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## Structure Reports

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## (Z)-{[3-(Hydroxymethyl)-1,3-thiazolidin-2-ylidene]amino}formonitrile

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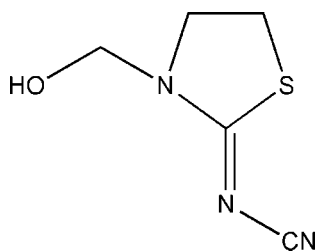
Received 13 June 2009; accepted 16 June 2009

 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.119; data-to-parameter ratio = 12.9.

In the title molecule,  $\text{C}_5\text{H}_7\text{N}_3\text{OS}$ , all the non-hydrogen atoms except the O atom are almost planar [maximum least squares plane deviation = 0.035 (3) Å for the N atom]. The crystal packing is stabilized by intermolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds, which link the molecules into inversion dimers.

### Related literature

For a related structure, see: Xie (2008). For the biological activity of thiazolidine-containing compounds, see: Iwata *et al.* (1988). For bond-length data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

 $\text{C}_5\text{H}_7\text{N}_3\text{OS}$ 
 $M_r = 157.20$ 

 Triclinic,  $P\bar{1}$   
 $a = 5.5321$  (11) Å  
 $b = 8.1790$  (16) Å  
 $c = 8.4978$  (17) Å  
 $\alpha = 101.56$  (3)°  
 $\beta = 100.39$  (3)°  
 $\gamma = 105.47$  (3)°

 $V = 351.75$  (16) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.39$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.22 \times 0.17 \times 0.13$  mm

#### Data collection

 Rigaku R-AXIS RAPID IP area-detector diffractometer  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.919$ ,  $T_{\max} = 0.951$ 

 2778 measured reflections  
 1234 independent reflections  
 1027 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.119$   
 $S = 1.19$   
 1234 reflections  
 96 parameters

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1A}\cdots\text{N3}^i$	0.80 (3)	2.04 (3)	2.839 (3)	174 (3)

 Symmetry code: (i)  $-x, -y + 1, -z + 2$ .

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2526).

### References

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 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Xie, B. (2008). *Acta Cryst.* **E64**, o1237.

## supporting information

*Acta Cryst.* (2009). E65, o1645 [doi:10.1107/S1600536809023095]

**(Z)-{[3-(Hydroxymethyl)-1,3-thiazolidin-2-ylidene]amino}formonitrile****Xin-Lin Liu and Yu-Ming Li****S1. Comment**

Thiazolidine is an important kind of group in organic chemistry. Many compounds containing Thiazolidine groups possess a broad spectrum of biological activities (Iwata *et al.*, 1988). Here, we report the title crystal structure.

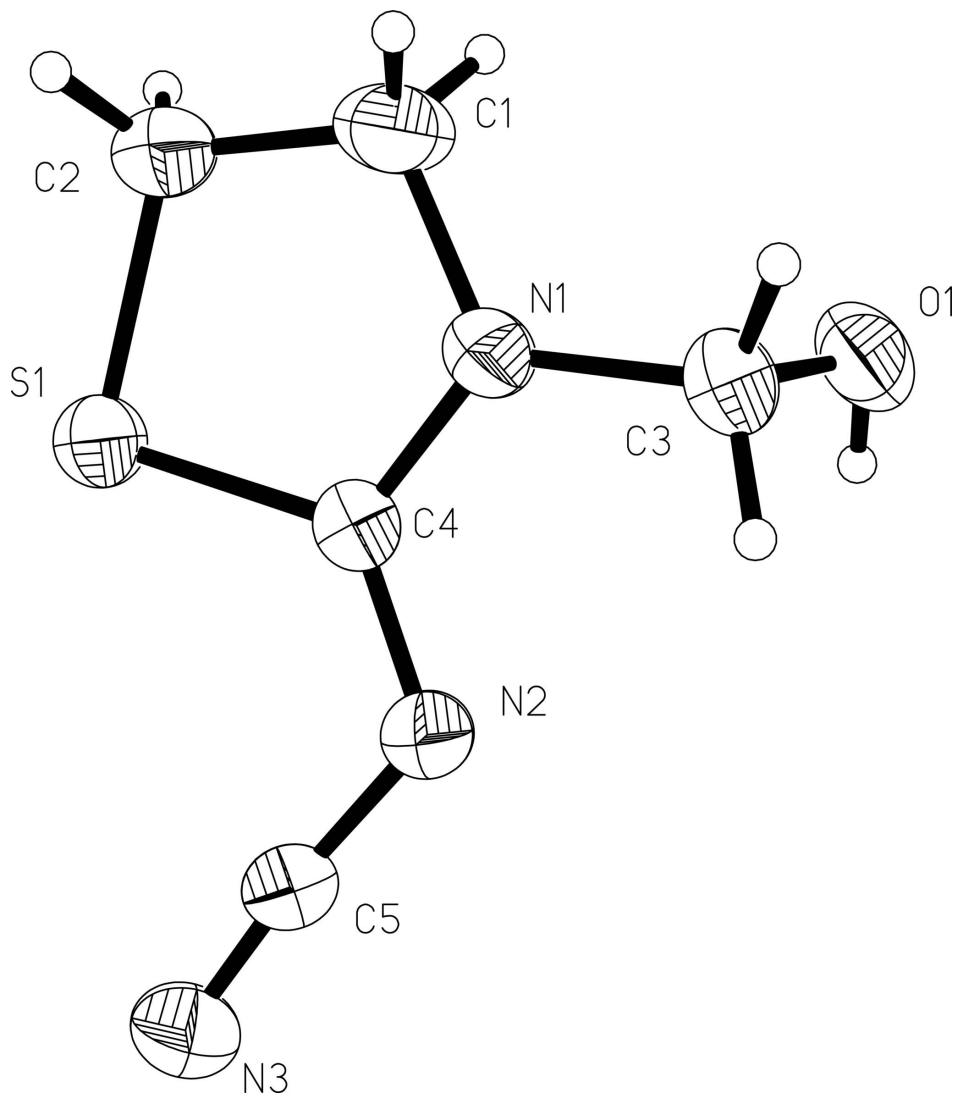
In (Z)-(3-(hydroxymethyl)thiazolidin-2-ylideneamino)formonitrile (Fig. 1), all bond lengths are normal (Allen *et al.*, 1987) and in a good agreement with those reported previously (Xie, 2008). It is known that the imino tautomers can exist as two geometrical isomers, *syn* (Z) and *anti* (E), but in this crystal, only Z isomers have been observed. The atoms of whole molecule except O atom (C1-C5/N1-N3/S1) are almost planar [maximum least squares plane deviation for N1 0.035 (3) Å]. The crystal packing is stabilized by intermolecular O—H···N hydrogen bonds, which link the molecules into dimers.

