

Sodium 2-mercaptoethanesulfonate monohydrate (coenzyme M sodium salt monohydrate)

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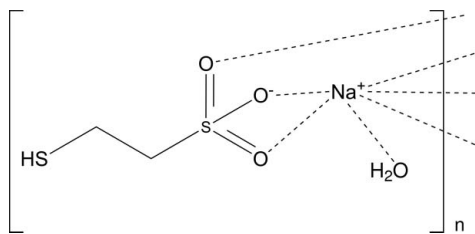
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Key indicators: single-crystal X-ray study; $T = 223$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.038; wR factor = 0.131; data-to-parameter ratio = 17.4.

The 2-thioethanesulfonate anion is the smallest known coenzyme in nature (HS-CoM) and plays a key role in methanogenesis by anaerobic archaea, as well as in the oxidation of alkenes by Gram-negative and Gram-positive eubacteria. The title compound, $\text{Na}^+\cdot\text{C}_2\text{H}_5\text{O}_3\text{S}_2^-\cdot\text{H}_2\text{O}$, is the Na^+ salt of HS-CoM crystallized as the monohydrate. Six O atoms form a distorted octahedral coordination geometry around the Na atom, at distances in the range 2.312 (4)–2.517 (3) Å. Two O atoms of the sulfonate group, one O atom of each of three other symmetry-related sulfonate groups plus the water O atom form the coordination environment of the Na^+ ion. This arrangement forms Na–O–Na layers in the crystal structure, parallel to (100).

Related literature

For related literature about HS-CoM, see: Allen *et al.* (1999); Bruchhausen *et al.* (1993); Günther & Hattendorf (2005); Graham *et al.* (2002); Latkoczy & Günther (2002); Mackay *et al.* (1999); Schramm *et al.* (1955); Thauer (1998). For the structure of the unhydrated Na HS-CoM salt, see: Bambiotti-Alberti *et al.* (2007).



Experimental

Crystal data

$\text{Na}^+\cdot\text{C}_2\text{H}_5\text{O}_3\text{S}_2^-\cdot\text{H}_2\text{O}$
 $M_r = 182.19$
 Orthorhombic, $Pna2_1$
 $a = 23.4301$ (8) Å
 $b = 5.0324$ (2) Å
 $c = 6.1254$ (2) Å
 $V = 722.24$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.74$ mm⁻¹
 $T = 223$ K
 $0.26 \times 0.20 \times 0.01$ mm

Data collection

Nonius KappaCCD diffractometer
 Absorption correction: none
 1647 measured reflections
 1534 independent reflections
 1263 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.065$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.131$
 $S = 0.95$
 1534 reflections
 88 parameters
 1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.25$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.37$ e Å⁻³
 Absolute structure: Flack (1983),
627 Friedel pairs
 Flack parameter: 0.13 (18)

Table 1

Selected bond lengths (Å).

Na9—O5 ⁱ	2.312 (4)	Na9—O6 ⁱⁱⁱ	2.416 (2)
Na9—O8 ⁱⁱ	2.322 (4)	Na9—O5	2.456 (3)
Na9—O7	2.404 (3)	Na9—O8	2.517 (3)

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

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek 2003); software used to prepare material for publication: *maXus* (Mackay *et al.*, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2190).

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supplementary materials

Acta Cryst. (2008). E64, m1476-m1477 [doi:10.1107/S1600536808031814]

Sodium 2-mercaptoethanesulfonate monohydrate (coenzyme M sodium salt monohydrate)

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Comment

The title compound includes 2-thioethanesulfonate ion, the smallest known coenzyme in nature, coenzyme M, which plays a key role in methanogenesis by anaerobic archaea (Thauer, 1998) and in the oxidation of alkenes by gram-negative and gram-positive eubacteria (Allen *et al.*, 1999). Furthermore its sodium salt (mesna) is medically used as mucolytics and to prevent urotoxic side effects of certain anticancer drugs (Bruchhausen *et al.*, 1993). Whereas the biosynthesis of coenzyme M starts by sulfitation of phosphoenolpyruvate (Graham *et al.*, 2002), the chemical synthesis begins from sodium 2-bromoethanesulfonate and thiourea in ammoniacal solution (Bruchhausen *et al.*, 1993). Since 2-thioethanesulfonic acid represents a highly viscous oil decomposing under release of hydrogen sulfide at room temperature, it is usually stored and sold as stable sodium or ammonium salt (Schramm *et al.*, 1955). The title compound is the monohydrate of the sodium salt.

