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Disodium 2,2′-dithiobis(ethanesulfonate) trihydrate (dimesna trihydrate)

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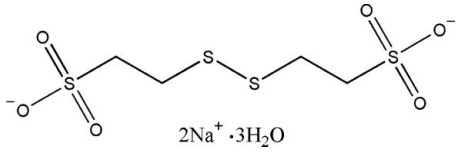
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.069; data-to-parameter ratio = 12.2.

The structure of the title compound, poly[[di-μ-aqua-μ_4-[2,2′-dithiobis(ethanesulfonato)]-disodium(I)] monohydrate], $\{[Na_2(C_4H_8O_6S_4)(H_2O)_2]\cdot H_2O\}_n$, otherwise known as dimesna trihydrate, exhibits layers formed by the anions parallel to the *ab* face, connected by layers formed by the Na^+ cations and coordinating water molecules.

Related literature

For related literature, see: Bambagiotti-Alberti *et al.* (2007); Bolte & Sakhaii (2004); Li *et al.* (2003); Ren & Zhao (2006); Verschraagen *et al.* (2004).



Experimental

Crystal data

$[Na_2(C_4H_8O_6S_4)(H_2O)_2]\cdot H_2O$
M_r = 380.37
Monoclinic, *Pa*
a = 5.7328 (2) Å
b = 10.9152 (4) Å
c = 11.2665 (4) Å
β = 97.106 (4)°
V = 699.58 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 7.22 mm^{-1}
T = 150 (2) K
0.15 × 0.10 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur PX Ultra CCD diffractometer
Absorption correction: multi-scan [*ABSPACK* from *CrysAlisPro RED* (Oxford Diffraction, 2006)]
T_{min} = 0.498, T_{max} = 1.000 (expected range = 0.347–0.697)
8713 measured reflections
2346 independent reflections
2246 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.04
2346 reflections
192 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983); 977 Friedel pairs
Flack parameter: 0.0 (4)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H72···O6	0.764 (15)	2.14 (3)	2.806 (3)	147 (6)
O7—H71···O7^{i}	0.763 (15)	2.27 (3)	2.9901 (15)	158 (6)
O8—H81···O3^{ii}	0.763 (15)	1.990 (15)	2.752 (3)	175 (4)
O8—H82···O3^{iii}	0.764 (15)	2.33 (3)	2.979 (3)	144 (4)
O9—H91···O6^{iv}	0.766 (15)	2.029 (17)	2.783 (3)	168 (4)

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

Data collection: *CrysAlisPro CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlisPro CCD*; data reduction: *CrysAlisPro RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2163).

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supplementary materials

Acta Cryst. (2007). E**63**, m1948 [**doi:10.1107/S1600536807029273**]

Disodium 2,2'-dithiobis(ethanesulfonate) trihydrate (dimesna trihydrate)

M. Bambagiotti-Alberti, G. Bartolucci, B. Bruni, M. Di Vaira and M. Passaponti

Comment

Dimesna, the disulfide readily formed from mesna (Bambagiotti-Alberti *et al.*, 2007) by oxidation (Li *et al.*, 2003), has been shown to protect against cisplatin-induced nephrotoxicity, due to its conversion in the kidneys into the monomeric mesna which, contrary to dimesna, is effective in inactivating urotoxic metabolites from cisplatin chemotherapy (Verschraagen *et al.*, 2004). On the other hand, direct use of mesna as an aid, instead of dimesna, is discouraged by owing to interference with chemotherapy.

Crystals of dimesna were obtained in the form of the trihydrate (I); the contents of the asymmetric unit are shown in Fig. 1. Corresponding bond distances in the two chemically equivalent parts of the anion are in substantial agreement, as they are with values previously found for mesna. The value of the S—S distance, 2.0338 (10) Å, agrees with values recently reported for this bond in similar environments [2.032 (1) Å (Ren & Zhao, 2006); 2.045 (1) Å (Bolte & Sakhaii, 2004)]. The S3 and S4 atoms are in antiperiplanar positions with respect to the connecting ethyl chain, whereas the S1 and S2 atoms in the other part of the anion are in an a-synclinal arrangement. In the crystal structure, the anionic portions of dimesna are arranged in layers parallel to the *ab*-face, with interposed layers formed by the cations and two of the water molecules (Fig. 2). The third water molecule (O7) occupies channels parallel to *a* in the anionic layer, forming chains of hydrogen-bonded water molecules which, in addition, are similarly linked to O atoms of sulfonate residues. The closest approach between S atoms of different anions in a layer is 3.845 (1) Å. Both Na^+ cations are six-coordinated by O atoms, four of these, in both coordination spheres, belonging to different anions, whereas two are common and are provided by the O8 and O9 water molecules. The latter water O atoms, as well as the sulfonate O1 and O5 atoms, bridge between symmetry-related cations, forming chains along *a*, whereas the O2 and O4 (also coordinating) sulfonate O atoms provide bridges between the chains. The sulfonate O3 and O6 sulfonate atoms, are not engaged in coordination to Na, but accept hydrogen bonds from water molecules.

