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catena-Poly[[aqua(1-methyl-1*H*-1,2,3,4-tetrazole-5-thiolato-κS)sodium]-di-μ-aqua-$\kappa^4 O$:*O*]

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The crystal structure of the title compound, $[Na(C_2H_3N_4S)(H_2O)_3]_n$, features polymeric chains made up of sodium coordination octahedra $NaS(H_2O)_5$, each of them sharing two μ-$H_2O\cdots\mu$-H_2O edges with two adjacent octahedra; the chains run along the *a* axis of the crystal structure. All three unsubstituted N atoms of the tetrazole ring are involved in the complex hydrogen-bonding system; however, none of them participate in the coordination of the sodium ion.

Key indicators

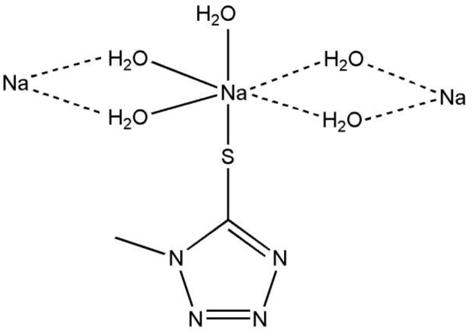
Single-crystal X-ray study
T = 296 K
Mean σ(N–C) = 0.002 Å
R factor = 0.027
wR factor = 0.072
Data-to-parameter ratio = 11.6

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

Comment

1-Methyl-1*H*-tetrazole-5-thiol (*L*) is a rather interesting and extensively studied compound, which exists either as a thiol or as a thione tautomer. Quite a few transition metal complexes of this ligand have been synthesized and structurally characterized (Nöth *et al.*, 1998; Wang *et al.*, 2006). Its complexes with the main group metals, however, are far more scarce, Ph_3SnL (Rodarte de Moura *et al.*, 1999) and [K(18-Crown-6)]*L* (Cea-Olivares *et al.*, 1995) being the only well documented cases. Both of these complexes have along with the tetrazolethiolate ligand *L* have additional organic ligands.

We report here the structure of the sodium salt of the ligand *L* in its trihydrated form; the tetrazolethiolate anion is the only organic ligand of the title complex, (I). A view of the asymmetric unit is shown in Fig. 1. The tetrazolethiolate anion coordinates to the Na^+ cation through its S atom (Table 1).



(I)

The Na1 ion has a distorted octahedral environment formed by a terminal water molecule O2, four bridging water molecules O1, O3, O1^{i} and O3^{ii} [symmetry codes (i): $-x$, $1-y$, $1-z$; (ii): $1-x$, $1-y$, $1-z$], and atom S1 of the tetrazolethiolate ligand. Each coordination octahedron shares common O1$\cdots$O3 and O1$^{i}\cdots$O3^{i} edges with each of the two adjacent octahedra, thus producing infinite chains running along the *a* axis of the crystal structure (Fig. 2). Similar chains of coordination octahedra of Na^+ ions were found in the

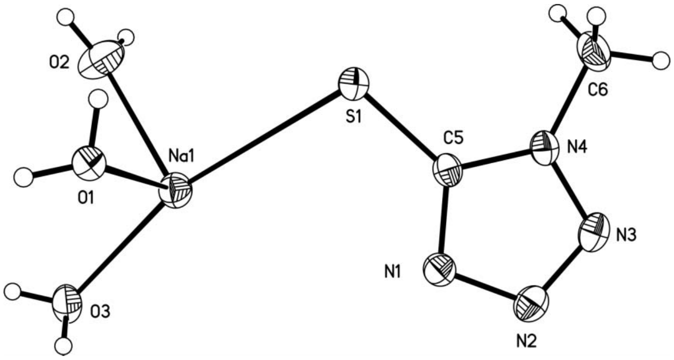


Figure 1
The asymmetric unit of the title compound with atomic labeling. Displacement ellipsoids are plotted at the 50% probability level.

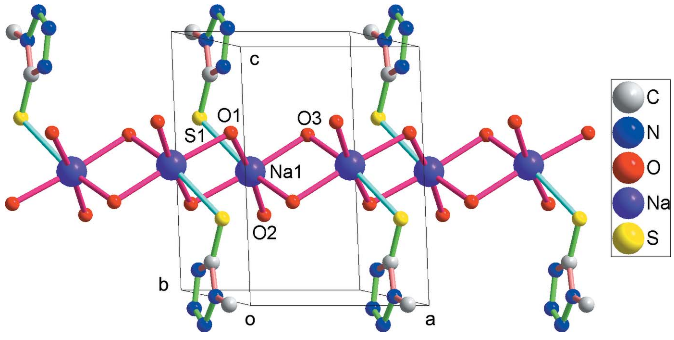


Figure 2
Part of the polymeric chain parallel to the *a* axis viewed down the *b* axis; H atoms have been omitted for clarity.

structure of sodium carboxynitrobenzoate tetrahydrate (Guo, 2004). In the crystal structure of the title compound, the chains are further linked into complex three-dimensional network *via* the O—H···N bonds, involving each of the three unsubstituted tetrazole N atoms (Table 2). It is noteworthy that none of the tetrazole N atoms participate in the coordination of the Na1 cation.

