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3-Amino-2-thioxothiazolidin-4-one

Qing-Li Zhou,[a] Zhen-Heng Zhang[b] and Zuo-Liang Jing[c]*

[a]College of Life Sciences and Engineering, Shaanxi University of Science and Technology, Shaanxi 712081, People's Republic of China, and Tianjin Food Engineering Centre, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China, [b]College of Food Engineering and Biotechnology, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China, and [c]College of Sciences, Tianjin University of Science and Technology, Tianjin 300457, People's Republic of China
Correspondence e-mail: jzl74@tust.edu.cn

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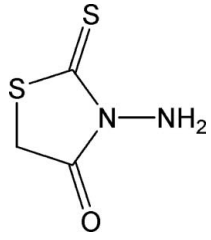
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 12.7.

The asymmetric unit of the title compound, $C_3H_4N_2OS_2$, contains two independent molecules, which differ in the orientation of the amino group by a 180° rotation around its bond with the thiazoline ring. The molecules are linked by N—H···O, N—H···N and N—H···S hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Belloni *et al.* (2005); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_3H_4N_2OS_2$
M_r = 148.20
Monoclinic, $P2_1/n$
a = 9.8257 (17) Å
b = 9.3118 (16) Å
c = 13.416 (2) Å
β = 105.924 (3)°
V = 1180.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 294 (2) K
0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.797, T_{max} = 0.857
5324 measured reflections
2052 independent reflections
1686 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.03
2052 reflections
161 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^{i}	0.899 (9)	2.38 (2)	3.049 (3)	131 (2)
N2—H2A···S1^{ii}	0.899 (9)	2.945 (15)	3.708 (2)	143.8 (19)
N2—H2B···N4^{iii}	0.909 (9)	2.246 (11)	3.130 (3)	164 (2)
N4—H4A···O1^{iv}	0.902 (9)	2.38 (2)	2.994 (3)	126 (2)
N4—H4B···N2^{iv}	0.902 (10)	2.40 (2)	3.061 (3)	130 (2)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2296).

References

Belloni, M., Kariuki, B. M., Manickam, M., Wilkie, J. & Preece, J. A. (2005). *Cryst. Growth Des.* **5**, 1443–1449.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tynan, E., Jensen, P., Lees, A. C., Moubaraki, B., Murray, K. S. & Kruger, P. E. (2005). *CrystEngComm*, **7**, 90–95.

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supplementary materials

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3-Amino-2-thioxothiazolidin-4-one

Q.-L. Zhou, Z.-H. Zhang and Z.-L. Jing

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry, we report the synthesis and structure of the title compound, (I).

The asymmetric unit of (I) comprises two independent molecules (Fig. 1), lying on the mirror planes, one at z = 0 and the other at z = 1/2. The two molecules differ in the orientation of the Amino group by a 180° rotation around its bond with the thiazoline ring. In both molecules the geometric parameters are normal. Each independent molecule is linked to a symmetry-equivalent molecule by intermolecular N—H···O and N—H···N hydrogen bonds,and linked to himself by N—H···S hydrogen bonds (Table 1), forming a three-dimensional network which leads to a stable crystal structure (Fig. 2).

Experimental

3-Amino-2-thioxo-thiazolidin-4-one (1 g) was added to an anhydrous ethanol (50 ml), with stirring at 350 K. The resulting colourless solution was filtered and the filtrate was allowed to stand in air at room temperature for 10 d, yielding colourless crystals of (I).

Refinement

H atoms of the amino group were found from difference Fourier map and refined freely. H atoms of the methylene group were placed in calculated positions with C—H = 0.97 Å and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

