Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(Hydroxymethyl)furan-2-carboxylic acid

Jun-Liang Liu and Qing-Yan Xu*

Laboratory of Microbial Pharmaceutical Engineering, Xiamen University, Xiamen 361005, People's Republic of China
Correspondence e-mail: xuqingyan@xmu.edu.cn

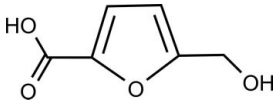
Received 21 May 2011; accepted 23 May 2011

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 11.1.

In the title compound, $C_6H_6O_4$, the furan ring is nearly coplanar with the carboxyl group, the maximum atomic deviation being 0.0248 (9) Å. The crystal packing is stabilized by classical O—H···O and weak C—H···O hydrogen bonding.

Related literature

For the biochemical significance of the title compound, see: Mrochek & Rainey (1972).



Experimental

Crystal data

$C_6H_6O_4$
M_r = 142.11
Orthorhombic, *Pbca*
a = 10.838 (3) Å
b = 7.2601 (17) Å
c = 15.526 (4) Å
V = 1221.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 294 K
0.32 × 0.22 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
5637 measured reflections
1098 independent reflections
1033 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.08
1098 reflections
99 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3^{i}	0.87 (2)	1.83 (2)	2.6951 (16)	169.2 (19)
O4—H4A···O1^{ii}	0.96 (2)	1.61 (2)	2.5643 (17)	171 (2)
C7—H7A···O4^{iii}	0.97	2.45	3.265 (2)	142

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support by the Fundamental Research Funds for the Central Universities, China (2010121092).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5218).

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Mrochek, J. & Rainey, W. (1972). *Clin. Chem.* **18**, 821-828.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o1548 [doi:10.1107/S1600536811019489]

5-(Hydroxymethyl)furan-2-carboxylic acid

Jun-Liang Liu and Qing-Yan Xu

S1. Comment

In the molecular structure of the compound, all the carbon atoms locate in the same plane. The crystal packing is stabilized by O—H···O and weak C—H···O hydrogen bonding (Table 1).

S2. Experimental

The title compound was obtained from the fermentation of *Aspergillus sp.* by column chromatography. The strain was isolated from a soil sample collected from Jinjiang salt-field, Fujian, China. The strain was cultured using half sea-water Potato Dextrose Agar medium at 28 degrees celsius for 14 days. The fermentation (40 liters) was extracted with ethyl acetate (EtOAc). The EtOAc extract (18.0 g) eluted with methanol-water (30%, 50%, 70%, 100%; V/V) to yield 12 fractions by column chromatography RP-18. Fraction 1 was further puried by Sephadex LH-20 (140 g) chromatography with methanol. Then 1–4 eluted with acetone by Sephadex LH-20 (80 g) chromatography, then the main components further puried by silica-gel column chromatography to afford the title compound (8.0 mg).

S3. Refinement

The carboxyl and hydroxy H atoms were located in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically and were treated as riding on their parent atoms, with C—H distances of 0.93–0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$.

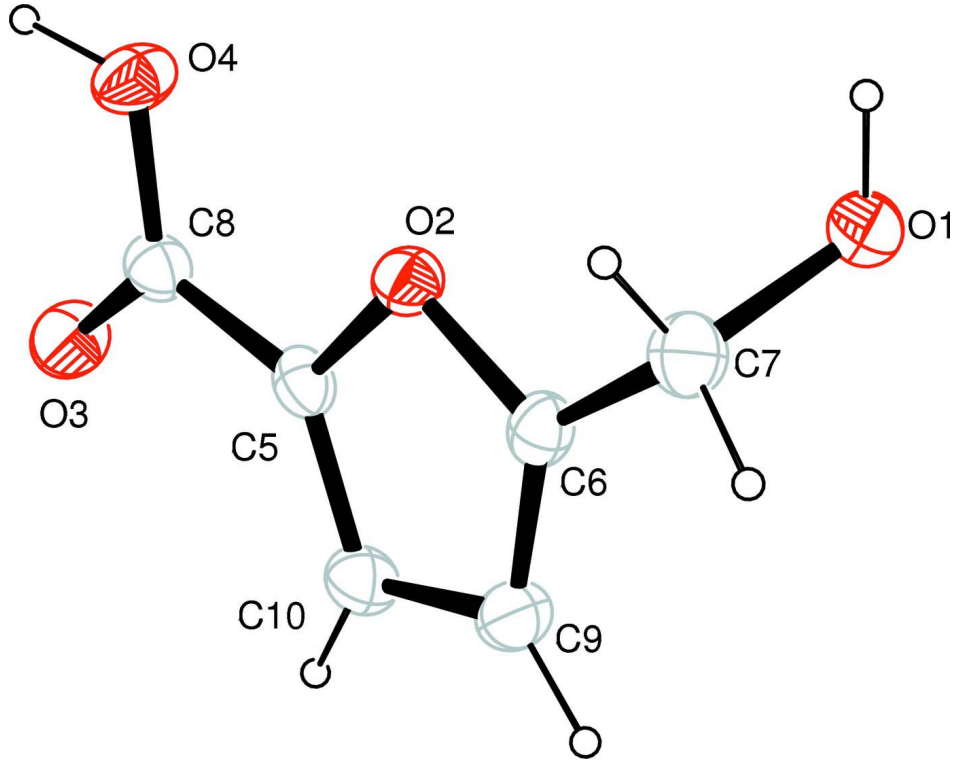


Figure 1

The molecular structure of the title compound with 50% probability ellipsoids.

