Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Lingqian Kong[a]* and Yanhong Liu[b]

[a]Dongchang College, Liaocheng University, Liaocheng 250059, People's Republic of China, and [b]Liaocheng No.3 Middle School, Liaocheng, People's Republic of China
Correspondence e-mail: konglingqian08@163.com

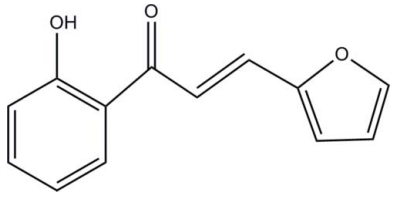
Received 13 September 2008; accepted 30 September 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.067; wR factor = 0.184; data-to-parameter ratio = 12.7.

In the title molecule, $C_{13}H_{10}O_3$, an intramolecular O—H···O hydrogen bond influences the molecular conformation, and the benzene and furan rings form a dihedral angle of 8.35 (7)°. Weak intermolecular C—H···O hydrogen bonds link molecules into sheets parallel to the *bc* plane.

Related literature

For a related crystal structure, see: Li *et al.* (1992).



Experimental

Crystal data

$C_{13}H_{10}O_3$
M_r = 214.21
Monoclinic, $P2_1/c$
a = 3.8560 (5) Å
b = 15.6565 (14) Å
c = 17.309 (2) Å
β = 95.065 (2)°
V = 1040.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.27 × 0.25 × 0.07 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.993
5153 measured reflections
1848 independent reflections
668 reflections with $I > 2\sigma(I)$
R_{int} = 0.126

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.184
S = 0.81
1848 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.82	1.84	2.544 (4)	144
C1—H1···O2^{i}	0.93	2.59	3.400 (5)	146
C3—H3A···O3^{ii}	0.93	2.59	3.504 (5)	169

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This project was supported by the Foundation of Dongchang College, Liaocheng University (grant No. LG0801).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2448).

References

Li, Z.-D., Huang, L.-Z., Su, G.-B. & Wang, H.-Y. (1992). *Chin. J. Struct. Chem.* **11**, 1–4.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2008). E**64**, o2161 [doi:10.1107/S1600536808031644]

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

Lingqian Kong and Yanhong Liu

S1. Comment

In continuation of our ongoing program directed to the development of environmentally benign methods of chemical synthesis, we describe in this paper a user-friendly, solvent-free protocol for the synthesis of chalcones starting from the fragrant aldehydes and fragrant ketones in the presence of NaOH under solvent-free conditions. Using this method, which can be considered as a a general method for the synthesis of chalcones, we obtained the title compound, (I). We present here its crystal structure.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in related compound (Li *et al.*, 1992). The benzene and furan rings form a dihedral angle of 8.35 (7)°. In the crystal, weak intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into sheets parallel to *bc* plane.

S2. Experimental

Furan-2-carbaldehyde (0.3 mmol) and 2-hydroxylacetophenone (0.3 mmol), NaOH (0.3 mmol) were mixed in 50 ml flash under sovlent-free conditions After stirring for 5 min at 373 K, the mixture was soilden slowly and afforded the title compound, then recrystallized from ethanol, affording the title compound as a colourless crystalline solid. Elemental analysis: calculated for $C_{13}H_{10}O_3$: C 72.90, H 4.71%; found: C 72.88, H 4.65%.

S3. Refinement

All H atoms were placed in geometrically idealized positions (O—H 0.85 Å, C—H 0.93 Å) and treated as riding, with U_{iso}(H) = 1.2 U_{eq}(C,O).