Six O atoms show a distorted octahedral coordination geometry around the Na atom at distances in the range of 2.312 (4)–2.517 (3) Å (Fig. 1). Two O atoms of a SO₃ group and one O of three other SO₃ groups plus the water O atom form the coordination sphere of the Na⁺ ion. This forms Na–O–Na layers parallel to (100) in the crystal (Fig. 2).

The crystal structure of the unhydrated form (Bambagiotti-Alberti *et al.*, 2007; CSD refcode *UDUVUL*) shows a similar six-fold coordination of the Na atom where the water O atom is replaced by an O-atom of a SO₃ group. The conformation of the S atoms is *antiperiplanar* in our compound and *gauche* in the unhydrated form.

Experimental

When adding pure ethanol to a concentrated solution of 2-thioethanesulfonic acid in water, we noticed a precipitating white crystalline mass never described before in the literature. Micro elementary analysis based on the empirical formula (C₂H₈O₄S₂) of the hydrated acid (HS–CoM⁺H₃O⁺) showed significantly low values for C and H. At the same time ¹H and ¹³C NMR analysis of the precipitate in D₂O ruled out any organic impurities. Investigations into the crystals by laser ablation inductively coupled plasma sector field mass spectrometry (LA-ICP-SF MS), however, clearly revealed the presence of sodium in hyperstoichiometric amounts: molar ratio (Na-23)/(S-32) = 1.34 (RSD: 8,5%, n = 9) (Günther & Hattendorf, 2005; Latkoczy & Günther, 2002). The white precipitate consisted of two different types of crystals, needles and thin plates. The needles were used for structure analysis by X-ray diffraction.

Refinement

H-positions for the methylene CH₂ groups have been calculated with fixed distance of 1.08 Å. H atoms for the water molecule and the thiol group have been taken from a difference map and were included in the refinement in their as-found positions.

Figures

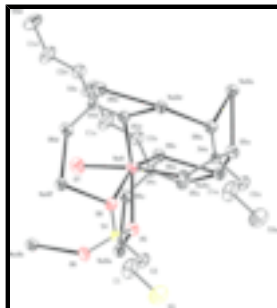


Fig. 1. The molecular structure of sodium 2-thioethanesulfonate hydrate with 50% probability displacement ellipsoids. H atoms are omitted for clarity. The complete coordination of the Na atom is shown. Symmetry codes: (a) $x, -1+y, z$; (b) $x, 1+y, z$; (c) $1/2-x, -1/2+y, -1/2+z$; (d) $1/2-x, -1/2+y, 1/2+z$; (e) $1/2-x, 1/2+y, -1/2+z$; (f) $1/2-x, 1/2+y, 1/2+z$.

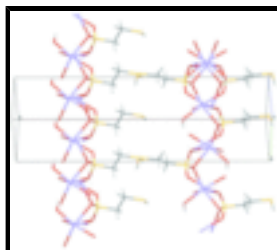
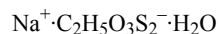


Fig. 2. Crystal structure viewed down the diagonal of the a - b axis, showing the layer structure of Na—O clusters.

sodium 2-mercaptoethanesulfonate monohydrate

Crystal data



$M_r = 182.19$

Orthorhombic, $Pna2_1$

Hall symbol: P 2c -2n

$a = 23.4301 (8) \text{ \AA}$

$b = 5.0324 (2) \text{ \AA}$

$c = 6.1254 (2) \text{ \AA}$

$V = 722.24 (4) \text{ \AA}^3$

$Z = 4$

$F_{000} = 376.0$

$D_x = 1.676 \text{ Mg m}^{-3}$

Melting point: 473 K

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5975 reflections

$\theta = 2.3\text{--}27.5^\circ$

$\mu = 0.74 \text{ mm}^{-1}$

$T = 223 \text{ K}$

Plate, colourless

$0.26 \times 0.20 \times 0.01 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer

