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DL-2-Amino-2-thiazoline-4-carboxylic acid trihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.082
Data-to-parameter ratio = 13.5

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

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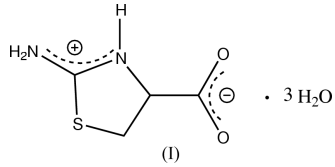
In the title compound, $C_4H_6N_2O_2S\cdot 3H_2O$, the 2-amino-2-thiazoline-4-carboxylic acid molecule is in a zwitterionic form and shows amino–imino tautomerism. There are intermolecular O—H···O, O—H···N, N—H···O and C—H···O interactions, forming a three-dimensional network.

Comment

Compounds with both amino and carboxylic acid groups in their molecular structure, such as amino acids, can exist as zwitterions and often cocrystallize with solvent molecules in the solid state. In a zwitterion, both charged groups, COO^- and NH_3^+ (or NH_2^+ or NH^+), may interact with each other and with the aqueous solvent by means of electrostatic, polarization and hydrogen-bonding interactions. In the 2-amino-2-thiazoline-4-carboxylic acid molecule, there are one amino-group, one imino N atom in the heterocycle, and one carboxylic acid group. To determine its specific structural features, we have performed an X-ray structural analysis of the title compound, (I).



(I)

This compound is a zwitterion, incorporating three water molecules as crystallization solvent (Fig. 1 and Table 1). The very similar bond distances of C3—N1 and C3—N2 indicate tautomerism between amino N2 and imino N1. The almost symmetric O1—C4—O2 group suggests also conjugation of the carboxylate.

A detailed analysis of the crystal packing shows that the hydrogen bonds involving O—H···O, C—H···O, N—H···O and O—H···N generate two-dimensional networks (Fig. 2 and Table 2). The hydrogen bonds O5—H5*A*···O4^{i}, O5—H5*B*···O4^{ii}, C1—H1*A*···O2^{i}, C2—H2···O2^{iv}, and N1—H1···O3^{iv} [symmetry codes: (i) $x-\frac{1}{2}, -\frac{1}{2}-y, z$; (ii) $x-\frac{1}{2}, -y, -z$; (iv) $\frac{1}{2}+x, -\frac{1}{2}-y, z$] connect adjacent two-dimensional networks (Fig. 3).

Experimental

The title compound was synthesized in our laboratory (Xuan *et al.*, 2003). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a saturated aqueous solution at room temperature.

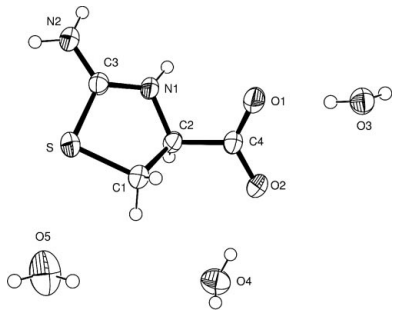


Figure 1
The molecular structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

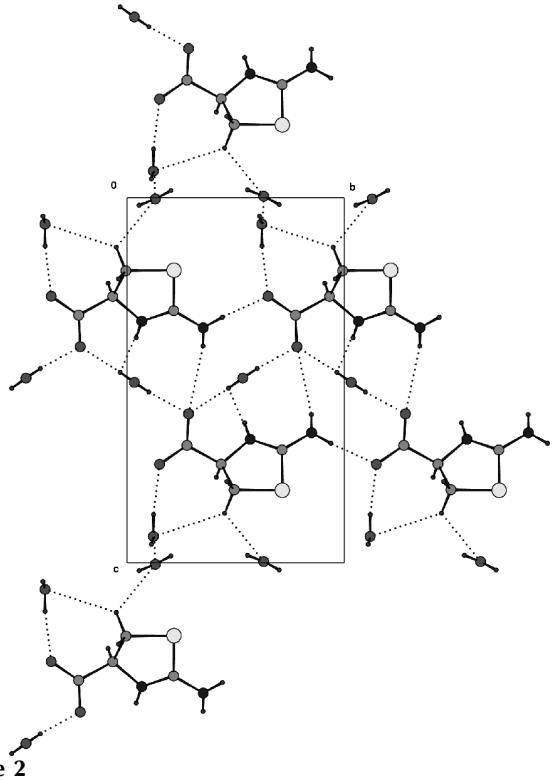


Figure 2
Packing diagram of (I), viewed along the *a* axis, showing, as dashed lines, the hydrogen-bonding and short-contact interactions within a two-dimensional molecular network.

