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

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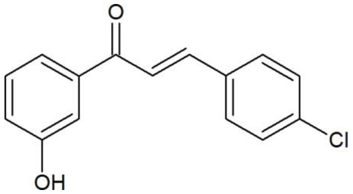
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.056; wR factor = 0.176; data-to-parameter ratio = 24.8.

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 = chloro, $C_{15}H_{11}ClO_2$, in the present paper, and one where R = methyl, $C_{16}H_{14}O_2$, in the preceding paper [Butcher, Jasinski, Narayana, Lakshmana & Yathirajan (2007). *Acta Cryst.* E**63**, o3660]. 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 hydrogen and the propyl-2-ketone oxygen.

Related literature

For the R = methyl structure and related references, see Butcher *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{11}ClO_2$
M_r = 258.69
Monoclinic, $P2_1/c$
a = 7.5910 (7) Å
b = 10.8509 (7) Å
c = 15.1544 (11) Å
β = 104.213 (8)°
V = 1210.05 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 203 K
0.47 × 0.38 × 0.17 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlisPro*; Oxford Diffraction, 2007)
T_{min} = 0.48, T_{max} = 0.95
15403 measured reflections
4072 independent reflections
2342 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
2 standard reflections every 50 reflections intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.176
S = 0.98
4072 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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	1.88	2.7029 (18)	172.2

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

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: BG2080).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o3661 [**doi:10.1107/S1600536807036653**]

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

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

Comment

Two new chalcones of general formula (2E)-1-(3-Hydroxyphenyl)-3-(4-*R*-phenyl)prop-2-en-1-one are reported, the one with *R*=Chloro ($C_{15}H_{11}ClO_2$) (II) in the present paper, the one with *R*=methyl ($C_{16}H_{14}O_2$) (I) in the preceeding one (Butcher *et al.*, 2007) to which the reader is referred for a general introduction.

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

The 3-hydroxyphenyl and 4-chlorophenyl groups are coplanar with each other and with the propyl 2 ketone group forming torsion angles 2.3 (3)°, C8—C9—C10—C11, and −2.7 (2)°, C8—C7—C1—C6, 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-chloroacetophenone (1.4 g, 0.01 mol) in ethanol (25 ml), a solution of potassium hydroxide (5%, 7.5 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 recrystallized from ethanol and the crystals were obtained from acetone by slow evaporation (yield: 78%; m.p.:425–426 K). Elemental analysis found: C: 69.52, H: 4.23%. $C_{15}H_{11}ClO_2$ requires C, 69.64, H: 4.29%.

Refinement

The larger than expected transmission factors range is probably due to inferior data quality and to the fact that the multi-scan correction deals with a number of factors, of which absorption is only one. All of the H atoms, except H1 which was located from a difference Fourier map, were inferred from neighbouring sites. All H atoms were included in the riding model approximation with C—H = 0.94 Å, and with $U_{iso}(H) = 1.19–1.20U_{eq}(C,O)$.

Figures

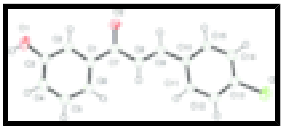

Fig. 1. Molecular structure of (II), showing atom labelling and 50% probability displacement ellipsoids.

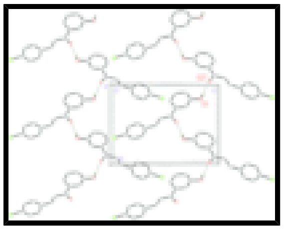

Fig. 2. Packing diagram of (II) viewed down the *a* axis. Dashed lines indicate O–H···O hydrogen bonds. Symmetry code: as in Table 1

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

Crystal data

$C_{15}H_{11}ClO_2$

$M_r = 258.69$

Monoclinic, $P2_1/c$

Hall symbol: -P 1 2ybc '