Experimental

Samples of dimesna, in microcrystalline form, were kindly provided by SIMS (SIMS srl, Reggello Firenze, Italy). Crystals suitable for X-ray diffraction were obtained by slow evaporation from water-methanol solutions of (I).

Refinement

The structure is pseudo centrosymmetric, but its intrinsically noncentrosymmetric nature is proved by the absence of symmetry for the symmetry–independent anion in the final model. It was refined as a racemic twin (thanks are expressed to a reviewer for pointing out this possibility), with 0.52 (2) main component. Aliphatic H atoms were in geometrically generated positions, riding. Assigned values of bond distances: secondary CH_2 0.99 Å. The positional parameters of water H atoms were refined, with a common soft restraint on O—H distances (0.76 (2) Å final value). The restraints $U(H) = 1.2U_{eq}(C)$ and $U(H) = 1.5U_{eq}(O)$ on thermal parameters were applied.

Figures

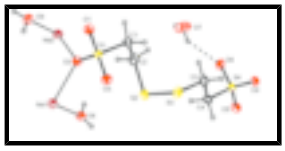

Fig. 1. A view of the contents of the asymmetric unit in (I). Displacement ellipsoids are drawn at the 50% probability level. Cordinative bonds to Na^+ ions are denoted by thin lines and a hydrogen bond by a dashed line.

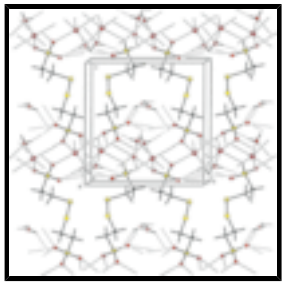

Fig. 2. A view of the crystal packing in (I), viewed along the *a* axis. Thin lines denote cordinative bonds to Na^+ ions and dashed lines represent hydrogen bonds.

poly[[di-μ-aqua-μ$_4$-[2,2'-dithiobis(ethanesulfonato)]-disodium(I)] monohydrate]

Crystal data

$[Na_2(C_4H_8O_6S_4)(H_2O)_2]\cdot H_2O$	F_{000} = 392
M_r = 380.37	D_x = 1.806 Mg m^{-3}
Monoclinic, *Pa*	Cu *K*α radiation λ = 1.54180 Å
Hall symbol: P -2ya	Cell parameters from 2793 reflections
a = 5.7328 (2) Å	θ = 11.1–44.5°
b = 10.9152 (4) Å	μ = 7.22 mm^{-1}
c = 11.2665 (4) Å	*T* = 150 (2) K
β = 97.106 (4)°	Prism, colourless
V = 699.58 (4) Å^3	0.15 × 0.10 × 0.05 mm
Z = 2	

Data collection

Oxford Diffraction Xcalibur PX Ultra CCD diffractometer	2346 independent reflections
Radiation source: fine-focus sealed tube	2246 reflections with $I > 2\sigma(I)$
Monochromator: Oxford Diffraction, Enhance ULTRA assembly	R_{int} = 0.034
T = 150(2) K	θ_{max} = 72.2°
ω scans	θ_{min} = 4.0°
Absorption correction: multi-scan [ABSPACK from CrysAlisPro RED (Oxford Diffraction, 2006)]	*h* = −7→5
T_{min} = 0.498, T_{max} = 1.000	*k* = −13→13
8713 measured reflections	*l* = −13→13

