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Aquabis[*N'*-(1,3-dithiolan-2-ylidene)-2-hydroxybenzohydrazidato(0.5-) κ^2 *N',O*]sodium(I)

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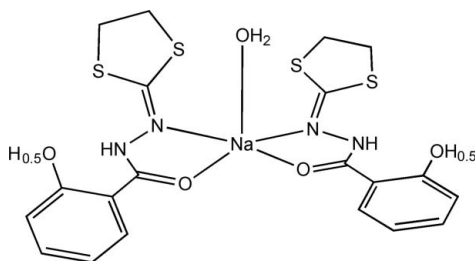
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 15.3.

The title compound, $[\text{Na}(\text{C}_{10}\text{H}_9.5\text{N}_2\text{O}_2\text{S}_2)_2(\text{H}_2\text{O})]$, is a molecular sodium complex with *N'*-(1,3-dithiolan-2-yl)-2-hydroxybenzohydrazide ligands with the negative charge spread evenly over both, and a water molecule. The Na^{I} ion coordination is distorted trigonal-bipyramidal, formed by two N and three O atoms, with the Na^{I} ion lying on a twofold rotation axis. Intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds occur. Molecules pack as discrete units and the crystal packing is stabilized by strong $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, which give rise to chains along [010]; the chains are interlinked by strong $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general background to the 2-salicylihydrazono-1,3-dithiolane ligand (H_2L) and its metal complexes, see: Beghidja *et al.* (2005, 2006); Bouchameni *et al.* (2011). For background to dithiocarbazates, see: Wang *et al.* (2002); Zhou *et al.* (2007) and for their biological activity, see: Tarafder *et al.* (2000, 2001).



Experimental

Crystal data

$[\text{Na}(\text{C}_{10}\text{H}_9.5\text{N}_2\text{O}_2\text{S}_2)_2(\text{H}_2\text{O})]$	$V = 1184.99$ (17) Å ³
$M_r = 548.68$	$Z = 2$
Monoclinic, $C2$	Mo $K\alpha$ radiation
$a = 16.6960$ (16) Å	$\mu = 0.46$ mm ⁻¹
$b = 5.9330$ (3) Å	$T = 298$ K
$c = 13.5240$ (12) Å	$0.14 \times 0.10 \times 0.08$ mm
$\beta = 117.804$ (3)°	

Data collection

Nonius KappaCCD diffractometer	2083 reflections with $I > 2\sigma(I)$
3660 measured reflections	$R_{\text{int}} = 0.050$
2463 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.126$	$\Delta\rho_{\text{max}} = 0.33$ e Å ⁻³
$S = 1.00$	$\Delta\rho_{\text{min}} = -0.43$ e Å ⁻³
2463 reflections	Absolute structure: Flack (1983), 970 Friedel pairs
161 parameters	Flack parameter: -0.06 (13)
5 restraints	

Table 1

Selected bond lengths (Å).

Na1—O1	2.320 (3)	Na1—N2	2.666 (4)
Na1—O3	2.214 (6)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1 \cdots O2	0.88	1.88	2.596 (4)	137
O2—H2 \cdots O2 ⁱⁱ	0.89 (5)	1.61 (9)	2.467 (4)	160 (14)
O3—H3 \cdots O1 ⁱⁱ	0.95 (4)	1.90 (4)	2.788 (5)	155 (4)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); 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: BQ2359).

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supporting information

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Aquabis[*N'*-(1,3-dithiolan-2-ylidene)-2-hydroxybenzohydrazidato(0.5-)- κ^2 *N',O*]sodium(I)

