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A redetermination of the structure of poly[[μ_4-(*R*)-2-ammonio-3-sulfonato-propanoato]aquasodium], originally reported as poly[[μ_7-L-cysteato(2−)]-disodium]

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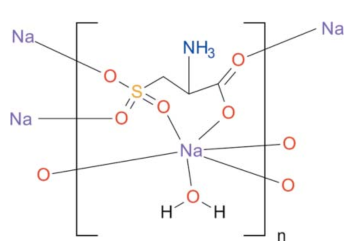
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.087; data-to-parameter ratio = 14.7.

The structure originally reported as poly[[μ_7-L-cysteato(2−)]-disodium], $[Na_2(C_3H_5NO_5S)]_n$ [Liu (2002). *Acta Cryst*. E**67**, m1346–m1347], has been redetermined with one of the sodium atoms replaced with a water molecule and an additional proton attached to the amine group, resulting in the revised formula $[Na\{CO_2CH(CH_2SO_3)NH_3\}(H_2O)]_n$. The agreement index, wR, has been reduced from 0.159 to 0.087 and the global instability index from 0.56 vu (valence units) to the acceptable value of 0.11 vu.

Related literature

The original structure determination of this compound was reported by Liu (2011). The bond-valence methods are described in Brown (2002).



Experimental

Crystal data

$[Na(C_3H_6NO_5S)(H_2O)]$
M_r = 209.15
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 = 0.48 mm^{-1}
T = 298 K
0.24 × 0.22 × 0.20 mm

Data collection

Rigaku SCX-Mini CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.894, T_{max} = 0.911
7845 measured reflections
1740 independent reflections
1463 reflections with $I > 2\Sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.087
S = 1.10
1740 reflections
118 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O4^{i}	2.3512 (19)	Na1—O2^{iii}	2.4272 (19)
Na1—O5^{ii}	2.3619 (19)	Na1—O1*W*	2.450 (2)
Na1—O3	2.4183 (18)	Na1—O1	2.4778 (18)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1*W*^{iv}	0.89	2.16	2.981 (3)	153
N1—H1*B*···O1^{v}	0.89	1.97	2.842 (2)	166
N1—H1*C*···O2^{iv}	0.89	1.88	2.766 (2)	173
O1*W*—H1*WA*···O3^{ii}	0.85 (1)	2.10 (1)	2.912 (3)	160 (4)
O1*W*—H1*WB*···O5^{vi}	0.85 (1)	2.08 (1)	2.930 (2)	178 (3)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); method used to solve structure: coordinates taken from the previous refinement (Liu, 2011); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

I wish to thank Dr Liu for supplying the original diffraction measurements through the editorial office of the journal.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5205).

References

Brown, I. D. (2002). *The Chemical Bond in Inorganic Chemistry, The Bond Valence Model*, IUCr Monographs on Crystallography 12, p. 166. Oxford University Press.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Liu, F.-H. (2011). *Acta Cryst.* E**67**, m1346–m1347.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2012). E**68**, m393   [https://doi.org/10.1107/S1600536812009683]

A redetermination of the structure of poly[[μ_4-(*R*)-2-ammonio-3-sulfonato-propanoato]aquasodium], originally reported as poly[[μ_7-L-cysteato(2−)]disodium]

I. David Brown

S1. Comment

In a recent issue of this journal, Liu (2011) reported the structure of the title compound, but a close examination of this structure shows a serious problem with the environment of one of the sodium atoms, Na2. In the Comment the author describes this atom as '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'. The Comment does not point out that the atomic displacement parameter of Na2 is almost three times larger than the next largest atomic displacement parameter, nor does it point out that the lengths of the four bonds around Na2 all lie in the range 2.90 to 3.03 Å, distances whose bond valence sum of 0.21 vu (valence unit) indicates that they are much longer than would be expected for a four-coordinate sodium cation. The global instability index [root mean square deviation of the bond valence sums of all atoms from their atomic valence, (Brown, 2002)] is 0.56 vu, much higher than the generally accepted limit of 0.20 vu for a stable structure. The environment of Na2 is, however, one that would be expected for a water molecule that forms moderate to weak hydrogen bonds. An additional hydrogen ion is required for charge neutrality, but protonating the water molecule is unlikely as this would require much shorter hydrogen bonds than are observed for this site, but protonating the amine group would not only increase the bond valence sum around the nitrogen from 2.51 vu to a value closer to the expected 3.00 vu, it would also result in an N—H bond positioned to form a hydrogen bond with the water molecule.

