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Poly[μ_2-aqua-aqua[μ_3-N-butyl-N-(2-hydroxyethyl)dithiocarbamato-$\kappa^3 O,O'$:S]sodium]

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In the title compound, [Na(C$_7$H$_{14}$NOS$_2$)(H$_2$O)$_2$]$_n$, 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.
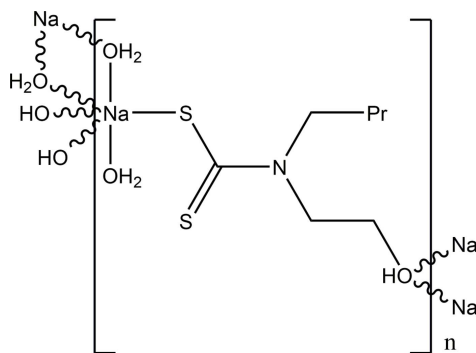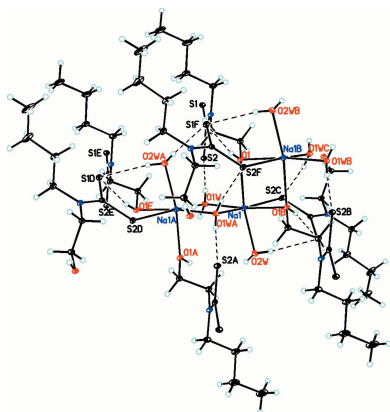
2. Structural commentary

The title compound is a two-dimensional polymer with formula [Na(μ_3-C$_7$H$_{14}$NOS$_2$)(μ_2-H$_2$O)(H$_2$O)]. Within this

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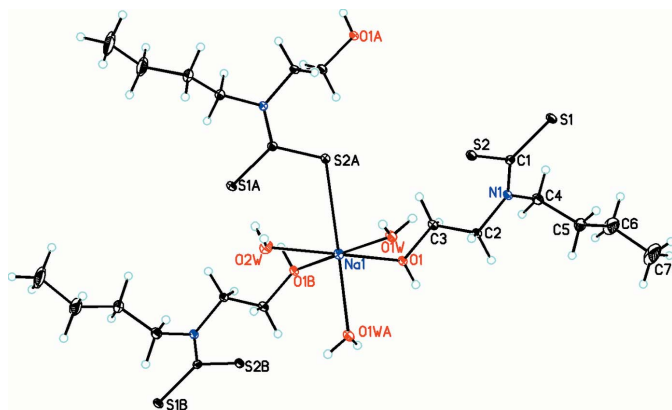
Figure 1
A portion of the title crystal structure showing the coordination environment for the Na^{I} cation and the atomic labels [symmetry codes: (A) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (B) $1 - x, -y, 1 - z$]. Displacement ellipsoids are drawn at the 30% probability level.

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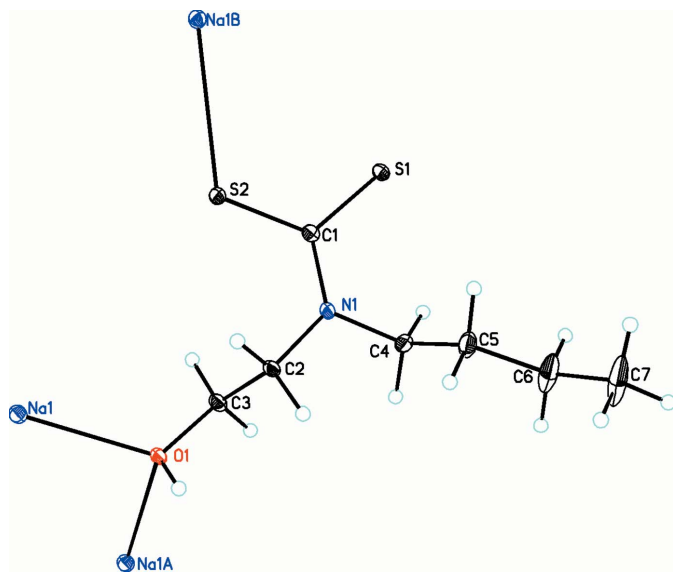
Table 1
Hydrogen-bond geometry (Å, °).

