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catena-Poly[[(3-methylsulfanyl-1,2,4-thiadiazole-5-thiolato)sodium]di-μ-aqua-κ^4O:O]

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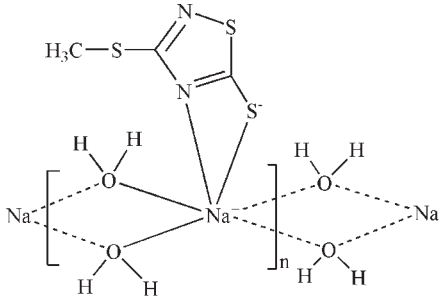
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(S–N) = 0.003 Å; R factor = 0.024; wR factor = 0.064; data-to-parameter ratio = 13.5.

The crystal structure of the title compound, $[Na(C_3H_3N_2S_3)(H_2O)_2]_n$, features polymeric chains made up of O···O edge-shared $NaSN(H_2O)_4$ units running along the b axis. The Na^+ ion and all non-H atoms of the thiadiazole ligand lie on a mirror plane.

Related literature

For related structures, see: Guo (2004); Wang *et al.* (2007).



Experimental

Crystal data

$[Na(C_3H_3N_2S_3)(H_2O)_2]$
M_r = 222.28
Monoclinic, $P2_1/m$
a = 7.5794 (8) Å
b = 6.9736 (6) Å
c = 8.6879 (12) Å
β = 102.027 (1)°
V = 449.13 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 298 K
0.39 × 0.27 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.739, T_{max} = 0.886
2256 measured reflections
862 independent reflections
728 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.064
S = 1.07
862 reflections
64 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O1	2.4493 (16)	Na1—O1^{i}	2.4736 (16)
Na1—N2	2.467 (2)	Na1—S3	3.1271 (14)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: CI2968).

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Wang, X.-H., Hu, M.-C. & Yang, Z.-Q. (2007). *Acta Cryst.* E**63**, m1527–m1529.

supporting information

Acta Cryst. (2010). E**66**, m15 [doi:10.1107/S1600536809051721]

catena-Poly[[(3-methylsulfanyl-1,2,4-thiadiazole-5-thiolato)sodium]di-μ-aqua-κ^4O:O]

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S1. Comment

In the title compound (Fig.1), each Na^+ ion has a six-coordinate environment formed by a S atom and a N atom of the 3-methylsulfanyl-1,2,4-thiadiazole-5-thiolate ligand, and four bridging water O atoms O1, O1A, O1B and O1C. The adjacent $NaSNO_4$ units share O1···O1A and O1B···O1C edges, producing chains running along the *b* axis (Fig. 2). Similar chains were found in the crystal structure of sodium carboxynitrobenzoate tetrahydrate (Guo, 2004). The Na—O [2.4493 (16) and 2.4736 (16) Å], Na—S [3.1271 (14) Å] and Na—N [2.467 (2) Å] distances are comparable to those observed in a related structure (Wang *et al.*, 2007).

S2. Experimental

To a solution of 3-methylmercapto-5-mercapto-1,2,4-thiadiazole (10 mmol) in 60 ml of doubly-distilled water, a solution of an equimolar amount (10 mmol) of sodium hydroxide in 40 ml of doubly-distilled water was added dropwise at room temperature. After vigorous stirring for 6 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. Two weeks later, colourless single crystals suitable for X-ray diffraction were obtained.

S3. Refinement

H atoms of the water molecules were initially located a difference Fourier map and later refined using a riding model with O-H = 0.85Å and U_{iso}(H) = 0.05 Å^2. C-bound H atoms were positioned geometrically and treated as riding on their parent atoms with C-H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C).