The Na1—O distances range from 2.3353 (15) Å to 2.4851 (14) Å with a mean value of 2.4293 Å. The C—N and N—N bond lengths are very close to those found in the dimeric free ligand (Cea-Olivares *et al.*, 1995). The C—S bond length measuring 1.7133 (14) Å lies in the range between the values for single [1.817 (5) Å] and double [1.555 (1) Å] C—S bonds (Dean, 1999), corresponding to partial π-bond character (Trinajstic, 1968; Huber *et al.*, 1982).

Experimental

To a solution of 1-methyl-1*H*-tetrazole-5-thione (10 mmol, 1.161 g) in 60 ml of doubly-distilled water, a solution of an equimolar amount (10 mmol, 0.400 g) of sodium hydroxide in 40 ml of doubly-distilled water was added dropwise at room temperature. After vigorous stirring for 4 h, the resulting mixture was evaporated *in vacuo* to a volume of about 20 ml and filtered hot. The filtrate was then set aside for crystallization at room temperature. Three weeks later, light-yellow crystals of the title compound suitable for X-ray analysis were isolated.

Crystal data

$[Na(C_2H_3N_4S)(H_2O)_3]$
$M_r = 192.18$
Triclinic, $P\bar{1}$
$a = 6.4420$ (7) Å
$b = 7.0072$ (8) Å
$c = 9.7713$ (11) Å
$\alpha = 105.519$ (1)°
$\beta = 97.098$ (1)°
$\gamma = 96.589$ (1)°
$V = 416.67$ (8) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.41$ mm^{-1}
$T = 296$ (2) K
0.42 × 0.39 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.848$, $T_{max} = 0.889$
2105 measured reflections
1463 independent reflections
1401 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.072$
$S = 1.00$
1463 reflections
126 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Na1—O1	2.4225 (14)	Na1—O3^{ii}	2.4851 (14)
Na1—O2	2.3353 (15)	Na1—S1	3.0163 (8)
Na1—O3	2.4493 (14)	S1—C5	1.7133 (14)
Na1—O1^{i}	2.4543 (13)		
O2—Na1—O1	92.10 (5)	O3—Na1—O3^{ii}	85.57 (5)
O2—Na1—O3	94.87 (6)	O1^{i}—Na1—O3^{ii}	99.43 (5)
O1—Na1—O3	100.02 (5)	O2—Na1—S1	98.58 (5)
O2—Na1—O1^{i}	172.45 (6)	O1—Na1—S1	84.02 (3)
O1—Na1—O1^{i}	81.04 (5)	O3—Na1—S1	165.82 (4)
O3—Na1—O1^{i}	83.29 (5)	O1^{i}—Na1—S1	83.94 (3)
O2—Na1—O3^{ii}	87.70 (5)	O3^{ii}—Na1—S1	90.47 (3)
O1—Na1—O3^{ii}	174.40 (5)		

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···S1^{iii}	0.822 (10)	2.560 (12)	3.3632 (16)	166 (3)
O2—H2*B*···N2^{iv}	0.814 (10)	2.298 (15)	3.084 (2)	163 (4)
O3—H3*B*···N3^{v}	0.813 (10)	2.225 (13)	3.0075 (18)	162 (2)
O3—H3*A*···S1^{i}	0.813 (10)	2.751 (17)	3.4769 (14)	150 (3)
O1—H1*B*···N1^{i}	0.822 (10)	1.998 (10)	2.8123 (18)	171 (2)
O1—H1*A*···S1^{vi}	0.822 (10)	2.540 (11)	3.3513 (12)	169 (2)

Symmetry codes: (i) $-x, -y+1, -z+1$; (iii) $-x+1, -y+2, -z+1$; (iv) $x, y, z-1$; (v) $x, y-1, z-1$; (vi) $-x, -y+2, -z+1$.

Methyl H atoms were placed in idealized positions and were included in the refinement in the riding model approximation with U_{iso} fixed at $1.5U_{eq}$(C) (C—H = 0.96 Å). H atoms associated with the water molecules were located in a difference Fourier map and refined isotropically with O—H bond lengths restrained to 0.82 (1) Å.

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Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XSHELL* (Bruker–Nonius, 2004) and *DIAMOND* (Brandenburg & Brendt, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 2003).

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