Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

5-Ethoxy-5-(1-hydroxyethyl)-1-methylpyrrolidin-2-one

Guo-Chun Ma, Hui-Min Liu and Wen-Qin Zhang*

Department of Chemistry, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: wqzhang@tju.edu.cn

Received 22 July 2004
Accepted 3 August 2004
Online 13 August 2004

In the title compound, $C_9H_{17}NO_3$, the pyrrolidine ring is almost planar, in contrast with the classical envelope conformation observed in other pyrrolidine-containing derivatives. The enantiomers are joined into a centrosymmetric dimer by complementary intermolecular O—H···O hydrogen bonds between the hydroxyl and carbonyl groups.

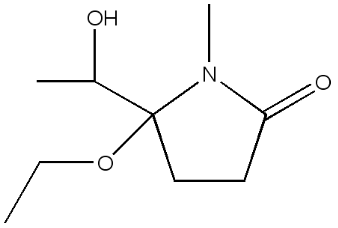
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.130
Data-to-parameter ratio = 16.8

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

Comment

Pyrrolidone derivatives are important pharmaceutical agents (Sasaki *et al.*, 1988). Some pyrrolidone derivatives serve as potential inhibitors of prostate cancer cell growth (Qiao *et al.*, 2001) and also as potent inhibitors of HIV-1 protease (Kazmierski *et al.*, 2002). Some derivatives, such as 5-alkoxyl-2-pyrrolidones, have been used as perfumes, cosmetics and food additives. In order to study the properties of these compounds, we have synthesized several new pyrrolidone derivatives by photolysis of succinimides, and we present here the crystal structure of one of them, the title compound, (I).



(I)

Due to conjugation between atom N1 and the C1═O1 bond, the pyrrolidine ring of (I) is almost planar, with a mean deviation from the plane of 0.0144 (3) Å (Fig. 1), which is in contrast with the classical envelope conformation observed in other pyrrolidine-containing derivatives (Thamotharan *et al.*, 2003; Zheng & Li, 2003). Atoms C7, O2, C4, C5 and O3 form a zigzag chain.

In the crystal structure of (I), strong intermolecular hydrogen bonds [O···O 2.732 (3) Å and O—H···O 174 (3)°] between the hydroxyl and carbonyl groups link the enantiomers of (I) into a centrosymmetric dimer (Fig. 2).

Experimental

The title compound was prepared by the photolysis of *N*-methylsuccinimide in ethanol. A solution of 1.0 g of *N*-methylsuccinimide in 100 ml ethanol was irradiated under a 254 nm low-pressure mercury lamp for 17 h, and then concentrated. The product was isolated by column chromatography. Single crystals of (I) suitable for X-ray analysis were grown from a solution in ethyl acetate (m.p. 393–395 K). Spectroscopic analysis: IR (KBr, ν, cm^{-1}): (1677, *s*, C═O),

DOI: 10.1107/S1600536804019026

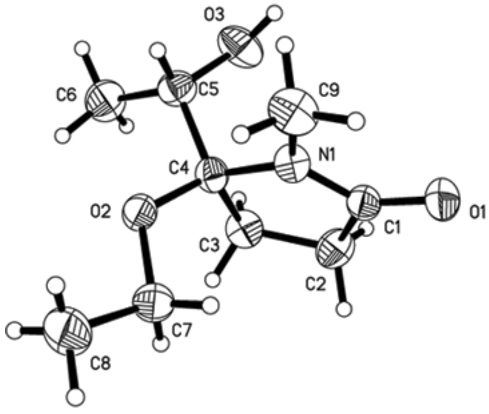


Figure 1
A view of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

(3287, *s*, OH); ^{1}H NMR (CDCl$_3$, δ, p.p.m.): 1.12 (*m*, 6H), 1.84 (*m*, 1H), 2.09–2.34 (*m*, 3H), 2.63 (*s*, 3H), 2.93 (*s*, 1H), 3.03 (*m*, 1H), 3.34 (*m*, 1H), 3.82 (*m*, 1H).

