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(2*E*)-1-(2-Hydroxyphenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

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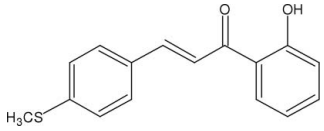
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.184; data-to-parameter ratio = 15.7.

Geometric parameters of the title compound, $C_{16}H_{14}O_2S$, a chalcone derivative, are in the usual ranges. The C=C double bond has a *trans* configuration. The essentially planar molecules (r.m.s. deviation for all non-H atoms = 0.034 Å) crystallize in planes parallel to the ($\bar{1}$40) plane. The molecular conformation is stabilized by an O—H···O hydrogen bond. The investigated crystal was a non-merohedral twin with a ratio of the twin components of 0.254 (1):0.746 (1).

Related literature

For related literature, see: Butcher *et al.* (2007); Conti (2006); Domínguez *et al.* (2005); Goto *et al.* (1991); Harrison *et al.* (2006); Indira *et al.* (2002); Lawrence *et al.* (2001); Nielsen *et al.* (2005); Pandey *et al.* (2005); Sarojini *et al.* (2006); Yathirajan, Mayekar, Narayana *et al.* (2007); Yathirajan, Mayekar, Sarojini *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{14}O_2S$
M_r = 270.33
Triclinic, $P\bar{1}$
a = 6.6516 (9) Å
b = 7.0223 (11) Å
c = 15.0248 (17) Å
α = 90.789 (11)°
β = 93.409 (11)°
γ = 105.718 (12)°
V = 673.98 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 173 (2) K
0.37 × 0.31 × 0.12 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.938, T_{max} = 0.982
13663 measured reflections
2807 independent reflections
2451 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.184
S = 1.10
2807 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O1	0.83 (5)	1.78 (5)	2.536 (3)	150 (5)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2443).

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supplementary materials

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(2*E*)-1-(2-Hydroxyphenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

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Comment

Chalcones are a class of naturally occurring compounds with various biological activities. They are known as the precursors of all flavonoid type natural products in biosynthesis. Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties such as cytotoxicity (Pandey *et al.*, 2005) and antiherpes activity and antitumour activity (Conti, 2006) and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.*, 2001). Chalcone derivatives are also used as antibiotics (Nielsen *et al.*, 2005) and as anti malerials (Domínguez *et al.*, 2005). Chalcone derivatives are recognized for NLO properties and have good crystallization ability (Goto *et al.* 1991; Indira *et al.* 2002; Sarojini *et al.*, 2006). Structures of few related chalcones *viz*. (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxy-3-methoxyphenyl)prop-2-en-1-one (Yathirajan, Mayekar, Narayana, *et al.*, 2007), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Yathirajan, Mayekar, Sarojini, *et al.* 2007), 3-[4-(methylsulfanyl)phenyl]-1-(4-nitrophenyl)prop-2-en-1-one (Harrison, Yathirajan, Mithun *et al.*, 2006), 2E)-1-(3-hydroxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one (Butcher *et al.* 2007). In continuation of our studies on chalcones, a new chalcone, $C_{16}H_{14}O_2S$, has been synthesized and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. The C—C double bond is *trans* configured. The essentially planar molecules [r.m.s. deviation for all non-H atoms 0.034 Å] crystallize in planes parallel to the (−1 4 0) plane. The molecular conformation is stabilized by a O—H···O hydrogen bond. The investigated crystal was a non-merohedral twin with a ratio of the twin components of 0.254 (1)/0.746 (1).

Experimental

To a solution of 2-hydroxyacetophenone (1.36 g, 0.01 mol) and 4-methylthiobenzaldehyde (1.52 g, 0.01 mol) in 20 ml of ethanol, 50% KOH (2.5 ml) was added at 273 K. The mixture was stirred overnight at room temperature and then poured on to ice water. The pH of this mixture was adjusted to 3–4 with 2 *M* HCl aqueous solution. A yellow precipitate was collected by filtration and purified by recrystallization in ethanol. The single crystals were grown from acetone by slow evaporation method. [m.p.: 338–343 K]. Analysis for $C_{16}H_{14}O_2S$: Found (Calculated): C 71.18 (71.08), H 5.25 (5.22), S 11.89% (11.86%).

