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# Poly[$\mu_2$-aqua-aqua[$\mu_3$-*N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamato-$\kappa^3O,O':S$]sodium]

**Muzzaffar A. Bhat,[a] Shalini Jain,[a] Sanjay K. Srivastava,[a] Ray J. Butcher[b]* and Jan Wikaira[c]**

[a]School of Studies in Chemistry, Jiwaji University, Gwalior 474 011, India, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, and [c]Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch, New Zealand. *Correspondence e-mail: rbutcher99@yahoo.com

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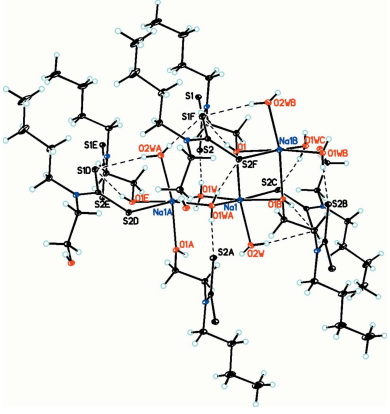
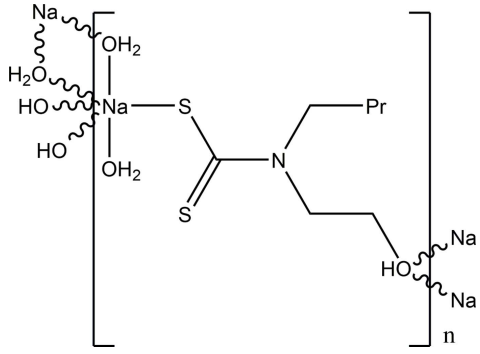
In the title compound, $[Na(C_7H_{14}NOS_2)(H_2O)_2]_n$, the $Na^I$ cation is coordinated by five O atoms [Na—O = 2.3142 (11)–2.4677 (10) Å] from three aqua and two *N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamate (*L*) ligands and one S atom [Na—S = 3.0074 (6) Å] from a third *L* ligand in a highly distorted octahedral geometry. Two aqua ligands related by an inversion center bridge two $Na^I$ cations, and each *L* ligand coordinates three $Na^I$ cations, leading to a layered arrangement aligned parallel to the *bc* plane. Intermolecular O—H···S hydrogen bonds are observed in the inner part of each polymeric layer; these are packed along the *a* axis and held together by weak van der Waals forces.

## 1. Chemical context

Dithiocarbamates have recently drawn more attention due to their application in group-transfer radical cyclization reactions (Grainger & Innocenti, 2007) and as ligands for chelating metals (Greenwood & Earnshaw, 1997). In recent years, their applications have not only become apparent as pesticides and fungicides, but they have also been widely used as vulcanization accelerators in the rubber industry (Svetlik *et al.*, 1955). Dithiocarbamates are also of biological importance due to their anticancer, antibacterial, antituberculosis and antifungal properties (Li *et al.*, 2015; Sim *et al.*, 2014; Chauhan *et al.*, 2012; Byrne *et al.*, 2007). Their anti-oxidant properties make them even more valuable compounds. As part of our investigations on organotindithio complexes (Srivastava *et al.*, 2007), we herein report the synthesis and structure of the title compound.






## 2. Structural commentary

The title compound is a two-dimensional polymer with formula $[Na(\mu_3\text{-}C_7H_{14}NOS_2)(\mu_2\text{-}H_2O)(H_2O)]$. Within this

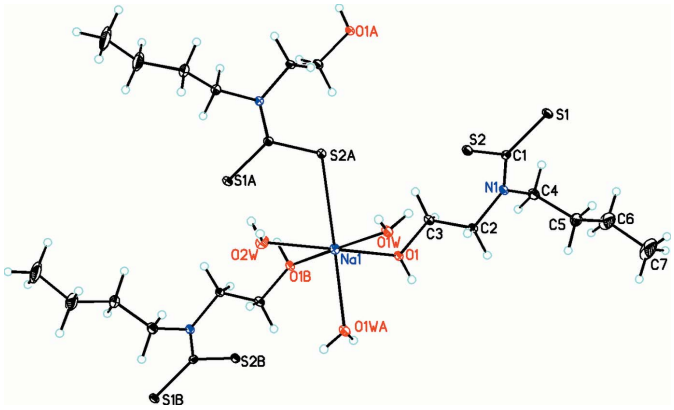



**Figure 1**
A portion of the title crystal structure showing the coordination environment for the $Na^{I}$ cation and the atomic labels [symmetry codes: (A) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (B) $1-x, -y, 1-z$]. Displacement ellipsoids are drawn at the 30% probability level.