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.069$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
2346 reflections	$\Delta\rho_{min} = -0.40$ e Å^{-3}
192 parameters	Extinction correction: none
8 restraints	Absolute structure: Flack & Bernardinelli (1999); 977 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.0 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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}
S1	0.44292 (10)	0.31465 (5)	0.07585 (5)	0.01495 (15)
O1	0.5960 (4)	0.41544 (17)	0.12214 (18)	0.0202 (4)
O2	0.2687 (4)	0.28386 (18)	0.15533 (17)	0.0193 (4)
O3	0.5760 (4)	0.20872 (19)	0.04342 (18)	0.0219 (4)
C1	0.2838 (5)	0.3722 (2)	−0.0587 (2)	0.0180 (6)
H11	0.2401	0.4585	−0.0457	0.022*
H12	0.3883	0.3714	−0.1224	0.022*
C2	0.0601 (6)	0.2998 (3)	−0.1022 (3)	0.0228 (6)
H21	−0.0269	0.3449	−0.1700	0.027*
H22	−0.0405	0.2983	−0.0368	0.027*
S2	0.10126 (14)	0.14314 (6)	−0.14969 (7)	0.02739 (18)
S3	0.32883 (13)	0.15983 (7)	−0.27364 (6)	0.02457 (16)
C3	0.1429 (6)	0.2132 (3)	−0.4068 (3)	0.0211 (6)
H31	0.0754	0.2937	−0.3894	0.025*
H32	0.2414	0.2250	−0.4721	0.025*

C4	−0.0557 (5)	0.1259 (2)	−0.4490 (2)	0.0181 (6)
H41	−0.1568	0.1147	−0.3847	0.022*
H42	0.0102	0.0451	−0.4668	0.022*
S4	−0.22768 (11)	0.18324 (5)	−0.57943 (5)	0.01576 (15)
O4	−0.0636 (4)	0.21572 (19)	−0.66323 (17)	0.0189 (4)
O5	−0.3898 (4)	0.08517 (19)	−0.62452 (17)	0.0227 (5)
O6	−0.3523 (4)	0.2900 (2)	−0.53982 (18)	0.0240 (5)
Na1	0.22800 (19)	0.09442 (9)	0.25452 (9)	0.0182 (2)
Na2	−0.02409 (19)	0.40532 (10)	0.23478 (10)	0.0192 (2)
O7	−0.3003 (5)	0.4610 (2)	−0.3525 (3)	0.0491 (7)
H71	−0.423 (5)	0.473 (6)	−0.335 (5)	0.074*
H72	−0.325 (11)	0.398 (3)	−0.381 (5)	0.074*
O8	−0.0935 (4)	0.03360 (18)	0.11922 (19)	0.0198 (4)
H81	−0.184 (6)	0.084 (3)	0.102 (4)	0.030*
H82	−0.074 (7)	−0.014 (3)	0.072 (3)	0.030*
O9	0.3065 (4)	0.45846 (17)	0.3702 (2)	0.0212 (4)
H91	0.391 (6)	0.406 (3)	0.388 (4)	0.032*
H92	0.297 (7)	0.488 (3)	0.431 (2)	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0134 (3)	0.0140 (3)	0.0169 (3)	0.0005 (2)	−0.0004 (2)	0.0005 (2)
O1	0.0185 (11)	0.0191 (10)	0.0218 (10)	−0.0035 (8)	−0.0019 (8)	−0.0010 (8)
O2	0.0186 (11)	0.0204 (9)	0.0192 (10)	0.0000 (8)	0.0040 (9)	0.0006 (8)
O3	0.0204 (11)	0.0197 (9)	0.0256 (11)	0.0053 (9)	0.0032 (9)	−0.0008 (8)
C1	0.0193 (15)	0.0162 (13)	0.0172 (13)	0.0011 (10)	−0.0036 (11)	0.0001 (10)
C2	0.0181 (16)	0.0301 (15)	0.0191 (14)	−0.0019 (12)	−0.0017 (12)	−0.0032 (11)
S2	0.0381 (5)	0.0249 (3)	0.0179 (3)	−0.0104 (3)	−0.0015 (3)	−0.0007 (3)
S3	0.0230 (4)	0.0286 (3)	0.0202 (3)	0.0046 (3)	−0.0052 (3)	−0.0050 (3)
C3	0.0220 (15)	0.0237 (13)	0.0174 (14)	−0.0011 (12)	0.0011 (11)	0.0019 (11)
C4	0.0198 (15)	0.0189 (13)	0.0148 (13)	−0.0006 (11)	−0.0012 (11)	0.0028 (10)
S4	0.0148 (3)	0.0180 (3)	0.0142 (3)	0.0006 (2)	0.0007 (2)	0.0008 (2)
O4	0.0191 (11)	0.0206 (9)	0.0175 (10)	0.0018 (8)	0.0049 (8)	0.0022 (7)
O5	0.0206 (12)	0.0248 (10)	0.0208 (11)	−0.0052 (8)	−0.0045 (9)	0.0018 (7)
O6	0.0243 (12)	0.0270 (10)	0.0205 (10)	0.0105 (9)	0.0015 (9)	−0.0017 (9)
Na1	0.0159 (6)	0.0188 (5)	0.0197 (5)	0.0001 (4)	0.0012 (5)	−0.0005 (4)
Na2	0.0167 (6)	0.0177 (5)	0.0221 (6)	0.0006 (4)	−0.0014 (5)	0.0003 (4)
O7	0.0488 (17)	0.0285 (13)	0.0649 (19)	−0.0014 (12)	−0.0139 (15)	−0.0125 (12)
O8	0.0162 (10)	0.0190 (10)	0.0233 (10)	0.0021 (8)	−0.0020 (8)	0.0002 (7)
O9	0.0180 (10)	0.0216 (10)	0.0233 (10)	0.0029 (8)	0.0000 (8)	−0.0028 (8)