$T = 223 \text{ K}$

CCD scans

Absorption correction: none

1647 measured reflections

1534 independent reflections

1263 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$

$\theta_{\text{max}} = 27.5^\circ$

$\theta_{\text{min}} = 3.4^\circ$

$h = -29 \rightarrow 30$

$k = -6 \rightarrow 6$

$l = -7 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
$wR(F^2) = 0.131$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{\max} < 0.001$
1534 reflections	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
88 parameters	$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 627 Friedel pairs
	Flack parameter: 0.13 (18)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S3	-0.00830 (4)	0.7465 (2)	0.8298 (4)	0.0483 (4)
H3	-0.0154	0.8542	0.6813	0.058*
S4	0.17410 (3)	0.75424 (11)	0.66676 (19)	0.0185 (2)
Na9	0.26442 (4)	0.3309 (2)	0.6658 (4)	0.0238 (3)
O5	0.19813 (10)	0.6264 (6)	0.4720 (5)	0.0239 (7)
O6	0.18238 (8)	1.0402 (4)	0.6710 (8)	0.0286 (5)
O7	0.33586 (10)	0.6737 (5)	0.6717 (8)	0.0338 (5)
H1	0.3259	0.8098	0.7595	0.023 (11)*
H2	0.3374	0.7465	0.5332	0.047 (16)*
O8	0.19475 (10)	0.6245 (6)	0.8649 (5)	0.0257 (7)
C1	0.06798 (17)	0.8051 (9)	0.8424 (9)	0.0464 (11)
H1A	0.0756	1.0166	0.8509	0.056*
H1B	0.0846	0.7169	0.9900	0.056*
C2	0.09943 (14)	0.6946 (6)	0.6517 (10)	0.0279 (8)
H2A	0.0829	0.7827	0.5039	0.033*
H2B	0.0920	0.4830	0.6431	0.033*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S3	0.0235 (5)	0.0688 (8)	0.0526 (8)	-0.0031 (4)	0.0074 (6)	0.0024 (6)
S4	0.0182 (4)	0.0178 (4)	0.0194 (4)	-0.00146 (19)	0.0008 (4)	0.0002 (7)
Na9	0.0267 (6)	0.0228 (6)	0.0219 (6)	0.0034 (4)	-0.0009 (9)	-0.0004 (10)
O5	0.0302 (16)	0.0223 (15)	0.0191 (18)	-0.0013 (11)	0.0050 (14)	-0.0031 (12)
O6	0.0325 (10)	0.0188 (10)	0.0344 (12)	-0.0029 (8)	0.0011 (17)	-0.003 (2)
O7	0.0398 (13)	0.0345 (11)	0.0271 (13)	0.0012 (10)	0.004 (2)	-0.005 (2)
O8	0.0301 (16)	0.0271 (17)	0.0197 (18)	0.0020 (12)	-0.0011 (13)	-0.0027 (14)
C1	0.0228 (17)	0.063 (3)	0.053 (3)	-0.0050 (17)	0.010 (2)	-0.013 (3)
C2	0.0182 (14)	0.0364 (16)	0.029 (2)	-0.0033 (12)	-0.001 (2)	-0.008 (2)

supplementary materials

Geometric parameters (Å, °)