polymer, each $Na^{I}$ ion exhibits a distorted octahedral geometry (Fig. 1) made up from coordination by the S atom of one *N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamate (*L*) anion, two hydroxy O atoms from two *L* ligands and three aqua ligands, of which two aqua ligands form bridging units between two $Na^{I}$ cations. The dithiocarbamate anion acts as a triply bridging ligand, where one S atom coordinates one sodium atom and the $O_{hydroxy}$ atom coordinates two sodium atoms (Fig. 2). The aforementioned feature of multiple coordination modes leads to the formation of polymeric layers parallel to the *bc* plane with the hydrophobic butyl arms protruding up and down. In the *L* ligand, while the two S atoms are not chemically equivalent as only one is involved in bonding to the Na cation, the C—S bond lengths are identical at 1.726 (1) Å.

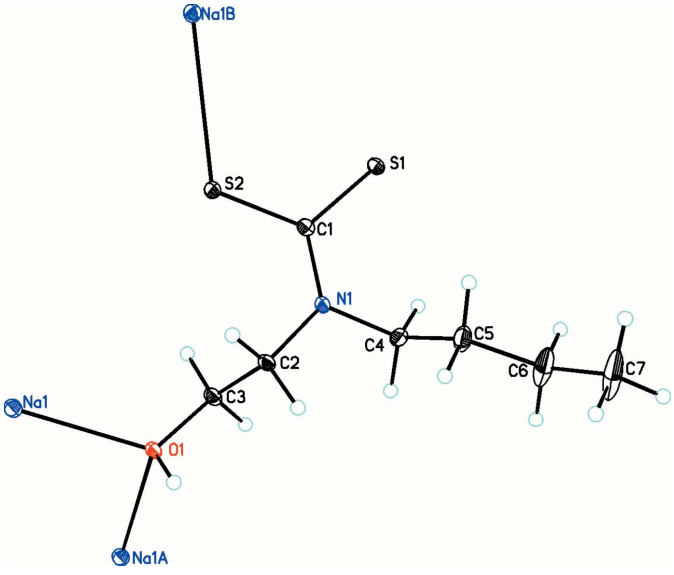



**Figure 2**
Diagram showing the triply bridging nature of the dithiocarbamate anion [symmetry codes: (A) $1-x, -y, 1-z$; (B) $1-x, y+\frac{1}{2}, \frac{1}{2}-z$].

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*O*···S1$^{i}$ | 0.82 (2) | 2.41 (2) | 3.2227 (10) | 167.6 (19) |
| O1*W*—H1*W*1···S2 | 0.82 (2) | 2.48 (2) | 3.2933 (10) | 168 (2) |
| O1*W*—H1*W*2···S2$^{ii}$ | 0.85 (3) | 2.42 (3) | 3.2605 (10) | 171 (2) |
| O2*W*—H2*W*2···S1$^{ii}$ | 0.78 (2) | 2.48 (2) | 3.2624 (11) | 173 (2) |

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

## 3. Supramolecular features

Intermolecular O—H···S hydrogen bonds (Table 1) are observed in the inner part of each polymeric layer (Fig. 3). The layers are further packed along the *a* axis and held together by weak van der Waals forces.

