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# Salicylideneacetone

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.060
*wR* factor = 0.145
Data-to-parameter ratio = 15.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, (*E*)-4-(2-hydroxyphenyl)but-3-en-2-one, $C_{10}H_{10}O_2$, was synthesized from salicylaldehyde and acetone. The molecule is essentially planar, suggesting a high degree of conjugation throughout the system. Intermolecular hydrogen bonds link adjacent molecules to form one-dimensional chains.

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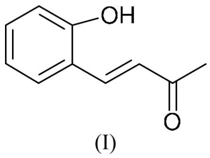
## Comment

All the bond lengths and angles (Table 1) in the title compound, (I), are within normal ranges (Allen *et al.*, 1987) and the structural data confirm the *E* configuration about the C=C bond. Atoms C7, C8, C9 and O1 constitute a well defined plane, with an average deviation of 0.005 (1) Å. The benzene ring plane is inclined at 4.2 (2)° to this plane, suggesting extensive delocalization in the molecular system. A weak intermolecular O2—H2···O1 hydrogen bond links adjacent molecules to form one-dimensional chains along the *c* axis (Fig. 2).



(I)

## Experimental

Salicylaldehyde (1.22 g, 10 mmol) was dissolved in acetone (10 ml). A few drops of dilute aqueous NaOH solution were added to the acetone solution, with stirring. The mixture was refluxed for 1h and then filtered. The filtrate was allowed to stand in air for a week, during which time about three-quarters of the orginal solvent volume evaporated and light-orange prismatic crystals of (I) were formed at the bottom of the vessel. These were filtered off, washed with acetone twice, and dried over $CaCl_2$ in a desiccator (yield 33%).

*Crystal data*

$C_{10}H_{10}O_2$
$M_r$ = 162.18
Triclinic, $P\overline{1}$
*a* = 7.350 (2) Å
*b* = 7.490 (2) Å
*c* = 8.810 (2) Å
α = 97.05 (3)°
β = 95.86 (3)°
γ = 115.34 (3)°
*V* = 428.5 (2) Å$^3$
*Z* = 2
$D_x$ = 1.257 Mg m$^{-3}$
Mo *K*α radiation
Cell parameters from 1525 reflections
θ = 6.6–28.0°
μ = 0.09 mm$^{-1}$
*T* = 293 (2) K
Prism, light orange
0.42 × 0.40 × 0.33 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.895, $T_{max}$ = 0.972
3464 measured reflections
1734 independent reflections
1438 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 26.5°
*h* = −9 → 9
*k* = −9 → 9
*l* = −11 → 11

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*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.145$
$S = 1.09$
1734 reflections
111 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.1545P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.30$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C9 | 1.220 (2) | C4—C5 | 1.370 (3) |
| O2—C1 | 1.359 (2) | C5—C6 | 1.395 (3) |
| C1—C2 | 1.387 (3) | C6—C7 | 1.458 (3) |
| C1—C6 | 1.401 (2) | C7—C8 | 1.327 (3) |
| C2—C3 | 1.373 (3) | C8—C9 | 1.456 (3) |
| C3—C4 | 1.380 (3) | C9—C10 | 1.491 (3) |
| | | | |
| O2—C1—C2 | 122.33 (18) | C5—C6—C7 | 122.81 (18) |
| O2—C1—C6 | 117.52 (17) | C1—C6—C7 | 119.44 (17) |
| C2—C1—C6 | 120.15 (18) | C8—C7—C6 | 126.98 (18) |
| C3—C2—C1 | 120.34 (19) | C7—C8—C9 | 124.91 (19) |
| C2—C3—C4 | 120.44 (19) | O1—C9—C8 | 119.5 (2) |
| C5—C4—C3 | 119.4 (2) | O1—C9—C10 | 119.5 (2) |
| C4—C5—C6 | 121.93 (19) | C8—C9—C10 | 120.93 (17) |
| C5—C6—C1 | 117.76 (18) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O1$^{i}$ | 0.82 | 1.91 | 2.715 (2) | 169 |

Symmetry code: (i) $x, y, 1 + z$.

H atoms were positioned geometrically and constrained to ride on their parent atoms at distances of C$sp^2$—H = 0.93 Å and C$sp^3$—H = 0.96 Å, with $U_{\rm iso} = 1.2U_{\rm eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

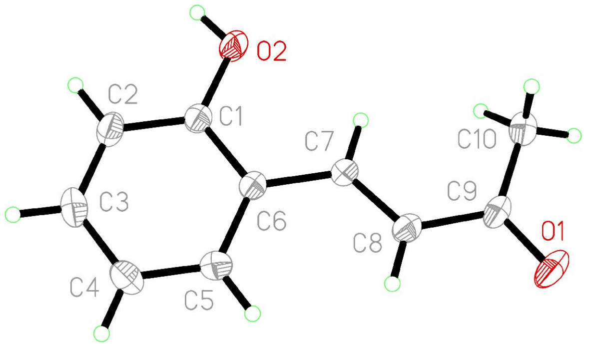

**Figure 1**
The structure of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

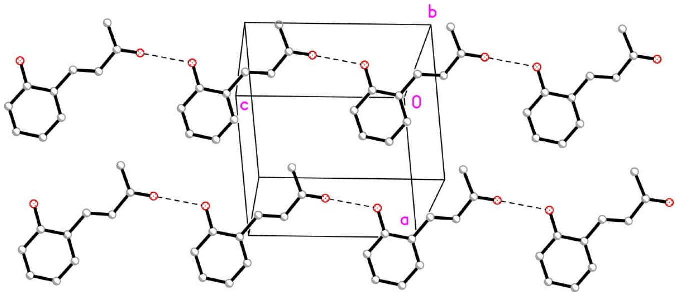

**Figure 2**
The molecular packing for (I), showing the one-dimensional chains formed along the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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