S3—C1	1.813 (4)	Na9—Na9 ⁱ	4.0207 (5)
S3—H3	1.0714	Na9—Na9 ⁱⁱ	4.0207 (5)
S4—O6	1.4522 (19)	Na9—Na9 ^v	4.0207 (5)
S4—O8	1.460 (4)	O5—Na9 ^v	2.312 (4)
S4—O5	1.468 (3)	O6—Na9 ^{vi}	2.416 (2)
S4—C2	1.778 (3)	O7—H1	0.9012
S4—Na9	3.0028 (13)	O7—H2	0.9247
Na9—O5 ⁱ	2.312 (4)	O8—Na9 ^{iv}	2.322 (4)
Na9—O8 ⁱⁱ	2.322 (4)	C1—C2	1.489 (6)
Na9—O7	2.404 (3)	C1—H1A	1.0800
Na9—O6 ⁱⁱⁱ	2.416 (2)	C1—H1B	1.0800
Na9—O5	2.456 (3)	C2—H2A	1.0800
Na9—O8	2.517 (3)	C2—H2B	1.0800
Na9—Na9 ^{iv}	4.0207 (5)		
C1—S3—H3	96.1	O8—Na9—Na9 ⁱ	83.64 (8)
O6—S4—O8	112.6 (2)	S4—Na9—Na9 ⁱ	108.91 (6)
O6—S4—O5	113.4 (2)	Na9 ^{iv} —Na9—Na9 ⁱ	77.477 (11)
O8—S4—O5	110.64 (11)	O5 ⁱ —Na9—Na9 ⁱⁱ	113.78 (8)
O6—S4—C2	107.43 (13)	O8 ⁱⁱ —Na9—Na9 ⁱⁱ	35.38 (7)
O8—S4—C2	107.1 (2)	O7—Na9—Na9 ⁱⁱ	125.28 (13)
O5—S4—C2	105.2 (2)	O6 ⁱⁱⁱ —Na9—Na9 ⁱⁱ	59.83 (11)
O6—S4—Na9	127.52 (9)	O5—Na9—Na9 ⁱⁱ	84.52 (8)
O8—S4—Na9	56.70 (12)	O8—Na9—Na9 ⁱⁱ	128.86 (8)
O5—S4—Na9	54.35 (12)	S4—Na9—Na9 ⁱⁱ	109.09 (5)
C2—S4—Na9	125.01 (11)	Na9 ^{iv} —Na9—Na9 ⁱⁱ	160.65 (6)
O5 ⁱ —Na9—O8 ⁱⁱ	106.77 (8)	Na9 ⁱ —Na9—Na9 ⁱⁱ	99.226 (14)
O5 ⁱ —Na9—O7	92.45 (14)	O5 ⁱ —Na9—Na9 ^v	163.76 (8)
O8 ⁱⁱ —Na9—O7	92.65 (14)	O8 ⁱⁱ —Na9—Na9 ^v	75.20 (9)
O5 ⁱ —Na9—O6 ⁱⁱⁱ	91.25 (13)	O7—Na9—Na9 ^v	71.31 (12)
O8 ⁱⁱ —Na9—O6 ⁱⁱⁱ	93.87 (12)	O6 ⁱⁱⁱ —Na9—Na9 ^v	104.78 (10)
O7—Na9—O6 ⁱⁱⁱ	171.25 (9)	O5—Na9—Na9 ^v	31.43 (7)
O5 ⁱ —Na9—O5	154.34 (14)	O8—Na9—Na9 ^v	83.84 (8)
O8 ⁱⁱ —Na9—O5	98.49 (14)	S4—Na9—Na9 ^v	55.88 (5)
O7—Na9—O5	90.75 (11)	Na9 ^{iv} —Na9—Na9 ^v	99.226 (14)
O6 ⁱⁱⁱ —Na9—O5	82.52 (10)	Na9 ⁱ —Na9—Na9 ^v	160.65 (6)
O5 ⁱ —Na9—O8	96.56 (14)	Na9 ⁱⁱ —Na9—Na9 ^v	77.476 (11)
O8 ⁱⁱ —Na9—O8	156.12 (14)	S4—O5—Na9 ^v	127.60 (18)
O7—Na9—O8	91.32 (12)	S4—O5—Na9	96.60 (16)
O6 ⁱⁱⁱ —Na9—O8	80.38 (10)	Na9 ^v —O5—Na9	114.93 (10)