## 4. Database survey

In a recent publication, Howie *et al.* (2008) reported a structurally similar compound where the butyl substituent was replaced by a propyl substituent. The crystal structures of other sodium salts of dithiocarbamates, $Na[S_2CN(C_2H_5)_2]\cdot 3H_2O$ (Colapietro *et al.*, 1968), $Na[S_2CN(CH_2)_4]\cdot 2H_2O$ (Albertsson *et al.*, 1980; Ymén, 1982), $Na[S_2CN(C_3H_7)_2]\cdot 5H_2O$ (Ymén, 1983) and $Na[S_2CN(CH_3)_2]\cdot 2H_2O$ (Oskarsson & Ymén, 1983), $Na[S_2CN(CH_2)_5]\cdot 2H_2O$ (Mafud & Gambardella,

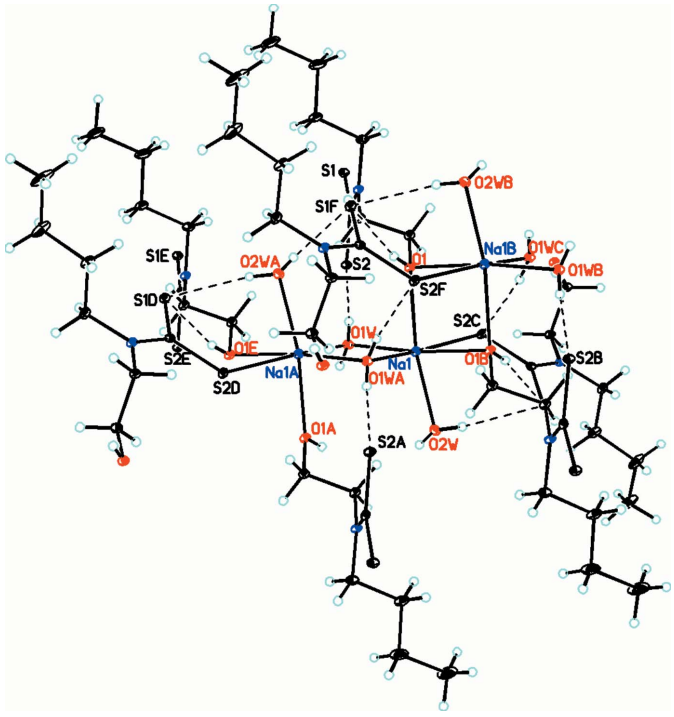



**Figure 3**
A portion of the crystal packing showing the O—H···S hydrogen bonds (dashed lines) in the inner part of the polymeric layer [symmetry codes: (A) $1-x, 1-y, 1-z$; (B) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (C) $1-x, -y, 1-z$; (D) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (E) $x, 1+y, z$; (F) $x, \frac{1}{2}-y, \frac{1}{2}+x$].

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Na(C_7H_{14}NOS_2)(H_2O)_2]$ |
| $M_r$ | 251.33 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 120 |
| $a, b, c$ (Å) | 15.6223 (3), 5.8379 (1), 14.7114 (3) |
| $\beta$ (°) | 101.868 (2) |
| $V$ (Å$^3$) | 1313.02 (4) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.90 |
| Crystal size (mm) | 0.39 × 0.31 × 0.24 |
| Data collection | |
| Diffractometer | Agilent SuperNova Dual Source diffractometer with an Atlas detector |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Agilent, 2012) |
| $T_{min}$, $T_{max}$ | 0.660, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 5973, 2731, 2617 |
| $R_{int}$ | 0.019 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.631 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.029, 0.080, 1.05 |
| No. of reflections | 2731 |
| No. of parameters | 149 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.29, −0.39 |

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

2011), $Na[S_2CN(C_8H_5NS)]\cdot 3H_2O$ (Téllez *et al.*, 2004) have been reported. All these structures are polymeric in nature and contain the $\mu(H_2O)_2Na_2$ unit.

## 5. Synthesis and crystallization

The title compound was prepared by the reaction of *N*-butyl *N*-hydroxyethyl amine (0.01 mol), carbon disulfide (0.01 mol) and sodium hydroxide (0.01 mol) in dry diethyl ether and was stirred for 4 h at 253 K. The crude product was recrystallized from isopropyl alcohol. It was then dissolved in a hexane:diethyl ether (1:1 *v*/*v*) mixture and put in a deep freezer overnight. Square transparent crystals suitable for X ray analysis were obtained in 80% yield (m.p.: 430 K). Analysis calculated for $C_7H_{18}NO_3S_2$ (%) S, 29.78; found: S, 29.84.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were idealized with C—H distances of 0.99 Å for $CH_2$ and 0.98 Å for $CH_3$ groups with atomic displacement parameters of $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms and 1.2$U_{eq}$(C) for other H atoms. The water and hydroxyl H atoms were freely refined.