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S1. Comment

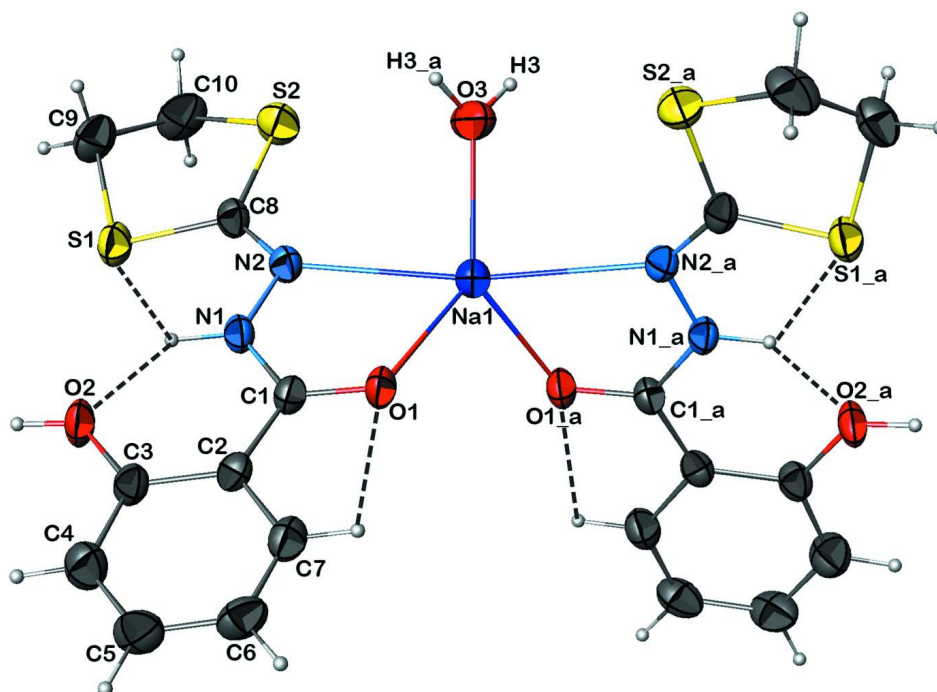
Dithiocarbazate R—NH₂NHCS₂ (DTC) and its substituted compounds remain of interest to researchers because of their wide variation in structure and properties (Zhou *et al.*, 2007; Wang *et al.*, 2002). Some of these compounds have been widely studied for their antibacterial and antifungal activities (Tarafer *et al.*, 2000; Tarafer *et al.*, 2001). The ligand H₂L was synthesized as previously described (Beghidja *et al.*, 2005). The molecular structure of the title compound is illustrated in Fig. 1. The sodium cation is chelated by two H_{1.5}L^{-1/2} bidentate anions coordinated by the hydrazide group *via* O1 and N2 atoms. Na1—O1 = 2.316 (3) Å, Na1—N2 = 2.664 (3) Å. The geometry around the metal is a distorted trigonal bipyramid with a water molecule lying in the axial position through O3. Na1—O3 = 2.213 (5) Å. The crystal structure can be described as a one-dimensional set of chains, interlinked by strong hydrogen-bonds type O—H \cdots O, along the *b* axis, between O3—H3 \cdots O1. These chains are interconnected along the *c* axis *via* strong hydrogen-bonds type O—H \cdots O between O2—H2 \cdots O2 (Fig 2).

S2. Experimental

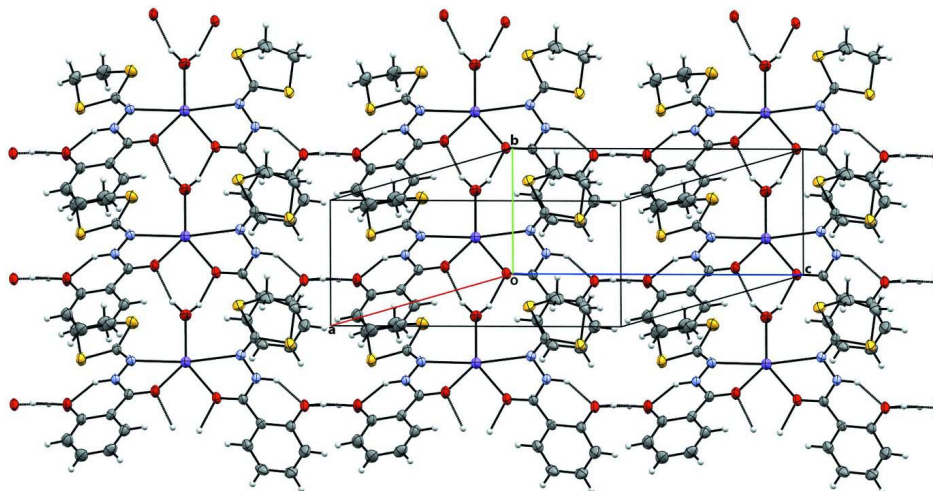
The reaction of H₂L (0.05 g, 2 × 10⁻⁴ mol) with Mn(OH)₃ (0.0106 g, 10⁻⁴ mol) and NaOH (0.01 g, 2 × 10⁻⁴ mol) in ethanol solution leads to a yellow solution which was left to stand undisturbed at room temperature. Several days later, x-ray quality colorless single crystals were obtained by slow evaporation, which were filtrated and characterized.

