

Related literature

For the biological properties of chalcones, see: Nowakowska (2007) and for their role in tubulin polymerization inhibition, see: Edwards *et al.* (1989). For related structures, see: Jasinski *et al.* (2010, 2011a,b); Butcher *et al.* (2007a,b); Narayana *et al.* (2007); Sarojini *et al.* (2007a,b). For standard bond lengths, see: Allen *et al.*, (1987).



Experimental

Crystal data

$C_{15}H_{11}ClO_2$ $V = 1207.97(6)$ Å³
 $M_r = 258.69$ $Z = 4$
 Monoclinic, $P2_1/n$ Mo $K\alpha$ radiation
 $a = 7.3570(2)$ Å $\mu = 0.31$ mm⁻¹
 $b = 15.6450(5)$ Å $T = 200$ K
 $c = 10.4954(3)$ Å $0.51 \times 0.45 \times 0.36$ mm
 $\beta = 90.518(3)^\circ$

Data collection

Oxford Diffraction Gemini diffractometer 10126 measured reflections
 Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007) 4020 independent reflections
 $T_{min} = 0.984, T_{max} = 1.000$ 2924 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$ 164 parameters
 $wR(F^2) = 0.115$ H-atom parameters constrained
 $S = 1.07$ $\Delta\rho_{max} = 0.38$ e Å⁻³
 4020 reflections $\Delta\rho_{min} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

D—H...A	D—H	H...A	D...A	D—H...A
O1—H1O...O2 ⁱ	0.84	1.83	2.6556 (12)	167
C6—H6A...O1 ⁱⁱ	0.95	2.57	3.5070 (13)	169
C11—H11A...O1 ⁱⁱⁱ	0.95	2.55	3.3382 (15)	141
C14—H14A...Cg1 ⁱⁱⁱ	0.95	2.79	3.7090 (14)	163

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

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.

BKS thanks the P. A. College of Engineering for the research facilities. RJB acknowledges the NSF MRI program (grant No. 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: SJ5108).

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supplementary materials

Acta Cryst. (2011). E67, o756 [doi:10.1107/S160053681100701X]

(2E)-3-(4-Chlorophenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one

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Comment

Chalcones, or 1,3-diaryl-2-propen-1-ones, belong to the flavonoid family. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β -unsaturated carbonyl system. The radical quenching properties of the phenolic groups present in many chalcones have raised interest in using the compounds or chalcone rich plant extracts as drugs or food preservatives. Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities (Nowakowska, 2007). Certain chalcone derivatives are reported to inhibit the polymerization of tubulin to form microtubules and are therefore antimitotic agents which can be used as antigout agents. The chalcone derivatives are also reported to inhibit the destruction of the myelin sheath in the central nervous system of multiple sclerosis patients and are thus useful in controlling the progressive nature of the disease (Edwards *et al.*, 1989).

In a continuation of our studies on the crystal structures of chalcones (Jasinski *et al.*, 2010, 2011a, 2011b), we report here the synthesis and crystal structure of the title compound, C₁₅H₁₁ClO₂, (I), Fig. 2. The dihedral angle between the mean planes of the chlorobenzene and hydroxybenzene rings is 6.5 (6)°. The mean plane of the prop-2-en-1-one group, the active site in this molecule, makes angles of 18.0 (1)° with the hydroxy benzene and 11.5 (1)° with the chlorobenzene rings, respectively. Bond lengths are normal (Allen *et al.*, 1987) and correspond to those observed in related compounds (Butcher *et al.*, 2007a, 2007b; Narayana *et al.*, 2007; Sarojini *et al.*, 2007a, 2007b). Crystal packing is stabilized by O—H...O hydrogen bonds, weak C—H...O, C—H...Cg π -ring (Table 1) and π — π intermolecular stacking interactions (Table 2 & Fig. 3).

Experimental

4-Hydroxyacetophenone (1.36 g, 0.01 mol) was mixed with 4-chlorobenzaldehyde (1.40 g, 0.01 mol) and dissolved in ethanol (20 ml) (Fig. 1). To this solution 4 ml of KOH (50%) (10 mL) was added at 0°C. The reaction mixture was stirred for 4 h 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 yellow solid was filtered, washed successively with dilute HCl solution and distilled water and finally recrystallized from ethanol (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 acetone. M.P:419 K. Composition: Found (Calculated) for C₁₅H₁₁ClO₂, C: 69.53 (69.64); H: 4.26 (4.29).

