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

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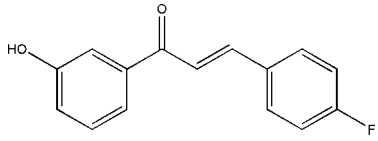
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.145; data-to-parameter ratio = 24.6.

In the title molecule, $C_{15}H_{11}FO_2$, the 3-hydroxyphenyl and 4-fluorophenyl groups are coplanar with each other and also with the plane of the prop-2-en-1-one linkage. Crystal packing is stabilized by intermolecular O—H···O hydrogen bonding between the hydroxyl H atom and the prop-2-en-1-one O atom, which links the molecules into a chain along the [010] direction.

Related literature

For related structures, see: Butcher *et al.* (2006); Yathirajan *et al.* (2006, 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

$C_{15}H_{11}FO_2$
M_r = 242.24
Monoclinic, $P2_1/n$
a = 7.4149 (4) Å
b = 11.3162 (6) Å
c = 14.7472 (8) Å
β = 104.311 (6)°
V = 1199.01 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 203 K
0.59 × 0.47 × 0.31 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.643, T_{max} = 1.000 (expected range 0.942–0.970)
16754 measured reflections
4038 independent reflections
1916 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
2 standard reflections
every 50 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.145
S = 1.06
4038 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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	2.7013 (13)	159

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2418).

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supplementary materials

Acta Cryst. (2007). E**63**, o3586 [**doi:10.1107/S1600536807034964**]

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

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

Comment

Chalcones are known for their anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. We have synthesized a new chalcone, the title compound. In view of the importance of the title compound, its crystal structure is reported here.

The 3-hydroxyphenyl and 4-fluorophenyl groups of the title molecule (Fig. 1) are coplanar [dihedral angle = 3.11 (8)°] with each other and also with the propyl-2-ketone group, forming torsion angles C8—C9—C10—C11 and C8—C7—C1—C6 of 4.9 (2)° and −1.75 (18)°, respectively.

Intermolecular O—H···O hydrogen bonding interactions (Table 1) involving the hydroxyl group and the carbonyl O atom link the molecules into a chain along the [0 1 0] direction (Fig. 2).

Experimental

To a mixture of 1-(3-hydroxyphenyl)ethanone (1.36 g, 0.01 mol) and 4-fluoroacetophenone (1.38 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 solid that precipitated was filtered off and washed with cold ethanol, dried and recrystallized from ethanol. X-ray quality crystals were obtained from ethyl acetate by slow evaporation (yield: 80%; m.p. 408–09 K). Analysis found: C 74.30, H 4.51%; $C_{15}H_{11}ClO_2$ requires: C 74.37, H 4.58%.

Refinement

All H atoms, except H1, were found in a difference map. But all H atoms were refined using a riding model with O—H = 0.83 Å and C—H = 0.94 Å, and with U_{iso}(H) = 1.19–1.20 U_{eq}(C,*O*). Owing to the poor diffraction quality of the crystal, the ratio of observed to unique reflections is low (47%).

Figures

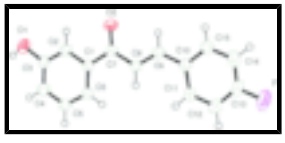

Fig. 1. Molecular structure of the title compound, showing atom labelling and 50% probability displacement ellipsoids.

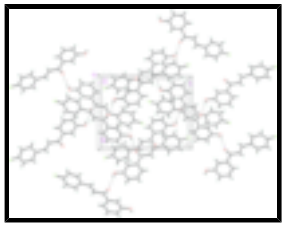

Fig. 2. Packing diagram of the title compound, viewed down the *a* axis. Dashed lines indicate O—H···O hydrogen bonds.