S3. Refinement

The positions of the H atoms of the water molecule and hydroxyl group were located in the electron density maps; other H atoms were placed in calculated positions and refined as riding with C—H = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic groups; N—H = 0.86 Å, U_{iso} = 1.2U_{eq}(N); O—H = 0.90–0.95 Å, U_{iso} = 1.5U_{eq}(O).

**Figure 1**

ORTEP view of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. The intramolecular hydrogen bond is shown as a dashed line. Symmetry code: (a) -x+1, y, -z+1.

**Figure 2**

Mercury view of the crystal structure of title compound along the *a* axis showing the two-dimensional network *via* a strong hydrogen bonds through O—H...O atoms.

Aquabis[*N'*-(1,3-dithiolan-2-ylidene)-2-hydroxybenzohydrazidato(0.5)- κ^2N',O]sodium(I)

Crystal data

[Na(C₁₀H_{9.5}N₂O₂S₂)₂(H₂O)] $M_r = 548.68$ Monoclinic, *C*2Hall symbol: *C* 2y $a = 16.6960$ (16) Å $b = 5.9330$ (3) Å $c = 13.5240$ (12) Å $\beta = 117.804$ (3)° $V = 1184.99$ (17) Å³ $Z = 2$ $F(000) = 568$ $D_x = 1.538$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2559 reflections

 $\theta = 1.0$ – 27.5° $\mu = 0.46$ mm⁻¹ $T = 298$ K

Plates, colorless

 $0.14 \times 0.10 \times 0.08$ mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: Rotating Anode

Horizontally mounted graphite crystal
monochromatorDetector resolution: 9 pixels mm⁻¹ φ scans, and ω scans with κ offsets

3660 measured reflections

2463 independent reflections

2083 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.050$ $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.7^\circ$ $h = -21 \rightarrow 21$ $k = -6 \rightarrow 7$ $l = -13 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.047$ $wR(F^2) = 0.126$ $S = 1.00$

2463 reflections

161 parameters

5 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 2.9944P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.021$ $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³Absolute structure: Flack (1983), 970 Friedel
pairsAbsolute structure parameter: -0.06 (13)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles**Refinement.** Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating $-R$ -factor-obs 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.34168 (7)	0.79324 (19)	0.76027 (8)	0.0330 (3)	
S2	0.33261 (8)	1.0904 (2)	0.57897 (10)	0.0388 (4)	
Na1	0.50000	0.7068 (4)	0.50000	0.0324 (8)	