O5—Na9—O8	57.90 (7)	S4—O6—Na9 ^{vi}	134.91 (12)
O5 ⁱ —Na9—S4	125.55 (10)	Na9—O7—H1	112.0
O8 ⁱⁱ —Na9—S4	127.54 (10)	Na9—O7—H2	107.3
O7—Na9—S4	88.94 (7)	H1—O7—H2	104.9
O6 ⁱⁱⁱ —Na9—S4	82.46 (6)	S4—O8—Na9 ^{iv}	126.59 (19)
O5—Na9—S4	29.05 (8)	S4—O8—Na9	94.29 (16)
O8—Na9—S4	29.01 (8)	Na9 ^{iv} —O8—Na9	112.33 (10)
O5 ⁱ —Na9—Na9 ^{iv}	74.00 (8)	C2—C1—S3	113.2 (3)
O8 ⁱⁱ —Na9—Na9 ^{iv}	162.52 (8)	C2—C1—H1A	108.9
O7—Na9—Na9 ^{iv}	69.91 (11)	S3—C1—H1A	108.9
O6 ⁱⁱⁱ —Na9—Na9 ^{iv}	103.59 (10)	C2—C1—H1B	108.9
O5—Na9—Na9 ^{iv}	83.28 (8)	S3—C1—H1B	108.9
O8—Na9—Na9 ^{iv}	32.29 (7)	H1A—C1—H1B	107.8
S4—Na9—Na9 ^{iv}	55.67 (5)	C1—C2—S4	112.5 (3)
O5 ⁱ —Na9—Na9 ⁱ	33.64 (7)	C1—C2—H2A	109.1
O8 ⁱⁱ —Na9—Na9 ⁱ	113.20 (9)	S4—C2—H2A	109.1
O7—Na9—Na9 ⁱ	123.68 (13)	C1—C2—H2B	109.1
O6 ⁱⁱⁱ —Na9—Na9 ⁱ	58.49 (11)	S4—C2—H2B	109.1
O5—Na9—Na9 ⁱ	129.85 (9)	H2A—C2—H2B	107.8
O6—S4—Na9—O5 ⁱ	91.9 (3)	O8—Na9—O5—S4	4.61 (8)
O8—S4—Na9—O5 ⁱ	-2.37 (19)	Na9 ^{iv} —Na9—O5—S4	-16.81 (12)
O5—S4—Na9—O5 ⁱ	-174.30 (19)	Na9 ⁱ —Na9—O5—S4	50.69 (17)
C2—S4—Na9—O5 ⁱ	-90.6 (3)	Na9 ⁱⁱ —Na9—O5—S4	148.14 (13)
O6—S4—Na9—O8 ⁱⁱ	-92.9 (3)	Na9 ^v —Na9—O5—S4	-137.0 (2)
O8—S4—Na9—O8 ⁱⁱ	172.8 (2)	O5 ⁱ —Na9—O5—Na9 ^v	147.7 (2)
O5—S4—Na9—O8 ⁱⁱ	0.92 (18)	O8 ⁱⁱ —Na9—O5—Na9 ^v	-42.28 (14)
C2—S4—Na9—O8 ⁱⁱ	84.6 (3)	O7—Na9—O5—Na9 ^v	50.50 (18)
O6—S4—Na9—O7	-0.3 (3)	O6 ⁱⁱⁱ —Na9—O5—Na9 ^v	-135.11 (15)
O8—S4—Na9—O7	-94.6 (2)	O8—Na9—O5—Na9 ^v	141.6 (2)
O5—S4—Na9—O7	93.4 (2)	S4—Na9—O5—Na9 ^v	137.0 (2)
C2—S4—Na9—O7	177.2 (2)	Na9 ^{iv} —Na9—O5—Na9 ^v	120.17 (13)
O6—S4—Na9—O6 ⁱⁱⁱ	178.0 (4)	Na9 ⁱ —Na9—O5—Na9 ^v	-172.34 (6)
O8—S4—Na9—O6 ⁱⁱⁱ	83.75 (18)	Na9 ⁱⁱ —Na9—O5—Na9 ^v	-74.88 (13)
O5—S4—Na9—O6 ⁱⁱⁱ	-88.17 (17)	O8—S4—O6—Na9 ^{vi}	67.2 (4)
C2—S4—Na9—O6 ⁱⁱⁱ	-4.5 (3)	O5—S4—O6—Na9 ^{vi}	-59.3 (4)
O6—S4—Na9—O5	-93.8 (3)	C2—S4—O6—Na9 ^{vi}	-175.1 (4)
O8—S4—Na9—O5	171.92 (14)	Na9—S4—O6—Na9 ^{vi}	2.7 (5)
C2—S4—Na9—O5	83.7 (3)	O6—S4—O8—Na9 ^{iv}	1.0 (3)
O6—S4—Na9—O8	94.3 (3)	O5—S4—O8—Na9 ^{iv}	129.03 (19)
O5—S4—Na9—O8	-171.92 (14)	C2—S4—O8—Na9 ^{iv}	-116.9 (2)
C2—S4—Na9—O8	-88.2 (3)	Na9—S4—O8—Na9 ^{iv}	122.0 (2)