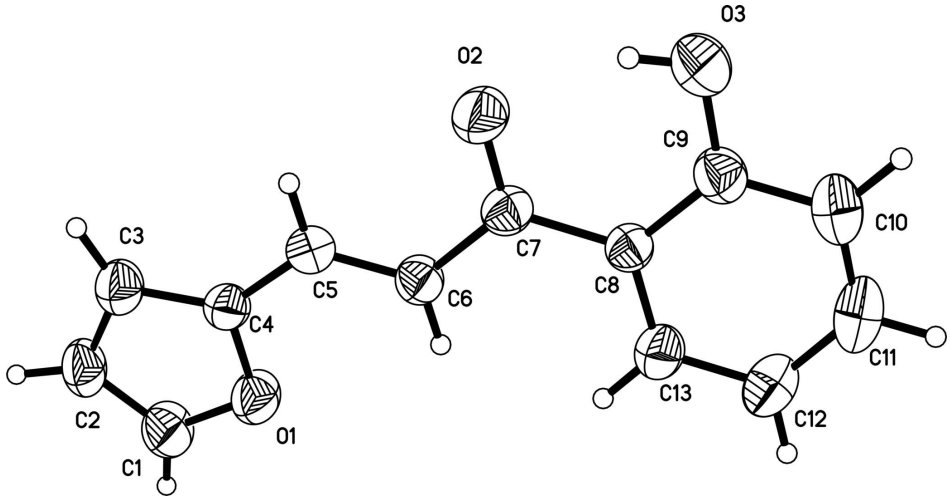


Figure 1

The molecular structure of (I) showing the atomic numbering and 40% probability displacement ellipsoids.

(E)-3-(2-Furyl)-1-(2-hydroxyphenyl)prop-2-en-1-one

Crystal data

$C_{13}H_{10}O_3$
$M_r = 214.21$
Monoclinic, $P2_1/c$
$a = 3.8560\ (5)$ Å
$b = 15.6565\ (14)$ Å
$c = 17.309\ (2)$ Å
$\beta = 95.065\ (2)°$
$V = 1040.9\ (2)$ Å^3
$Z = 4$
$F(000) = 448$
$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 438 reflections
$\theta = 2.4–18.4°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.27 × 0.25 × 0.07 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: φ and ω pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.974$, $T_{max} = 0.993$
5153 measured reflections
1848 independent reflections
668 reflections with $I > 2\sigma(I)$
$R_{int} = 0.126$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -4\rightarrow4$
$k = -7\rightarrow18$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.184$
$S = 0.81$
1848 reflections
146 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
O1	1.0561 (7)	0.73465 (16)	0.48262 (15)	0.0794 (9)

O2	0.8017 (8)	0.83794 (18)	0.74522 (15)	0.0885 (11)
O3	0.5477 (10)	0.9672 (2)	0.80912 (17)	0.1030 (12)
H3	0.6546	0.9220	0.8087	0.154*
C1	1.1454 (12)	0.6735 (3)	0.4327 (2)	0.0842 (15)
H1	1.1472	0.6811	0.3794	0.101*
C2	1.2297 (11)	0.6018 (3)	0.4699 (3)	0.0769 (13)
H2	1.3018	0.5510	0.4485	0.092*
C3	1.1887 (11)	0.6177 (3)	0.5478 (2)	0.0748 (13)
H3A	1.2271	0.5788	0.5882	0.090*
C4	1.0842 (10)	0.6991 (2)	0.5544 (2)	0.0584 (10)
C5	0.9983 (9)	0.7493 (2)	0.6177 (2)	0.0608 (11)
H5	1.0222	0.7240	0.6665	0.073*
C6	0.8860 (10)	0.8300 (2)	0.6137 (2)	0.0598 (11)
H6	0.8676	0.8578	0.5661	0.072*
C7	0.7918 (10)	0.8754 (2)	0.6822 (2)	0.0600 (11)
C8	0.6700 (9)	0.9648 (2)	0.6757 (2)	0.0553 (10)
C9	0.5559 (11)	1.0064 (3)	0.7399 (2)	0.0690 (12)
C10	0.4467 (12)	1.0901 (3)	0.7358 (3)	0.0835 (14)
H10	0.3697	1.1170	0.7790	0.100*
C11	0.4529 (13)	1.1329 (3)	0.6679 (3)	0.0930 (16)
H11	0.3769	1.1893	0.6649	0.112*
C12	0.5685 (12)	1.0951 (3)	0.6033 (3)	0.0839 (14)
H12	0.5747	1.1256	0.5573	0.101*
C13	0.6745 (11)	1.0117 (3)	0.6079 (2)	0.0702 (12)
H13	0.7518	0.9858	0.5642	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.111 (3)	0.0632 (19)	0.0648 (18)	0.0106 (16)	0.0132 (16)	−0.0022 (16)
O2	0.138 (3)	0.067 (2)	0.0625 (18)	0.0095 (18)	0.0190 (18)	0.0029 (15)
O3	0.150 (4)	0.087 (3)	0.076 (2)	0.010 (2)	0.033 (2)	−0.0105 (18)
C1	0.112 (4)	0.076 (3)	0.065 (3)	0.008 (3)	0.015 (3)	−0.014 (3)
C2	0.080 (4)	0.057 (3)	0.095 (3)	0.008 (2)	0.012 (3)	−0.016 (3)
C3	0.086 (4)	0.061 (3)	0.078 (3)	0.008 (2)	0.011 (2)	−0.004 (2)
C4	0.065 (3)	0.053 (2)	0.058 (2)	−0.002 (2)	0.010 (2)	−0.001 (2)
C5	0.063 (3)	0.059 (2)	0.061 (2)	0.001 (2)	0.010 (2)	0.004 (2)
C6	0.067 (3)	0.058 (2)	0.054 (2)	0.002 (2)	0.005 (2)	−0.003 (2)
C7	0.064 (3)	0.057 (3)	0.059 (2)	−0.005 (2)	0.004 (2)	0.001 (2)
C8	0.055 (3)	0.053 (2)	0.058 (2)	−0.0020 (19)	0.006 (2)	−0.001 (2)
C9	0.071 (3)	0.069 (3)	0.068 (3)	−0.001 (2)	0.009 (2)	−0.009 (2)
C10	0.080 (4)	0.073 (3)	0.095 (4)	0.008 (3)	0.001 (3)	−0.023 (3)
C11	0.093 (4)	0.061 (3)	0.122 (4)	0.014 (3)	−0.014 (3)	−0.013 (3)
C12	0.099 (4)	0.063 (3)	0.086 (3)	0.000 (3)	−0.008 (3)	0.007 (3)
C13	0.078 (3)	0.056 (3)	0.076 (3)	−0.004 (2)	0.007 (2)	−0.005 (2)