Refinement

All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 $U_{eq}(C_{methyl})$] using a riding model with C—H = 0.95Å or 0.98Å for $C_{aromatic}$—H and C_{methyl}—H, respectively. The hydroxyl H atom was freely refined. The investigated crystal was a non-merohedral twin with a ratio of the twin components of 0.254 (1)/0.746 (1).

Figures

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

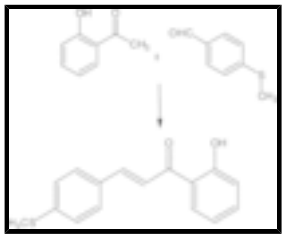

Fig. 2. The formation of the title compound.

(2E)-1-(2-Hydroxyphenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

Crystal data

$C_{16}H_{14}O_2S$	$Z = 2$
$M_r = 270.33$	$F_{000} = 284$
Triclinic, $P\overline{1}$	$D_x = 1.332$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.6516$ (9) Å	Cell parameters from 5613 reflections
$b = 7.0223$ (11) Å	$\theta = 3.7$–26.1°
$c = 15.0248$ (17) Å	$\mu = 0.23$ mm^{-1}
$\alpha = 90.789$ (11)°	$T = 173$ (2) K
$\beta = 93.409$ (11)°	Plate, yellow
$\gamma = 105.718$ (12)°	0.37 × 0.31 × 0.12 mm
$V = 673.98$ (16) Å^3	

Data collection

Stoe IPDSII two-circle diffractometer	2807 independent reflections
Radiation source: fine-focus sealed tube	2451 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.077$
$T = 173$(2) K	$\theta_{max} = 26.6^\circ$
ω scans	$\theta_{min} = 3.6^\circ$
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -8 \rightarrow 8$
$T_{min} = 0.938$, $T_{max} = 0.982$	$k = -8 \rightarrow 8$
13663 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.103P)^2 + 0.6276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.184$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.59$ e Å^{-3}
2807 reflections	$\Delta\rho_{min} = -0.43$ e Å^{-3}
179 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.056 (11)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.96299 (11)	0.85185 (11)	0.24466 (4)	0.0293 (3)
O1	0.0262 (3)	0.6428 (3)	0.64803 (13)	0.0311 (5)
O2	−0.1191 (3)	0.6145 (3)	0.80106 (15)	0.0341 (5)
H2O	−0.117 (8)	0.615 (8)	0.746 (3)	0.072 (15)*
C1	0.2112 (4)	0.6915 (4)	0.68040 (17)	0.0219 (5)
C2	0.3848 (4)	0.7324 (4)	0.62090 (17)	0.0238 (5)
H2	0.5252	0.7788	0.6452	0.029*
C3	0.3447 (4)	0.7040 (4)	0.53205 (17)	0.0230 (5)
H3	0.2015	0.6561	0.5117	0.028*
C11	0.2534 (4)	0.7082 (4)	0.77907 (17)	0.0224 (5)
C12	0.0818 (4)	0.6681 (4)	0.83462 (18)	0.0256 (6)
C13	0.1188 (5)	0.6841 (4)	0.92739 (19)	0.0334 (7)
H13	0.0040	0.6608	0.9643	0.040*
C14	0.3208 (6)	0.7333 (5)	0.96593 (19)	0.0383 (7)
H14	0.3438	0.7419	1.0290	0.046*
C15	0.4904 (5)	0.7705 (5)	0.91268 (19)	0.0377 (7)
H15	0.6291	0.8040	0.9393	0.045*
C16	0.4565 (4)	0.7584 (4)	0.82031 (18)	0.0296 (6)
H16	0.5731	0.7847	0.7844	0.036*
C21	0.4959 (4)	0.7383 (4)	0.46331 (16)	0.0216 (5)
C22	0.4208 (4)	0.7199 (4)	0.37357 (17)	0.0247 (5)
H22	0.2739	0.6841	0.3594	0.030*