**S2. Experimental**

A mixture of (Z)-(thiazolidin-2-ylideneamino)formonitrile 10 mmol (1.27 g), paraformaldehyde (0.36 g, 12 mmol) and 0.01 g triethylamine were refluxed in absolute EtOH (20 mL) for 3 h. On cooling, the product crystallizes and was filtered and then recrystallized from absolute ethanol. Yield 1.51 g (96%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

**S3. Refinement**

All H atoms were found on difference maps. The hydroxyl H atoms were refined freely, giving an O—H bond distance of 0.80 Å. The remaining H atoms were placed in calculated positions, with C—H = 0.97 Å with  $U_{\text{iso}}(\text{H}) = 1.2$  times  $U_{\text{eq}}(\text{C})$ .

**Figure 1**

The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

**(Z)-{[3-(Hydroxymethyl)-1,3-thiazolidin-2-ylidene]amino}formonitrile**

*Crystal data*

$C_5H_7N_3OS$

$M_r = 157.20$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 5.5321$  (11) Å

$b = 8.1790$  (16) Å

$c = 8.4978$  (17) Å

$\alpha = 101.56$  (3)°

$\beta = 100.39$  (3)°

$\gamma = 105.47$  (3)°

$V = 351.75$  (16) Å<sup>3</sup>

$Z = 2$

$F(000) = 164$

$D_x = 1.484$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2501 reflections

$\theta = 2.3$ – $25.1$ °

$\mu = 0.39$  mm<sup>-1</sup>

$T = 293$  K

Needle, colorless

$0.22 \times 0.17 \times 0.13$  mm

*Data collection*

Rigaku R-AXIS RAPID IP area-detector  
diffractometer  
Radiation source: Rotating Anode  
Graphite monochromator  
 $\omega$  oscillation scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.919$ ,  $T_{\max} = 0.951$

2778 measured reflections  
1234 independent reflections  
1027 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$   
 $\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 3.2^\circ$   
 $h = -6 \rightarrow 6$   
 $k = -9 \rightarrow 9$   
 $l = -10 \rightarrow 10$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.119$   
 $S = 1.19$   
1234 reflections  
96 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.06P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$   
Extinction correction: *SHELXTL* (Sheldrick,  
2008),  $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.052 (16)

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.15141 (12)	0.91511 (8)	0.84635 (8)	0.0509 (3)
O1	0.3210 (4)	0.3944 (2)	0.6397 (3)	0.0640 (6)
N1	0.3875 (3)	0.6968 (2)	0.7503 (2)	0.0450 (5)
N2	0.2714 (4)	0.6719 (2)	0.9942 (2)	0.0490 (5)
N3	0.0736 (5)	0.7702 (3)	1.2185 (3)	0.0640 (6)
C1	0.3729 (7)	0.7839 (5)	0.6182 (4)	0.0724 (9)
H1B	0.2783	0.6980	0.5138	0.087*
H1C	0.5460	0.8400	0.6090	0.087*
C2	0.2400 (6)	0.9180 (4)	0.6529 (3)	0.0592 (7)
H2B	0.0866	0.8916	0.5642	0.071*
H2C	0.3545	1.0335	0.6600	0.071*
C3	0.4959 (5)	0.5525 (3)	0.7414 (3)	0.0529 (6)
H3A	0.6495	0.5809	0.6993	0.063*
H3B	0.5477	0.5389	0.8521	0.063*
C4	0.2782 (4)	0.7467 (3)	0.8711 (3)	0.0395 (5)