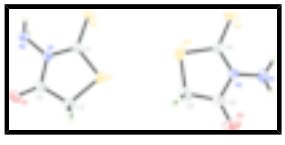

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

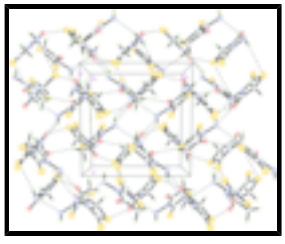

Fig. 2. The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

3-Amino-2-thioxothiazolidin-4-one

Crystal data

$C_3H_4N_2OS_2$	F_{000} = 608
M_r = 148.20	D_x = 1.668 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2513 reflections
a = 9.8257 (17) Å	θ = 3.1–26.2º
b = 9.3118 (16) Å	μ = 0.80 mm^{-1}
c = 13.416 (2) Å	T = 294 (2) K
β = 105.924 (3)º	Block, colourless
V = 1180.4 (3) Å^3	0.30 × 0.26 × 0.20 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	2052 independent reflections
Radiation source: fine-focus sealed tube	1686 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→9
T_{min} = 0.797, T_{max} = 0.857	k = −9→11
5324 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.085	$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.5975P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2052 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
161 parameters	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.42862 (7)	0.22451 (7)	0.88952 (5)	0.0471 (2)
S2	0.45652 (7)	0.17983 (7)	1.11280 (5)	0.0469 (2)
S3	0.74095 (8)	0.46329 (7)	0.97871 (6)	0.0562 (2)
S4	0.94214 (8)	0.65599 (8)	1.12373 (5)	0.0547 (2)
O1	0.13941 (19)	−0.0621 (2)	0.80930 (12)	0.0521 (5)
O2	0.8082 (2)	0.6549 (2)	0.74386 (13)	0.0655 (6)
N1	0.28161 (19)	0.03994 (19)	0.95556 (13)	0.0320 (4)
N2	0.2236 (2)	−0.0421 (2)	1.02200 (14)	0.0384 (5)
N3	0.87489 (19)	0.66393 (19)	0.91821 (13)	0.0332 (4)
N4	0.9526 (2)	0.7909 (2)	0.92041 (18)	0.0447 (5)
C1	0.3843 (2)	0.1415 (2)	0.99099 (17)	0.0326 (5)
C2	0.2310 (2)	0.0216 (3)	0.84990 (17)	0.0368 (5)
C3	0.3057 (3)	0.1194 (3)	0.79385 (17)	0.0436 (6)
H3A	0.2381	0.1814	0.7470	0.052*
H3B	0.3554	0.0638	0.7537	0.052*
C4	0.8593 (2)	0.6040 (2)	1.00653 (17)	0.0356 (5)
C5	0.7091 (3)	0.4857 (3)	0.8416 (2)	0.0552 (7)
H5A	0.7339	0.3987	0.8108	0.066*
H5B	0.6099	0.5064	0.8098	0.066*
C6	0.7985 (3)	0.6077 (3)	0.82491 (18)	0.0427 (6)
H2A	0.295 (2)	−0.080 (3)	1.0717 (15)	0.067 (9)*
H2B	0.174 (2)	0.021 (2)	1.0505 (17)	0.060 (8)*
H4A	0.974 (3)	0.788 (3)	0.8592 (10)	0.076 (10)*
H4B	1.0315 (17)	0.790 (3)	0.9741 (12)	0.065 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0468 (4)	0.0497 (4)	0.0476 (4)	−0.0103 (3)	0.0177 (3)	0.0000 (3)
S2	0.0439 (4)	0.0494 (4)	0.0388 (3)	0.0025 (3)	−0.0031 (3)	−0.0089 (3)
S3	0.0545 (5)	0.0407 (4)	0.0734 (5)	−0.0070 (3)	0.0178 (4)	0.0075 (3)
S4	0.0518 (4)	0.0744 (5)	0.0339 (3)	0.0148 (4)	0.0048 (3)	−0.0048 (3)

O1	0.0526 (11)	0.0622 (12)	0.0380 (9)	−0.0170 (9)	0.0066 (8)	−0.0129 (8)
O2	0.1022 (17)	0.0598 (12)	0.0319 (9)	0.0172 (11)	0.0136 (10)	0.0003 (9)
N1	0.0328 (10)	0.0334 (10)	0.0291 (9)	0.0017 (8)	0.0074 (8)	−0.0010 (8)
N2	0.0419 (12)	0.0391 (11)	0.0347 (10)	−0.0022 (9)	0.0114 (9)	0.0031 (9)
N3	0.0347 (11)	0.0297 (10)	0.0338 (10)	0.0020 (8)	0.0073 (8)	−0.0014 (8)
N4	0.0437 (13)	0.0348 (11)	0.0580 (14)	−0.0057 (10)	0.0178 (11)	0.0014 (10)
C1	0.0285 (12)	0.0301 (11)	0.0379 (12)	0.0056 (10)	0.0069 (9)	−0.0031 (9)
C2	0.0357 (13)	0.0411 (13)	0.0326 (12)	0.0047 (11)	0.0078 (10)	−0.0041 (10)
C3	0.0495 (15)	0.0491 (15)	0.0343 (12)	0.0028 (12)	0.0149 (11)	0.0000 (11)
C4	0.0328 (13)	0.0355 (12)	0.0390 (12)	0.0091 (10)	0.0108 (10)	0.0028 (10)
C5	0.0480 (16)	0.0411 (14)	0.0646 (18)	0.0005 (13)	−0.0048 (13)	−0.0139 (13)
C6	0.0501 (15)	0.0366 (13)	0.0363 (13)	0.0111 (11)	0.0036 (11)	−0.0054 (11)

Geometric parameters (Å, °)

