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Poly[[μ_7-L-cysteato(2−)]disodium]

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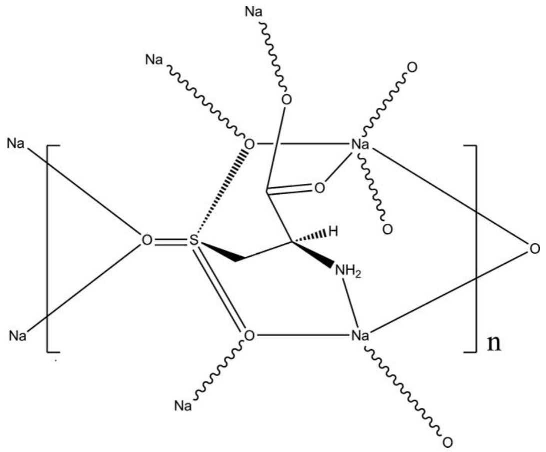
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.159; data-to-parameter ratio = 16.0.

The title compound {systematic name: poly[[μ_7-(2R)-2-amino-3-sulfonatopropanoato]disodium]}, $[Na_2(C_3H_5NO_5S)]_n$, was obtained through solvent-thermal reaction of L-cysteic acid and aqueous sodium hydroxide. The monomer consists of two Na^+ cations that are coordinated to the deprotonated amino acid. The latter acts as donor utilizing all available coordination sites, *viz.* the amino, the carboxylate and the sulfonate residues, so producing a monomeric framework in which the two coordinated Na^+ ions have different coordination spheres and geometries. One of the Na^+ ions has an O_5 coordination sphere with a typical geometric arrangement, intermediate between trigonal–bipyramidal and square–pyramidal; all the O atoms from the amino acid (three from the sulfonate and two from the caboxylate residues) act as donors. The second Na^+ ion is tetracoordinated within an NO_3 coordination sphere. The Na^+ ion binds to the amino N atom, to one of the O atom of the carboxylic residue and to two O atoms of the sulfonate group in a distorted tetrahedral arrangement. As the sulfonate O atoms bind to both Na^+ ions, a three-dimensional polymeric framework is obtained.

Related literature

For L-cysteic acid in coordination compounds, see: Hendrickson & Karle (1971); Ramanadham *et al.* (1973). For metal-organic frameworks of L-Cysteic acid, see: Bharadwaj *et al.* (1985); Riley *et al.* (2002); Huang *et al.* (2009).



Experimental

Crystal data

$[Na_2(C_3H_5NO_5S)]$
M_r = 213.13
Monoclinic, $P2_1/c$
a = 5.7574 (12) Å
b = 11.875 (2) Å
c = 11.691 (3) Å
β = 109.15 (3)°
V = 755.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 298 K
0.24 × 0.22 × 0.20 mm

Data collection

Rigaku SCX-MINI diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.885, T_{max} = 0.903
7845 measured reflections
1740 independent reflections
1463 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.159
S = 1.06
1740 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O1	2.478 (3)	Na2—N1	2.976 (5)
Na1—O2^{i}	2.427 (3)	Na2—O3^{iv}	2.905 (5)
Na1—O3	2.415 (4)	Na2—O4	3.028 (5)
Na1—O4^{ii}	2.351 (4)	Na2—O5^{iii}	2.922 (5)
Na1—O5^{iii}	2.364 (3)		

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2024).

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supplementary materials

Acta Cryst. (2011). E**67**, m1346-m1347 [**doi:10.1107/S1600536811035525**]

Poly[[μ_7-L-cysteato(2-)]disodium]

F.-H. Liu

Comment

Amino acids are of interest in coordination chemistry because they have a large number of highly flexible derivatives capable of forming a wide range of metal compexes. Recently, L-Cysteic acid, (Hendrickson *et al.*, 1971), (Ramanadham *et al.* 1973) has become an important ligand in the coordination and construction of metal-organic frameworks (MOFs), as a result, some of these frameworks with unusual topologies have been reported by (Bharadwaj *et al.*, 1985, Riley *et al.*, 2002, and Huang *et al.* 2009). As a part of our work in amino acid coordination research we chose L-Cysteic acid as our ligand. The title compound has recently been prepared in our laboratory and its structure is reported here.

The molecular structure of $[C_3H_5NNa_2O_5S]_n$ is presented in Fig.1**a-c.** Fig.1**a** shows that two Na^+ cations are coordinated to one L-Cysteic acid while Fig.1**b** shows the μ7 connectivity of each L-Cysteic acid. Each L-Cysteic acid chelates one Na^+ cation with its O-donor of sulfonate group and of the carboxylate one, and chelates the other Na^+ cation with another O-donor from the same sulfonate group and the amine N-donor. Fig.1**c** shows the coordination environment of the two Na^+ cations: for Na1 it is five coordinated while for Na2 forms a 4 coordinated Na node. Moreover, Na1 and Na2 are bridged by one O atom from sulfonyl group. In conclusion, the Na cation and the L-Cysteic acid ligand construct a three-dimensional frameword with space group P21/c, Fig.2.

