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Sodium selenite pentahydrate, Na₂SeO₃·5H₂O

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Key indicators: single-crystal X-ray study; T = 100 K; mean σ (Se–O) = 0.001 Å; R factor = 0.015; wR factor = 0.039; data-to-parameter ratio = 16.9.

In the crystal structure of Na₂SeO₃·5H₂O [disodium selenate(IV) pentahydrate], two Se, two selenite O atoms and one water O atom are located on a mirror plane, and one water O atom is located on a twofold rotation axis. The coordination of one Na⁺ cation is distorted trigonal bipyramidal, formed by three equatorial H₂O ligands and two axial selenite O atoms. The other Na⁺ cation has an octahedral coordination by six water molecules. The two independent SeO₃ groups form almost undistorted trigonal pyramids, with Se-O bond lengths in the range 1.6856 (7)–1.7202 (10) Å and O-Se-Oangles in the range 101.98 (3)–103.11 (5)°, and both are μ_2 -O:O-bonded to a pair of Na⁺ cations. Hydrogen bonds involving all water molecules and selenite O atoms consolidate the crystal packing. Although anhydrous Na2SeO3 and Na_2TeO_3 are isotypic, the title compound is surprisingly not isotypic with Na₂TeO₃·5H₂O. In the tellurite hydrate, all Na⁺ cations have an octahedral coordination and the TeO₃ groups are bonded to Na⁺ only via one of their three O atoms.

Related literature

For the crystal structure of Na₂TeO₃·5H₂O, see: Philippot *et al.* (1979). For crystal structure of anhydrous Na₂SeO₃ and Na₂TeO₃, see: Wickleder (2002); Masse et al. (1980). For the crystal structures of the isotypic series MgSO₃·6H₂O, MgSeO₃·6H₂O, MgTeO₃·6H₂O, and Mg(HPO₃)·6H₂O, see: Andersen & Lindqvist (1984); Andersen et al. (1984); Powell et al. (1994). For Na₂(HPO₃)·5H₂O, see: Brodalla et al. (1978). For pharmaceutical aspects of Na₂SeO₃·5H₂O, see: European Pharmacopoeia (2013). For van der Waals radii, see: Rowland & Taylor (1996).

 $V = 1676.70 (10) \text{ Å}^3$

 $0.35 \times 0.21 \times 0.14 \text{ mm}$

23979 measured reflections

2529 independent reflections

2435 reflections with $I > 2\sigma(I)$

Mo $K\alpha$ radiation $\mu = 4.58 \text{ mm}^-$

Z = 8

T = 100 K

 $R_{\rm int} = 0.022$

Experimental

Crystal data

Na ₂ SeO ₃ ·5H ₂ O
$M_r = 263.02$
Orthorhombic, Pbcm
a = 6.5865 (2) Å
b = 17.2263 (6) Å
c = 14.7778 (6) Å

Data collection

Bruker SMART CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2003) $T_{\min} = 0.503, T_{\max} = 0.746$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.015$	70 restraints
$wR(F^2) = 0.039$	All H-atom parameters refined
S = 1.07	$\Delta \rho_{\rm max} = 0.64 \text{ e} \text{ Å}^{-3}$
2529 reflections	$\Delta \rho_{\rm min} = -0.58 \text{ e} \text{ Å}^{-3}$
150 parameters	

Table 1			
Selected	bond	lengths	(Å).

Na1-O7W	2.3266 (9)	$Na2-O7W^{ii}$	2.4056 (9)
Na1-O6W	2.3600 (9)	Na2-O9W	2.5108 (9)
Na1-O2	2.3650 (9)	Se1-O2	1.6857 (7)
Na1-O5W	2.3781 (10)	Se1-O2 ⁱⁱⁱ	1.6857 (7)
Na1-O4	2.4119 (9)	Se1-O1	1.7164 (10)
$Na2 - O9W^{i}$	2.3458 (9)	Se2-O4	1.6856 (7)
Na2-O6W	2.3520 (9)	Se2-O4 ⁱⁱⁱ	1.6856 (7)
Na2-O10W	2.3852 (9)	Se2-O3	1.7202 (10)
Na2-O8W	2.3930 (9)		

Symmetry codes: (i) $x, -y + \frac{1}{2}, -z + 1$; (ii) x - 1, y, z; (iii) $x, y, -z + \frac{3}{2}$.