O1	0.5618 (2)	0.4475 (5)	0.6448 (2)	0.0318 (9)	
O2	0.5000 (2)	0.3636 (5)	0.9088 (2)	0.0348 (10)	
O3	0.50000	1.0799 (9)	0.50000	0.057 (2)	
N1	0.4834 (2)	0.5736 (6)	0.7318 (2)	0.0245 (10)	
N2	0.4434 (2)	0.7412 (6)	0.6540 (3)	0.0261 (10)	
C1	0.5421 (3)	0.4301 (7)	0.7235 (3)	0.0261 (12)	
C2	0.5809 (3)	0.2538 (7)	0.8092 (3)	0.0249 (11)	
C3	0.5575 (3)	0.2237 (7)	0.8968 (3)	0.0282 (11)	
C4	0.5962 (3)	0.0414 (8)	0.9695 (4)	0.0393 (16)	
C5	0.6562 (3)	-0.1025 (9)	0.9594 (4)	0.0400 (16)	
C6	0.6809 (3)	-0.0701 (8)	0.8755 (4)	0.0373 (14)	
C7	0.6425 (3)	0.1041 (8)	0.8012 (3)	0.0325 (12)	
C8	0.3821 (3)	0.8554 (7)	0.6639 (3)	0.0262 (11)	
C9	0.2806 (3)	1.0562 (9)	0.7390 (4)	0.0400 (16)	
C10	0.2425 (3)	1.1176 (9)	0.6176 (4)	0.0453 (16)	
H1	0.47040	0.56020	0.78750	0.0290*	
H2	0.512 (8)	0.379 (19)	0.980 (3)	0.0680*	0.500
H3	0.470 (4)	1.171 (8)	0.435 (3)	0.0680*	
H4	0.58030	0.01670	1.02760	0.0470*	
H5	0.68110	-0.22480	1.01000	0.0480*	
H6	0.72380	-0.16700	0.86960	0.0450*	
H7	0.65820	0.12360	0.74260	0.0390*	
H9A	0.23110	1.03850	0.75920	0.0480*	
H9B	0.32190	1.17610	0.78640	0.0480*	
H10A	0.21950	1.27430	0.60530	0.0540*	
H10B	0.19180	1.01580	0.57130	0.0540*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0373 (6)	0.0381 (6)	0.0316 (5)	0.0081 (5)	0.0228 (5)	0.0031 (5)
S2	0.0465 (7)	0.0349 (6)	0.0353 (6)	0.0119 (5)	0.0194 (5)	0.0097 (5)
Na1	0.0457 (14)	0.0278 (13)	0.0329 (12)	0.0000	0.0260 (11)	0.0000
O1	0.0435 (17)	0.0330 (17)	0.0300 (15)	0.0067 (13)	0.0265 (14)	0.0027 (12)
O2	0.0449 (18)	0.0407 (19)	0.0274 (15)	0.0150 (15)	0.0240 (15)	0.0072 (13)
O3	0.113 (5)	0.029 (3)	0.040 (3)	0.0000	0.044 (3)	0.0000
N1	0.0286 (17)	0.0287 (18)	0.0195 (15)	0.0012 (15)	0.0139 (13)	0.0016 (14)
N2	0.0321 (18)	0.0259 (19)	0.0225 (16)	0.0035 (15)	0.0145 (14)	0.0029 (12)
C1	0.030 (2)	0.028 (2)	0.025 (2)	-0.0002 (17)	0.0167 (17)	-0.0024 (16)
C2	0.0249 (18)	0.027 (2)	0.0217 (17)	-0.0008 (16)	0.0100 (14)	-0.0048 (15)
C3	0.030 (2)	0.033 (2)	0.0213 (18)	0.0045 (17)	0.0116 (16)	0.0001 (16)
C4	0.046 (3)	0.041 (3)	0.029 (2)	0.008 (2)	0.016 (2)	0.0058 (18)
C5	0.045 (3)	0.036 (3)	0.029 (2)	0.012 (2)	0.009 (2)	0.0066 (19)
C6	0.036 (2)	0.033 (3)	0.037 (2)	0.011 (2)	0.012 (2)	-0.002 (2)
C7	0.033 (2)	0.036 (2)	0.033 (2)	-0.001 (2)	0.0193 (18)	-0.005 (2)
C8	0.029 (2)	0.030 (2)	0.0190 (18)	-0.0005 (16)	0.0108 (16)	0.0010 (15)
C9	0.038 (2)	0.044 (3)	0.043 (3)	0.009 (2)	0.023 (2)	-0.003 (2)
C10	0.040 (2)	0.045 (3)	0.045 (3)	0.022 (2)	0.015 (2)	0.003 (2)

Geometric parameters (Å, °)