C23	0.5558 (4)	0.7527 (4)	0.30451 (16)	0.0249 (5)
H23	0.5011	0.7397	0.2442	0.030*
C24	0.7725 (4)	0.8047 (4)	0.32437 (16)	0.0218 (5)
C25	0.8500 (4)	0.8217 (4)	0.41452 (17)	0.0231 (5)
H25	0.9967	0.8564	0.4287	0.028*
C26	0.7137 (4)	0.7881 (4)	0.48237 (16)	0.0230 (5)
H26	0.7681	0.7990	0.5427	0.028*
C27	0.8098 (5)	0.8098 (5)	0.13936 (18)	0.0341 (7)
H27A	0.7278	0.6708	0.1336	0.051*
H27B	0.9034	0.8406	0.0904	0.051*
H27C	0.7150	0.8951	0.1369	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0311 (4)	0.0328 (4)	0.0258 (4)	0.0106 (3)	0.0068 (3)	0.0035 (3)
O1	0.0208 (9)	0.0398 (12)	0.0308 (10)	0.0057 (9)	−0.0011 (7)	0.0014 (9)
O2	0.0240 (10)	0.0397 (12)	0.0398 (12)	0.0089 (9)	0.0092 (8)	0.0023 (10)
C1	0.0224 (12)	0.0179 (12)	0.0263 (12)	0.0073 (10)	0.0011 (9)	0.0008 (10)
C2	0.0224 (12)	0.0213 (12)	0.0269 (12)	0.0049 (10)	0.0007 (10)	−0.0013 (10)
C3	0.0236 (12)	0.0192 (12)	0.0263 (12)	0.0059 (10)	0.0013 (9)	0.0020 (10)
C11	0.0250 (12)	0.0190 (12)	0.0253 (12)	0.0089 (10)	0.0034 (10)	0.0000 (9)
C12	0.0286 (13)	0.0189 (12)	0.0313 (13)	0.0087 (10)	0.0077 (10)	0.0005 (10)
C13	0.0447 (17)	0.0290 (14)	0.0308 (14)	0.0150 (13)	0.0143 (12)	0.0051 (11)
C14	0.0540 (19)	0.0390 (17)	0.0257 (13)	0.0191 (15)	0.0024 (13)	0.0009 (12)
C15	0.0376 (16)	0.0471 (18)	0.0293 (14)	0.0152 (14)	−0.0056 (12)	−0.0035 (13)
C16	0.0274 (13)	0.0353 (15)	0.0280 (13)	0.0122 (12)	0.0015 (10)	−0.0026 (11)
C21	0.0246 (12)	0.0169 (11)	0.0230 (12)	0.0055 (10)	−0.0008 (9)	0.0000 (9)
C22	0.0219 (12)	0.0255 (13)	0.0255 (12)	0.0055 (10)	−0.0052 (9)	−0.0012 (10)
C23	0.0286 (13)	0.0258 (13)	0.0199 (11)	0.0076 (11)	−0.0037 (9)	−0.0019 (10)
C24	0.0265 (12)	0.0184 (12)	0.0210 (11)	0.0068 (10)	0.0014 (9)	0.0001 (9)
C25	0.0207 (11)	0.0217 (12)	0.0252 (12)	0.0036 (10)	−0.0034 (9)	−0.0013 (10)
C26	0.0259 (13)	0.0220 (12)	0.0200 (11)	0.0055 (10)	−0.0033 (9)	−0.0013 (9)
C27	0.0504 (18)	0.0318 (15)	0.0235 (13)	0.0164 (14)	0.0050 (12)	0.0014 (11)

Geometric parameters (Å, °)

S1—C24	1.765 (3)	C14—H14	0.9500
S1—C27	1.806 (3)	C15—C16	1.391 (4)
O1—C1	1.250 (3)	C15—H15	0.9500
O2—C12	1.351 (3)	C16—H16	0.9500
O2—H2O	0.83 (5)	C21—C22	1.402 (3)
C1—C2	1.472 (3)	C21—C26	1.406 (3)
C1—C11	1.489 (3)	C22—C23	1.394 (4)
C2—C3	1.347 (4)	C22—H22	0.9500
C2—H2	0.9500	C23—C24	1.400 (4)
C3—C21	1.461 (3)	C23—H23	0.9500
C3—H3	0.9500	C24—C25	1.412 (3)
C11—C16	1.403 (4)	C25—C26	1.385 (4)