Table 2	
Hydrogen-bond geometry (Å, °).	

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
O5W−H5A···O3 ^{iv}	0.83 (1)	2.12 (1)	2.9468 (16)	173 (3)
$O5W-H5B\cdots O1^{iv}$	0.83 (1)	2.58 (2)	3.3631 (17)	158 (3)
$O6W-H6A\cdots O1$	0.83 (1)	1.95 (1)	2.7704 (12)	176 (2)
$O6W - H6B \cdot \cdot \cdot O3$	0.83 (1)	2.05(1)	2.8660 (11)	169 (2)
$O7W - H7A \cdots O4^{v}$	0.83 (1)	1.89 (1)	2.7252 (11)	176 (2)
$O7W - H7B \cdot \cdot \cdot O10W^{v}$	0.83 (1)	2.09 (1)	2.8740 (12)	157 (2)
$O8W - H8AB \cdots O2$	0.84(1)	1.96 (1)	2.7744 (9)	166 (1)
$O9W - H9A \cdots O1$	0.83 (1)	1.99 (1)	2.8027 (11)	168 (2)
$O9W - H9B \cdot \cdot \cdot O2^{ii}$	0.83(1)	1.91 (1)	2.7259 (11)	168 (2)
$O10W - H10A \cdots O4^{v}$	0.83 (1)	1.96 (1)	2.7672 (11)	164 (2)
$O10W-H10B\cdots O3^{vi}$	0.83 (1)	2.01 (1)	2.8374 (11)	174 (2)

Symmetry codes: (ii) x - 1, y, z; (iv) x + 1, y, z; (v) -x + 1, -y + 1, -z + 1; (vi) -x, -v + 1, -z + 1

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2012); software used to prepare material for publication: SHELXL97 and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6939).

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supporting information

Acta Cryst. (2013). E69, i77-i78 [doi:10.1107/S1600536813028602]

Sodium selenite pentahydrate, Na₂SeO₃·5H₂O

Kurt Mereiter

S1. Comment

During an investigation of some simple salt hydrates the question for the crystal structure of the title compound Na₂SeO₃.5H₂O arose. Although this solid is a commercial commodity, nutrition supplement, fertilizer additive, and therapeutic substance (European Pharmacopoeia, 2013), its crystallography turned out to be barren land. In order to close this gap, a crystal structure determination of the title compound was carried out.