This proposed model has been refined and is reported in this paper. The bond valence sum of 0.21 vu around the original Na2 has been replaced by a sum of 1.94 vu around the oxygen of water, and the sum around the N1 atom has been increased to 3.17 vu. Moreover, Na1 now has a meaningful octahedral environment (Fig. 1) with a Na1—O1W contact of 2.450 (2) Å instead of a Na1—Na2 contact as in the original model.

Based on the rerefinement of the structure, this crystal must be reformulated as sodium (*R*)-2-ammonium-3-sulfo-propanoate monohydrate, $Na(CO_2CH(CH_2SO_3)NH_3)(H_2O)$.

S2. Experimental

The preparation of the compound is detailed in the original report (Liu, 2011).

S3. Refinement

The structure was refined using the original diffraction measurements of Liu (2011). For re-refinement of the original model, all H atoms were removed in the first refinement cycle and the doubtful atom Na2 replaced by an O atom (O1W). All H atoms were discernible from difference maps. H atoms attached to C atoms were finally included in calculated positions using a riding model with bond lengths C—H = 0.97 or 0.98 Å and U_{iso}(H) = 1.2 times U_{eq}(C); H atoms attached to the ammonium group were constrained to bond lengths N—H = 0.89 Å with $U_{iso}(H) = 1.5$ times $U_{eq}(N)$. The water H atoms were restrained to bond lengths of 0.85 (1) Å.

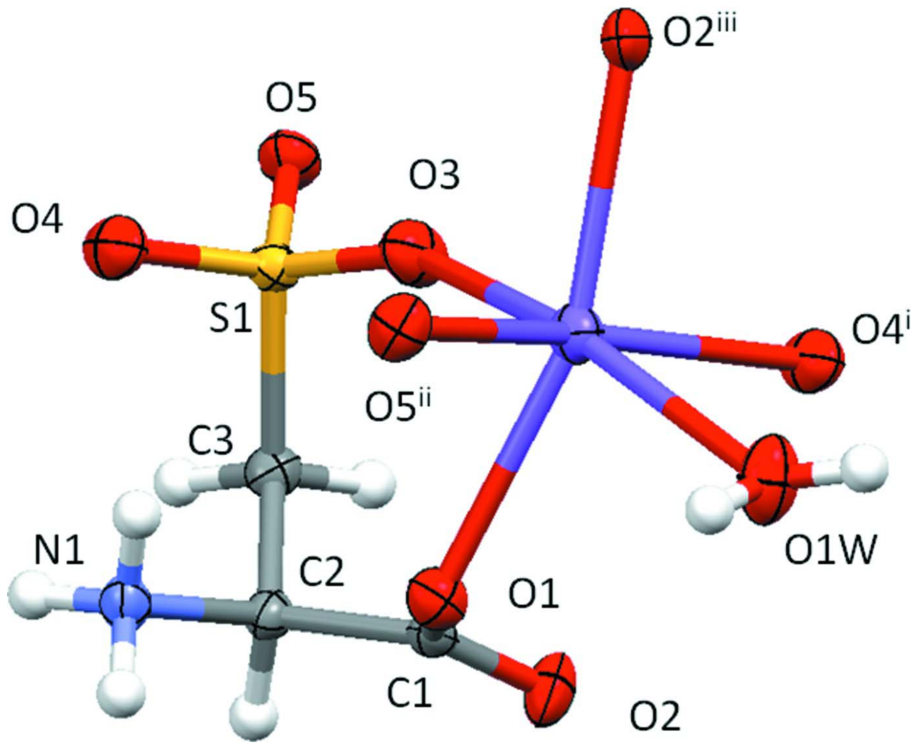


Figure 1

The environment of the Na^+ cation with atomic displacement parameters drawn at the 50% probability level. [Symmetry codes: (i) *x* - 1, *y*, *z*; (ii) *x*, -*y* + 3/2, *z* + 1/2; (iii) -*x*, *y* - 1/2, -*z* + 1/2.]