## Acknowledgements

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# supporting information

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## Poly[$\mu_2$-aqua-aqua[$\mu_3$-*N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamato-$\kappa^3O,O':S$]sodium]

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### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### Poly[$\mu_2$-aqua-aqua[$\mu_3$-*N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamato-$\kappa^3O,O':S$]sodium]

*Crystal data*

$[Na(C_7H_{14}NOS_2)(H_2O)_2]$
$M_r = 251.33$
Monoclinic, $P2_1/c$
$a = 15.6223$ (3) Å
$b = 5.8379$ (1) Å
$c = 14.7114$ (3) Å
$\beta = 101.868$ (2)°
$V = 1313.02$ (4) Å$^3$
$Z = 4$
$F(000) = 536$
$D_x = 1.271$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 4003 reflections
$\theta = 3.1$–$76.6°$
$\mu = 3.90$ mm$^{-1}$
$T = 120$ K
Chunk, colorless
0.39 × 0.31 × 0.24 mm

*Data collection*

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube
Detector resolution: 10.6501 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.660$, $T_{max} = 1.000$
5973 measured reflections
2731 independent reflections
2617 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 76.4°$, $\theta_{min} = 2.9°$
$h = -19 \rightarrow 17$
$k = -7 \rightarrow 4$
$l = -18 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.080$
$S = 1.05$
2731 reflections
149 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2 + 0.3898P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{min} = -0.39$ e Å$^{-3}$
Extinction correction: *SHELXL2014* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0041 (4)