Fig. 1 shows a characteristic part of the structure. The atoms Se1, O1, Se2, O3, O5w and its two hydrogen atoms H5a and H5b are located on a mirror plane at x, y, 3/4. The water oxygen O8w is located on a twofold axis at x, 1/4, 1/2. All other atoms are in the general position. There are two independent selenite groups in the structure. Both have point symmetry C_s -m and an almost undistorted trigonal pyramidal geometry with Se-O bond distances of 1.6857 (7) – 1.7202 (10) Å (mean value 1.697 (2) Å) and O—Se—O angles of 101.98 (3) – 103.11 (5)° (mean value 102.4 (5)°; Fig. 1 and Table 1). Comparable dimensions have been reported for anhydrous Na₂SeO₃ (Wickleder, 2002), MgSeO₃.6H₂O (Andersen et al., 1984) and numerous other simple selenites. In the title compound the two selenite groups are bonded to a pair of mirror related Na1 atoms, which have a distorted trigonal dipyramidal coordination by three water molecules (O5w, O6w, O7w) in equatorial positions and two selenite oxygen atoms (O2 of Se1 and O4 of Se2) in apical positions. The two pentagonal bipyramids share a common corner *via* the water molecule O5w. Thus a compact group $\{(Na1)_2(H_2O)_3(SeO_3)_2\}$ is formed, which is reinforced by four internal hydrogen bonds donated by O6w and O6wⁱ to O1 and O3 (Fig. 1). The second sodium atom, Na2, has an octahedral coordination by water molecules only. This Na $2(H_2O)_6$ octahedron shares a face with a second Na2 octahedron related by a twofold axis through O8w to form a double octahedron $\{(Na2)_2(H_2O)_9\}$. The two building blocks of the structure, $\{(Na1)_2(H_2O)_5(SeO_3)_2\}$ and $\{(Na2)_2(H_2O)_9\}$, are then mutually linked via four common water molecules (two O6w and two O7w) to form corrugated layers of the composition Na₂SeO₃.5H₂O extending at $y \simeq 1/4$ and $y \simeq 3/4$ parallel to (010). A top and a side view of a Na₂SeO₃.5H₂O layer including hydrogen bonds is depicted in Fig. 2. All water molecules have approximately tetrahedral coordination figures, either by two Na and two hydrogen bond acceptors (O5w, O6w, O7w, O8w, O9w) or by one Na, one hydrogen bond donor and two hydrogen bond acceptors (O10w). Hydrogen bond data given in Table 2 show normal values for all water molecules except O5w, which has one weak and one very weak interaction (O = 2.9468 (16) and 3.3631 (17) Å) with the selenite oxygen atoms O1 and O3 belonging to the same Na₂SeO₃.5H₂O layer. All other hydrogen bonds have O···O distances in the narrow range of 2.7252 (11) to 2.8660 (11) Å with O—H···O angles between 157 (2)° and 176 (2)°. The water molecules of O5w, O6w, O8w (has two symmetry equivalent H-bonds and therefore only one entry in Table 2), and O9w feature exclusively intra-layer hydrogen bonds. Only O7w and O10w donate four inter-layer hydrogen bonds, which explains the observed good cleavage of the crystals along (010). Figures 3, 4 and 5 show projections of the crystal structure. Fig. 3 gives a view parallel to the a axis, this is parallel to two Na₂SeO₃.5H₂O layers. It reveals that the electron lone-pairs of Se1 and Se2 point to an open space between the layers. The shortest distance between adjacent Se atoms of two different Na₂SeO₃.5H₂O layers is Se1...Se2(1 - x, 1/2 - y, 3/2 - z) = 3.438 Å and corresponds to a mutual off-set of the

two Se by 2.152 Å along [100]. This Se1...Se2 distance is *ca* 0.2 Å smaller than the sum of the van der Waals radii for two Se (2×1.80 Å; Rowland & Taylor, 1996) and might indicate a weak mutual interaction.

The crystal structure of anhydrous Na₂SeO₃ is known (Wickleder, 2002). This monoclinic structure can be seen as a distorted NaCl lattice (Masse et al., 1980), where Se replacing one out of three Na is shifted along a body diagonal of the NaCl lattice so that it has only three facial instead of six octahedral Se-O bonds while two Na atoms maintain their octahedral NaO₆ coordination of the NaCl lattice. In reality the oxygen atoms are shifted more than Na and Se because they compensate arising voids and bond length differences between <Na-O> = 2.48 Å and <Se-O> = 1.70 Å. Anhydrous Na₂TeO₃ (Masse et al., 1980) is isostructural with Na₂SeO₃ but is more regular because of the larger size of Te (<Te-O> = 1.88 Å) within the host lattice of the NaO₆ octahedra with <Na-O> = 2.50 Å. Both salts furnish on crystallization from water pentahydrates, namely the title compound Na₂SeO₃.5H₂O and Na₂TeO₃.5H₂O. In view of the isomorphism of the anhydrous couple it is somewhat unexpected that Na₂TeO₃.5H₂O does not adopt the crystal structure of the title compound or vice versa. The tellurite hydrate crystallizes in the monoclinic space group C2/c (Philippot et al., 1979). It features a framework structure of the composition $Na_4(H_2O)_{10}(TeO_3)_2$ containing three different kinds of Na. Two of these Na have relative regular octahedral coordination figures by water molecules and form infinite chains $Na_3(H_2O)_{10} \equiv (H_2O)_3Na_1(H_2O)_3Na_2(H_2O)_3Na_1$ with two face- and one edge-sharing links per section. A third kind of Na with a strongly deformed centrosymmetric octahedral coordination by four H₂O and two O bridges the chains via four corner-sharing links and carries simultaneously two TeO₃ groups bonded to it η^1 -O-mode, *i.e. via* only one of their three O atoms. A reasonable alternative for the structures of Na₂SeO₃.5H₂O and Na₂TeO₃.5H₂O could be the structure of Na₂(HPO₃).5H₂O, a phosphonate with a layered structure of Na(H₂O)₅ square pyramids, Na(H₂O)₅(O) octahedra, and n^{1} -O-bonded HPO₃ groups linked together only via shared edges and corners (Brodalla et al., 1978). In it the P-bonded phosphonate H atom occupies that space which the electron lone-pair lobes of Se or Te would favour. A proof for this concept and good example for a single common structure type of four different pyramidal XO_3^{2-} anions is the series MgSO₃.6H₂O (Andersen & Lindqvist, 1984), MgSeO₃.6H₂O (Andersen et al., 1984), MgTeO₃.6H₂O (Andersen et al., 1984), and Mg(HPO₃).6H₂O (Powell et al., 1994) consisting of Mg(H₂O)₆ octahedra and XO₃ pyramids (disregarding the H in HPO₃) bound together by an elastic system of hydrogen bonds into a trigonal lattice of space group R3.