S1—C8	1.764 (5)	N1—H1	0.8800
S1—C9	1.812 (6)	C1—C2	1.469 (6)
S2—C8	1.750 (4)	C2—C3	1.421 (6)
S2—C10	1.815 (6)	C2—C7	1.401 (7)
Na1—O1	2.320 (3)	C3—C4	1.401 (6)
Na1—O3	2.214 (6)	C4—C5	1.371 (8)
Na1—N2	2.666 (4)	C5—C6	1.390 (7)
Na1—O1 ⁱ	2.320 (3)	C6—C7	1.374 (6)
Na1—N2 ⁱ	2.666 (4)	C9—C10	1.503 (7)
O1—C1	1.256 (5)	C4—H4	0.9500
O2—C3	1.335 (6)	C5—H5	0.9500
O2—H2	0.89 (5)	C6—H6	0.9500
O3—H3 ⁱ	0.95 (4)	C7—H7	0.9500
O3—H3	0.95 (4)	C9—H9A	0.9900
N1—N2	1.373 (5)	C9—H9B	0.9900
N1—C1	1.342 (6)	C10—H10A	0.9900
N2—C8	1.285 (6)	C10—H10B	0.9900
S1…N1	2.880 (4)	C3…H1	2.5100
S1…C4 ⁱⁱ	3.614 (5)	C3…H2 ^{ix}	2.60 (11)
S2…C10 ⁱⁱⁱ	3.660 (5)	C4…H9B ^{xii}	3.0300
S2…O3	3.4263 (15)	C4…H2 ^{ix}	2.98 (12)
S1…H1	2.4300	C4…H4 ^{ix}	2.9700
S1…H7 ^{iv}	3.1300	C6…H5 ^{xiii}	2.9300
S1…H4 ⁱⁱ	2.8600	C7…H5 ^{xiii}	3.0300
S2…H10A ⁱⁱⁱ	2.9100	C7…H3 ^{viii}	2.88 (4)
S2…H10B ^v	3.1500	C9…H6 ^{xiv}	2.8800
Na1…C10 ^{vi}	3.633 (6)	C9…H4 ⁱⁱ	2.9300
Na1…C10 ⁱⁱⁱ	3.633 (6)	H1…S1	2.4300
Na1…H10B ^{vi}	3.1000	H1…O2	1.8800
Na1…H10B ⁱⁱⁱ	3.1000	H1…C3	2.5100
O1…O3 ^{vii}	2.788 (5)	H1…H2	2.5900
O1…N2	2.681 (5)	H2…H1	2.5900
O1…C9 ^{vi}	3.323 (7)	H2…H4	2.3800
O1…O3 ^{viii}	2.788 (5)	H2…O2 ^{ix}	1.61 (9)
O1…C10 ^{vi}	3.360 (7)	H2…C3 ^{ix}	2.60 (11)
O2…C4 ^{ix}	3.378 (6)	H2…C4 ^{ix}	2.98 (12)
O2…N1	2.596 (4)	H3…O1 ^{xi}	1.90 (4)
O2…C3 ^{ix}	3.298 (5)	H3…C1 ^{xi}	2.57 (4)
O2…O2 ^{ix}	2.467 (4)	H3…C2 ^{xi}	3.04 (4)
O3…O1 ^x	2.788 (5)	H3…C7 ^{xi}	2.88 (4)
O3…S2 ⁱ	3.4263 (15)	H3…H7 ^{xi}	2.3700
O3…O1 ^{xi}	2.788 (5)	H4…H2	2.3800
O3…S2	3.4263 (15)	H4…S1 ^{xii}	2.8600
O1…H7	2.4600	H4…O2 ^{ix}	2.8000
O1…H10B ^{vi}	2.8100	H4…C4 ^{ix}	2.9700