Refinement

The hydroxyl hydrogen (H1O) was located by a Fourier map, fixed at 0.84 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 Atom—H lengths of 0.95 Å (CH). Isotropic displacement parameters for these atoms were set to 1.18–1.21 (CH) or 1.18 (OH) times U_{eq} of the parent atom.

Figures

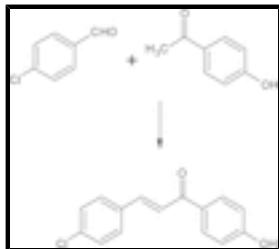


Fig. 1. Reaction scheme for the preparation of (I).

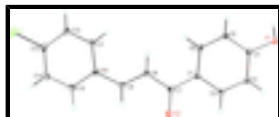


Fig. 2. Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.



Fig. 3. Packing diagram of the title compound viewed down the *a* axis. Dashed lines indicate O—H...O hydrogen bonds and weak C—H...O intermolecular interactions.

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Crystal data

$C_{15}H_{11}ClO_2$

$M_r = 258.69$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.3570$ (2) Å

$b = 15.6450$ (5) Å

$c = 10.4954$ (3) Å

$\beta = 90.518$ (3)°

$V = 1207.97$ (6) Å³

$Z = 4$

$F(000) = 536$

$D_x = 1.422$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4738 reflections

$\theta = 4.7$ – 32.4 °

$\mu = 0.31$ mm⁻¹

$T = 200$ K

Irregular chunk, colorless

$0.51 \times 0.45 \times 0.36$ mm

Data collection

Oxford Diffraction Gemini diffractometer

Radiation source: fine-focus sealed tube graphite

Detector resolution: 10.5081 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)

4020 independent reflections

2924 reflections with $I > 2\sigma(I)$

$R_{int} = 0.022$

$\theta_{max} = 32.6$ °, $\theta_{min} = 4.7$ °

$h = -10 \rightarrow 10$

$k = -23 \rightarrow 17$

$T_{\min} = 0.984$, $T_{\max} = 1.000$
10126 measured reflections

$l = -11 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.115$

$S = 1.07$

4020 reflections

164 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl	0.13335 (5)	0.12309 (2)	0.03417 (3)	0.03910 (12)
O1	0.83226 (11)	-0.31714 (6)	-0.88736 (8)	0.0269 (2)
H1O	0.7288	-0.3393	-0.8952	0.032*
O2	1.03166 (11)	-0.08981 (6)	-0.40899 (9)	0.0300 (2)
C1	0.86149 (15)	-0.16357 (7)	-0.56445 (10)	0.0217 (2)
C2	1.01626 (15)	-0.18219 (7)	-0.63990 (11)	0.0233 (2)
H2A	1.1307	-0.1587	-0.6162	0.028*
C3	1.00442 (15)	-0.23337 (7)	-0.74638 (11)	0.0240 (2)
H3A	1.1090	-0.2440	-0.7964	0.029*
C4	0.83821 (15)	-0.26923 (7)	-0.77995 (11)	0.0218 (2)
C5	0.68456 (15)	-0.25387 (8)	-0.70399 (11)	0.0249 (2)
H5A	0.5718	-0.2800	-0.7253	0.030*
C6	0.69667 (15)	-0.20111 (8)	-0.59876 (11)	0.0250 (2)
H6A	0.5916	-0.1903	-0.5494	0.030*
C7	0.88030 (15)	-0.10548 (7)	-0.45464 (11)	0.0228 (2)
C8	0.71613 (16)	-0.06563 (8)	-0.39876 (11)	0.0257 (2)