S2. Experimental

 Na_2SeO_3 (p.A. Merck) was dissolved in a small amount of deionized water. The solution was then slowly evaporated at T ≈ 285 K and gave after seeding colourless prsimatic crystals of $Na_2SeO_3.5H_2O$, which were placed of filter paper in order to remove adherent mother liquor. A crystal was then immediately mounted under Paratone oil on a MiTeGen MicroLoopTM and transferred to a Bruker SMART APEX diffractometer equipped with a Bruker Kryoflex cooler.

S3. Refinement

All hydrogen atoms were clearly visible in a difference Fourier synthesis and refined satisfactorily without restraints. In the final refinement all water molecules were restrained to have similar O—H and similar intramolecular H···H distances using two SADI ($\sigma = 0.01$ Å) restraints (Sheldrick, 2008). The isotropic U_{iso} (H) were freely refined.



View of a characteristic part of the crystal structure of Na₂SeO₃.5H₂O. Thermal displacement ellipsoids are shown at the 70% probability level. Symmetry operators are given on the lower right.



Two perspective representations of one Na₂SeO₃.5H₂O layer parallel to (010) at $y \sim 1/4$, viewed along [010] (top) and along [100] (bottom). Hydrogen bonds are indicated by blue lines. Symmetry operators are given on the lower right.



Projection of the structure of $Na_2SeO_3.5H_2O$ along [100] with hydrogen bonds shown as dashed lines. Symmetry codes and the letter O for oxygen atoms have been omitted for legibility.



Projection of the structure of Na₂SeO₃.5H₂O parallel to [010] with hydrogen bonds shown as dashed lines. Some coinciding sites have been labeled as guidance.



Figure 5

Projection of the structure of Na₂SeO₃.5H₂O parallel to [001] with hydrogen bonds shown as dashed lines. Symmetry codes and the letter O for oxygen atoms have been omitted for legibility.

Disodium selenate(IV) pentahydrate

Crystal data	
Na ₂ SeO ₃ ·5H ₂ O	Orthorhombic, Pbcm
$M_r = 263.02$	Hall symbol: -P 2c 2b

Mo *K* α radiation, $\lambda = 0.71073$ Å

 $\theta = 2.4 - 30.0^{\circ}$

 $\mu = 4.58 \text{ mm}^{-1}$ T = 100 K

Prism, colourless

 $0.35 \times 0.21 \times 0.14 \text{ mm}$

Cell parameters from 7917 reflections

a = 6.5865 (2) Å b = 17.2263 (6) Å c = 14.7778 (6) Å V = 1676.70 (10) Å³ Z = 8 F(000) = 1040 $D_x = 2.084$ Mg m⁻³

Data collection

Bruker SMART CCD	23979 measured reflections
diffractometer	2529 independent reflections
Radiation source: fine-focus sealed tube	2435 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.022$
ω and φ scans	$\theta_{\rm max} = 30.0^\circ, \theta_{\rm min} = 2.4^\circ$
Absorption correction: multi-scan	$h = -9 \rightarrow 9$
(SADABS; Bruker, 2003)	$k = -22 \rightarrow 24$
$T_{\min} = 0.503, \ T_{\max} = 0.746$	$l = -20 \rightarrow 16$