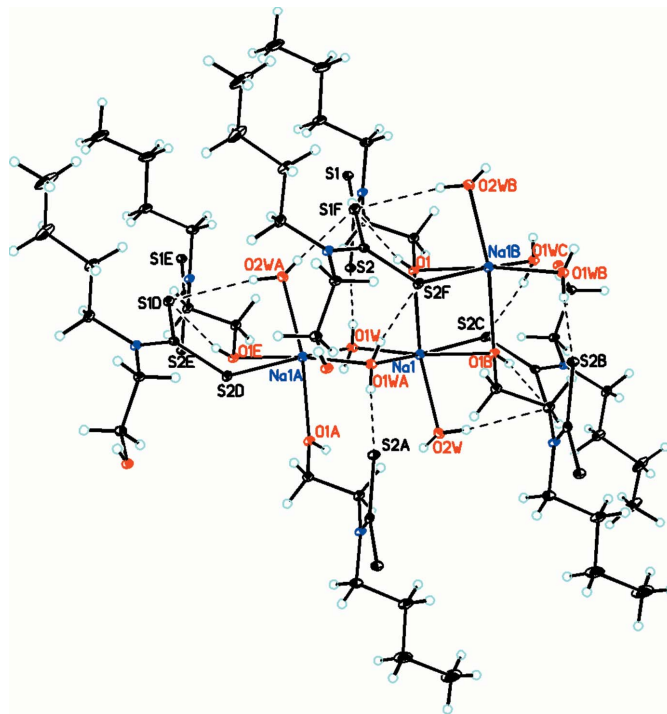| $D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1—H1$O\cdots$S1^{i}	0.82 (2)	2.41 (2)	3.2227 (10)	167.6 (19)
O1W—H1W1$\cdots$S2	0.82 (2)	2.48 (2)	3.2933 (10)	168 (2)
O1W—H1W2$\cdots$S2^{ii}	0.85 (3)	2.42 (3)	3.2605 (10)	171 (2)
O2W—H2W2$\cdots$S1^{ii}	0.78 (2)	2.48 (2)	3.2624 (11)	173 (2)

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$\cdots$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$_2$CN(C$_2$H$_5$)$_2$]·3H$_2$O (Colapietro *et al.*, 1968), Na[S$_2$CN(CH$_2$)$_4$]·2H$_2$O (Albertsson *et al.*, 1980; Ymén, 1982), Na[S$_2$CN(C$_3$H$_7$)$_2$]·5H$_2$O (Ymén, 1983) and Na[S$_2$CN(CH$_3$)$_2$]·2H$_2$O (Oskarsson & Ymén, 1983), Na[S$_2$CN(CH$_2$)$_5$]·2H$_2$O (Mafud & Gambardella,

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

Figure 3
A portion of the crystal packing showing the O—H$\cdots$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) $x, \frac{1}{2} - y, \frac{1}{2} + x$].

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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)
β (°)	101.868 (2)
V (Å³)	1313.02 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm⁻¹)	3.90
Crystal size (mm)	$0.39 \times 0.31 \times 0.24$
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[S₂CN(C₈H₅NS)]·3H₂O (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 C₇H₁₈NO₃S₂ (%) 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 CH₂ and 0.98 Å for CH₃ groups with atomic displacement parameters of $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms. The water and hydroxyl H atoms were freely refined.