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

Crystal data

$C_{15}H_{11}FO_2$	F_{000} = 504
M_r = 242.24	D_x = 1.342 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5107 reflections
a = 7.4149 (4) Å	θ = 4.8–32.5º
b = 11.3162 (6) Å	μ = 0.10 mm^{-1}
c = 14.7472 (8) Å	T = 203 K
β = 104.311 (6)º	Prism, colourless
V = 1199.01 (11) Å^3	0.59 × 0.47 × 0.31 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R diffractometer	R_{int} = 0.042
Radiation source: fine-focus sealed tube	θ_{max} = 32.5º
Monochromator: graphite	θ_{min} = 4.8º
T = 203 K	h = −11→11
φ and ω scans	k = −16→17
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	l = −21→22
T_{min} = 0.643, T_{max} = 1.000	2 standard reflections
16754 measured reflections	every 50 reflections
4038 independent reflections	intensity decay: none
1916 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.145	$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001

4038 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -0.17$ 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}
F	0.53494 (15)	0.34667 (10)	−0.46126 (6)	0.0827 (4)
O1	0.71674 (13)	0.81902 (9)	0.33109 (6)	0.0491 (3)
H1	0.6731	0.8786	0.3507	0.059*
O2	0.83919 (12)	0.53556 (8)	0.10376 (6)	0.0449 (3)
C1	0.65119 (16)	0.70409 (10)	0.09520 (8)	0.0318 (3)
C2	0.71346 (16)	0.71937 (11)	0.19185 (8)	0.0339 (3)
H2A	0.7999	0.6658	0.2270	0.041*
C3	0.65035 (17)	0.81164 (12)	0.23650 (8)	0.0360 (3)
C4	0.52401 (19)	0.89189 (12)	0.18486 (9)	0.0436 (3)
H4A	0.4812	0.9555	0.2148	0.052*
C5	0.4616 (2)	0.87745 (13)	0.08907 (10)	0.0488 (4)
H5A	0.3759	0.9317	0.0543	0.059*
C6	0.52293 (19)	0.78494 (12)	0.04362 (9)	0.0426 (3)
H6A	0.4790	0.7762	−0.0215	0.051*
C7	0.72278 (15)	0.60043 (10)	0.05300 (8)	0.0321 (3)
C8	0.65602 (16)	0.57558 (11)	−0.04758 (8)	0.0327 (3)
H8A	0.5600	0.6220	−0.0841	0.039*
C9	0.72904 (16)	0.48853 (11)	−0.08792 (9)	0.0347 (3)
H9A	0.8244	0.4445	−0.0485	0.042*
C10	0.67813 (16)	0.45384 (11)	−0.18606 (9)	0.0344 (3)
C11	0.54868 (19)	0.51720 (12)	−0.25370 (9)	0.0427 (3)
H11A	0.4933	0.5852	−0.2358	0.051*
C12	0.5007 (2)	0.48226 (14)	−0.34577 (10)	0.0523 (4)
H12A	0.4133	0.5252	−0.3908	0.063*
C13	0.5838 (2)	0.38287 (15)	−0.37027 (10)	0.0522 (4)
C14	0.7107 (2)	0.31840 (14)	−0.30732 (11)	0.0514 (4)
H14A	0.7654	0.2508	−0.3263	0.062*
C15	0.75793 (18)	0.35409 (12)	−0.21479 (10)	0.0418 (3)