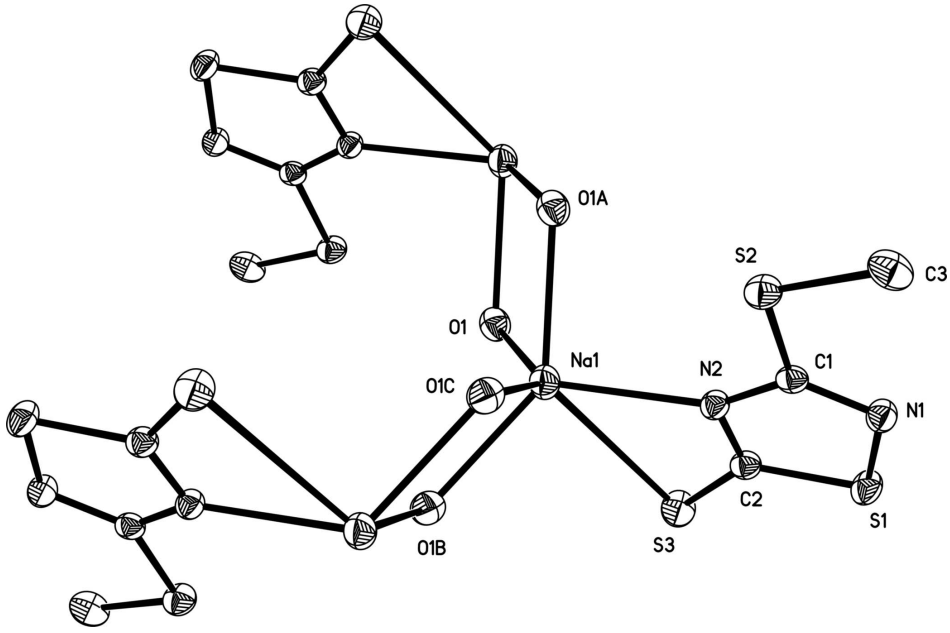

Figure 1

The coordination environment around the Na^+ ion. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (A) -*x*, -*y*, 2-*z*; (B) *x*, 1/2-*y*, *z*; (C) -*x*, 1/2+*y*, 2-*z*].

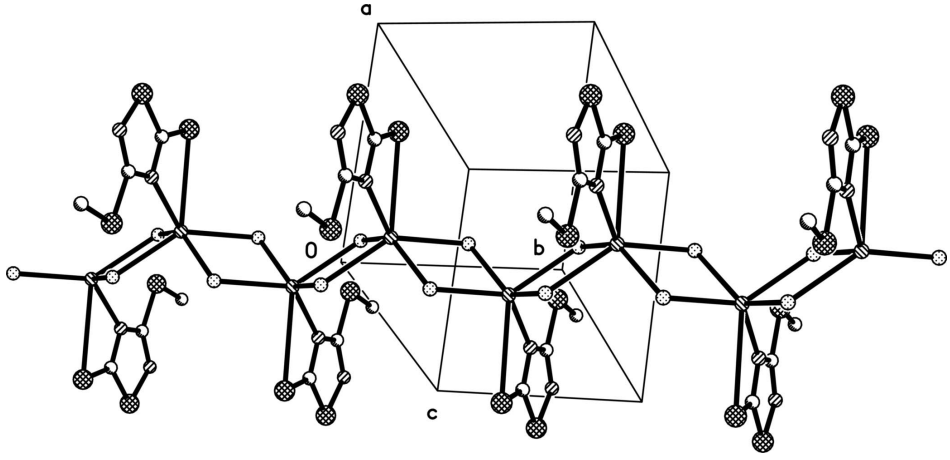

Figure 2

Part of the polymeric chain parallel to the *b* axis. H atoms have been omitted for clarity.

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$M_r = 222.28$
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
$a = 7.5794$ (8) Å
$b = 6.9736$ (6) Å
$c = 8.6879$ (12) Å
$\beta = 102.027$ (1)°
$V = 449.13$ (9) Å^3
$Z = 2$
$F(000) = 228$
$D_x = 1.644$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1437 reflections
$\theta = 2.4$–27.9°
$\mu = 0.83$ mm^{-1}

T = 298 K
Block, colourless

0.39 × 0.27 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.739, T_{max} = 0.886

2256 measured reflections
862 independent reflections
728 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°, θ_{min} = 2.4°
$h = -7 \rightarrow 9$
$k = -8 \rightarrow 8$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.064
S = 1.07
862 reflections
64 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 0.2249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Na1	0.07064 (15)	0.2500	0.93636 (13)	0.0400 (3)	
N1	0.1651 (3)	0.2500	0.4084 (3)	0.0339 (5)	
N2	0.1364 (3)	0.2500	0.6700 (2)	0.0291 (5)	
O1	0.16585 (17)	−0.0019 (2)	1.13259 (15)	0.0413 (4)	
H1A	0.1666	0.0502	1.2212	0.050*	
H1B	0.2701	−0.0493	1.1374	0.050*	
S1	0.37894 (9)	0.2500	0.51077 (9)	0.0386 (2)	
S2	−0.17326 (9)	0.2500	0.46612 (9)	0.0378 (2)	
S3	0.46031 (10)	0.2500	0.86933 (9)	0.0448 (2)	
C1	0.0626 (3)	0.2500	0.5131 (3)	0.0283 (6)	
C2	0.3165 (3)	0.2500	0.6910 (3)	0.0310 (6)	
C3	−0.2220 (4)	0.2500	0.2548 (3)	0.0470 (8)	
H3A	−0.3503	0.2500	0.2163	0.071*	
H3B	−0.1709	0.1376	0.2175	0.071*	0.50

