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# Sodium selenite pentahydrate, $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot \mathbf{5 \mathrm { H } _ { 2 } \mathrm { O }}$ 

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Key indicators: single-crystal X-ray study; $T=100 \mathrm{~K}$; mean $\sigma(\mathrm{Se}-\mathrm{O})=0.001 \AA$; $R$ factor $=0.015 ; w R$ factor $=0.039$; data-to-parameter ratio $=16.9$.

In the crystal structure of $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ [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 $\mathrm{Na}^{+}$cation is distorted trigonal bipyramidal, formed by three equatorial $\mathrm{H}_{2} \mathrm{O}$ ligands and two axial selenite O atoms. The other $\mathrm{Na}^{+}$cation has an octahedral coordination by six water molecules. The two independent $\mathrm{SeO}_{3}$ groups form almost undistorted trigonal pyramids, with $\mathrm{Se}-\mathrm{O}$ bond lengths in the range 1.6856 (7)-1.7202 (10) $\AA$ and $\mathrm{O}-\mathrm{Se}-\mathrm{O}$ angles in the range 101.98 (3) $-103.11(5)^{\circ}$, and both are $\mu_{2^{-}}$ $O: O$-bonded to a pair of $\mathrm{Na}^{+}$cations. Hydrogen bonds involving all water molecules and selenite O atoms consolidate the crystal packing. Although anhydrous $\mathrm{Na}_{2} \mathrm{SeO}_{3}$ and $\mathrm{Na}_{2} \mathrm{TeO}_{3}$ are isotypic, the title compound is surprisingly not isotypic with $\mathrm{Na}_{2} \mathrm{TeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$. In the tellurite hydrate, all $\mathrm{Na}^{+}$ cations have an octahedral coordination and the $\mathrm{TeO}_{3}$ groups are bonded to $\mathrm{Na}^{+}$only via one of their three O atoms.

## Related literature

For the crystal structure of $\mathrm{Na}_{2} \mathrm{TeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$, see: Philippot et al. (1979). For crystal structure of anhydrous $\mathrm{Na}_{2} \mathrm{SeO}_{3}$ and $\mathrm{Na}_{2} \mathrm{TeO}_{3}$, see: Wickleder (2002); Masse et al. (1980). For the crystal structures of the isotypic series $\mathrm{MgSO}_{3} \cdot 6 \mathrm{H}_{2} \mathrm{O}$, $\mathrm{MgSeO}_{3} \cdot 6 \mathrm{H}_{2} \mathrm{O}, \mathrm{MgTeO}_{3} \cdot 6 \mathrm{H}_{2} \mathrm{O}$, and $\mathrm{Mg}\left(\mathrm{HPO}_{3}\right) \cdot 6 \mathrm{H}_{2} \mathrm{O}$, see: Andersen \& Lindqvist (1984); Andersen et al. (1984); Powell et al. (1994). For $\mathrm{Na}_{2}\left(\mathrm{HPO}_{3}\right) \cdot 5 \mathrm{H}_{2} \mathrm{O}$, see: Brodalla et al. (1978). For pharmaceutical aspects of $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$, see: European Pharmacopoeia (2013). For van der Waals radii, see: Rowland \& Taylor (1996).

## Experimental

Crystal data
$\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$
$M_{r}=263.02$
Orthorhombic, Pbcm
$a=6.5865$ (2) $\AA$
$b=17.2263$ (6) A
$c=14.7778$ (6) $\AA$

## Data collection

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

## Refinement

$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.015$
$w R\left(F^{2}\right)=0.039$
$S=1.07$
2529 reflections
150 parameters
$V=1676.70(10) \AA^{3}$
$Z=8$
Mo $K \alpha$ radiation
$\mu=4.58 \mathrm{~mm}^{-1}$
$T=100 \mathrm{~K}$
$0.35 \times 0.21 \times 0.14 \mathrm{~mm}$