poly[[μ_4-(*R*)-2-ammonio-3-sulfonatopropanoato]aquasodium]

Crystal data

$[Na(C_3H_6NO_5S)(H_2O)]$
$M_r = 209.15$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.7574$ (12) Å
$b = 11.875$ (2) Å
$c = 11.691$ (3) Å
$\beta = 109.15$ (3)°
$V = 755.1$ (3) Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.840$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7309 reflections
$\theta = 3.4$–27.5°
$\mu = 0.48$ mm^{-1}
$T = 298$ K
Prism, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Rigaku SCX-Mini CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.894$, $T_{max} = 0.911$
7845 measured reflections
1740 independent reflections
1463 reflections with $I > 2\Sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -7 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.087$
$S = 1.10$
1740 reflections
118 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.5281P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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}
Na1	0.04743 (15)	0.74874 (7)	0.32550 (8)	0.0227 (2)
C1	0.2113 (4)	1.00587 (18)	0.31408 (19)	0.0187 (4)
C2	0.4306 (4)	1.03306 (18)	0.27159 (19)	0.0183 (4)
H2	0.4392	1.1153	0.2677	0.022*
C3	0.3962 (4)	0.98919 (18)	0.14342 (19)	0.0202 (5)
H3A	0.5201	1.0241	0.1155	0.024*
H3B	0.2371	1.0146	0.0905	0.024*
N1	0.6664 (3)	0.99540 (16)	0.36077 (16)	0.0229 (4)
H1A	0.6638	0.9210	0.3694	0.034*
H1B	0.6869	1.0284	0.4318	0.034*
H1C	0.7900	1.0143	0.3347	0.034*
O1	0.2380 (3)	0.93424 (13)	0.39576 (13)	0.0244 (4)
O2	0.0199 (3)	1.06104 (14)	0.26136 (16)	0.0294 (4)
O3	0.2321 (3)	0.78831 (14)	0.17151 (15)	0.0310 (4)
O4	0.6636 (3)	0.80928 (14)	0.19436 (15)	0.0300 (4)
O5	0.3578 (3)	0.82358 (14)	−0.00367 (13)	0.0251 (4)
S1	0.41302 (9)	0.84075 (4)	0.12587 (5)	0.01761 (15)
O1W	−0.1946 (4)	0.76543 (17)	0.46236 (17)	0.0356 (4)
H1WA	−0.090 (5)	0.759 (4)	0.5329 (15)	0.090 (15)*
H1WB	−0.326 (3)	0.740 (3)	0.471 (3)	0.058 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0214 (5)	0.0242 (5)	0.0216 (5)	0.0005 (4)	0.0058 (4)	0.0015 (4)

C1	0.0195 (11)	0.0171 (10)	0.0209 (11)	−0.0036 (9)	0.0087 (9)	−0.0060 (9)
C2	0.0178 (10)	0.0169 (10)	0.0221 (11)	0.0000 (8)	0.0091 (9)	−0.0003 (8)
C3	0.0228 (11)	0.0187 (11)	0.0209 (11)	0.0011 (9)	0.0094 (9)	0.0013 (9)
N1	0.0174 (9)	0.0297 (10)	0.0223 (10)	−0.0022 (8)	0.0073 (8)	−0.0045 (8)
O1	0.0275 (9)	0.0259 (8)	0.0216 (8)	−0.0031 (7)	0.0105 (7)	0.0012 (7)
O2	0.0195 (8)	0.0306 (9)	0.0411 (10)	0.0060 (7)	0.0139 (7)	0.0091 (8)
O3	0.0366 (10)	0.0311 (9)	0.0319 (9)	−0.0106 (8)	0.0203 (8)	−0.0026 (7)
O4	0.0256 (9)	0.0286 (9)	0.0291 (9)	0.0075 (7)	0.0000 (7)	−0.0007 (7)
O5	0.0264 (8)	0.0309 (9)	0.0184 (8)	−0.0045 (7)	0.0079 (7)	−0.0053 (6)
S1	0.0193 (3)	0.0179 (3)	0.0160 (3)	−0.0013 (2)	0.0063 (2)	−0.0006 (2)
O1W	0.0274 (10)	0.0517 (12)	0.0302 (10)	0.0023 (9)	0.0127 (9)	0.0119 (9)