supplementary materials

O6—S4—Na9—Na9 ^{iv}	65.9 (3)	O6—S4—O8—Na9	-121.06 (16)
O8—S4—Na9—Na9 ^{iv}	-28.43 (14)	O5—S4—O8—Na9	7.01 (12)
O5—S4—Na9—Na9 ^{iv}	159.65 (14)	C2—S4—O8—Na9	121.08 (15)
C2—S4—Na9—Na9 ^{iv}	-116.6 (2)	O5 ⁱ —Na9—O8—S4	178.06 (16)
O6—S4—Na9—Na9 ⁱ	125.1 (3)	O8 ⁱⁱ —Na9—O8—S4	-14.1 (4)
O8—S4—Na9—Na9 ⁱ	30.82 (14)	O7—Na9—O8—S4	85.44 (17)
O5—S4—Na9—Na9 ⁱ	-141.11 (14)	O6 ⁱⁱⁱ —Na9—O8—S4	-91.78 (16)
C2—S4—Na9—Na9 ⁱ	-57.4 (2)	O5—Na9—O8—S4	-4.62 (8)
O6—S4—Na9—Na9 ⁱⁱ	-127.6 (3)	Na9 ^{iv} —Na9—O8—S4	132.6 (2)
O8—S4—Na9—Na9 ⁱⁱ	138.14 (14)	Na9 ⁱ —Na9—O8—S4	-150.81 (13)
O5—S4—Na9—Na9 ⁱⁱ	-33.78 (14)	Na9 ⁱⁱ —Na9—O8—S4	-54.07 (17)
C2—S4—Na9—Na9 ⁱⁱ	49.9 (2)	Na9 ^v —Na9—O8—S4	14.40 (12)
O6—S4—Na9—Na9 ^v	-68.3 (3)	O5 ⁱ —Na9—O8—Na9 ^{iv}	45.45 (13)
O8—S4—Na9—Na9 ^v	-162.63 (14)	O8 ⁱⁱ —Na9—O8—Na9 ^{iv}	-146.7 (2)
O5—S4—Na9—Na9 ^v	25.45 (14)	O7—Na9—O8—Na9 ^{iv}	-47.17 (17)
C2—S4—Na9—Na9 ^v	109.2 (2)	O6 ⁱⁱⁱ —Na9—O8—Na9 ^{iv}	135.61 (15)
O6—S4—O5—Na9 ^v	-8.3 (3)	O5—Na9—O8—Na9 ^{iv}	-137.2 (2)
O8—S4—O5—Na9 ^v	-135.9 (2)	S4—Na9—O8—Na9 ^{iv}	-132.6 (2)
C2—S4—O5—Na9 ^v	108.8 (2)	Na9 ⁱ —Na9—O8—Na9 ^{iv}	76.58 (13)
Na9—S4—O5—Na9 ^v	-128.7 (2)	Na9 ⁱⁱ —Na9—O8—Na9 ^{iv}	173.32 (6)
O6—S4—O5—Na9	120.40 (17)	Na9 ^v —Na9—O8—Na9 ^{iv}	-118.21 (13)
O8—S4—O5—Na9	-7.21 (12)	S3—C1—C2—S4	179.9 (2)
C2—S4—O5—Na9	-122.50 (16)	O6—S4—C2—C1	-60.6 (4)
O5 ⁱ —Na9—O5—S4	10.8 (4)	O8—S4—C2—C1	60.6 (4)
O8 ⁱⁱ —Na9—O5—S4	-179.26 (15)	O5—S4—C2—C1	178.3 (3)
O7—Na9—O5—S4	-86.47 (18)	Na9—S4—C2—C1	121.5 (3)
O6 ⁱⁱⁱ —Na9—O5—S4	87.92 (15)		