23979 measured reflections 2529 independent reflections 2435 reflections with $I>2 \sigma(I)$ $R_{\text {int }}=0.022$

70 restraints
All H -atom parameters refined
$\Delta \rho_{\text {max }}=0.64 \mathrm{e}^{-3}$
$\Delta \rho_{\text {min }}=-0.58 \mathrm{e}^{-3}$

Table 1
Selected bond lengths ( $\AA$ ).

| $\mathrm{Na} 1-\mathrm{O} 7 W$ | $2.3266(9)$ | $\mathrm{Na} 2-\mathrm{O} 7 W^{\mathrm{ii}}$ | $2.4056(9)$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{Na} 1-\mathrm{O} 6 W$ | $2.3600(9)$ | $\mathrm{Na} 2-\mathrm{O} 9 W^{2}$ | $2.5108(9)$ |
| $\mathrm{Na} 1-\mathrm{O} 2$ | $2.3650(9)$ | $\mathrm{Se} 1-\mathrm{O} 2$ | $1.6857(7)$ |
| $\mathrm{Na} 1-\mathrm{O} 5 W$ | $2.3781(10)$ | $\mathrm{Se} 1-\mathrm{O} 2^{\text {iii }}$ | $1.6857(7)$ |
| $\mathrm{Na} 1-\mathrm{O} 4$ | $2.4119(9)$ | $\mathrm{Se} 1-\mathrm{O} 1$ | $1.7164(10)$ |
| $\mathrm{Na} 2-\mathrm{O} 9 W^{\mathrm{i}}$ | $2.3458(9)$ | $\mathrm{Se} 2-\mathrm{O} 4$ | $1.6856(7)$ |
| $\mathrm{Na} 2-\mathrm{O} 6 W$ | $2.3520(9)$ | $\mathrm{Se} 2-\mathrm{O} 4^{\mathrm{iii}}$ | $1.6856(7)$ |
| $\mathrm{Na} 2-\mathrm{O} 10 W$ | $2.3852(9)$ | $\mathrm{Se} 2-\mathrm{O} 3$ | $1.7202(10)$ |
| $\mathrm{Na} 2-\mathrm{O} 8 W$ | $2.3930(9)$ |  |  |

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 ( $\AA^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | D-H | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{O} 5 W-\mathrm{H} 54 \cdots \mathrm{O} 3^{\text {iv }}$ | 0.83 (1) | 2.12 (1) | 2.9468 (16) | 173 (3) |
| $\mathrm{O} 5 W-\mathrm{H} 5 B \cdots \mathrm{O} 1^{\text {iv }}$ | 0.83 (1) | 2.58 (2) | 3.3631 (17) | 158 (3) |
| $\mathrm{O} 6 W-\mathrm{H} 6 A \cdots \mathrm{O} 1$ | 0.83 (1) | 1.95 (1) | 2.7704 (12) | 176 (2) |
| $\mathrm{O} 6 W-\mathrm{H} 6 B \cdots \mathrm{O}$ | 0.83 (1) | 2.05 (1) | 2.8660 (11) | 169 (2) |
| $\mathrm{O} 7 W-\mathrm{H} 7 A \cdots \mathrm{O} 4^{\text {v }}$ | 0.83 (1) | 1.89 (1) | 2.7252 (11) | 176 (2) |
| $\mathrm{O} 7 W-\mathrm{H} 7 B \cdots \mathrm{O} 10 W^{\mathrm{v}}$ | 0.83 (1) | 2.09 (1) | 2.8740 (12) | 157 (2) |
| $\mathrm{O} 8 W-\mathrm{H} 8 A B \cdots \mathrm{O} 2$ | 0.84 (1) | 1.96 (1) | 2.7744 (9) | 166 (1) |
| $\mathrm{O} 9 W-\mathrm{H} 9 A \cdots \mathrm{O} 1$ | 0.83 (1) | 1.99 (1) | 2.8027 (11) | 168 (2) |
| $\mathrm{O} 9 W-\mathrm{H} 9 \mathrm{~B} \cdots \mathrm{O} 2^{\text {ii }}$ | 0.83 (1) | 1.91 (1) | 2.7259 (11) | 168 (2) |
| $\mathrm{O} 10 W-\mathrm{H} 10 A \cdots \mathrm{O}^{\text {v }}$ | 0.83 (1) | 1.96 (1) | 2.7672 (11) | 164 (2) |
| $\mathrm{O} 10 W-\mathrm{H} 10 \mathrm{~B} \cdots \mathrm{O}^{\text {vi }}$ | 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) $-x,-y+1,-z+1$.