$a = 7.5910$ (7) Å

$b = 10.8509$ (7) Å

$c = 15.1544$ (11) Å

$\beta = 104.213$ (8)°

$V = 1210.05$ (16) Å^3

$Z = 4$

$F_{000} = 536$

$D_x = 1.420$ Mg m^{-3}

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

Cell parameters from 5848 reflections

$\theta = 4.7–32.4$°

$\mu = 0.31$ mm^{-1}

$T = 203$ K

Plate, colorless

0.47 × 0.38 × 0.17 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: multi-scan (*CrysAlisPro*; Oxford Diffraction, 2007)

$T_{min} = 0.48$, $T_{max} = 0.95$

15403 measured reflections

4072 independent reflections

2342 reflections with $I > 2\sigma(I)$

$R_{int} = 0.069$

$\theta_{max} = 32.6$°

$\theta_{min} = 4.7$°

$h = -11 \rightarrow 10$

$k = -16 \rightarrow 15$

$l = -22 \rightarrow 22$

2 standard reflections

every 50 reflections

intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.176$

$S = 0.98$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1075P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

4072 reflections	$\Delta\rho_{max}$ = 0.75 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.36 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 > 2sigma(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}
Cl	0.51228 (7)	0.67123 (5)	0.02769 (3)	0.0498 (2)
O1	1.10564 (19)	0.18538 (12)	0.82766 (8)	0.0408 (3)
H1	1.1559	0.1197	0.8478	0.049*
O2	0.75857 (17)	0.46703 (11)	0.60068 (8)	0.0371 (3)
C1	0.9418 (2)	0.29521 (14)	0.59612 (11)	0.0275 (3)
C2	0.9721 (2)	0.28277 (15)	0.69002 (11)	0.0293 (4)
H2A	0.9177	0.3384	0.7228	0.035*
C3	1.0821 (2)	0.18899 (15)	0.73585 (11)	0.0308 (4)
C4	1.1593 (2)	0.10554 (15)	0.68772 (13)	0.0369 (4)
H4A	1.2330	0.0416	0.7184	0.044*
C5	1.1278 (3)	0.11638 (16)	0.59428 (13)	0.0394 (4)
H5A	1.1796	0.0588	0.5617	0.047*
C6	1.0214 (2)	0.21064 (16)	0.54781 (12)	0.0348 (4)
H6A	1.0028	0.2178	0.4844	0.042*
C7	0.8283 (2)	0.39982 (14)	0.55349 (10)	0.0270 (3)
C8	0.7987 (2)	0.42422 (14)	0.45573 (10)	0.0275 (3)
H8A	0.8609	0.3770	0.4210	0.033*
C9	0.6852 (2)	0.51211 (14)	0.41560 (10)	0.0277 (3)
H9A	0.6264	0.5566	0.4533	0.033*
C10	0.6412 (2)	0.54776 (13)	0.31968 (10)	0.0260 (3)
C11	0.7139 (2)	0.48648 (15)	0.25585 (11)	0.0307 (4)
H11A	0.7919	0.4190	0.2745	0.037*
C12	0.6737 (2)	0.52297 (16)	0.16603 (11)	0.0340 (4)
H12A	0.7233	0.4810	0.1235	0.041*
C13	0.5594 (2)	0.62216 (16)	0.13965 (11)	0.0322 (4)
C14	0.4848 (2)	0.68418 (15)	0.20078 (13)	0.0342 (4)
H14A	0.4059	0.7510	0.1816	0.041*
C15	0.5269 (2)	0.64728 (15)	0.29067 (12)	0.0326 (4)