Geometric parameters (Å, º)

Na1—O4^{i}	2.3512 (19)	C3—S1	1.781 (2)
Na1—O5^{ii}	2.3619 (19)	C3—H3A	0.9700
Na1—O3	2.4183 (18)	C3—H3B	0.9700
Na1—O2^{iii}	2.4272 (19)	N1—H1A	0.8900
Na1—O1W	2.450 (2)	N1—H1B	0.8900
Na1—O1	2.4778 (18)	N1—H1C	0.8900
C1—O1	1.250 (3)	O3—S1	1.4567 (16)
C1—O2	1.256 (3)	O4—S1	1.4505 (17)
C1—C2	1.535 (3)	O5—S1	1.4561 (16)
C2—N1	1.484 (3)	O1W—H1WA	0.8499 (11)
C2—C3	1.537 (3)	O1W—H1WB	0.8500 (11)
C2—H2	0.9800		
O4^{i}—Na1—O5^{ii}	162.02 (7)	C2—C3—H3A	108.1
O4^{i}—Na1—O3	90.22 (7)	S1—C3—H3A	108.1
O5^{ii}—Na1—O3	107.74 (7)	C2—C3—H3B	108.1
O4^{i}—Na1—O2^{iii}	91.21 (7)	S1—C3—H3B	108.1
O5^{ii}—Na1—O2^{iii}	89.57 (7)	H3A—C3—H3B	107.3
O3—Na1—O2^{iii}	85.17 (6)	C2—N1—H1A	109.5
O4^{i}—Na1—O1W	77.69 (7)	C2—N1—H1B	109.5
O5^{ii}—Na1—O1W	84.94 (7)	H1A—N1—H1B	109.5
O3—Na1—O1W	162.46 (7)	C2—N1—H1C	109.5
O2^{iii}—Na1—O1W	107.49 (7)	H1A—N1—H1C	109.5
O4^{i}—Na1—O1	99.41 (7)	H1B—N1—H1C	109.5
O5^{ii}—Na1—O1	85.01 (6)	C1—O1—Na1	114.94 (13)
O3—Na1—O1	79.58 (6)	C1—O2—Na1^{iv}	132.70 (14)
O2^{iii}—Na1—O1	161.39 (6)	S1—O3—Na1	153.84 (11)
O1W—Na1—O1	89.79 (7)	S1—O4—Na1^{v}	172.12 (12)
O1—C1—O2	126.7 (2)	S1—O5—Na1^{vi}	140.97 (10)
O1—C1—C2	118.85 (19)	O4—S1—O5	112.10 (10)
O2—C1—C2	114.45 (18)	O4—S1—O3	112.88 (11)
N1—C2—C1	111.67 (17)	O5—S1—O3	112.51 (10)
N1—C2—C3	112.25 (17)	O4—S1—C3	105.86 (10)
C1—C2—C3	112.80 (17)	O5—S1—C3	104.88 (10)

N1—C2—H2	106.5	O3—S1—C3	107.96 (10)
C1—C2—H2	106.5	Na1—O1W—H1WA	105 (3)
C3—C2—H2	106.5	Na1—O1W—H1WB	140 (2)
C2—C3—S1	116.96 (15)	H1WA—O1W—H1WB	103 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1*W*^{v}	0.89	2.16	2.981 (3)	153
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Poly[[μ_7-L-cysteato(2−)]disodium]

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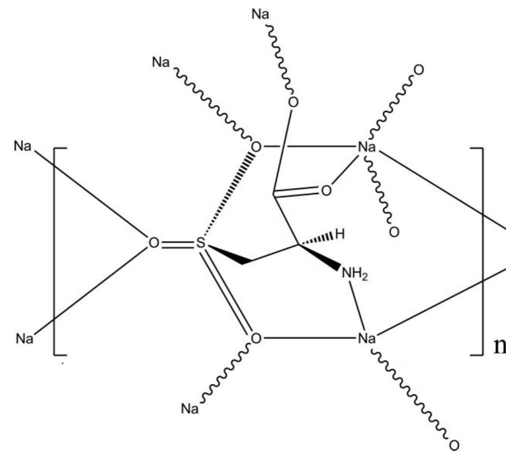
Received 25 August 2011; accepted 31 August 2011

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-(2*R*)-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).