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier Least-squares matrix: full map $R[F^2 > 2\sigma(F^2)] = 0.015$ Hydrogen site location: inferred from $wR(F^2) = 0.039$ neighbouring sites S = 1.07All H-atom parameters refined 2529 reflections $w = 1/[\sigma^2(F_o^2) + (0.0224P)^2 + 0.7143P]$ 150 parameters where $P = (F_o^2 + 2F_c^2)/3$ 70 restraints $(\Delta/\sigma)_{\rm max} = 0.003$ $\Delta \rho_{\rm max} = 0.64 \ {\rm e} \ {\rm \AA}^{-3}$ Primary atom site location: structure-invariant $\Delta \rho_{\rm min} = -0.58 \ {\rm e} \ {\rm \AA}^{-3}$ direct methods

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 $F^2 > \sigma(F^2)$ 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 eq	uivalent	isotropic	displacemen	t parameters	(Å	2)
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	x	y	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Nal	0.51942 (7)	0.40815 (3)	0.62757 (3)	0.01543 (9)	
Na2	0.00865 (7)	0.34328 (2)	0.49775 (3)	0.01121 (8)	
Se1	0.36729 (2)	0.233898 (8)	0.7500	0.00946 (4)	
01	0.13882 (15)	0.28182 (7)	0.7500	0.01128 (19)	
O2	0.48606 (11)	0.27444 (4)	0.66069 (5)	0.01294 (14)	
Se2	0.30596 (2)	0.578291 (8)	0.7500	0.00853 (4)	
O3	0.08542 (15)	0.52480 (6)	0.7500	0.01135 (19)	
O4	0.43189 (11)	0.54110 (4)	0.66066 (5)	0.01209 (14)	
O5W	0.7537 (2)	0.41001 (7)	0.7500	0.0182 (2)	
H5A	0.840 (3)	0.4453 (11)	0.7500	0.051 (9)*	

H5B	0.821 (4)	0.3692 (10)	0.7500	0.112 (17)*	
O6W	0.16164 (12)	0.40116 (4)	0.62475 (6)	0.01327 (15)	
H6A	0.149 (3)	0.3651 (7)	0.6612 (9)	0.030 (5)*	
H6B	0.142 (3)	0.4410 (6)	0.6550 (10)	0.038 (5)*	
O7W	0.73311 (12)	0.43467 (5)	0.50608 (5)	0.01336 (14)	
H7A	0.682 (2)	0.4442 (10)	0.4557 (8)	0.030 (4)*	
H7B	0.783 (2)	0.4762 (7)	0.5234 (10)	0.030 (4)*	
O8W	0.27783 (17)	0.2500	0.5000	0.0132 (2)	
H8AB	0.3565 (17)	0.2526 (12)	0.5444 (5)	0.035 (5)*	
O9W	-0.12523 (11)	0.24467 (5)	0.60772 (6)	0.01310 (15)	
H9A	-0.053 (2)	0.2498 (10)	0.6531 (9)	0.030 (5)*	
H9B	-0.2434 (15)	0.2472 (11)	0.6262 (11)	0.035 (5)*	
O10W	0.17400 (12)	0.42733 (5)	0.39277 (6)	0.01412 (15)	
H10A	0.2910 (15)	0.4283 (10)	0.3722 (11)	0.031 (5)*	
H10B	0.099 (2)	0.4383 (11)	0.3494 (9)	0.030 (5)*	

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0141 (2)	0.0175 (2)	0.0148 (2)	-0.00088 (16)	0.00163 (16)	0.00129 (16)
Na2	0.01154 (18)	0.01093 (18)	0.01114 (19)	0.00028 (14)	-0.00033 (14)	-0.00044 (14)
Se1	0.00905 (7)	0.01022 (7)	0.00911 (7)	0.00145 (4)	0.000	0.000
01	0.0073 (4)	0.0151 (5)	0.0114 (5)	0.0017 (4)	0.000	0.000
O2	0.0110 (3)	0.0179 (4)	0.0099 (3)	0.0010 (3)	0.0022 (3)	0.0016 (3)
Se2	0.00845 (7)	0.00848 (7)	0.00867 (7)	-0.00085 (4)	0.000	0.000
03	0.0080 (4)	0.0127 (5)	0.0133 (5)	-0.0022 (4)	0.000	0.000
O4	0.0111 (3)	0.0150 (3)	0.0101 (3)	-0.0005 (3)	0.0018 (3)	-0.0014 (3)
O5W	0.0184 (5)	0.0175 (6)	0.0186 (6)	-0.0028 (5)	0.000	0.000
O6W	0.0166 (4)	0.0106 (4)	0.0126 (4)	-0.0008 (3)	-0.0011 (3)	-0.0007 (3)
O7W	0.0151 (3)	0.0140 (3)	0.0110 (3)	0.0005 (3)	-0.0004 (3)	0.0001 (3)
O8W	0.0116 (5)	0.0181 (5)	0.0099 (5)	0.000	0.000	-0.0010 (4)
O9W	0.0092 (3)	0.0189 (4)	0.0112 (3)	-0.0001 (3)	0.0004 (3)	-0.0018 (3)
O10W	0.0108 (3)	0.0183 (4)	0.0132 (4)	-0.0008 (3)	0.0001 (3)	0.0022 (3)