Geometric parameters (Å, º)

O1—C1	1.354 (4)	C6—C7	1.455 (5)
O1—C4	1.357 (4)	C6—H6	0.9300
O2—C7	1.237 (4)	C7—C8	1.476 (5)
O3—C9	1.349 (4)	C8—C13	1.386 (5)
O3—H3	0.8200	C8—C9	1.393 (5)
C1—C2	1.321 (5)	C9—C10	1.377 (6)
C1—H1	0.9300	C10—C11	1.354 (5)
C2—C3	1.394 (5)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.374 (6)
C3—C4	1.343 (5)	C11—H11	0.9300
C3—H3A	0.9300	C12—C13	1.368 (5)
C4—C5	1.413 (5)	C12—H12	0.9300
C5—C6	1.335 (5)	C13—H13	0.9300
C5—H5	0.9300		
C1—O1—C4	106.9 (3)	O2—C7—C8	120.1 (4)
C9—O3—H3	109.5	C6—C7—C8	120.1 (3)
C2—C1—O1	110.8 (3)	C13—C8—C9	117.1 (4)
C2—C1—H1	124.6	C13—C8—C7	122.6 (3)
O1—C1—H1	124.6	C9—C8—C7	120.3 (4)
C1—C2—C3	106.0 (4)	O3—C9—C10	116.6 (4)
C1—C2—H2	127.0	O3—C9—C8	122.0 (4)
C3—C2—H2	127.0	C10—C9—C8	121.4 (4)
C4—C3—C2	108.2 (4)	C11—C10—C9	119.2 (4)
C4—C3—H3A	125.9	C11—C10—H10	120.4
C2—C3—H3A	125.9	C9—C10—H10	120.4
C3—C4—O1	108.2 (3)	C10—C11—C12	121.6 (4)
C3—C4—C5	133.3 (4)	C10—C11—H11	119.2
O1—C4—C5	118.5 (3)	C12—C11—H11	119.2
C6—C5—C4	125.7 (3)	C13—C12—C11	118.8 (4)
C6—C5—H5	117.1	C13—C12—H12	120.6
C4—C5—H5	117.1	C11—C12—H12	120.6
C5—C6—C7	121.6 (3)	C12—C13—C8	122.0 (4)
C5—C6—H6	119.2	C12—C13—H13	119.0
C7—C6—H6	119.2	C8—C13—H13	119.0
O2—C7—C6	119.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.82	1.84	2.544 (4)	144
C1—H1···O2^{i}	0.93	2.59	3.400 (5)	146
C3—H3*A*···O3^{ii}	0.93	2.59	3.504 (5)	169

Symmetry codes: (i) x, $-y+3/2$, $z-1/2$; (ii) $-x+2$, $y-1/2$, $-z+3/2$.