C5	0.1620 (5)	0.7289 (3)	1.1096 (3)	0.0482 (6)
H1A	0.216 (6)	0.353 (4)	0.686 (4)	0.080 (10)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0639 (4)	0.0564 (4)	0.0506 (4)	0.0356 (3)	0.0251 (3)	0.0217 (3)
O1	0.0818 (13)	0.0500 (10)	0.0697 (13)	0.0227 (9)	0.0443 (11)	0.0109 (9)
N1	0.0543 (11)	0.0508 (10)	0.0416 (11)	0.0272 (9)	0.0206 (9)	0.0158 (8)
N2	0.0661 (12)	0.0492 (11)	0.0457 (12)	0.0278 (9)	0.0249 (9)	0.0202 (9)
N3	0.0854 (16)	0.0641 (13)	0.0531 (14)	0.0263 (12)	0.0342 (12)	0.0195 (11)
C1	0.101 (2)	0.102 (2)	0.0584 (17)	0.0688 (19)	0.0462 (16)	0.0452 (16)
C2	0.0827 (17)	0.0620 (15)	0.0481 (15)	0.0335 (14)	0.0262 (13)	0.0240 (12)
C3	0.0601 (14)	0.0561 (14)	0.0562 (15)	0.0318 (12)	0.0255 (12)	0.0166 (12)
C4	0.0416 (11)	0.0386 (10)	0.0389 (12)	0.0140 (9)	0.0111 (9)	0.0087 (9)
C5	0.0622 (14)	0.0462 (12)	0.0421 (14)	0.0191 (11)	0.0171 (11)	0.0179 (10)

*Geometric parameters (Å, °)*

S1—C4	1.735 (2)	N3—C5	1.156 (3)
S1—C2	1.801 (3)	C1—C2	1.486 (4)
O1—C3	1.392 (3)	C1—H1B	0.9700
O1—H1A	0.80 (3)	C1—H1C	0.9700
N1—C4	1.331 (3)	C2—H2B	0.9700
N1—C1	1.447 (3)	C2—H2C	0.9700
N1—C3	1.455 (3)	C3—H3A	0.9700
N2—C5	1.314 (3)	C3—H3B	0.9700
N2—C4	1.315 (3)		
C4—S1—C2	92.28 (11)	S1—C2—H2B	110.0
C3—O1—H1A	111 (2)	C1—C2—H2C	110.0
C4—N1—C1	116.2 (2)	S1—C2—H2C	110.0
C4—N1—C3	122.77 (19)	H2B—C2—H2C	108.4
C1—N1—C3	120.8 (2)	O1—C3—N1	112.3 (2)
C5—N2—C4	118.1 (2)	O1—C3—H3A	109.1
N1—C1—C2	110.0 (2)	N1—C3—H3A	109.1
N1—C1—H1B	109.7	O1—C3—H3B	109.1
C2—C1—H1B	109.7	N1—C3—H3B	109.1
N1—C1—H1C	109.7	H3A—C3—H3B	107.9
C2—C1—H1C	109.7	N2—C4—N1	121.5 (2)
H1B—C1—H1C	108.2	N2—C4—S1	125.35 (17)
C1—C2—S1	108.30 (18)	N1—C4—S1	113.20 (17)
C1—C2—H2B	110.0	N3—C5—N2	174.2 (3)
C4—N1—C1—C2	1.7 (4)	C1—N1—C4—N2	177.4 (2)
C3—N1—C1—C2	176.5 (2)	C3—N1—C4—N2	2.8 (3)
N1—C1—C2—S1	-0.2 (3)	C1—N1—C4—S1	-2.5 (3)
C4—S1—C2—C1	-0.9 (2)	C3—N1—C4—S1	-177.14 (17)

C4—N1—C3—O1	95.2 (3)	C2—S1—C4—N2	-178.0 (2)
C1—N1—C3—O1	-79.2 (3)	C2—S1—C4—N1	1.95 (18)
C5—N2—C4—N1	179.5 (2)	C4—N2—C5—N3	-171 (3)
C5—N2—C4—S1	-0.6 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 <i>A</i> $\cdots$ N3 <sup>i</sup>	0.80 (3)	2.04 (3)	2.839 (3)	174 (3)

Symmetry code: (i)  $-x, -y+1, -z+2$ .