H15A	0.8454	0.3101	−0.1706	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F	0.1133 (9)	0.0953 (8)	0.0383 (6)	0.0028 (7)	0.0166 (5)	−0.0175 (5)
O1	0.0562 (6)	0.0548 (6)	0.0317 (5)	−0.0022 (5)	0.0020 (4)	−0.0099 (4)
O2	0.0462 (5)	0.0447 (5)	0.0384 (5)	0.0093 (4)	0.0005 (4)	0.0028 (4)
C1	0.0304 (6)	0.0350 (6)	0.0298 (6)	−0.0055 (5)	0.0069 (5)	0.0015 (5)
C2	0.0295 (6)	0.0384 (7)	0.0308 (6)	−0.0058 (5)	0.0020 (5)	0.0010 (5)
C3	0.0350 (7)	0.0418 (7)	0.0300 (7)	−0.0106 (5)	0.0057 (5)	−0.0054 (5)
C4	0.0456 (8)	0.0418 (8)	0.0424 (8)	0.0012 (6)	0.0093 (6)	−0.0070 (6)
C5	0.0557 (9)	0.0475 (8)	0.0388 (8)	0.0148 (7)	0.0030 (6)	0.0024 (6)
C6	0.0470 (8)	0.0464 (8)	0.0316 (7)	0.0058 (6)	0.0046 (6)	0.0023 (6)
C7	0.0288 (6)	0.0336 (6)	0.0335 (6)	−0.0046 (5)	0.0067 (5)	0.0035 (5)
C8	0.0306 (6)	0.0360 (7)	0.0311 (6)	−0.0016 (5)	0.0066 (5)	0.0018 (5)
C9	0.0304 (6)	0.0378 (7)	0.0354 (7)	−0.0016 (5)	0.0073 (5)	0.0030 (5)
C10	0.0285 (6)	0.0377 (7)	0.0382 (7)	−0.0057 (5)	0.0104 (5)	−0.0024 (5)
C11	0.0442 (7)	0.0459 (8)	0.0382 (8)	0.0042 (6)	0.0103 (6)	−0.0012 (6)
C12	0.0578 (9)	0.0619 (10)	0.0345 (8)	0.0037 (8)	0.0062 (7)	0.0031 (7)
C13	0.0629 (10)	0.0619 (10)	0.0328 (8)	−0.0047 (8)	0.0140 (7)	−0.0086 (7)
C14	0.0573 (9)	0.0512 (9)	0.0497 (9)	0.0007 (7)	0.0209 (7)	−0.0149 (7)
C15	0.0388 (7)	0.0414 (8)	0.0455 (8)	0.0003 (6)	0.0107 (6)	−0.0030 (6)

Geometric parameters (Å, °)

F—C13	1.3635 (16)	C7—C8	1.4700 (17)
O1—C3	1.3622 (15)	C8—C9	1.3330 (17)
O1—H1	0.83	C8—H8A	0.94
O2—C7	1.2348 (14)	C9—C10	1.4564 (17)
C1—C2	1.3962 (16)	C9—H9A	0.94
C1—C6	1.4009 (17)	C10—C15	1.3884 (18)
C1—C7	1.4861 (17)	C10—C11	1.3989 (18)
C2—C3	1.3766 (18)	C11—C12	1.3739 (19)
C2—H2A	0.94	C11—H11A	0.94
C3—C4	1.3890 (18)	C12—C13	1.373 (2)
C4—C5	1.3832 (18)	C12—H12A	0.94
C4—H4A	0.94	C13—C14	1.359 (2)
C5—C6	1.379 (2)	C14—C15	1.3825 (19)
C5—H5A	0.94	C14—H14A	0.94
C6—H6A	0.94	C15—H15A	0.94
C3—O1—H1	109.5	C9—C8—H8A	119.4
C2—C1—C6	118.83 (11)	C7—C8—H8A	119.4
C2—C1—C7	117.59 (11)	C8—C9—C10	127.49 (12)
C6—C1—C7	123.58 (11)	C8—C9—H9A	116.3
C3—C2—C1	121.10 (11)	C10—C9—H9A	116.3
C3—C2—H2A	119.4	C15—C10—C11	117.91 (12)
C1—C2—H2A	119.4	C15—C10—C9	119.80 (12)