Experimental

The title complex was synthesized through solvent-thermal reaction by L-Cysteic acid with NaOH aqueous as following method: 84.58 mg (0.5 mmol) of L-Cysteic acid, 10 mL 0.5% NaOH aqueous, were added to a 20 ml Teflon vessel. The vessel was sealed and placed inside a stainless steel autoclave, which was kept at 140°C for 72 h. Then the crystal suiting for X-ray single-crystal analysis was obtained.

Refinement

H atoms bonded to N atom were located in a difference map and refined with distance restraints of N—H = 0.899–0.900 Å, and with $U_{\rm iso}$(H) = 1.2Ueq(N). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.970–0.981 Å and with $U_{\rm iso}$(H) = 1.2 times $U_{\rm eq}$(C).

Figures

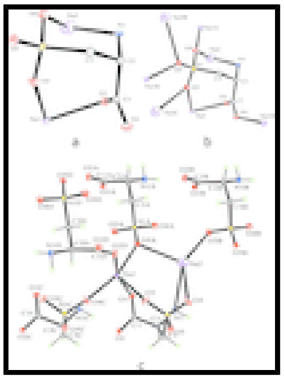


Fig. 1. The *ORTEP-3* view of the title complex with atom labels and 50% probability displacement ellipsoids for non-H atoms. **a**. The asymmetric unit of the title complex. **b**. The μ7 connectivity of each L-Cysteic acid. Other Na^+ cations are hidden for breifness. **c**. The coordination mode for Na1 and Na2. The other L-Cysteic acid is hidden for breifness.

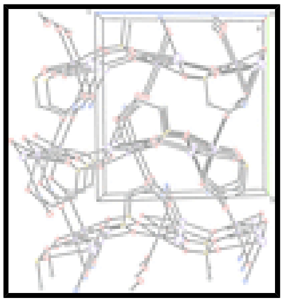


Fig. 2. The 2x2x2 packing view of the title complex, viewed down the *a* axis for non-H atoms.

poly[[μ$_7$-(2*R*)-2-amino-3-sulfonatopropanoato]disodium]

Crystal data

$[Na_2(C_3H_5NO_5S)]$	$F(000) = 432$
$M_r = 213.13$	$D_x = 1.875$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 7309 reflections
$a = 5.7574$ (12) Å	$\theta = 3.4$–$27.5°$
$b = 11.875$ (2) Å	$\mu = 0.52$ mm^{-1}
$c = 11.691$ (3) Å	$T = 298$ K
$\beta = 109.15$ (3)°	Prism, colourless
$V = 755.1$ (3) Å^3	0.24 × 0.22 × 0.20 mm
$Z = 4$	

Data collection

Rigaku SCX-MINI diffractometer	1740 independent reflections
Radiation source: fine-focus sealed tube, Rigaku SCX-MINI	1463 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.044$
ω scans	$\theta_{\rm max} = 27.5°$, $\theta_{\rm min} = 3.4°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -7\rightarrow7$

$T_{\min} = 0.885$, $T_{\max} = 0.903$	$k = -15 \rightarrow 15$
7845 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.060$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.159$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 2.942P]$ where $P = (F_o^2 + 2F_c^2)/3$
1740 reflections	$(\Delta/\sigma)_{\max} < 0.001$
109 parameters	$\Delta\rho_{\max} = 0.82$ e Å^{-3}
0 restraints	$\Delta\rho_{\min} = -0.94$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Na2	0.8052 (6)	0.7652 (3)	0.4635 (3)	0.0831 (9)
Na1	0.0476 (3)	0.74867 (13)	0.32535 (13)	0.0217 (4)
C1	0.2111 (7)	1.0060 (3)	0.3139 (3)	0.0182 (7)
C2	0.4308 (6)	1.0333 (3)	0.2716 (3)	0.0172 (7)
H2	0.4404	1.1156	0.2680	0.021*
C3	0.3963 (7)	0.9894 (3)	0.1434 (3)	0.0193 (7)
H3A	0.5202	1.0242	0.1154	0.023*
H3B	0.2372	1.0147	0.0904	0.023*
N1	0.6663 (6)	0.9944 (3)	0.3610 (3)	0.0220 (7)
H1A	0.7827	1.0134	0.3287	0.026*
H1B	0.6904	1.0396	0.4257	0.026*
O1	0.2379 (5)	0.9342 (2)	0.3959 (2)	0.0237 (6)
O2	0.0199 (5)	1.0610 (2)	0.2616 (3)	0.0286 (7)
O3	0.2320 (6)	0.7884 (3)	0.1716 (3)	0.0304 (7)
O4	0.6639 (5)	0.8093 (2)	0.1942 (3)	0.0293 (7)
O5	0.3581 (5)	0.8235 (2)	−0.0035 (2)	0.0246 (6)