Crystal data

$C_9H_{17}NO_3$
$M_r = 187.24$
Monoclinic, $P2_1/c$
$a = 7.188$ (2) Å
$b = 17.363$ (5) Å
$c = 8.297$ (2) Å
$\beta = 93.267$ (5)°
$V = 1033.8$ (5) Å^3
$Z = 4$
$D_x = 1.203$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 848 reflections
$\theta = 2.4$–24.8°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.20 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.971$, $T_{\max} = 0.991$
5897 measured reflections
2122 independent reflections
1362 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 26.5°$
$h = -9 \rightarrow 8$
$k = -21 \rightarrow 18$
$l = -10 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.130$
$S = 1.02$
2122 reflections
126 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.2892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.011 (3)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.333 (3)	O2—C4	1.416 (2)
N1—C4	1.461 (2)	O3—C5	1.417 (3)
O1—C1	1.225 (2)		
C1—N1—C4	114.92 (16)	N1—C1—C2	109.03 (18)
C4—O2—C7	116.73 (15)	O2—C4—N1	110.49 (15)
O1—C1—N1	125.3 (2)	O2—C4—C5	104.17 (16)
C4—N1—C1—O1	177.35 (19)	C7—O2—C4—C5	179.87 (17)
C4—N1—C1—C2	−3.0 (2)	O2—C4—C5—O3	176.80 (16)

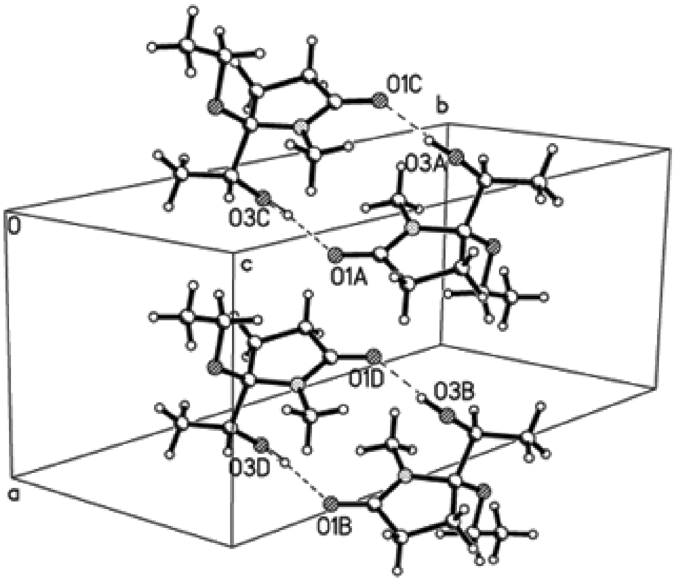


Figure 2
A view of the packing in (I), with the hydrogen bonds shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1$^{\rm i}$	0.91 (4)	1.83 (4)	2.732 (3)	174 (3)

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

H3 was found in a difference map and refined freely. All other H atoms were positioned geometrically and refined as riding, with O—H = 0.91 Å and C—H = 0.96–0.98 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent) for OH, CH and CH$_2$ H atoms, or 1.5$U_{\rm eq}$(parent) for CH$_3$ H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Sasaki, H., Kojima, M., Mori, Y., Nakamura, J. & Shibasaki, J. (1988). *Int. J. Pharm.* **44**, 15–24.
Qiao, L. X., Zhao, L. Y., Rong, S. B., Wu, X. W., Wang, S. M., Fujii, T., Kazanietz, M. G., Rauser, L., Savage, J., Roth, B. L., Flippen-Anderson, J. & Kozikowski, A. P. (2001). *Bioorg. Med. Chem. Lett.* **11**, 955–959.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Thamotharan, S., Parthasarathi, V., Gupta, P., Jindal, D. P., Piplani, P. & Linden, A. (2003). *Acta Cryst.* E**59**, o1334–o1335.
Kazmierski, W. M., Furfine, E., Spaltenstein, A. & Wright, L. L. (2002). *Bioorg. Med. Chem. Lett.* **12**, 3431–3433.
Zheng, P. W. & Li, C. B. (2003). *Acta Cryst.* E**59**, o1621–o1623.