Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (*Z*)-3-(2-Oxo-1,3-oxazolidin-3-ylcarbonyl)-prop-2-enoic acid

**Yu-Dong Shen, Yu Wang, Zhi-Li Xiao, Hong-Tao Lei and Yuan-Ming Sun***

The Key Laboratory of Food Quality and Safety, Education Department of Guangdong Province, Food Quality and Safety Research Institute, South China Agricultural University, Guangzhou, Guangdong Province 510642, People's Republic of China

Correspondence e-mail: shenyudong@scau.edu.cn

Received 3 January 2007
Accepted 11 January 2007

**Key indicators**

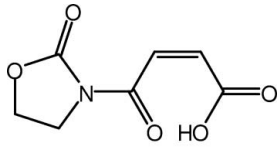
Single-crystal X-ray study
*T* = 173 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.036
*wR* factor = 0.109
Data-to-parameter ratio = 14.1

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

In the title compound, $C_7H_7NO_5$, intermolecular O—H···O hydrogen bonds connect two symmetry-related molecules, forming a pseudo-dimer.

## Comment

In the past, furazolidone [*N*-(5-nitro-2-furfurylidenenamino)-2-oxazolidinone] was once used as a veterinary drug for its obvious growth-promotion effect and good antibacterial activity. Since 1995, the use of furazolidone has been prohibited in food-animal production in many countries because of its carcinogenicity and mutagenicity (European Commission Regulation, 1995; Cooper *et al.*, 2004). However, as a result of the low costs of furazolidone and its treatment benefits, it has been proven by detecting the metabolites AOZ (3-amino-2-oxazolidinone) in animal-origin food that illegal abuse of furazolidone is still active (European Commission, 2005; Cooper *et al.*, 2004).




(I)

Among analytical methods for detecting AOZ residue, immunoassay is an efficient screening technique for the monitoring of illegal furazolidone. However, immunoassay formats reported are mainly based on the detection of the AOZ derivative NPAOZ (3-(2-nitrobenzylideneamino)oxazolidin-2-one), which must undergo a troublesome derivati-

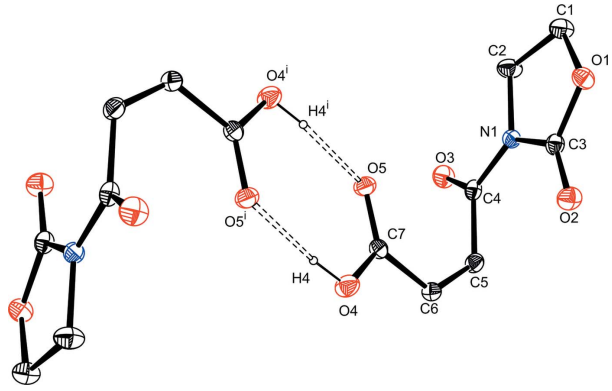



**Figure 1**
The structure of the dimer. Displacement ellipsoids are drawn at the 30% probability level. O—H···O hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

zation step (Cooper *et al.*, 2004; Franek *et al.*, 2006). As part of our investigation of immunoassay methods for directly detecting AOZ itself, we report here the synthesis and crystal structure of a new hapten, (I), for producing a specific antibody of AOZ.

The title compound is a non-aromatic AOZ analogue with a free carboxylic acid group, as shown in Fig. 1. The three C—O distances [C3—O2 = 1.198 (2), C4—O3 = 1.212 (2) and C7—O5 = 1.224 (2) Å] fall within the normal double-bond range; the C5—C6 bond length is 1.321 (2) Å, showing double-bond character. The bond distances within the O1/C1/C2/N1/C3 five-membered ring vary from 1.343 (2) to 1.506 (2) Å, indicating a non-aromatic character, which is also consistent with the NMR experiment. O—H···O hydrogen bonds (Table 1) link two adjacent molecules, forming a centrosymmetric dimer (Fig. 1).

## Experimental

To a solution of oxazolidinone (1.74 g, 0.02 mol), lithium chloride (0.84 g, 0.02 mol), and triethylamine (2.02 g, 0.02 mol) in dry THF (20 ml) was added maleic anhydride (2.35 g, 0.024 mol) at 253 K. The mixture was allowed to warm to 263 K and stirred overnight. THF was removed *in vacuo*. The residue was treated with saturated $NaHCO_3$ and adjusted to pH = 2 with concentrated hydrochloric acid. The mixture was then extracted with EtOAc, and the organic layer was washed with saturated NaCl and subsequently dried with $Na_2SO_4$. The solvents were removed under reduced pressure. The resulting solid was recrystallized from dichloromethane to give (I) in 92% yield. Crystals suitable for X-ray analysis were grown from an acetone–dichloromethane (1:2) solution.

*Crystal data*

$C_7H_7NO_5$
$M_r$ = 185.14
Monoclinic, $P2_1/c$
$a$ = 8.4248 (16) Å
$b$ = 5.0585 (9) Å
$c$ = 18.060 (3) Å
$\beta$ = 91.128 (3)°
$V$ = 769.5 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.598 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.14 mm$^{-1}$
$T$ = 173 (2) K
Block, colourless
0.48 × 0.46 × 0.35 mm

*Data collection*

Bruker SMART diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.935, $T_{max}$ = 0.953
4303 measured reflections
1679 independent reflections
1325 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 27.1°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
$S$ = 1.08
1679 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.1606P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H4···O5$^{i}$ | 0.82 | 1.87 | 2.6817 (16) | 168 |

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and O—H = 0.82 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C,O).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

The work was supported by the Natural Science Foundation of Guangdong Province (Nos. 06300421 and 06300423), the Headmaster's Science Fund of High Schools (5100–k06133) and Public Bidding Items Fund for a Great Breakthrough in Key Fields (No. 2006A25005002). The authors thank Dr Xi Liu in Chongqing Normal University for help.

## References

Bruker (2001). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*, Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Cooper, K. M., Elliott, C. T. & Kennedy, D. G. (2004). *Food Additives Contam.* **21**, 841–848.
European Commission (2005). *Rapid Alert System for Food and Feed*, Annual Report 2004.
European Commission Regulation (1995). (EC), 1442/95 (1995) 26/06; *Off. J. Eur. Commun.* **L143**, 26–30.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Franek, M., Diblikova, I., Vass, M., Kotkova, L., Stastny, K., Frgalova, K. & Hruska, K. (2006). *Vet. Med.* **51**, 248–257.
Siemens (1994). *SHELXTL*. Version 5. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.