

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

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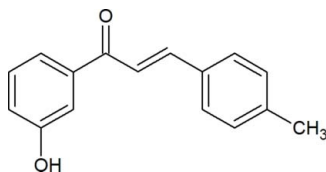
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Key indicators: single-crystal X-ray study; $T = 203$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.116; data-to-parameter ratio = 25.6.

Two new chalcones of general type (2E)-1-(3-hydroxyphenyl)-3-(4-*R*-phenyl)prop-2-en-1-one are reported, one where *R* = methyl, $\text{C}_{16}\text{H}_{14}\text{O}_2$, in the present paper, and one where *R* = chloro, $\text{C}_{15}\text{H}_{11}\text{ClO}_2$, in the following paper [Butcher, Jasinski, Narayana, Lakshmana & Yathirajan (2007). *Acta Cryst.* **E63**, 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

$\text{C}_{16}\text{H}_{14}\text{O}_2$	$V = 1250.42$ (12) Å ³
$M_r = 238.27$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.6363$ (5) Å	$\mu = 0.08$ mm ⁻¹
$b = 11.0786$ (5) Å	$T = 203$ K
$c = 15.2355$ (8) Å	$0.51 \times 0.47 \times 0.32$ mm
$\beta = 104.038$ (6)°	

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^i$	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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supplementary materials

Acta Cryst. (2007). E63, o3660 [doi:10.1107/S1600536807036641]

(2E)-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 (C₁₆H₁₄O₂) (I), reported in the present paper, and *R*=Chloro (C₁₅H₁₁ClO₂) (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 nearly 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%. C₁₆H₁₄O₂ 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 $U_{iso}(H) = 1.18–1.50U_{eq}(C, O)$.

Figures

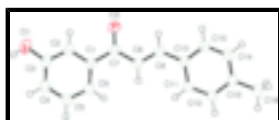


Fig. 1. Molecular structure of (I), showing atom labelling and 50% probability displacement ellipsoids.

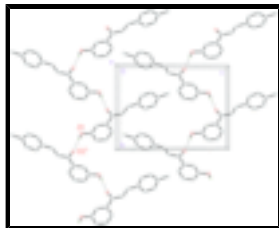


Fig. 2. Packing diagram of (I) viewed down the *a* axis. Dashed lines indicate O–H···O hydrogen bonds. Symmetry code: as in Table 1

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

Crystal data

$C_{16}H_{14}O_2$

$M_r = 238.27$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 7.6363$ (5) Å

$b = 11.0786$ (5) Å

$c = 15.2355$ (8) Å

$\beta = 104.038$ (6)°

$V = 1250.42$ (12) Å³

$Z = 4$

$F_{000} = 504$

$D_x = 1.266$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4283 reflections

$\theta = 4.6$ – 32.5 °

$\mu = 0.08$ mm⁻¹

$T = 203$ K

Prism, colorless

$0.51 \times 0.47 \times 0.32$ mm

Data collection

Oxford Diffraction Gemini R diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 203$ K

φ and ω scans

Absorption correction: none

17875 measured reflections

4225 independent reflections

1758 reflections with $I > 2\sigma(I)$

$R_{int} = 0.041$

$\theta_{max} = 32.5$ °

$\theta_{min} = 4.6$ °

$h = -11$ → 11

$k = -15$ → 16

$l = -22$ → 22

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.116$

$S = 0.85$

4225 reflections

165 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2]$

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

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

$\Delta\rho_{max} = 0.17$ e Å⁻³

$\Delta\rho_{min} = -0.25$ 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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

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H16C 0.5325 0.2511 0.4568 0.085*

Atomic displacement parameters (\AA^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 (\AA , $^\circ$)

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, °)

<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—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

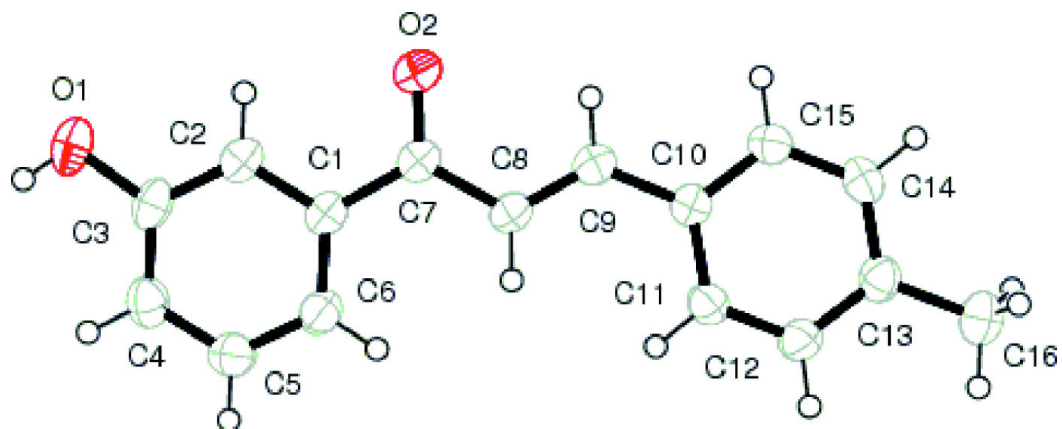


Fig. 2