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Na1 | 0.44835 (3) | 0.26004 (8) | 0.45654 (3) | 0.01595 (14) |
| S1 | 0.76058 (2) | 0.34854 (5) | 0.14289 (2) | 0.01645 (11) |
| S2 | 0.60961 (2) | 0.50629 (5) | 0.22351 (2) | 0.01569 (11) |
| O1 | 0.59309 (6) | 0.09872 (16) | 0.47496 (6) | 0.0155 (2) |
| H1O | 0.6306 (14) | 0.125 (4) | 0.5218 (15) | 0.035 (5)* |
| O1W | 0.50061 (6) | 0.58495 (17) | 0.39025 (6) | 0.0172 (2) |
| H1W1 | 0.5325 (15) | 0.551 (4) | 0.3542 (15) | 0.039 (6)* |
| H1W2 | 0.4670 (16) | 0.686 (4) | 0.3609 (16) | 0.046 (6)* |
| O2W | 0.30199 (7) | 0.34773 (19) | 0.44462 (7) | 0.0220 (2) |
| H2W1 | 0.2792 (15) | 0.233 (4) | 0.4121 (16) | 0.041 (6)* |
| H2W2 | 0.2843 (15) | 0.462 (4) | 0.4197 (15) | 0.036 (6)* |
| N1 | 0.73937 (7) | 0.23989 (18) | 0.31192 (7) | 0.0149 (2) |
| C1 | 0.70580 (8) | 0.3542 (2) | 0.23350 (8) | 0.0138 (2) |
| C2 | 0.70139 (8) | 0.2560 (2) | 0.39489 (8) | 0.0154 (3) |
| H2A | 0.6735 | 0.4079 | 0.3964 | 0.019* |
| H2B | 0.7485 | 0.2424 | 0.4510 | 0.019* |
| C3 | 0.63355 (8) | 0.0692 (2) | 0.39629 (8) | 0.0167 (3) |
| H3A | 0.5884 | 0.0758 | 0.3383 | 0.020* |
| H3B | 0.6621 | −0.0828 | 0.3996 | 0.020* |
| C4 | 0.82101 (9) | 0.1072 (2) | 0.32374 (9) | 0.0197 (3) |
| H4A | 0.8270 | 0.0440 | 0.2629 | 0.024* |
| H4B | 0.8184 | −0.0229 | 0.3662 | 0.024* |
| C5 | 0.90068 (9) | 0.2546 (3) | 0.36299 (10) | 0.0269 (3) |
| H5A | 0.9006 | 0.3906 | 0.3228 | 0.032* |
| H5B | 0.8963 | 0.3091 | 0.4256 | 0.032* |
| C6 | 0.98645 (11) | 0.1266 (4) | 0.36977 (15) | 0.0465 (5) |
| H6A | 0.9929 | 0.0811 | 0.3067 | 0.056* |
| H6B | 0.9852 | −0.0147 | 0.4067 | 0.056* |
| C7 | 1.06488 (12) | 0.2721 (5) | 0.41491 (19) | 0.0658 (8) |
| H7A | 1.1185 | 0.1809 | 0.4213 | 0.099* |
| H7B | 1.0576 | 0.3224 | 0.4764 | 0.099* |
| H7C | 1.0689 | 0.4063 | 0.3760 | 0.099* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Na1 | 0.0155 (3) | 0.0175 (3) | 0.0152 (2) | −0.00088 (18) | 0.00403 (19) | 0.00032 (18) |
| S1 | 0.01710 (17) | 0.02187 (18) | 0.01177 (17) | 0.00208 (11) | 0.00623 (12) | 0.00148 (10) |
| S2 | 0.01414 (17) | 0.02106 (18) | 0.01238 (17) | 0.00310 (10) | 0.00394 (11) | 0.00173 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0133 (4) | 0.0226 (5) | 0.0114 (4) | −0.0007 (3) | 0.0044 (3) | 0.0013 (3) |
| O1W | 0.0175 (4) | 0.0200 (5) | 0.0152 (4) | 0.0025 (4) | 0.0061 (4) | 0.0011 (4) |
| O2W | 0.0203 (5) | 0.0190 (5) | 0.0257 (5) | 0.0024 (4) | 0.0024 (4) | −0.0033 (4) |