Geometric parameters (Å, °)

Na1—O7W	2.3266 (9)	Se2—O3	1.7202 (10)
Na1—O6W	2.3600 (9)	O5W—Na1 ⁱⁱⁱ	2.3781 (10)
Na1—O2	2.3650 (9)	O5W—H5A	0.831 (10)
Na1—O5W	2.3781 (10)	O5W—H5B	0.833 (10)
Na1—O4	2.4119 (9)	O6W—H6A	0.826 (9)
Na2—O9W ⁱ	2.3458 (9)	O6W—H6B	0.830 (9)
Na2—O6W	2.3520 (9)	O7W—Na2 ^{iv}	2.4057 (9)
Na2—O10W	2.3852 (9)	O7W—H7A	0.833 (9)
Na2—O8W	2.3930 (9)	O7W—H7B	0.829 (9)
Na2—O7W ⁱⁱ	2.4056 (9)	O8W—Na2 ⁱ	2.3930 (9)
Na2—O9W	2.5108 (9)	O8W—H8AB	0.837 (8)
Sel—O2	1.6857 (7)	O9W—Na2 ⁱ	2.3457 (9)

Se1—O2 ⁱⁱⁱ	1.6857 (7)	O9W—H9A	0.825 (9)
Sel—O1	1.7164 (10)	O9W—H9B	0.826 (9)
Se2—O4	1.6856 (7)	O10W—H10A	0.828 (9)
Se2—O4 ⁱⁱⁱ	1.6856 (7)	O10W—H10B	0.829 (9)
07W—Na1—06W	126 90 (3)	Na1—O5W—Na1 ⁱⁱⁱ	99.06 (5)
07W—Na1— 02	11403(3)	Na1—O5W—H5A	1169(10)
06W—Na1— 02	82 02 (3)	Nal ⁱⁱⁱ —O5W—H5A	116.9(10)
0.00 Na1 -0.5 W	101.06(4)	Na1—O5W—H5B	109.6(13)
O6W—Na1— $O5W$	131.46 (4)	Na1 ⁱⁱⁱ —O5W—H5B	109.6(13)
02—Na1— $05W$	85.18 (4)	H5A—O5W—H5B	104.6 (15)
07W—Na1—04	96.58 (3)	Na2—O6W—Na1	117.62 (4)
O6W—Na1—O4	79.24 (3)	Na2—O6W—H6A	99.2 (11)
02—Na1—O4	149.39 (3)	Na1—O6W—H6A	97.2 (12)
O5W—Na1—O4	89.32 (4)	Na2—O6W—H6B	135.6 (12)
O9W ⁱ —Na2—O6W	164.81 (3)	Na1—O6W—H6B	95.9 (13)
O9W ⁱ —Na2—O10W	97.56 (3)	H6A—O6W—H6B	104.8 (12)
O6W—Na2—O10W	93.79 (3)	Na1—O7W—Na2 ^{iv}	111.55 (3)
O9W ⁱ —Na2—O8W	81.60 (3)	Na1—O7W—H7A	119.0 (12)
O6W—Na2—O8W	87.49 (3)	Na2 ^{iv} —O7W—H7A	112.8 (12)
O10W—Na2—O8W	94.49 (3)	Na1—O7W—H7B	99.9 (12)
O9W ⁱ —Na2—O7W ⁱⁱ	99.97 (3)	Na2 ^{iv} —O7W—H7B	106.4 (12)
O6W—Na2—O7W ⁱⁱ	90.29 (3)	H7A—O7W—H7B	105.4 (12)
O10W—Na2—O7W ⁱⁱ	88.88 (3)	H8AB ⁱ —O8W—Na2 ⁱ	115.7 (11)
O8W—Na2—O7W ⁱⁱ	176.07 (3)	H8AB ⁱ —O8W—Na2	118.9 (12)
O9W ⁱ —Na2—O9W	82.01 (3)	Na2 ⁱ —O8W—Na2	84.39 (4)
O6W—Na2—O9W	85.46 (3)	H8AB ⁱ —O8W—H8AB	103.5 (14)
O10W—Na2—O9W	172.76 (3)	Na2 ⁱ —O8W—H8AB	118.9 (12)
O8W—Na2—O9W	78.28 (3)	Na2—O8W—H8AB	115.7 (11)
O7W ⁱⁱ —Na2—O9W	98.32 (3)	Na2 ⁱ —O9W—Na2	82.82 (3)
O2 ⁱⁱⁱ —Se1—O2	103.06 (5)	Na2 ⁱ —O9W—H9A	113.2 (12)
O2 ⁱⁱⁱ —Se1—O1	101.98 (3)	Na2—O9W—H9A	104.5 (12)
O2—Se1—O1	101.98 (3)	Na2 ⁱ —O9W—H9B	127.4 (12)
Se1—O2—Na1	127.49 (4)	Na2—O9W—H9B	120.6 (13)
O4 ⁱⁱⁱ —Se2—O4	103.11 (5)	H9A—O9W—H9B	105.5 (12)
O4 ⁱⁱⁱ —Se2—O3	102.24 (3)	Na2—O10W—H10A	132.5 (12)
O4—Se2—O3	102.24 (3)	Na2—O10W—H10B	111.7 (12)
Se2—O4—Na1	129.59 (4)	H10A—O10W—H10B	105.2 (12)