O1...H3 ^{viii}	1.90 (4)	H4...C9 ^{xii}	2.9300
O1...H9A ^{vi}	2.5700	H4...H4 ^{ix}	2.4200
O2...H2 ^{ix}	1.61 (8)	H4...H9B ^{xiii}	2.4600
O2...H9B ^{vii}	2.8700	H5...C6 ^{xv}	2.9300
O2...H4 ^{ix}	2.8000	H5...C7 ^{xv}	3.0300
O2...H1	1.8800	H6...C9 ^{xvi}	2.8800
N1...S1	2.880 (4)	H6...H9A ^{xvi}	2.3400
N1...O1	2.257 (5)	H6...H9B ^{xvi}	2.5600
N1...O2	2.596 (4)	H7...O1	2.4600
N2...O1	2.681 (5)	H7...H3 ^{viii}	2.3700
C3...O2 ^{ix}	3.298 (5)	H7...S1 ^{vi}	3.1300
C4...O2 ^{ix}	3.378 (6)	H9A...O1 ^{iv}	2.5700
C4...S1 ^{xii}	3.614 (5)	H9A...C1 ^{iv}	3.0300
C4...C9 ^{xii}	3.495 (7)	H9A...H6 ^{xiv}	2.3400
C9...O1 ^{iv}	3.323 (7)	H9B...O2 ^x	2.8700
C9...C4 ⁱⁱ	3.495 (7)	H9B...C4 ⁱⁱ	3.0300
C10...O1 ^{iv}	3.360 (7)	H9B...H4 ⁱⁱ	2.4600
C10...Na1 ^{iv}	3.633 (6)	H9B...H6 ^{xiv}	2.5600
C10...Na1 ^v	3.633 (6)	H10A...S2 ^v	2.9100
C10...S2 ^v	3.660 (5)	H10B...Na1 ^{iv}	3.1000
C1...H9A ^{vi}	3.0300	H10B...O1 ^{iv}	2.8100
C1...H3 ^{viii}	2.57 (4)	H10B...S2 ⁱⁱⁱ	3.1500
C2...H3 ^{viii}	3.04 (4)	H10B...Na1 ^v	3.1000
C8—S1—C9	94.8 (2)	O2—C3—C2	121.1 (4)
C8—S2—C10	94.8 (2)	O2—C3—C4	121.2 (4)
O1—Na1—O3	131.54 (8)	C3—C4—C5	122.0 (5)
O1—Na1—N2	64.63 (11)	C4—C5—C6	120.3 (5)
O1—Na1—O1 ⁱ	96.91 (13)	C5—C6—C7	119.1 (5)
O1—Na1—N2 ⁱ	122.01 (13)	C2—C7—C6	122.0 (4)
O3—Na1—N2	85.61 (9)	S1—C8—S2	115.2 (3)
O1 ⁱ —Na1—O3	131.54 (8)	S1—C8—N2	124.4 (3)
O3—Na1—N2 ⁱ	85.61 (9)	S2—C8—N2	120.5 (3)
O1 ⁱ —Na1—N2	122.01 (13)	S1—C9—C10	107.6 (4)
N2—Na1—N2 ⁱ	171.22 (15)	S2—C10—C9	107.9 (4)
O1 ⁱ —Na1—N2 ⁱ	64.63 (11)	C3—C4—H4	119.00
Na1—O1—C1	125.5 (3)	C5—C4—H4	119.00
C3—O2—H2	113 (8)	C4—C5—H5	120.00
Na1—O3—H3	125 (3)	C6—C5—H5	120.00
Na1—O3—H3 ⁱ	125 (3)	C5—C6—H6	120.00
H3—O3—H3 ⁱ	111 (4)	C7—C6—H6	120.00
N2—N1—C1	120.6 (3)	C2—C7—H7	119.00
Na1—N2—N1	108.7 (2)	C6—C7—H7	119.00
Na1—N2—C8	135.3 (3)	S1—C9—H9A	110.00
N1—N2—C8	115.4 (4)	S1—C9—H9B	110.00
C1—N1—H1	120.00	C10—C9—H9A	110.00
N2—N1—H1	120.00	C10—C9—H9B	110.00
N1—C1—C2	117.2 (4)	H9A—C9—H9B	108.00