H15A	0.4774	0.6902	0.3328	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0649 (4)	0.0536 (3)	0.0289 (2)	0.0138 (2)	0.0080 (2)	0.00854 (19)
O1	0.0468 (8)	0.0458 (7)	0.0286 (6)	−0.0020 (6)	0.0068 (6)	0.0106 (5)
O2	0.0450 (8)	0.0380 (6)	0.0314 (6)	0.0067 (5)	0.0150 (5)	−0.0010 (5)
C1	0.0273 (8)	0.0277 (7)	0.0269 (8)	−0.0065 (6)	0.0057 (6)	0.0011 (6)
C2	0.0294 (9)	0.0313 (8)	0.0283 (8)	−0.0077 (6)	0.0089 (7)	0.0009 (6)
C3	0.0295 (9)	0.0364 (9)	0.0267 (8)	−0.0096 (7)	0.0073 (6)	0.0062 (6)
C4	0.0334 (10)	0.0346 (9)	0.0425 (10)	0.0024 (7)	0.0092 (8)	0.0111 (8)
C5	0.0436 (11)	0.0353 (9)	0.0426 (10)	0.0070 (8)	0.0169 (8)	0.0024 (8)
C6	0.0393 (10)	0.0352 (9)	0.0312 (8)	0.0029 (7)	0.0114 (7)	0.0017 (7)
C7	0.0270 (8)	0.0284 (7)	0.0263 (8)	−0.0071 (6)	0.0079 (6)	−0.0008 (6)
C8	0.0308 (9)	0.0270 (7)	0.0254 (7)	−0.0026 (6)	0.0084 (6)	−0.0008 (6)
C9	0.0296 (9)	0.0283 (8)	0.0262 (7)	−0.0026 (6)	0.0086 (6)	−0.0017 (6)
C10	0.0260 (8)	0.0260 (7)	0.0267 (7)	−0.0030 (6)	0.0077 (6)	0.0004 (6)
C11	0.0299 (9)	0.0326 (8)	0.0290 (7)	0.0060 (7)	0.0060 (6)	0.0030 (7)
C12	0.0350 (10)	0.0395 (9)	0.0288 (8)	0.0050 (7)	0.0102 (7)	−0.0031 (7)
C13	0.0343 (9)	0.0345 (9)	0.0262 (8)	−0.0001 (7)	0.0044 (7)	0.0020 (6)
C14	0.0324 (9)	0.0323 (8)	0.0376 (9)	0.0071 (7)	0.0080 (7)	0.0046 (7)
C15	0.0352 (10)	0.0305 (8)	0.0346 (9)	0.0044 (7)	0.0132 (7)	−0.0005 (7)

Geometric parameters (Å, °)

Cl—C13	1.7298 (16)	C7—C8	1.467 (2)
O1—C3	1.3591 (19)	C8—C9	1.328 (2)
O1—H1	0.8300	C8—H8A	0.9400
O2—C7	1.2284 (19)	C9—C10	1.461 (2)
C1—C2	1.391 (2)	C9—H9A	0.9400
C1—C6	1.400 (2)	C10—C15	1.387 (2)
C1—C7	1.475 (2)	C10—C11	1.395 (2)
C2—C3	1.389 (2)	C11—C12	1.378 (2)
C2—H2A	0.9400	C11—H11A	0.9400
C3—C4	1.380 (3)	C12—C13	1.379 (2)
C4—C5	1.382 (3)	C12—H12A	0.9400
C4—H4A	0.9400	C13—C14	1.374 (2)
C5—C6	1.384 (2)	C14—C15	1.380 (2)
C5—H5A	0.9400	C14—H14A	0.9400
C6—H6A	0.9400	C15—H15A	0.9400
C3—O1—H1	109.5	C9—C8—H8A	119.6
C2—C1—C6	119.13 (15)	C7—C8—H8A	119.6
C2—C1—C7	117.06 (14)	C8—C9—C10	127.58 (14)
C6—C1—C7	123.80 (14)	C8—C9—H9A	116.2
C3—C2—C1	120.71 (15)	C10—C9—H9A	116.2
C3—C2—H2A	119.6	C15—C10—C11	118.34 (14)
C1—C2—H2A	119.6	C15—C10—C9	119.59 (14)