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Rigaku SCX-MINI diffractometer
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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).

References

Bharadwaj, P. K., Cohen, B., Zhang, D., Potenza, J. A. & Schugar, H. J. (1985). *Acta Cryst.* C**41**, 1033–1035.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hendrickson, W. A. & Karle, J. (1971). *Acta Cryst.* B**27**, 427–431.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Huang, F. P., Li, H. Y., Tian, J. L., Gu, W., Jiang, Y. M., Yan, S. P. & Liao, D. Z. (2009). *Cryst. Growth Des.* **7**, 3191–3196.
Ramanadham, M., Sikka, S. K. & Chidambaram, R. (1973). *Acta Cryst.* B**29**, 1167–1170.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Riley, P. J., Reid, J. L., Cote, A. P. & Shimizu, G. K. H. (2002). *Can. J. Chem.* **80**, 1584–1591.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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Poly[[μ_7-L-cysteato(2−)]disodium]

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S1. 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.

S2. 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.

S3. 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_{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_{iso}(H) = 1.2 times U_{eq}(C).

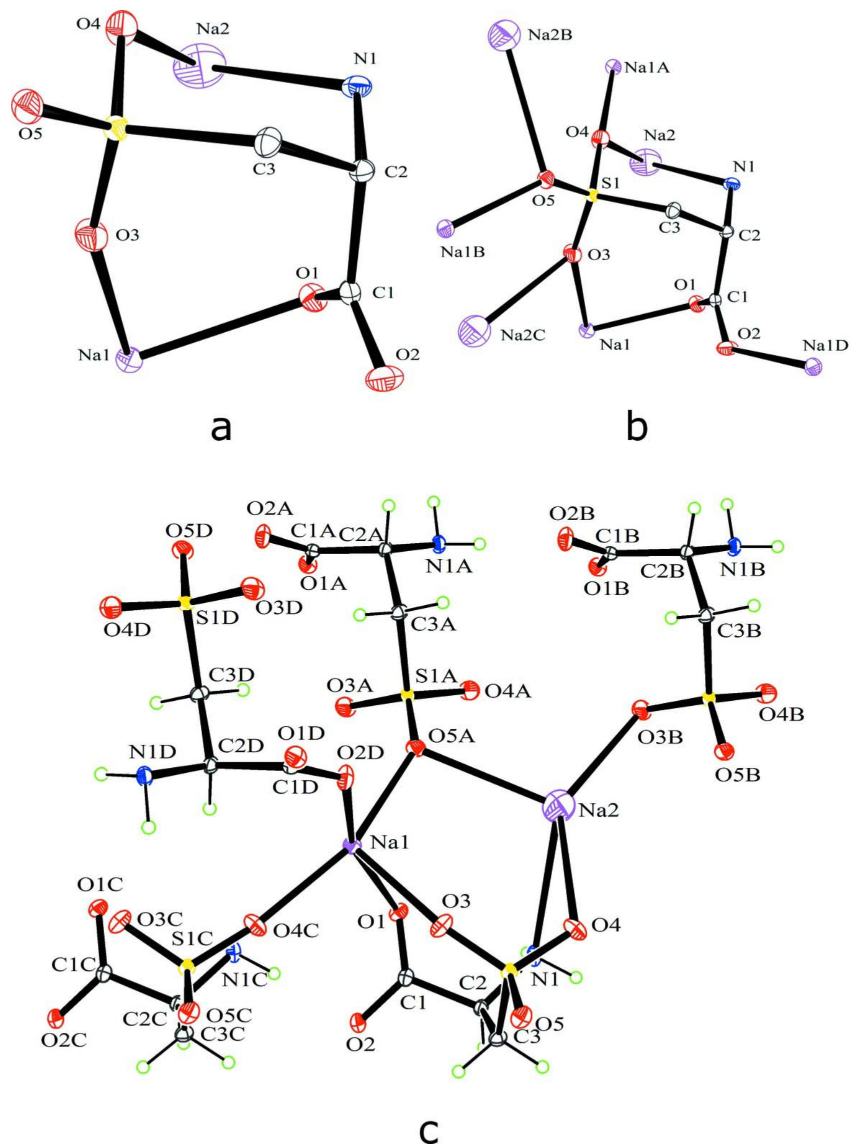

Figure 1

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.