Crystal data

$C_4H_6N_2O_2S\cdot 3H_2O$
$M_r = 200.22$
Orthorhombic, $P2_1ab$
$a = 8.0835\ (4)$ Å
$b = 8.1546\ (3)$ Å
$c = 13.7591\ (7)$ Å
$V = 906.97\ (7)$ Å^3
$Z = 4$
$D_x = 1.466$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11305 reflections
$\theta = 2.5$–27.4°
$\mu = 0.35$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
0.30 × 0.29 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.849$, $T_{max} = 0.917$
8161 measured reflections
1968 independent reflections
1620 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 27.4^\circ$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -17 \rightarrow 17$

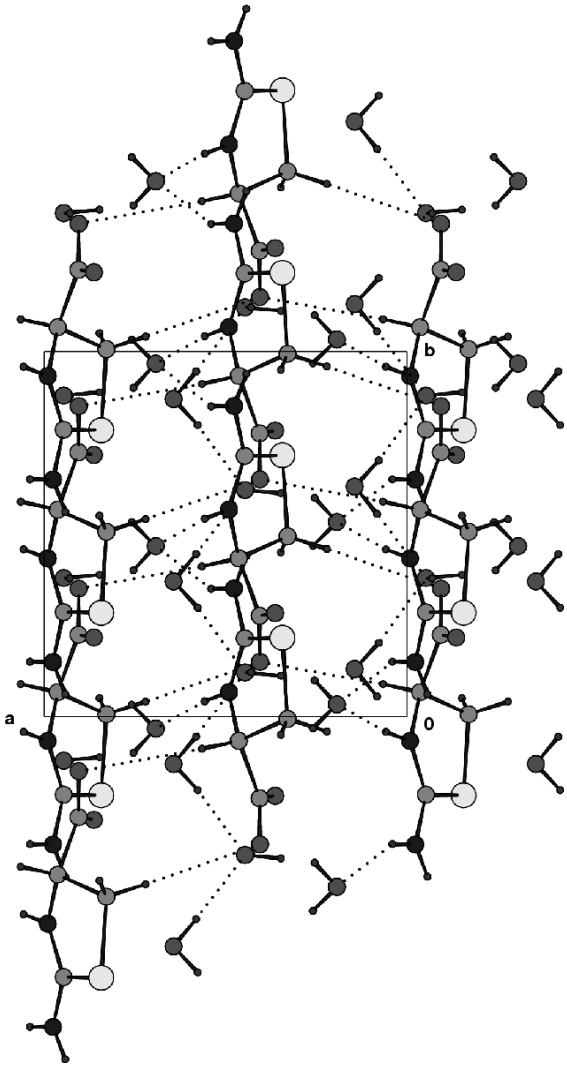


Figure 3
Packing diagram of (I), viewed along the *c* axis, showing, as dashed lines. the hydrogen-bonding interactions between adjacent molecular networks.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.082$
$S = 1.07$
1968 reflections
146 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.010 (2)
Absolute structure: Flack (1983), 852 Friedel pairs
Flack parameter = 0.49 (9)

Table 1
Selected geometric parameters (Å, °).

S—C3	1.738 (2)	C1—C2	1.533 (4)
S—C1	1.814 (2)	C3—N2	1.308 (3)
O1—C4	1.243 (3)	C4—O2	1.250 (3)
N1—C3	1.313 (3)	C4—C2	1.534 (3)
N1—C2	1.454 (3)		
O1—C4—C2	118.88 (19)	O2—C4—C2	115.5 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O4^{i}	0.825 (19)	1.94 (2)	2.759 (3)	175 (4)
O5—H5B···O4^{ii}	0.854 (19)	1.94 (2)	2.787 (3)	174 (4)
O4—H4B···O2	0.839 (18)	1.915 (19)	2.749 (3)	173 (4)
O3—H3A···O1^{iii}	0.846 (18)	1.97 (2)	2.802 (3)	166 (4)
O3—H3B···O1	0.821 (18)	1.920 (19)	2.731 (3)	169 (3)
O3—H3A···N1^{iii}	0.846 (18)	2.80 (3)	3.343 (3)	123 (3)
N1—H1···O3^{iv}	0.848 (17)	1.972 (18)	2.816 (3)	173 (3)
N2—H2A···O2^{v}	0.867 (18)	1.914 (19)	2.772 (3)	170 (3)
N2—H2B···O1^{vi}	0.856 (17)	2.98 (3)	3.411 (3)	114 (2)
N2—H2B···O3^{vii}	0.856 (17)	2.08 (2)	2.862 (3)	152 (3)
C1—H1B···O5	0.97	2.86	3.288 (4)	108
C1—H1B···O4	0.97	2.93	3.640 (3)	131
C1—H1A···O2^{i}	0.97	2.78	3.744 (4)	175
C2—H2···O2^{iv}	0.98	2.84	3.637 (3)	140

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

H atoms bonded to N and O atoms were located in difference Fourier maps and refined isotropically. Refined distances were O—H = 0.846 (18)–0.855 (19) Å and N—H = 0.848 (17)–0.867 (18) Å. H atoms bonded to C atoms were placed at calculated positions, refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent atom), and C—H distances were constrained to 0.97–0.98 Å. The Flack (1983) parameter indicates that the sample, itself a racemate in a space group with glide planes, is twinned by inversion.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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