O1—C3—C4	123.78 (16)	C11—C10—C9	122.06 (14)
O1—C3—C2	116.41 (15)	C12—C11—C10	121.24 (15)
C4—C3—C2	119.82 (15)	C12—C11—H11A	119.4
C3—C4—C5	119.78 (16)	C10—C11—H11A	119.4
C3—C4—H4A	120.1	C11—C12—C13	118.80 (15)
C5—C4—H4A	120.1	C11—C12—H12A	120.6
C4—C5—C6	121.12 (17)	C13—C12—H12A	120.6
C4—C5—H5A	119.4	C14—C13—C12	121.39 (15)
C6—C5—H5A	119.4	C14—C13—Cl	119.36 (13)
C5—C6—C1	119.42 (16)	C12—C13—Cl	119.23 (13)
C5—C6—H6A	120.3	C13—C14—C15	119.30 (16)
C1—C6—H6A	120.3	C13—C14—H14A	120.3
O2—C7—C8	119.99 (15)	C15—C14—H14A	120.3
O2—C7—C1	119.39 (14)	C14—C15—C10	120.92 (15)
C8—C7—C1	120.62 (13)	C14—C15—H15A	119.5
C9—C8—C7	120.88 (14)	C10—C15—H15A	119.5

C6—C1—C2—C3	1.0 (2)	C1—C7—C8—C9	174.62 (15)
C7—C1—C2—C3	−178.02 (14)	C7—C8—C9—C10	179.95 (14)
C1—C2—C3—O1	179.11 (14)	C8—C9—C10—C15	−176.19 (16)
C1—C2—C3—C4	−1.3 (2)	C8—C9—C10—C11	2.3 (3)
O1—C3—C4—C5	−179.99 (16)	C15—C10—C11—C12	−0.2 (3)
C2—C3—C4—C5	0.5 (3)	C9—C10—C11—C12	−178.68 (15)
C3—C4—C5—C6	0.7 (3)	C10—C11—C12—C13	0.1 (3)
C4—C5—C6—C1	−1.1 (3)	C11—C12—C13—C14	−0.4 (3)
C2—C1—C6—C5	0.3 (2)	C11—C12—C13—Cl	178.41 (13)
C7—C1—C6—C5	179.16 (16)	C12—C13—C14—C15	0.8 (3)
C2—C1—C7—O2	−3.6 (2)	Cl—C13—C14—C15	−178.03 (14)
C6—C1—C7—O2	177.48 (15)	C13—C14—C15—C10	−0.9 (3)
C2—C1—C7—C8	176.21 (14)	C11—C10—C15—C14	0.6 (3)
C6—C1—C7—C8	−2.7 (2)	C9—C10—C15—C14	179.11 (15)
O2—C7—C8—C9	−5.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2$^{\mathrm{i}}$	0.83	1.88	2.7029 (18)	172.2

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+3/2.

Fig. 1

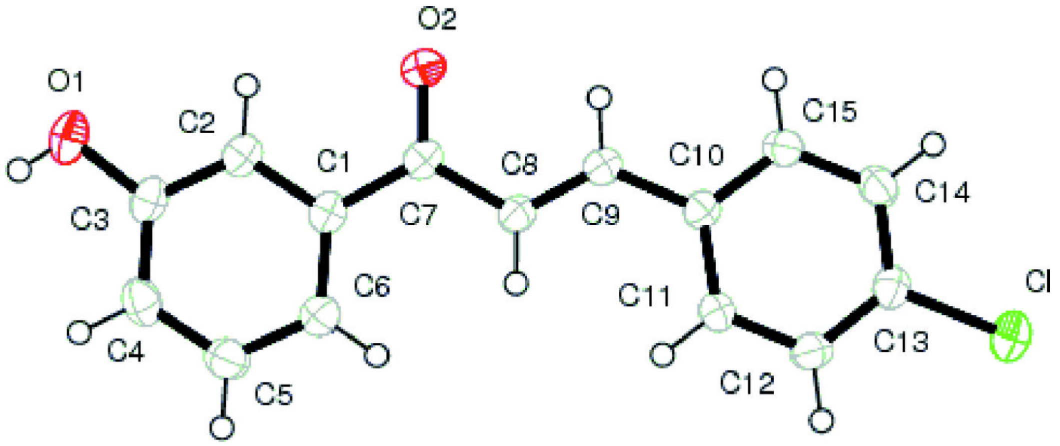

Fig. 2