S1	0.41314 (16)	0.84073 (7)	0.12588 (8)	0.0166 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na2	0.081 (2)	0.097 (2)	0.0771 (19)	0.0052 (17)	0.0339 (16)	0.0134 (17)
Na1	0.0211 (8)	0.0228 (8)	0.0202 (8)	0.0001 (6)	0.0056 (6)	0.0015 (6)
C1	0.0185 (17)	0.0158 (17)	0.0214 (18)	−0.0033 (14)	0.0080 (14)	−0.0051 (14)
C2	0.0168 (16)	0.0161 (17)	0.0210 (17)	0.0001 (13)	0.0095 (14)	0.0002 (13)
C3	0.0240 (18)	0.0179 (17)	0.0187 (17)	0.0005 (14)	0.0104 (15)	0.0002 (14)
N1	0.0144 (14)	0.0333 (18)	0.0184 (15)	−0.0015 (13)	0.0054 (12)	−0.0058 (13)
O1	0.0263 (14)	0.0257 (14)	0.0208 (13)	−0.0038 (11)	0.0102 (11)	0.0012 (11)
O2	0.0187 (13)	0.0296 (15)	0.0399 (17)	0.0049 (11)	0.0128 (12)	0.0082 (13)
O3	0.0358 (17)	0.0297 (16)	0.0319 (16)	−0.0108 (13)	0.0195 (14)	−0.0023 (13)
O4	0.0251 (15)	0.0282 (15)	0.0276 (15)	0.0067 (12)	−0.0010 (12)	−0.0012 (12)
O5	0.0268 (14)	0.0298 (15)	0.0180 (13)	−0.0052 (11)	0.0084 (11)	−0.0049 (11)
S1	0.0180 (4)	0.0170 (4)	0.0151 (4)	−0.0012 (3)	0.0059 (3)	−0.0006 (3)

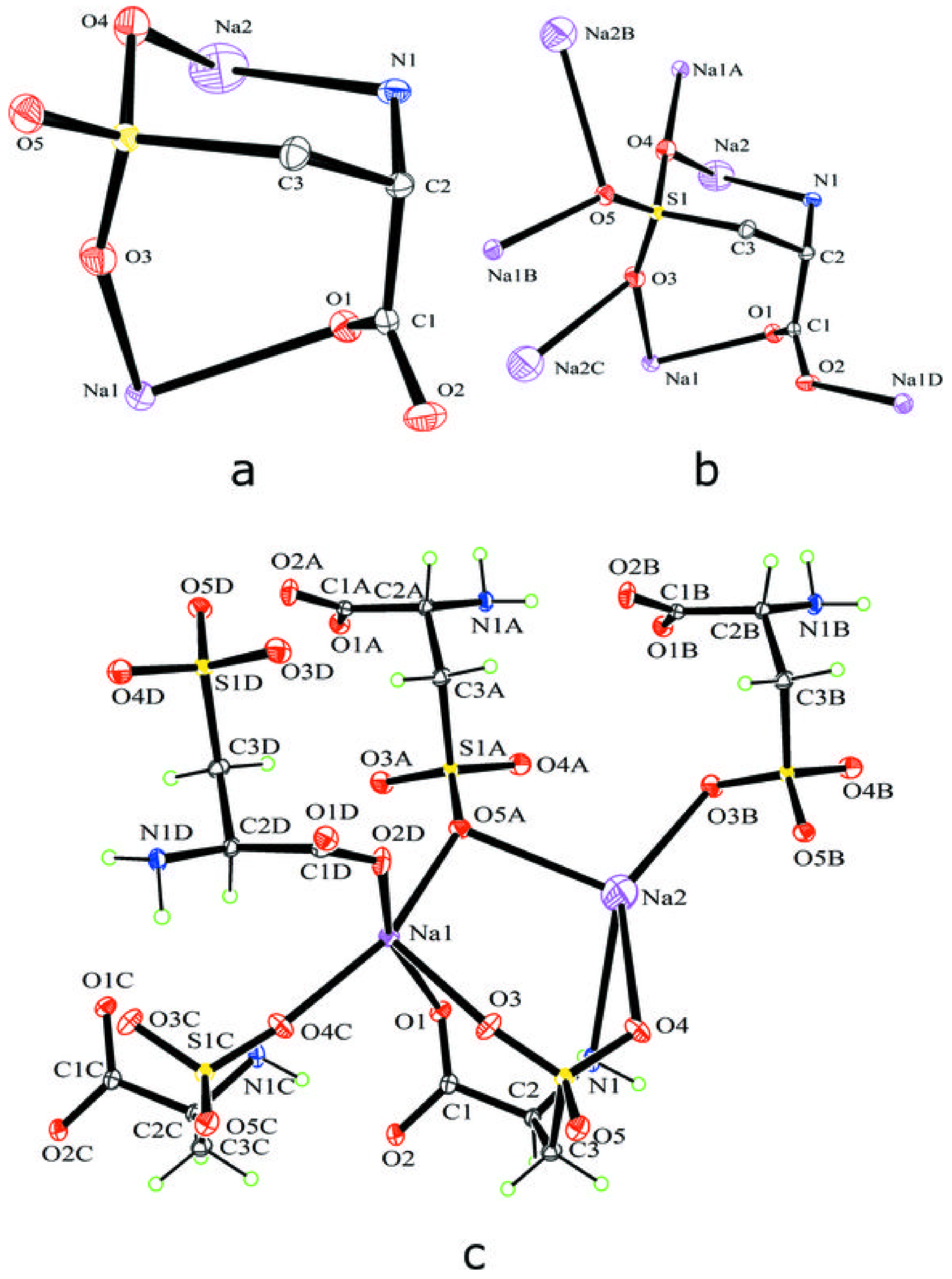
Geometric parameters (Å, °)