Symmetry codes: (i) *x*, -*y*+1/2, -*z*+1; (ii) *x*-1, *y*, *z*; (iii) *x*, *y*, -*z*+3/2; (iv) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	Н…А	D····A	<i>D</i> —H… <i>A</i>
O5 <i>W</i> —H5 <i>A</i> ···O3 ^{iv}	0.83 (1)	2.12 (1)	2.9468 (16)	173 (3)
O5W—H5B···O1 ^{iv}	0.83 (1)	2.58 (2)	3.3631 (17)	158 (3)
O6 <i>W</i> —H6 <i>A</i> ···O1	0.83 (1)	1.95 (1)	2.7704 (12)	176 (2)
O6 <i>W</i> —H6 <i>B</i> ···O3	0.83 (1)	2.05 (1)	2.8660 (11)	169 (2)

supporting information

a a a (4)	4 9 9 (4)		
0.83 (1)	1.89 (1)	2.7252 (11)	176 (2)
0.83 (1)	2.09 (1)	2.8740 (12)	157 (2)
0.84 (1)	1.96 (1)	2.7744 (9)	166 (1)
0.83 (1)	1.99 (1)	2.8027 (11)	168 (2)
0.83 (1)	1.91 (1)	2.7259 (11)	168 (2)
0.83 (1)	1.96 (1)	2.7672 (11)	164 (2)
0.83 (1)	2.01 (1)	2.8374 (11)	174 (2)
	0.83 (1) 0.83 (1) 0.84 (1) 0.83 (1) 0.83 (1) 0.83 (1) 0.83 (1)	$\begin{array}{cccc} 0.83 \ (1) & 1.89 \ (1) \\ 0.83 \ (1) & 2.09 \ (1) \\ 0.84 \ (1) & 1.96 \ (1) \\ 0.83 \ (1) & 1.99 \ (1) \\ 0.83 \ (1) & 1.91 \ (1) \\ 0.83 \ (1) & 1.96 \ (1) \\ 0.83 \ (1) & 2.01 \ (1) \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Symmetry codes: (ii) *x*-1, *y*, *z*; (iv) *x*+1, *y*, *z*; (v) -*x*+1, -*y*+1, -*z*+1; (vi) -*x*, -*y*+1, -*z*+1.