| N1 | 0.0121 (5) | 0.0214 (5) | 0.0118 (5) | 0.0007 (4) | 0.0040 (4) | 0.0013 (4) |
| C1 | 0.0136 (6) | 0.0157 (6) | 0.0118 (5) | −0.0035 (4) | 0.0020 (4) | −0.0014 (4) |
| C2 | 0.0141 (6) | 0.0226 (6) | 0.0100 (5) | −0.0014 (5) | 0.0036 (4) | 0.0014 (4) |
| C3 | 0.0174 (6) | 0.0211 (6) | 0.0130 (6) | −0.0013 (5) | 0.0062 (4) | −0.0006 (5) |
| C4 | 0.0166 (6) | 0.0260 (6) | 0.0167 (6) | 0.0060 (5) | 0.0038 (5) | 0.0034 (5) |
| C5 | 0.0143 (7) | 0.0410 (9) | 0.0250 (7) | 0.0026 (6) | 0.0027 (5) | −0.0022 (6) |
| C6 | 0.0172 (8) | 0.0670 (13) | 0.0528 (11) | 0.0100 (8) | 0.0015 (7) | −0.0184 (10) |
| C7 | 0.0139 (8) | 0.0942 (19) | 0.0856 (18) | 0.0041 (10) | 0.0015 (9) | −0.0321 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Na1—O2W | 2.3142 (11) | N1—C1 | 1.3425 (16) |
| Na1—O1W | 2.3544 (11) | N1—C2 | 1.4658 (15) |
| Na1—O1W$^{i}$ | 2.4074 (11) | N1—C4 | 1.4717 (16) |
| Na1—O1 | 2.4128 (10) | C2—C3 | 1.5237 (17) |
| Na1—O1$^{ii}$ | 2.4677 (10) | C2—H2A | 0.9900 |
| Na1—S2$^{iii}$ | 3.0074 (6) | C2—H2B | 0.9900 |
| Na1—Na1$^{i}$ | 3.3527 (10) | C3—H3A | 0.9900 |
| Na1—Na1$^{ii}$ | 3.5509 (10) | C3—H3B | 0.9900 |
| Na1—H2W1 | 2.59 (2) | C4—C5 | 1.525 (2) |
| S1—C1 | 1.7261 (13) | C4—H4A | 0.9900 |
| S2—C1 | 1.7256 (13) | C4—H4B | 0.9900 |
| S2—Na1$^{iv}$ | 3.0073 (6) | C5—C6 | 1.519 (2) |
| O1—C3 | 1.4386 (14) | C5—H5A | 0.9900 |
| O1—Na1$^{ii}$ | 2.4677 (10) | C5—H5B | 0.9900 |
| O1—H1O | 0.82 (2) | C6—C7 | 1.526 (3) |
| O1W—Na1$^{i}$ | 2.4074 (10) | C6—H6A | 0.9900 |
| O1W—H1W1 | 0.82 (2) | C6—H6B | 0.9900 |
| O1W—H1W2 | 0.85 (3) | C7—H7A | 0.9800 |
| O2W—H2W1 | 0.86 (2) | C7—H7B | 0.9800 |
| O2W—H2W2 | 0.78 (2) | C7—H7C | 0.9800 |
| | | | |
| O2W—Na1—O1W | 102.22 (4) | Na1$^{i}$—O1W—H1W2 | 105.5 (16) |
| O2W—Na1—O1W$^{i}$ | 96.88 (4) | H1W1—O1W—H1W2 | 103 (2) |
| O1W—Na1—O1W$^{i}$ | 90.49 (4) | Na1—O2W—H2W1 | 99.2 (15) |
| O2W—Na1—O1 | 169.54 (4) | Na1—O2W—H2W2 | 118.2 (16) |
| O1W—Na1—O1 | 87.95 (4) | H2W1—O2W—H2W2 | 110 (2) |
| O1W$^{i}$—Na1—O1 | 85.37 (4) | C1—N1—C2 | 122.02 (10) |
| O2W—Na1—O1$^{ii}$ | 83.15 (4) | C1—N1—C4 | 122.61 (11) |
| O1W—Na1—O1$^{ii}$ | 174.49 (4) | C2—N1—C4 | 115.15 (10) |
| O1W$^{i}$—Na1—O1$^{ii}$ | 90.05 (4) | N1—C1—S2 | 120.56 (9) |
| O1—Na1—O1$^{ii}$ | 86.64 (3) | N1—C1—S1 | 119.09 (9) |
| O2W—Na1—S2$^{iii}$ | 85.90 (3) | S2—C1—S1 | 120.36 (7) |
| O1W—Na1—S2$^{iii}$ | 95.69 (3) | N1—C2—C3 | 111.54 (10) |
| O1W$^{i}$—Na1—S2$^{iii}$ | 172.54 (3) | N1—C2—H2A | 109.3 |