Geometric parameters (Å, °)

S1—O3	1.457 (2)	O4—Na1^{iii}	2.406 (2)
S1—O2	1.461 (2)	O5—Na1^{iv}	2.435 (2)
S1—O1	1.4626 (19)	O5—Na1^{v}	2.527 (2)
S1—C1	1.784 (3)	Na1—O8	2.338 (2)

O1—Na2^{i}	2.384 (2)	Na1—O8^{vi}	2.389 (2)
O1—Na2^{ii}	2.476 (2)	Na1—O4^{vii}	2.406 (2)
O2—Na1	2.376 (2)	Na1—O5^{viii}	2.435 (2)
O2—Na2	2.397 (2)	Na1—O5^{ix}	2.527 (2)
C1—C2	1.534 (4)	Na1—Na1^{x}	3.5305 (12)
C1—H11	0.9900	Na1—Na1^{vi}	3.5305 (12)
C1—H12	0.9900	Na2—O9	2.354 (2)
C2—S2	1.816 (3)	Na2—O1^{xi}	2.384 (2)
C2—H21	0.9900	Na2—O4^{vii}	2.392 (2)
C2—H22	0.9900	Na2—O9^{xii}	2.419 (2)
S2—S3	2.0338 (10)	Na2—O1^{xii}	2.476 (2)
S3—C3	1.825 (3)	Na2—Na2^{ii}	3.5339 (12)
C3—C4	1.515 (4)	Na2—Na2^{xii}	3.5339 (12)
C3—H31	0.9900	O7—H71	0.763 (15)
C3—H32	0.9900	O7—H72	0.764 (15)
C4—S4	1.779 (3)	O8—Na1^{x}	2.389 (2)
C4—H41	0.9900	O8—H81	0.763 (15)
C4—H42	0.9900	O8—H82	0.764 (15)
S4—O4	1.456 (2)	O9—Na2^{ii}	2.419 (2)
S4—O6	1.465 (2)	O9—H91	0.766 (15)
S4—O5	1.467 (2)	O9—H92	0.763 (15)
O4—Na2^{iii}	2.392 (2)		
O3—S1—O2	112.97 (12)	O8—Na1—O5^{ix}	83.66 (7)
O3—S1—O1	112.14 (12)	O2—Na1—O5^{ix}	167.79 (8)
O2—S1—O1	112.34 (12)	O8^{vi}—Na1—O5^{ix}	93.13 (8)
O3—S1—C1	107.16 (12)	O4^{vii}—Na1—O5^{ix}	88.53 (7)
O2—S1—C1	106.57 (13)	O5^{viii}—Na1—O5^{ix}	87.02 (7)
O1—S1—C1	105.04 (12)	O8—Na1—Na1^{x}	42.24 (6)
S1—O1—Na2^{i}	128.56 (12)	O2—Na1—Na1^{x}	129.43 (6)
S1—O1—Na2^{ii}	125.78 (12)	O8^{vi}—Na1—Na1^{x}	94.03 (6)
Na2^{i}—O1—Na2^{ii}	93.29 (7)	O4^{vii}—Na1—Na1^{x}	73.65 (5)
S1—O2—Na1	127.08 (12)	O5^{viii}—Na1—Na1^{x}	130.55 (6)
S1—O2—Na2	131.69 (12)	O5^{ix}—Na1—Na1^{x}	43.60 (5)
Na1—O2—Na2	101.06 (8)	O8—Na1—Na1^{vi}	114.13 (7)
C2—C1—S1	114.2 (2)	O2—Na1—Na1^{vi}	112.41 (6)
C2—C1—H11	108.7	O8^{vi}—Na1—Na1^{vi}	41.13 (6)
S1—C1—H11	108.7	O4^{vii}—Na1—Na1^{vi}	157.52 (5)
C2—C1—H12	108.7	O5^{viii}—Na1—Na1^{vi}	45.69 (5)
S1—C1—H12	108.7	O5^{ix}—Na1—Na1^{vi}	79.53 (6)
H11—C1—H12	107.6	Na1^{x}—Na1—Na1^{vi}	108.56 (5)
C1—C2—S2	116.4 (2)	O9—Na2—O1^{xi}	160.56 (8)
C1—C2—H21	108.2	O9—Na2—O4^{vii}	91.05 (8)