supplementary materials

H8A	0.5998	-0.0789	-0.4335	0.031*
C9	0.72854 (16)	-0.01152 (7)	-0.30074 (11)	0.0244 (2)
H9A	0.8482	0.0042	-0.2753	0.029*
C10	0.57985 (15)	0.02682 (7)	-0.22700 (11)	0.0232 (2)
C11	0.39739 (16)	0.00729 (8)	-0.25006 (12)	0.0269 (3)
H11A	0.3655	-0.0270	-0.3215	0.032*
C12	0.26083 (16)	0.03728 (8)	-0.16994 (12)	0.0286 (3)
H12A	0.1376	0.0221	-0.1856	0.034*
C13	0.30593 (17)	0.08902 (8)	-0.06791 (11)	0.0267 (3)
C14	0.48422 (18)	0.11178 (8)	-0.04434 (12)	0.0296 (3)
H14A	0.5144	0.1483	0.0250	0.036*
C15	0.61975 (17)	0.08026 (8)	-0.12423 (12)	0.0277 (3)
H15A	0.7427	0.0957	-0.1080	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0429 (2)	0.0418 (2)	0.03272 (18)	0.01436 (15)	0.01185 (14)	0.00176 (13)
O1	0.0232 (4)	0.0314 (5)	0.0261 (4)	-0.0042 (3)	0.0043 (3)	-0.0055 (3)
O2	0.0223 (4)	0.0345 (5)	0.0330 (5)	0.0028 (4)	-0.0034 (3)	-0.0045 (4)
C1	0.0207 (5)	0.0229 (5)	0.0216 (5)	0.0009 (4)	0.0022 (4)	0.0022 (4)
C2	0.0175 (5)	0.0265 (6)	0.0259 (6)	-0.0006 (4)	0.0006 (4)	0.0022 (5)
C3	0.0190 (5)	0.0280 (6)	0.0250 (6)	0.0004 (4)	0.0053 (4)	0.0015 (4)
C4	0.0236 (5)	0.0218 (5)	0.0203 (5)	0.0008 (4)	0.0022 (4)	0.0034 (4)
C5	0.0185 (5)	0.0296 (6)	0.0265 (6)	-0.0049 (4)	0.0031 (4)	0.0009 (5)
C6	0.0204 (5)	0.0296 (6)	0.0250 (6)	-0.0003 (4)	0.0057 (4)	0.0003 (5)
C7	0.0219 (5)	0.0241 (6)	0.0226 (5)	0.0012 (4)	0.0013 (4)	0.0033 (4)
C8	0.0203 (5)	0.0312 (6)	0.0257 (6)	0.0018 (5)	-0.0001 (4)	-0.0020 (5)
C9	0.0221 (5)	0.0250 (6)	0.0262 (6)	-0.0004 (4)	-0.0004 (4)	0.0004 (5)
C10	0.0243 (5)	0.0210 (5)	0.0241 (5)	0.0009 (4)	0.0001 (4)	-0.0003 (4)
C11	0.0265 (6)	0.0274 (6)	0.0267 (6)	0.0013 (5)	-0.0025 (5)	-0.0048 (5)
C12	0.0226 (6)	0.0319 (6)	0.0312 (6)	0.0027 (5)	-0.0010 (5)	-0.0002 (5)
C13	0.0311 (6)	0.0239 (6)	0.0251 (6)	0.0074 (5)	0.0041 (5)	0.0028 (5)
C14	0.0381 (7)	0.0244 (6)	0.0263 (6)	0.0012 (5)	-0.0021 (5)	-0.0048 (5)
C15	0.0273 (6)	0.0268 (6)	0.0290 (6)	-0.0029 (5)	-0.0031 (5)	-0.0029 (5)

Geometric parameters (\AA , $^\circ$)

Cl—C13	1.7517 (12)	C7—C8	1.4846 (15)
O1—C4	1.3541 (14)	C8—C9	1.3348 (16)
O1—H1O	0.8400	C8—H8A	0.9500
O2—C7	1.2328 (14)	C9—C10	1.4734 (15)
C1—C6	1.3917 (16)	C9—H9A	0.9500
C1—C2	1.4230 (14)	C10—C15	1.3939 (16)
C1—C7	1.4733 (16)	C10—C11	1.3957 (17)
C2—C3	1.3770 (16)	C11—C12	1.3971 (16)
C2—H2A	0.9500	C11—H11A	0.9500
C3—C4	1.3879 (16)	C12—C13	1.3804 (18)
C3—H3A	0.9500	C12—H12A	0.9500