O1—C1—N1	120.6 (4)	S2—C10—H10A	110.00
O1—C1—C2	122.3 (4)	S2—C10—H10B	110.00
C1—C2—C7	117.4 (4)	C9—C10—H10A	110.00
C3—C2—C7	118.8 (4)	C9—C10—H10B	110.00
C1—C2—C3	123.8 (4)	H10A—C10—H10B	108.00
C2—C3—C4	117.8 (4)		
C9—S1—C8—S2	-11.2 (3)	N2—N1—C1—C2	-179.2 (4)
C9—S1—C8—N2	168.7 (4)	Na1—N2—C8—S1	163.7 (2)
C8—S1—C9—C10	35.8 (4)	Na1—N2—C8—S2	-16.4 (6)
C10—S2—C8—S1	-11.6 (3)	N1—N2—C8—S1	-5.8 (5)
C10—S2—C8—N2	168.5 (4)	N1—N2—C8—S2	174.1 (3)
C8—S2—C10—C9	36.2 (4)	O1—C1—C2—C3	-177.5 (4)
O3—Na1—O1—C1	60.2 (4)	O1—C1—C2—C7	0.7 (6)
N2—Na1—O1—C1	2.4 (3)	N1—C1—C2—C3	2.1 (6)
O1 ⁱ —Na1—O1—C1	-119.8 (3)	N1—C1—C2—C7	-179.8 (4)
N2 ⁱ —Na1—O1—C1	175.9 (3)	C1—C2—C3—O2	-2.7 (7)
O1—Na1—N2—N1	-1.8 (2)	C1—C2—C3—C4	176.8 (4)
O1—Na1—N2—C8	-171.8 (5)	C7—C2—C3—O2	179.1 (4)
O3—Na1—N2—N1	-142.4 (2)	C7—C2—C3—C4	-1.4 (6)
O3—Na1—N2—C8	47.6 (4)	C1—C2—C7—C6	-178.4 (4)
O1 ⁱ —Na1—N2—N1	80.2 (3)	C3—C2—C7—C6	-0.1 (7)
O1 ⁱ —Na1—N2—C8	-89.8 (4)	O2—C3—C4—C5	-179.2 (4)
Na1—O1—C1—N1	-2.7 (6)	C2—C3—C4—C5	1.3 (7)
Na1—O1—C1—C2	176.9 (3)	C3—C4—C5—C6	0.3 (8)
C1—N1—N2—Na1	1.5 (4)	C4—C5—C6—C7	-1.8 (8)
C1—N1—N2—C8	173.7 (4)	C5—C6—C7—C2	1.7 (7)
N2—N1—C1—O1	0.4 (6)	S1—C9—C10—S2	-48.2 (4)

Symmetry codes: (i) $-x+1, y, -z+1$; (ii) $-x+1, y+1, -z+2$; (iii) $-x+1/2, y-1/2, -z+1$; (iv) $x-1/2, y+1/2, z$; (v) $-x+1/2, y+1/2, -z+1$; (vi) $x+1/2, y-1/2, z$; (vii) $x, y-1, z$; (viii) $-x+1, y-1, -z+1$; (ix) $-x+1, y, -z+2$; (x) $x, y+1, z$; (xi) $-x+1, y+1, -z+1$; (xii) $-x+1, y-1, -z+2$; (xiii) $-x+3/2, y+1/2, -z+2$; (xiv) $x-1/2, y+3/2, z$; (xv) $-x+3/2, y-1/2, -z+2$; (xvi) $x+1/2, y-3/2, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots S1	0.8800	2.4300	2.880 (4)	112.00
N1—H1 \cdots O2	0.8800	1.8800	2.596 (4)	137.00
O2—H2 \cdots O2 ^{ix}	0.89 (5)	1.61 (9)	2.467 (4)	160 (14)
O3—H3 \cdots O1 ^{xi}	0.95 (4)	1.90 (4)	2.788 (5)	155 (4)
C4—H4 \cdots S1 ^{xii}	0.95	2.86	3.614 (5)	137
C7—H7 \cdots O1	0.95	2.46	2.790 (5)	100
C9—H9A \cdots O1 ^{iv}	0.99	2.57	3.323 (7)	133

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