S2—C2—H21	108.2	O1^{xi}—Na2—O4^{vii}	99.28 (8)
C1—C2—H22	108.2	O9—Na2—O2	80.42 (8)
S2—C2—H22	108.2	O1^{xi}—Na2—O2	117.56 (8)
H21—C2—H22	107.3	O4^{vii}—Na2—O2	79.24 (7)
C2—S2—S3	103.64 (11)	O9—Na2—O9^{xii}	78.08 (7)
C3—S3—S2	103.52 (11)	O1^{xi}—Na2—O9^{xii}	84.01 (8)
C4—C3—S3	113.44 (19)	O4^{vii}—Na2—O9^{xii}	99.18 (8)
C4—C3—H31	108.9	O2—Na2—O9^{xii}	158.42 (9)
S3—C3—H31	108.9	O9—Na2—O1^{xii}	83.39 (8)
C4—C3—H32	108.9	O1^{xi}—Na2—O1^{xii}	89.09 (7)
S3—C3—H32	108.9	O4^{vii}—Na2—O1^{xii}	168.28 (9)
H31—C3—H32	107.7	O2—Na2—O1^{xii}	89.64 (7)
C3—C4—S4	110.91 (18)	O9^{xii}—Na2—O1^{xii}	89.79 (7)
C3—C4—H41	109.5	O9—Na2—Na2^{ii}	42.94 (6)
S4—C4—H41	109.5	O1^{xi}—Na2—Na2^{ii}	131.34 (6)
C3—C4—H42	109.5	O4^{vii}—Na2—Na2^{ii}	129.14 (6)
S4—C4—H42	109.5	O2—Na2—Na2^{ii}	73.63 (5)
H41—C4—H42	108.0	O9^{xii}—Na2—Na2^{ii}	91.69 (6)
O4—S4—O6	112.47 (13)	O1^{xii}—Na2—Na2^{ii}	42.33 (5)
O4—S4—O5	112.68 (12)	O9—Na2—Na2^{xii}	116.35 (6)
O6—S4—O5	111.96 (13)	O1^{xi}—Na2—Na2^{xii}	44.37 (5)
O4—S4—C4	106.54 (13)	O4^{vii}—Na2—Na2^{xii}	112.40 (6)
O6—S4—C4	105.63 (13)	O2—Na2—Na2^{xii}	158.24 (5)
O5—S4—C4	106.99 (12)	O9^{xii}—Na2—Na2^{xii}	41.53 (6)
S4—O4—Na2^{iii}	129.00 (12)	O1^{xii}—Na2—Na2^{xii}	79.32 (6)
S4—O4—Na1^{iii}	130.60 (12)	Na2^{ii}—Na2—Na2^{xii}	108.41 (6)
Na2^{iii}—O4—Na1^{iii}	100.33 (8)	H71—O7—H72	97 (6)
S4—O5—Na1^{iv}	130.65 (12)	Na1—O8—Na1^{x}	96.63 (9)
S4—O5—Na1^{v}	123.57 (13)	Na1—O8—H81	115 (3)
Na1^{iv}—O5—Na1^{v}	90.70 (7)	Na1^{x}—O8—H81	104 (3)
O8—Na1—O2	93.20 (8)	Na1—O8—H82	119 (3)
O8—Na1—O8^{vi}	77.48 (7)	Na1^{x}—O8—H82	99 (3)
O2—Na1—O8^{vi}	97.72 (8)	H81—O8—H82	118 (4)
O8—Na1—O4^{vii}	82.99 (8)	Na2—O9—Na2^{ii}	95.53 (9)
O2—Na1—O4^{vii}	79.37 (7)	Na2—O9—H91	115 (3)
O8^{vi}—Na1—O4^{vii}	160.09 (8)	Na2^{ii}—O9—H91	110 (3)
O8—Na1—O5^{viii}	159.28 (9)	Na2—O9—H92	123 (3)
O2—Na1—O5^{viii}	99.53 (8)	Na2^{ii}—O9—H92	113 (3)
O8^{vi}—Na1—O5^{viii}	84.62 (8)	H91—O9—H92	101 (4)
O4^{vii}—Na1—O5^{viii}	115.29 (8)		
O3—S1—O1—Na2^{i}	−32.55 (19)	Na2—O2—Na1—O8^{vi}	159.45 (8)