C4—C5	1.4098 (15)	C13—C14	1.3793 (18)
C5—C6	1.3811 (17)	C14—C15	1.3984 (17)
C5—H5A	0.9500	C14—H14A	0.9500
C6—H6A	0.9500	C15—H15A	0.9500
C4—O1—H1O	109.5	C9—C8—H8A	119.3
C6—C1—C2	117.99 (10)	C7—C8—H8A	119.3
C6—C1—C7	122.56 (10)	C8—C9—C10	128.11 (11)
C2—C1—C7	119.45 (10)	C8—C9—H9A	115.9
C3—C2—C1	121.71 (10)	C10—C9—H9A	115.9
C3—C2—H2A	119.1	C15—C10—C11	117.45 (10)
C1—C2—H2A	119.1	C15—C10—C9	119.90 (11)
C2—C3—C4	119.35 (10)	C11—C10—C9	122.49 (11)
C2—C3—H3A	120.3	C10—C11—C12	121.18 (11)
C4—C3—H3A	120.3	C10—C11—H11A	119.4
O1—C4—C3	117.18 (10)	C12—C11—H11A	119.4
O1—C4—C5	123.03 (10)	C13—C12—C11	119.66 (11)
C3—C4—C5	119.78 (10)	C13—C12—H12A	120.2
C6—C5—C4	120.52 (11)	C11—C12—H12A	120.2
C6—C5—H5A	119.7	C14—C13—C12	120.79 (11)
C4—C5—H5A	119.7	C14—C13—C1	120.34 (10)
C5—C6—C1	120.59 (10)	C12—C13—C1	118.84 (10)
C5—C6—H6A	119.7	C13—C14—C15	118.92 (12)
C1—C6—H6A	119.7	C13—C14—H14A	120.5
O2—C7—C1	120.32 (10)	C15—C14—H14A	120.5
O2—C7—C8	119.88 (11)	C10—C15—C14	121.95 (11)
C1—C7—C8	119.80 (10)	C10—C15—H15A	119.0
C9—C8—C7	121.37 (11)	C14—C15—H15A	119.0
C6—C1—C2—C3	2.13 (17)	C1—C7—C8—C9	-178.78 (11)
C7—C1—C2—C3	-177.42 (11)	C7—C8—C9—C10	-173.67 (11)
C1—C2—C3—C4	-1.28 (17)	C8—C9—C10—C15	177.89 (12)
C2—C3—C4—O1	178.21 (10)	C8—C9—C10—C11	2.43 (19)
C2—C3—C4—C5	-0.86 (17)	C15—C10—C11—C12	-2.62 (18)
O1—C4—C5—C6	-176.85 (11)	C9—C10—C11—C12	172.94 (12)
C3—C4—C5—C6	2.17 (18)	C10—C11—C12—C13	1.71 (19)
C4—C5—C6—C1	-1.29 (18)	C11—C12—C13—C14	0.26 (19)
C2—C1—C6—C5	-0.81 (17)	C11—C12—C13—C1	-178.00 (10)
C7—C1—C6—C5	178.72 (11)	C12—C13—C14—C15	-1.18 (19)
C6—C1—C7—O2	162.67 (11)	C1—C13—C14—C15	177.05 (10)
C2—C1—C7—O2	-17.81 (17)	C11—C10—C15—C14	1.68 (18)
C6—C1—C7—C8	-17.34 (17)	C9—C10—C15—C14	-174.00 (11)
C2—C1—C7—C8	162.18 (11)	C13—C14—C15—C10	0.19 (19)
O2—C7—C8—C9	1.20 (18)		

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>
O1—H1O...O2 ⁱ	0.84	1.83	2.6556 (12)	167
C6—H6A...O1 ⁱⁱ	0.95	2.57	3.5070 (13)	169

supplementary materials

C11—H11A...O1 ⁱⁱ	0.95	2.55	3.3382 (15)	141
C14—H14A...Cg1 ⁱⁱⁱ	0.95	2.79	3.7090 (14)	163

Symmetry codes: (i) $x-1/2, -y-1/2, z-1/2$; (ii) $x-1/2, -y-1/2, z+1/2$; (iii) $-x+3/2, y+1/2, -z+3/2$.