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supporting information

Poly[μ_2-aqua-aqua[μ_3-*N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamato-κ^3*O*,*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[μ_2-aqua-aqua[μ_3-*N*-butyl-*N*-(2-hydroxyethyl)dithiocarbamato-κ^3*O*,*O*′:*S*]sodium]

Crystal data

[Na(C$_7$H$_{14}$NOS$_2$)(H$_2$O)$_2$]
M_r = 251.33
Monoclinic, $P2_1/c$
a = 15.6223 (3) Å
b = 5.8379 (1) Å
c = 14.7114 (3) Å
β = 101.868 (2)°
V = 1313.02 (4) Å^3
Z = 4

$F(000)$ = 536
D_x = 1.271 Mg m^{-3}
Cu *Kα* radiation, λ = 1.54184 Å
Cell parameters from 4003 reflections
θ = 3.1–76.6°
μ = 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}
ω 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
θ_{max} = 76.4°, θ_{min} = 2.9°
h = −19→17
k = −7→4
l = −18→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^2λ^3/sin(2θ)]$^{-1/4}$
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 (Å^2)

	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 (Å^2)

	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—S2ⁱⁱⁱ	90.69 (3)	C3—C2—H2A	109.3
O1ⁱⁱ—Na1—S2ⁱⁱⁱ	83.39 (3)	N1—C2—H2B	109.3
O2W—Na1—Na1ⁱ	103.57 (4)	C3—C2—H2B	109.3
O1W—Na1—Na1ⁱ	45.89 (3)	H2A—C2—H2B	108.0
O1Wⁱ—Na1—Na1ⁱ	44.60 (3)	O1—C3—C2	110.32 (10)
O1—Na1—Na1ⁱ	85.23 (3)	O1—C3—H3A	109.6
O1ⁱⁱ—Na1—Na1ⁱ	134.40 (3)	C2—C3—H3A	109.6
S2ⁱⁱⁱ—Na1—Na1ⁱ	141.41 (3)	O1—C3—H3B	109.6
O2W—Na1—Na1ⁱⁱ	125.82 (4)	C2—C3—H3B	109.6
O1W—Na1—Na1ⁱⁱ	131.86 (3)	H3A—C3—H3B	108.1
O1Wⁱ—Na1—Na1ⁱⁱ	86.89 (3)	N1—C4—C5	111.56 (12)
O1—Na1—Na1ⁱⁱ	43.93 (2)	N1—C4—H4A	109.3
O1ⁱⁱ—Na1—Na1ⁱⁱ	42.71 (2)	C5—C4—H4A	109.3
S2ⁱⁱⁱ—Na1—Na1ⁱⁱ	85.882 (19)	N1—C4—H4B	109.3
Na1ⁱ—Na1—Na1ⁱⁱ	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)
O1Wⁱ—Na1—H2W1	112.5 (5)	C6—C5—H5A	109.0
O1—Na1—H2W1	152.6 (6)	C4—C5—H5A	109.0
O1ⁱⁱ—Na1—H2W1	73.3 (5)	C6—C5—H5B	109.0
S2ⁱⁱⁱ—Na1—H2W1	69.0 (5)	C4—C5—H5B	109.0
Na1ⁱ—Na1—H2W1	122.2 (5)	H5A—C5—H5B	107.8
Na1ⁱⁱ—Na1—H2W1	113.8 (5)	C5—C6—C7	111.93 (18)
C1—S2—Na1ⁱᵛ	115.32 (4)	C5—C6—H6A	109.2
C3—O1—Na1	120.87 (7)	C7—C6—H6A	109.2
C3—O1—Na1ⁱⁱ	115.00 (8)	C5—C6—H6B	109.2
Na1—O1—Na1ⁱⁱ	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
Na1ⁱⁱ—O1—H1O	91.1 (15)	C6—C7—H7B	109.5
Na1—O1W—Na1ⁱ	89.50 (4)	H7A—C7—H7B	109.5
Na1—O1W—H1W1	112.5 (16)	C6—C7—H7C	109.5
Na1ⁱ—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)	Na1ⁱⁱ—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)
Na1ⁱᵛ—S2—C1—N1	178.00 (8)	C2—N1—C4—C5	−85.29 (13)
Na1ⁱᵛ—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.