O2—S1—O1—Na2^{i}	95.97 (16)	S1—O2—Na1—O4^{vii}	175.00 (14)
C1—S1—O1—Na2^{i}	−148.59 (15)	Na2—O2—Na1—O4^{vii}	−0.59 (9)
O3—S1—O1—Na2^{ii}	−164.23 (12)	S1—O2—Na1—O5^{viii}	60.84 (16)
O2—S1—O1—Na2^{ii}	−35.72 (17)	Na2—O2—Na1—O5^{viii}	−114.75 (8)
C1—S1—O1—Na2^{ii}	79.73 (16)	S1—O2—Na1—O5^{ix}	−177.4 (3)
O3—S1—O2—Na1	9.99 (19)	Na2—O2—Na1—O5^{ix}	7.0 (4)
O1—S1—O2—Na1	−118.08 (14)	S1—O2—Na1—Na1^{x}	−126.68 (13)
C1—S1—O2—Na1	127.41 (14)	Na2—O2—Na1—Na1^{x}	57.72 (10)
O3—S1—O2—Na2	−175.80 (14)	S1—O2—Na1—Na1^{vi}	15.03 (16)
O1—S1—O2—Na2	56.13 (19)	Na2—O2—Na1—Na1^{vi}	−160.57 (5)
C1—S1—O2—Na2	−58.39 (18)	S1—O2—Na2—O9	−81.77 (16)
O3—S1—C1—C2	79.0 (2)	Na1—O2—Na2—O9	93.52 (9)
O2—S1—C1—C2	−42.2 (2)	S1—O2—Na2—O1^{xi}	90.38 (17)
O1—S1—C1—C2	−161.6 (2)	Na1—O2—Na2—O1^{xi}	−94.33 (9)
S1—C1—C2—S2	−65.8 (3)	S1—O2—Na2—O4^{vii}	−174.69 (15)
C1—C2—S2—S3	−53.8 (2)	Na1—O2—Na2—O4^{vii}	0.60 (9)
C2—S2—S3—C3	−77.94 (14)	S1—O2—Na2—O9^{xii}	−86.9 (3)
S2—S3—C3—C4	−59.4 (2)	Na1—O2—Na2—O9^{xii}	88.3 (2)
S3—C3—C4—S4	−179.55 (16)	S1—O2—Na2—O1^{xii}	1.59 (17)
C3—C4—S4—O4	50.4 (2)	Na1—O2—Na2—O1^{xii}	176.88 (8)
C3—C4—S4—O6	−69.4 (2)	S1—O2—Na2—Na2^{ii}	−38.18 (14)
C3—C4—S4—O5	171.12 (19)	Na1—O2—Na2—Na2^{ii}	137.11 (8)
O6—S4—O4—Na2^{iii}	−11.5 (2)	S1—O2—Na2—Na2^{xii}	60.6 (3)
O5—S4—O4—Na2^{iii}	116.17 (15)	Na1—O2—Na2—Na2^{xii}	−124.15 (16)
C4—S4—O4—Na2^{iii}	−126.80 (15)	O2—Na1—O8—Na1^{x}	−152.21 (8)
O6—S4—O4—Na1^{iii}	171.83 (14)	O8^{vi}—Na1—O8—Na1^{x}	110.59 (12)
O5—S4—O4—Na1^{iii}	−60.48 (19)	O4^{vii}—Na1—O8—Na1^{x}	−73.34 (7)
C4—S4—O4—Na1^{iii}	56.55 (18)	O5^{viii}—Na1—O8—Na1^{x}	79.7 (3)
O4—S4—O5—Na1^{iv}	−88.73 (18)	O5^{ix}—Na1—O8—Na1^{x}	15.95 (8)
O6—S4—O5—Na1^{iv}	39.24 (19)	Na1^{vi}—Na1—O8—Na1^{x}	91.46 (8)
C4—S4—O5—Na1^{iv}	154.52 (15)	O1^{xi}—Na2—O9—Na2^{ii}	−82.5 (3)
O4—S4—O5—Na1^{v}	37.37 (16)	O4^{vii}—Na2—O9—Na2^{ii}	155.11 (8)
O6—S4—O5—Na1^{v}	165.33 (12)	O2—Na2—O9—Na2^{ii}	76.21 (7)
C4—S4—O5—Na1^{v}	−79.39 (16)	O9^{xii}—Na2—O9—Na2^{ii}	−105.73 (11)
S1—O2—Na1—O8	−102.75 (15)	O1^{xii}—Na2—O9—Na2^{ii}	−14.54 (7)
Na2—O2—Na1—O8	81.66 (9)	Na2^{xii}—Na2—O9—Na2^{ii}	−89.14 (8)
S1—O2—Na1—O8^{vi}	−24.95 (16)		