| | | | |
|---|---|---|---|
| O1—Na1—S2$^{iii}$ | 90.69 (3) | C3—C2—H2A | 109.3 |
| O1$^{ii}$—Na1—S2$^{iii}$ | 83.39 (3) | N1—C2—H2B | 109.3 |
| O2W—Na1—Na1$^{i}$ | 103.57 (4) | C3—C2—H2B | 109.3 |
| O1W—Na1—Na1$^{i}$ | 45.89 (3) | H2A—C2—H2B | 108.0 |
| O1W$^{i}$—Na1—Na1$^{i}$ | 44.60 (3) | O1—C3—C2 | 110.32 (10) |
| O1—Na1—Na1$^{i}$ | 85.23 (3) | O1—C3—H3A | 109.6 |
| O1$^{ii}$—Na1—Na1$^{i}$ | 134.40 (3) | C2—C3—H3A | 109.6 |
| S2$^{iii}$—Na1—Na1$^{i}$ | 141.41 (3) | O1—C3—H3B | 109.6 |
| O2W—Na1—Na1$^{ii}$ | 125.82 (4) | C2—C3—H3B | 109.6 |
| O1W—Na1—Na1$^{ii}$ | 131.86 (3) | H3A—C3—H3B | 108.1 |
| O1W$^{i}$—Na1—Na1$^{ii}$ | 86.89 (3) | N1—C4—C5 | 111.56 (12) |
| O1—Na1—Na1$^{ii}$ | 43.93 (2) | N1—C4—H4A | 109.3 |
| O1$^{ii}$—Na1—Na1$^{ii}$ | 42.71 (2) | C5—C4—H4A | 109.3 |
| S2$^{iii}$—Na1—Na1$^{ii}$ | 85.882 (19) | N1—C4—H4B | 109.3 |
| Na1$^{i}$—Na1—Na1$^{ii}$ | 115.45 (3) | C5—C4—H4B | 109.3 |
| O2W—Na1—H2W1 | 19.0 (5) | H4A—C4—H4B | 108.0 |
| O1W—Na1—H2W1 | 111.5 (5) | C6—C5—C4 | 112.80 (14) |
| O1W$^{i}$—Na1—H2W1 | 112.5 (5) | C6—C5—H5A | 109.0 |
| O1—Na1—H2W1 | 152.6 (6) | C4—C5—H5A | 109.0 |
| O1$^{ii}$—Na1—H2W1 | 73.3 (5) | C6—C5—H5B | 109.0 |
| S2$^{iii}$—Na1—H2W1 | 69.0 (5) | C4—C5—H5B | 109.0 |
| Na1$^{i}$—Na1—H2W1 | 122.2 (5) | H5A—C5—H5B | 107.8 |
| Na1$^{ii}$—Na1—H2W1 | 113.8 (5) | C5—C6—C7 | 111.93 (18) |
| C1—S2—Na1$^{iv}$ | 115.32 (4) | C5—C6—H6A | 109.2 |
| C3—O1—Na1 | 120.87 (7) | C7—C6—H6A | 109.2 |
| C3—O1—Na1$^{ii}$ | 115.00 (8) | C5—C6—H6B | 109.2 |
| Na1—O1—Na1$^{ii}$ | 93.36 (3) | C7—C6—H6B | 109.2 |
| C3—O1—H1O | 109.9 (14) | H6A—C6—H6B | 107.9 |
| Na1—O1—H1O | 120.7 (14) | C6—C7—H7A | 109.5 |
| Na1$^{ii}$—O1—H1O | 91.1 (15) | C6—C7—H7B | 109.5 |
| Na1—O1W—Na1$^{i}$ | 89.50 (4) | H7A—C7—H7B | 109.5 |
| Na1—O1W—H1W1 | 112.5 (16) | C6—C7—H7C | 109.5 |
| Na1$^{i}$—O1W—H1W1 | 124.5 (15) | H7A—C7—H7C | 109.5 |
| Na1—O1W—H1W2 | 122.7 (16) | H7B—C7—H7C | 109.5 |
| | | | |
| C2—N1—C1—S2 | −5.92 (16) | Na1—O1—C3—C2 | 102.88 (10) |
| C4—N1—C1—S2 | 179.80 (9) | Na1$^{ii}$—O1—C3—C2 | −146.38 (8) |
| C2—N1—C1—S1 | 173.66 (9) | N1—C2—C3—O1 | −176.02 (9) |
| C4—N1—C1—S1 | −0.62 (16) | C1—N1—C4—C5 | 89.35 (15) |
| Na1$^{iv}$—S2—C1—N1 | 178.00 (8) | C2—N1—C4—C5 | −85.29 (13) |
| Na1$^{iv}$—S2—C1—S1 | −1.57 (9) | N1—C4—C5—C6 | −176.06 (13) |
| C1—N1—C2—C3 | 91.65 (14) | C4—C5—C6—C7 | −176.34 (18) |
| C4—N1—C2—C3 | −93.68 (13) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*O*···S1$^{v}$ | 0.82 (2) | 2.41 (2) | 3.2227 (10) | 167.6 (19) |
| O1*W*—H1*W*1···S2 | 0.82 (2) | 2.48 (2) | 3.2933 (10) | 168 (2) |
| O1*W*—H1*W*2···S2$^{iv}$ | 0.85 (3) | 2.42 (3) | 3.2605 (10) | 171 (2) |
| O2*W*—H2*W*2···S1$^{iv}$ | 0.78 (2) | 2.48 (2) | 3.2624 (11) | 173 (2) |

Symmetry codes: (iv) −*x*+1, *y*+1/2, −*z*+1/2; (v) *x*, −*y*+1/2, *z*+1/2.