S1—C1	1.722 (2)	N2—H2B	0.909 (9)
S1—C3	1.793 (2)	N3—C4	1.356 (3)
S2—C1	1.633 (2)	N3—C6	1.374 (3)
S3—C4	1.724 (2)	N3—N4	1.403 (3)
S3—C5	1.792 (3)	N4—H4A	0.902 (9)
S4—C4	1.633 (2)	N4—H4B	0.902 (10)
O1—C2	1.202 (3)	C2—C3	1.495 (3)
O2—C6	1.201 (3)	C3—H3A	0.9700
N1—C1	1.370 (3)	C3—H3B	0.9700
N1—C2	1.378 (3)	C5—C6	1.490 (4)
N1—N2	1.408 (3)	C5—H5A	0.9700
N2—H2A	0.899 (9)	C5—H5B	0.9700
C1—S1—C3	93.10 (11)	N1—C2—C3	110.7 (2)
C4—S3—C5	92.92 (11)	C2—C3—S1	107.43 (15)
C1—N1—C2	117.77 (19)	C2—C3—H3A	110.2
C1—N1—N2	122.88 (17)	S1—C3—H3A	110.2
C2—N1—N2	119.31 (19)	C2—C3—H3B	110.2
N1—N2—H2A	108.4 (19)	S1—C3—H3B	110.2
N1—N2—H2B	105.7 (17)	H3A—C3—H3B	108.5
H2A—N2—H2B	109.9 (14)	N3—C4—S4	125.01 (18)
C4—N3—C6	118.4 (2)	N3—C4—S3	110.78 (16)
C4—N3—N4	121.30 (19)	S4—C4—S3	124.21 (14)
C6—N3—N4	119.9 (2)	C6—C5—S3	107.41 (17)
N3—N4—H4A	102.4 (19)	C6—C5—H5A	110.2
N3—N4—H4B	110.5 (19)	S3—C5—H5A	110.2
H4A—N4—H4B	111.3 (14)	C6—C5—H5B	110.2
N1—C1—S2	125.08 (17)	S3—C5—H5B	110.2
N1—C1—S1	110.96 (15)	H5A—C5—H5B	108.5
S2—C1—S1	123.96 (14)	O2—C6—N3	121.8 (2)
O1—C2—N1	124.1 (2)	O2—C6—C5	127.7 (2)
O1—C2—C3	125.2 (2)	N3—C6—C5	110.5 (2)
C2—N1—C1—S2	179.48 (16)	C6—N3—C4—S4	179.53 (17)
N2—N1—C1—S2	1.5 (3)	N4—N3—C4—S4	−8.4 (3)
C2—N1—C1—S1	−0.6 (2)	C6—N3—C4—S3	0.2 (3)

N2—N1—C1—S1	−178.61 (15)	N4—N3—C4—S3	172.31 (16)
C3—S1—C1—N1	−0.33 (17)	C5—S3—C4—N3	−0.39 (18)
C3—S1—C1—S2	179.58 (15)	C5—S3—C4—S4	−179.72 (16)
C1—N1—C2—O1	−178.7 (2)	C4—S3—C5—C6	0.45 (19)
N2—N1—C2—O1	−0.6 (3)	C4—N3—C6—O2	−179.4 (2)
C1—N1—C2—C3	1.4 (3)	N4—N3—C6—O2	8.4 (3)
N2—N1—C2—C3	179.52 (18)	C4—N3—C6—C5	0.2 (3)
O1—C2—C3—S1	178.6 (2)	N4—N3—C6—C5	−172.1 (2)
N1—C2—C3—S1	−1.5 (2)	S3—C5—C6—O2	179.1 (2)
C1—S1—C3—C2	1.05 (18)	S3—C5—C6—N3	−0.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.899 (9)	2.38 (2)	3.049 (3)	131 (2)
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N2—H2B···N4^{iii}	0.909 (9)	2.246 (11)	3.130 (3)	164 (2)
N4—H4A···O1^{iv}	0.902 (9)	2.38 (2)	2.994 (3)	126 (2)
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Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+2; (iv) *x*+1, *y*+1, *z*.

Fig. 1

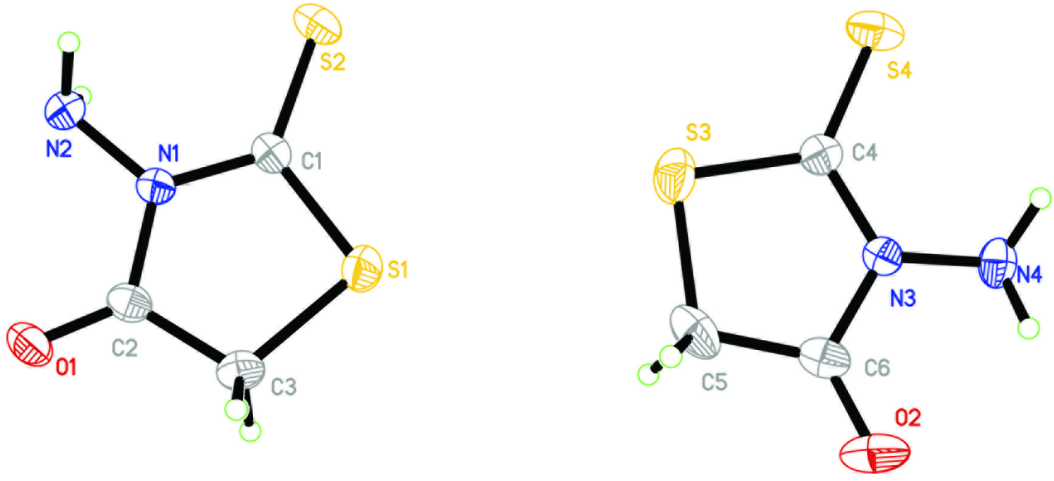

Fig. 2