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

Fig. 1

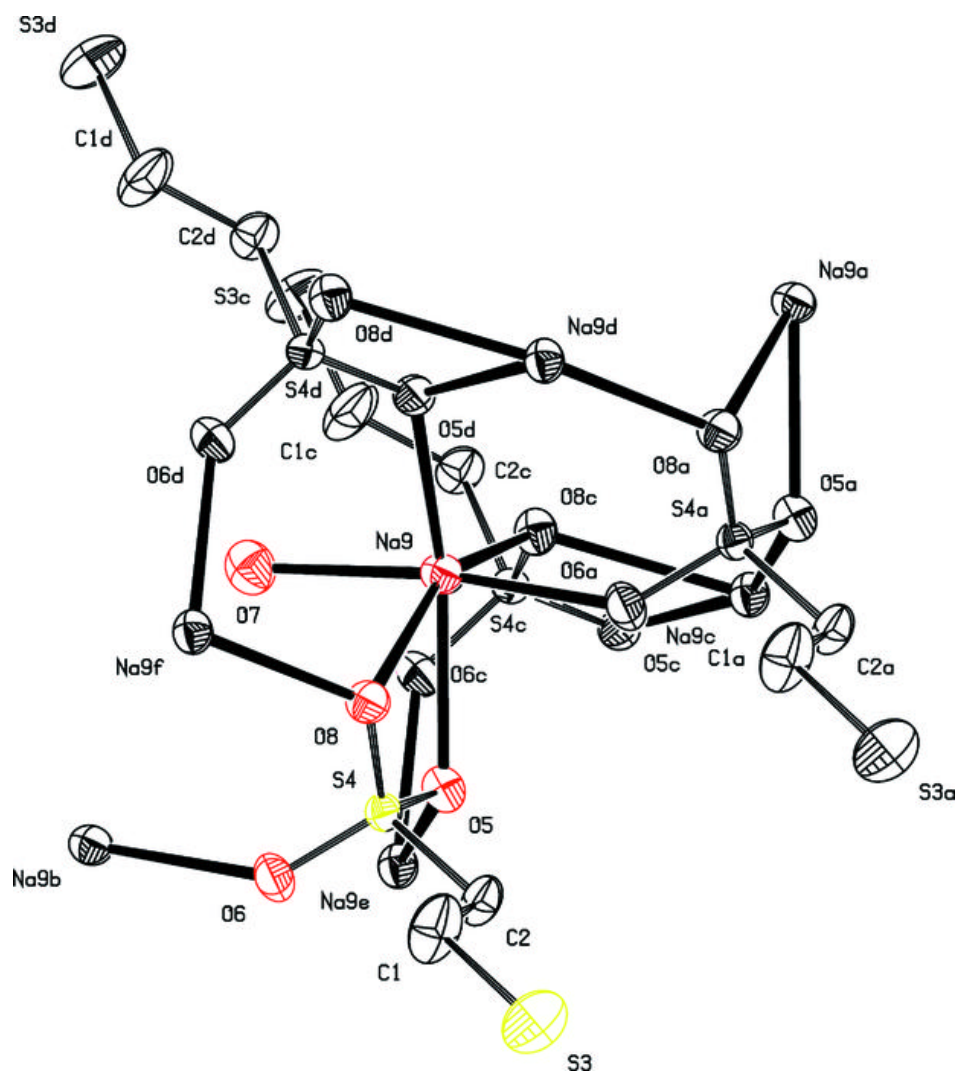


Fig. 2