H3C	−0.1709	0.3624	0.2175	0.071*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0488 (7)	0.0382 (7)	0.0350 (6)	0.000	0.0134 (5)	0.000
N1	0.0315 (12)	0.0391 (14)	0.0321 (13)	0.000	0.0085 (10)	0.000
N2	0.0261 (11)	0.0318 (12)	0.0302 (12)	0.000	0.0074 (9)	0.000
O1	0.0393 (8)	0.0461 (9)	0.0374 (8)	0.0029 (6)	0.0054 (6)	−0.0041 (7)
S1	0.0274 (4)	0.0514 (5)	0.0394 (4)	0.000	0.0122 (3)	0.000
S2	0.0256 (4)	0.0444 (5)	0.0423 (4)	0.000	0.0043 (3)	0.000
S3	0.0319 (4)	0.0626 (6)	0.0364 (4)	0.000	−0.0009 (3)	0.000
C1	0.0286 (13)	0.0214 (13)	0.0350 (15)	0.000	0.0067 (11)	0.000
C2	0.0280 (13)	0.0295 (15)	0.0358 (15)	0.000	0.0070 (11)	0.000
C3	0.0439 (17)	0.0468 (19)	0.0426 (18)	0.000	−0.0088 (14)	0.000

Geometric parameters (Å, º)

Na1—O1^{i}	2.4493 (16)	N2—C1	1.361 (3)
Na1—O1	2.4493 (16)	O1—Na1^{ii}	2.4736 (16)
Na1—N2	2.467 (2)	O1—H1A	0.85
Na1—O1^{ii}	2.4736 (16)	O1—H1B	0.85
Na1—O1^{iii}	2.4736 (16)	S1—C2	1.727 (3)
Na1—S3	3.1271 (14)	S2—C1	1.749 (3)
Na1—Na1^{ii}	3.8756 (10)	S2—C3	1.796 (3)
Na1—Na1^{iv}	3.8756 (10)	S3—C2	1.698 (3)
N1—C1	1.314 (3)	C3—H3A	0.96
N1—S1	1.679 (2)	C3—H3B	0.96
N2—C2	1.340 (3)	C3—H3C	0.96
O1^{i}—Na1—O1	91.62 (8)	Na1^{ii}—Na1—Na1^{iv}	128.23 (6)
O1^{i}—Na1—N2	124.42 (5)	C1—N1—S1	106.14 (18)
O1—Na1—N2	124.42 (5)	C2—N2—C1	109.3 (2)
O1^{i}—Na1—O1^{ii}	139.79 (5)	C2—N2—Na1	105.76 (16)
O1—Na1—O1^{ii}	76.14 (5)	C1—N2—Na1	144.92 (16)
N2—Na1—O1^{ii}	92.90 (6)	Na1—O1—Na1^{ii}	103.86 (5)
O1^{i}—Na1—O1^{iii}	76.14 (5)	Na1—O1—H1A	105.7
O1—Na1—O1^{iii}	139.79 (5)	Na1^{ii}—O1—H1A	112.7
N2—Na1—O1^{iii}	92.90 (6)	Na1—O1—H1B	116.7
O1^{ii}—Na1—O1^{iii}	88.79 (7)	Na1^{ii}—O1—H1B	111.0
O1^{i}—Na1—S3	88.68 (4)	H1A—O1—H1B	106.9
O1—Na1—S3	88.68 (4)	N1—S1—C2	93.66 (12)
N2—Na1—S3	56.09 (5)	C1—S2—C3	102.79 (14)
O1^{ii}—Na1—S3	128.30 (4)	C2—S3—Na1	73.65 (9)
O1^{iii}—Na1—S3	128.30 (4)	N1—C1—N2	121.0 (2)
O1^{i}—Na1—Na1^{ii}	120.36 (6)	N1—C1—S2	124.2 (2)
O1—Na1—Na1^{ii}	38.29 (3)	N2—C1—S2	114.86 (18)
N2—Na1—Na1^{ii}	112.92 (3)	N2—C2—S3	124.5 (2)

O1^{ii}—Na1—Na1^{ii}	37.85 (3)	N2—C2—S1	109.90 (19)
O1^{iii}—Na1—Na1^{ii}	117.98 (6)	S3—C2—S1	125.60 (16)
S3—Na1—Na1^{ii}	112.39 (3)	S2—C3—H3A	109.5
O1^{i}—Na1—Na1^{iv}	38.29 (3)	S2—C3—H3B	109.5
O1—Na1—Na1^{iv}	120.36 (6)	H3A—C3—H3B	109.5
N2—Na1—Na1^{iv}	112.92 (3)	S2—C3—H3C	109.5
O1^{ii}—Na1—Na1^{iv}	117.98 (6)	H3A—C3—H3C	109.5
O1^{iii}—Na1—Na1^{iv}	37.85 (4)	H3B—C3—H3C	109.5
S3—Na1—Na1^{iv}	112.39 (3)		

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