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1/2, −*y*+1, *z*; (iii) *x*, *y*, *z*−1; (iv) *x*−1, *y*, *z*−1; (v) *x*−1/2, −*y*, *z*−1; (vi) *x*+1/2, −*y*, *z*; (vii) *x*, *y*, *z*+1; (viii) *x*+1, *y*, *z*+1; (ix) *x*+1/2, −*y*, *z*+1; (x) *x*−1/2, −*y*, *z*; (xi) *x*−1, *y*, *z*; (xii) *x*−1/2, −*y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H72···O6	0.764 (15)	2.14 (3)	2.806 (3)	147 (6)
O7—H71···O7^{xii}	0.763 (15)	2.27 (3)	2.9901 (15)	158 (6)
O8—H81···O3^{xi}	0.763 (15)	1.990 (15)	2.752 (3)	175 (4)
O8—H82···O3^{x}	0.764 (15)	2.33 (3)	2.979 (3)	144 (4)
O9—H91···O6^{viii}	0.766 (15)	2.029 (17)	2.783 (3)	168 (4)

Symmetry codes: (xii) $x-1/2, -y+1, z$; (xi) $x-1, y, z$; (x) $x-1/2, -y, z$; (viii) $x+1, y, z+1$.

Fig. 1

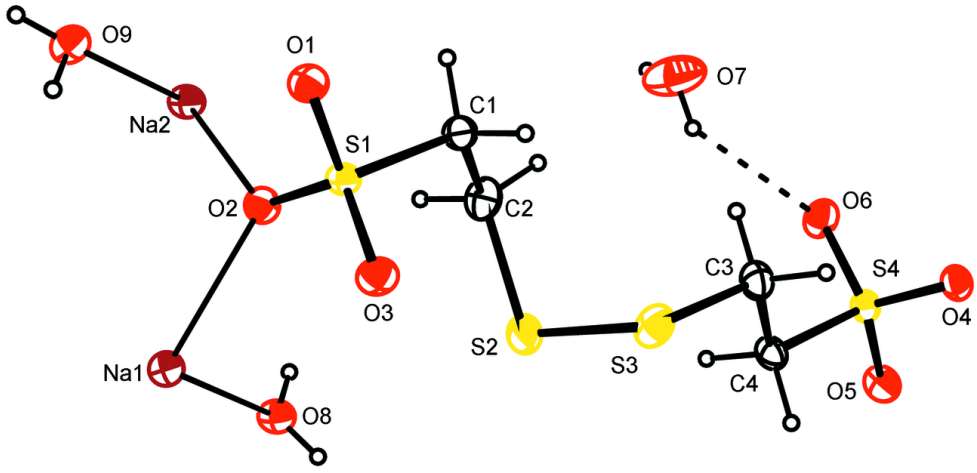

Fig. 2