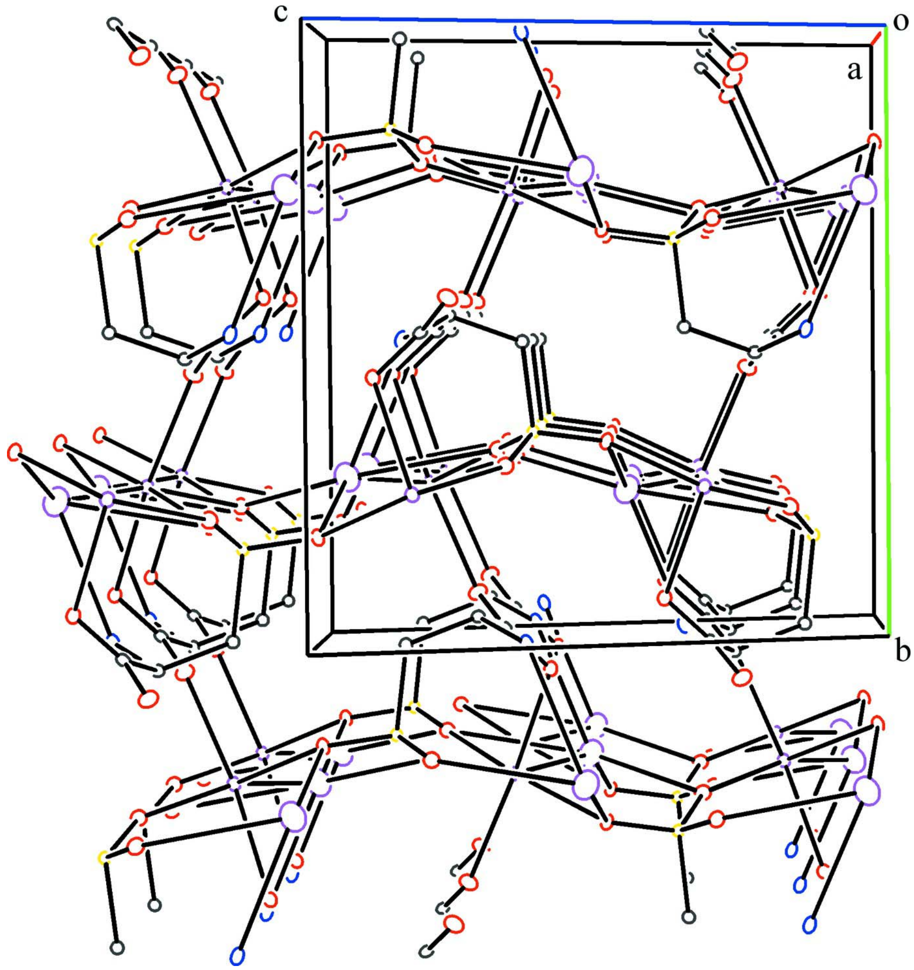

Figure 2

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

$[Na_2(C_3H_5NO_5S)]$
M_r = 213.13
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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
$F(000)$ = 432
D_x = 1.875 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7309 reflections
θ = 3.4–27.5°
μ = 0.52 mm^{-1}
T = 298 K
Prism, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Rigaku SCX-MINI diffractometer
Radiation source: fine-focus sealed tube, Rigaku SCX-MINI
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.885, T_{max} = 0.903
7845 measured reflections

1740 independent reflections
1463 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -7 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.159$
$S = 1.06$
1740 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 2.942P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ 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 (Å²)

	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, º)

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.