C11—C12	1.423 (4)	C25—H25	0.9500
C12—C13	1.399 (4)	C26—H26	0.9500
C13—C14	1.382 (5)	C27—H27A	0.9800
C13—H13	0.9500	C27—H27B	0.9800
C14—C15	1.391 (5)	C27—H27C	0.9800
C24—S1—C27	103.57 (13)	C15—C16—H16	119.3
C12—O2—H2O	107 (4)	C11—C16—H16	119.3
O1—C1—C2	119.9 (2)	C22—C21—C26	118.0 (2)
O1—C1—C11	119.5 (2)	C22—C21—C3	118.6 (2)
C2—C1—C11	120.7 (2)	C26—C21—C3	123.4 (2)
C3—C2—C1	120.0 (2)	C23—C22—C21	121.7 (2)
C3—C2—H2	120.0	C23—C22—H22	119.1
C1—C2—H2	120.0	C21—C22—H22	119.1
C2—C3—C21	127.6 (2)	C22—C23—C24	119.7 (2)
C2—C3—H3	116.2	C22—C23—H23	120.1
C21—C3—H3	116.2	C24—C23—H23	120.1
C16—C11—C12	118.0 (2)	C23—C24—C25	119.1 (2)
C16—C11—C1	122.8 (2)	C23—C24—S1	125.08 (19)
C12—C11—C1	119.2 (2)	C25—C24—S1	115.84 (19)
O2—C12—C13	117.8 (2)	C26—C25—C24	120.5 (2)
O2—C12—C11	122.3 (2)	C26—C25—H25	119.8
C13—C12—C11	119.9 (3)	C24—C25—H25	119.8
C14—C13—C12	120.7 (3)	C25—C26—C21	121.0 (2)
C14—C13—H13	119.7	C25—C26—H26	119.5
C12—C13—H13	119.7	C21—C26—H26	119.5
C13—C14—C15	120.3 (3)	S1—C27—H27A	109.5
C13—C14—H14	119.9	S1—C27—H27B	109.5
C15—C14—H14	119.9	H27A—C27—H27B	109.5
C16—C15—C14	119.8 (3)	S1—C27—H27C	109.5
C16—C15—H15	120.1	H27A—C27—H27C	109.5
C14—C15—H15	120.1	H27B—C27—H27C	109.5
C15—C16—C11	121.4 (3)		
O1—C1—C2—C3	−4.6 (4)	C12—C11—C16—C15	−0.5 (4)
C11—C1—C2—C3	175.6 (2)	C1—C11—C16—C15	−179.2 (3)
C1—C2—C3—C21	179.4 (2)	C2—C3—C21—C22	−173.2 (3)
O1—C1—C11—C16	178.8 (3)	C2—C3—C21—C26	7.1 (4)
C2—C1—C11—C16	−1.4 (4)	C26—C21—C22—C23	−1.0 (4)
O1—C1—C11—C12	0.1 (4)	C3—C21—C22—C23	179.2 (2)
C2—C1—C11—C12	179.9 (2)	C21—C22—C23—C24	0.2 (4)
C16—C11—C12—O2	−178.5 (2)	C22—C23—C24—C25	0.5 (4)
C1—C11—C12—O2	0.2 (4)	C22—C23—C24—S1	−179.7 (2)
C16—C11—C12—C13	1.5 (4)	C27—S1—C24—C23	−1.5 (3)
C1—C11—C12—C13	−179.7 (2)	C27—S1—C24—C25	178.3 (2)
O2—C12—C13—C14	178.3 (3)	C23—C24—C25—C26	−0.3 (4)
C11—C12—C13—C14	−1.8 (4)	S1—C24—C25—C26	179.9 (2)
C12—C13—C14—C15	0.9 (5)	C24—C25—C26—C21	−0.5 (4)
C13—C14—C15—C16	0.2 (5)	C22—C21—C26—C25	1.2 (4)
C14—C15—C16—C11	−0.3 (5)	C3—C21—C26—C25	−179.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2O···O1	0.83 (5)	1.78 (5)	2.536 (3)	150 (5)

Fig. 1

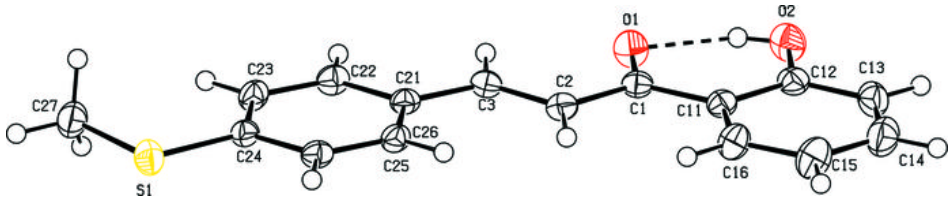
O1
O2
C23
C22
C21
C3
C2
C1
C11
C12
C13
C27
C24
C26
C25
C16
C15
C14
S1

Fig. 2