Na1—O1	2.478 (3)	C2—N1	1.488 (5)
Na1—O2^{i}	2.427 (3)	C2—C3	1.538 (5)
Na1—O3	2.415 (4)	C2—H2	0.9800
Na1—O4^{ii}	2.351 (4)	C3—S1	1.783 (4)
Na1—O5^{iii}	2.364 (3)	C3—H3A	0.9700
Na2—N1	2.976 (5)	C3—H3B	0.9700
Na2—O3^{iv}	2.905 (5)	N1—H1A	0.9000
Na2—O4	3.028 (5)	N1—H1B	0.9000
Na2—O5^{iii}	2.922 (5)	O3—S1	1.457 (3)
C1—O2	1.253 (5)	O4—S1	1.451 (3)
C1—O1	1.254 (5)	O5—S1	1.455 (3)
C1—C2	1.537 (5)		
O1—Na1—O5^{iii}	84.93 (10)	C1—C2—H2	106.7
O1—Na1—O3	79.62 (12)	C3—C2—H2	106.7
O3—Na1—O4^{ii}	90.18 (13)	C2—C3—S1	117.0 (3)
O4^{ii}—Na1—O5^{iii}	162.00 (13)	C2—C3—H3A	108.1
O3^{iv}—Na2—N1	125.41 (16)	S1—C3—H3A	108.1
O3^{iv}—Na2—O4	140.68 (16)	C2—C3—H3B	108.1
O3^{iv}—Na2—O5^{iii}	110.50 (14)	S1—C3—H3B	108.1
O4—Na2—N1	58.54 (11)	H3A—C3—H3B	107.3
O4—Na2—O5^{iii}	104.59 (13)	C2—N1—H1A	105.0
O5^{iii}—Na2—N1	104.53 (14)	C2—N1—H1B	105.0
O2—C1—O1	126.6 (3)	H1A—N1—H1B	105.9
O2—C1—C2	114.6 (3)	O4—S1—O5	111.96 (17)
O1—C1—C2	118.8 (3)	O4—S1—O3	113.02 (19)
N1—C2—C1	111.4 (3)	O5—S1—O3	112.53 (17)

N1—C2—C3	112.1 (3)	O4—S1—C3	105.86 (18)
C1—C2—C3	112.7 (3)	O5—S1—C3	104.89 (17)
N1—C2—H2	106.7	O3—S1—C3	107.93 (17)

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*−1, *y*, *z*; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) *x*+1, −*y*+3/2, *z*+1/2.

Fig. 1


O4
Na2
N1
O5
C3
C2
O3
O1
C1
Na1
O2
a
Na2B
Na1A
O4
Na2
N1
S1
O5
C3
C2
Na1B
O3
O1
C1
Na2C
Na1
O2
Na1D
b
O2A
C1A
C2A
N1A
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O5D
O3D
S1D
O4D
O2B
C1B
C2B
N1B
O1B
C3A
C3B
C3D
S1A
O3A
O4A
O5A
O4B
O3B
O5B
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O1D
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O3C
S1C
O4C
O1
O3
O4
N1C
C1C
C2
N1
C1
C2C
O5C
C3C
O5
C3
O2C
O2
c

Fig. 2