O1—C3—C2	117.18 (11)	C11—C10—C9	122.28 (12)
O1—C3—C4	123.05 (12)	C12—C11—C10	121.45 (13)
C2—C3—C4	119.77 (12)	C12—C11—H11A	119.3
C5—C4—C3	119.51 (13)	C10—C11—H11A	119.3
C5—C4—H4A	120.2	C13—C12—C11	118.18 (14)
C3—C4—H4A	120.2	C13—C12—H12A	120.9
C6—C5—C4	121.25 (13)	C11—C12—H12A	120.9
C6—C5—H5A	119.4	C14—C13—F	118.79 (14)
C4—C5—H5A	119.4	C14—C13—C12	122.68 (13)
C5—C6—C1	119.53 (12)	F—C13—C12	118.53 (14)
C5—C6—H6A	120.2	C13—C14—C15	118.74 (14)
C1—C6—H6A	120.2	C13—C14—H14A	120.6
O2—C7—C8	120.57 (11)	C15—C14—H14A	120.6
O2—C7—C1	118.94 (11)	C14—C15—C10	121.04 (13)
C8—C7—C1	120.49 (10)	C14—C15—H15A	119.5
C9—C8—C7	121.27 (11)	C10—C15—H15A	119.5
C6—C1—C2—C3	0.27 (18)	C1—C7—C8—C9	174.75 (11)
C7—C1—C2—C3	−178.49 (11)	C7—C8—C9—C10	−179.81 (10)
C1—C2—C3—O1	179.23 (10)	C8—C9—C10—C15	−174.46 (12)
C1—C2—C3—C4	−0.65 (19)	C8—C9—C10—C11	4.9 (2)
O1—C3—C4—C5	−179.26 (12)	C15—C10—C11—C12	0.2 (2)
C2—C3—C4—C5	0.6 (2)	C9—C10—C11—C12	−179.18 (12)
C3—C4—C5—C6	−0.2 (2)	C10—C11—C12—C13	−0.2 (2)
C4—C5—C6—C1	−0.2 (2)	C11—C12—C13—C14	0.0 (2)
C2—C1—C6—C5	0.15 (19)	C11—C12—C13—F	179.08 (13)
C7—C1—C6—C5	178.82 (13)	F—C13—C14—C15	−178.96 (12)
C2—C1—C7—O2	−3.07 (16)	C12—C13—C14—C15	0.1 (2)
C6—C1—C7—O2	178.24 (11)	C13—C14—C15—C10	−0.1 (2)
C2—C1—C7—C8	176.94 (10)	C11—C10—C15—C14	−0.10 (19)
C6—C1—C7—C8	−1.75 (18)	C9—C10—C15—C14	179.32 (12)
O2—C7—C8—C9	−5.25 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.83	1.91	2.7013 (13)	159

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

Fig. 1

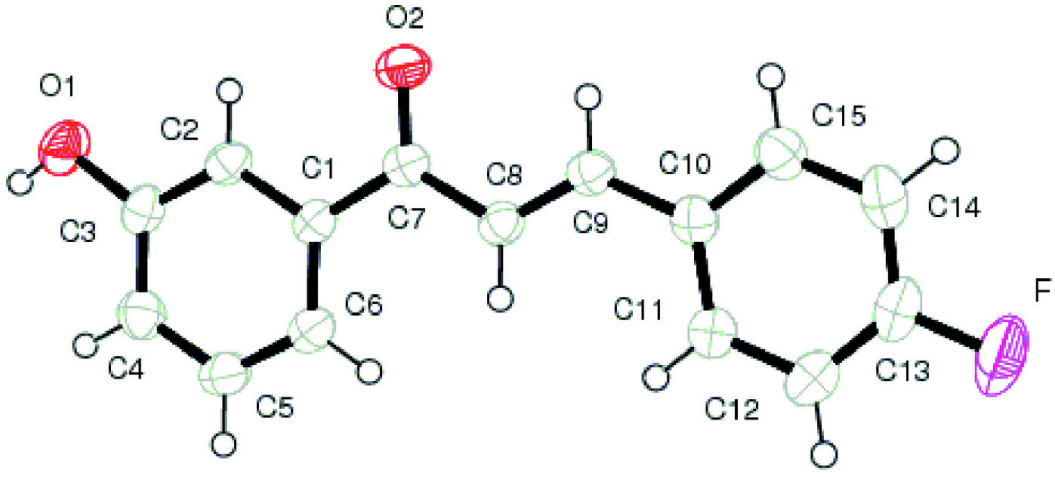

Fig. 2