5-(Hydroxymethyl)furan-2-carboxylic acid

Crystal data

$C_6H_6O_4$
$M_r = 142.11$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 10.838\ (3)$ Å
$b = 7.2601\ (17)$ Å
$c = 15.526\ (4)$ Å
$V = 1221.7\ (5)$ Å^3
$Z = 8$
$F(000) = 592$
$D_x = 1.545$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10988 reflections
$\theta = 2.6$–$25.2°$
$\mu = 0.13$ mm^{-1}
$T = 294$ K
Block, colourless
0.32 × 0.22 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
5637 measured reflections
1098 independent reflections
1033 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.2°$, $\theta_{min} = 2.6°$
$h = -12 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -18 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.090$
$S = 1.08$
1098 reflections
99 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.5232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.93802 (10)	0.18266 (16)	0.31353 (7)	0.0276 (3)
O2	0.84194 (9)	0.14583 (14)	0.49749 (6)	0.0216 (3)
O3	0.68657 (9)	0.30625 (16)	0.68473 (7)	0.0300 (3)
O4	0.88618 (9)	0.26469 (16)	0.65427 (7)	0.0282 (3)
C5	0.74292 (13)	0.19201 (19)	0.54835 (9)	0.0204 (3)
C6	0.79370 (13)	0.08250 (18)	0.42169 (8)	0.0208 (3)
C7	0.88366 (14)	0.0247 (2)	0.35516 (9)	0.0262 (4)
H7A	0.9481	−0.0487	0.3817	0.031*
H7B	0.8424	−0.0510	0.3125	0.031*
C8	0.76830 (13)	0.2598 (2)	0.63503 (9)	0.0219 (3)
C9	0.66913 (13)	0.0865 (2)	0.42436 (9)	0.0243 (4)
H9A	0.6155	0.0498	0.3809	0.029*
C10	0.63590 (14)	0.1574 (2)	0.50616 (9)	0.0242 (3)
H10A	0.5564	0.1765	0.5268	0.029*
H4A	0.898 (2)	0.290 (3)	0.7143 (16)	0.060 (6)*
H1A	1.018 (2)	0.179 (3)	0.3204 (13)	0.051 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0203 (6)	0.0392 (7)	0.0235 (6)	−0.0018 (5)	0.0007 (4)	0.0040 (5)
O2	0.0178 (5)	0.0265 (6)	0.0205 (5)	0.0012 (4)	0.0005 (4)	−0.0004 (4)
O3	0.0213 (5)	0.0445 (7)	0.0242 (6)	0.0059 (5)	0.0039 (4)	−0.0031 (5)
O4	0.0188 (5)	0.0425 (7)	0.0231 (6)	0.0034 (5)	−0.0003 (4)	−0.0070 (5)

C5	0.0189 (7)	0.0215 (7)	0.0209 (7)	0.0024 (5)	0.0044 (6)	0.0035 (5)
C6	0.0257 (8)	0.0178 (7)	0.0188 (7)	−0.0001 (6)	−0.0015 (6)	0.0010 (5)
C7	0.0273 (8)	0.0281 (8)	0.0232 (8)	0.0002 (6)	0.0018 (6)	−0.0014 (6)
C8	0.0188 (7)	0.0223 (7)	0.0246 (7)	0.0016 (6)	0.0018 (6)	0.0030 (6)
C9	0.0237 (8)	0.0251 (8)	0.0242 (8)	−0.0019 (6)	−0.0038 (6)	−0.0003 (6)
C10	0.0179 (7)	0.0282 (8)	0.0265 (8)	0.0002 (6)	0.0021 (6)	0.0022 (6)

Geometric parameters (Å, º)

O1—C7	1.4421 (19)	C5—C8	1.459 (2)
O1—H1A	0.88 (2)	C6—C9	1.351 (2)
O2—C6	1.3675 (17)	C6—C7	1.481 (2)
O2—C5	1.3739 (16)	C7—H7A	0.9700
O3—C8	1.2224 (18)	C7—H7B	0.9700
O4—C8	1.3124 (18)	C9—C10	1.417 (2)
O4—H4A	0.96 (2)	C9—H9A	0.9300
C5—C10	1.355 (2)	C10—H10A	0.9300
C7—O1—H1A	109.0 (13)	O1—C7—H7B	109.5
C6—O2—C5	106.15 (11)	C6—C7—H7B	109.5
C8—O4—H4A	111.1 (13)	H7A—C7—H7B	108.1
C10—C5—O2	110.21 (12)	O3—C8—O4	123.66 (14)
C10—C5—C8	132.03 (13)	O3—C8—C5	122.60 (13)
O2—C5—C8	117.72 (12)	O4—C8—C5	113.74 (12)
C9—C6—O2	110.38 (12)	C6—C9—C10	106.82 (13)
C9—C6—C7	133.27 (13)	C6—C9—H9A	126.6
O2—C6—C7	116.35 (12)	C10—C9—H9A	126.6
O1—C7—C6	110.88 (12)	C5—C10—C9	106.44 (13)
O1—C7—H7A	109.5	C5—C10—H10A	126.8
C6—C7—H7A	109.5	C9—C10—H10A	126.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3^{i}	0.87 (2)	1.83 (2)	2.6951 (16)	169.2 (19)
O4—H4*A*···O1^{ii}	0.96 (2)	1.61 (2)	2.5643 (17)	171 (2)
C7—H7*A*···O4^{iii}	0.97	2.45	3.265 (2)	142

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