Table 2

Selected geometric parameters (Å): Cg...Cg π stacking interactions, Cg1, Cg2 are the centroids of rings C1—C6 and C10—C15 [Symmetry codes: (i) 1-x, 2-y, 1-z; (ii) 1-x, 2-y, 2-z]

Cg1...CgJ	Cg...Cg (Å)	Cg1 Perp (Å)	Cgj Perp (Å)	Slippage (Å)
Cg1...Cg2 ⁱ	3.7771 (7)	3.3144 (5)	3.4958 (5)	
Cg2...Cg2 ⁱⁱ	3.6917 (7)	-3.3684 (5)	-3.3683 (5)	1.51 (1)

Fig. 1

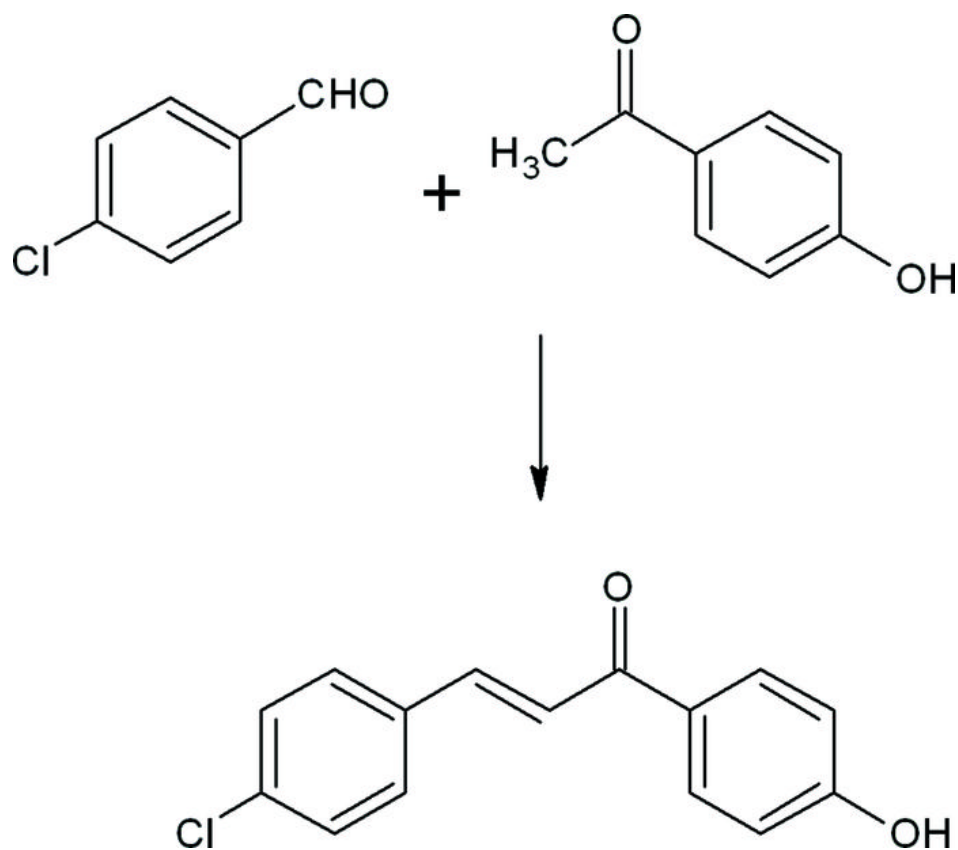


Fig. 2

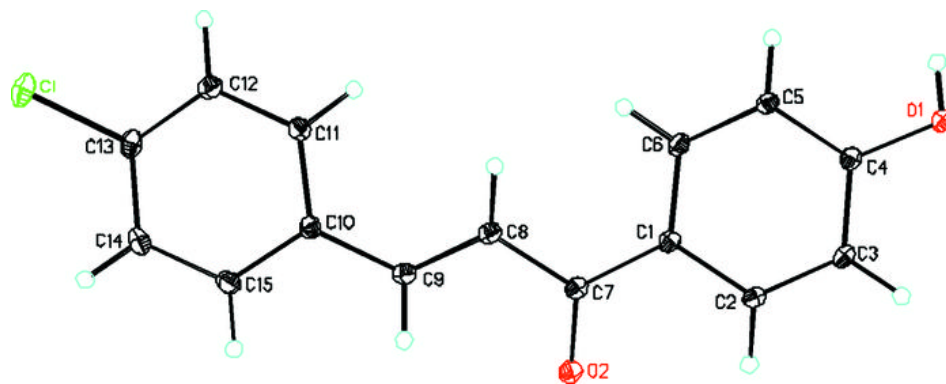


Fig. 3