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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## inorganic compounds

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, $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$

## Kurt Mereiter

## S1. Comment

During an investigation of some simple salt hydrates the question for the crystal structure of the title compound $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ 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 $\mathrm{Se} 1, \mathrm{O} 1, \mathrm{Se} 2, \mathrm{O}, \mathrm{O} 5 \mathrm{w}$ and its two hydrogen atoms H 5 a and H 5 b are located on a mirror plane at $x, y, 3 / 4$. The water oxygen O 8 w 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 $C_{\mathrm{s}}-\mathrm{m}$ and an almost undistorted trigonal pyramidal geometry with $\mathrm{Se}-\mathrm{O}$ bond distances of 1.6857 (7) 1.7202 (10) $\AA$ (mean value 1.697 (2) $\AA$ ) and $\mathrm{O}-\mathrm{Se}-\mathrm{O}$ angles of 101.98 (3) - 103.11 (5) ${ }^{\circ}$ (mean value 102.4 (5) ${ }^{\circ}$; Fig. 1 and Table 1). Comparable dimensions have been reported for anhydrous $\mathrm{Na}_{2} \mathrm{SeO}_{3}$ (Wickleder, 2002), $\mathrm{MgSeO}_{3} .6 \mathrm{H}_{2} \mathrm{O}$ (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 ( $\mathrm{O} 5 \mathrm{w}, \mathrm{O} 6 \mathrm{w}, \mathrm{O} 7 \mathrm{w}$ ) in equatorial positions and two selenite oxygen atoms ( O 2 of Se 1 and O 4 of Se 2 ) in apical positions. The two pentagonal bipyramids share a common corner via the water molecule O5w. Thus a compact group $\left\{(\mathrm{Na} 1)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{5}\left(\mathrm{SeO}_{3}\right)_{2}\right\}$ is formed, which is reinforced by four internal hydrogen bonds donated by O 6 w and $\mathrm{O}^{\mathrm{w}}{ }^{\mathrm{i}}$ to O 1 and O3 (Fig. 1). The second sodium atom, Na 2 , has an octahedral coordination by water molecules only. This $\mathrm{Na} 2\left(\mathrm{H}_{2} \mathrm{O}\right)_{6}$ octahedron shares a face with a second Na 2 octahedron related by a twofold axis through O 8 w to form a double octahedron $\left\{(\mathrm{Na} 2)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{9}\right\}$. The two building blocks of the structure, $\left\{(\mathrm{Na} 1)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{5}\left(\mathrm{SeO}_{3}\right)_{2}\right\}$ and $\left\{(\mathrm{Na} 2)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{9}\right\}$, are then mutually linked via four common water molecules (two O6w and two O 7 w ) to form corrugated layers of the composition $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ extending at $y \simeq 1 / 4$ and $y \simeq 3 / 4$ parallel to ( 010 ). A top and a side view of a $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ 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 O 5 w , which has one weak and one very weak interaction $(\mathrm{O} \cdots \mathrm{O}=2.9468$ (16) and 3.3631 (17) $\AA$ ) with the selenite oxygen atoms O 1 and O 3 belonging to the same $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ layer. All other hydrogen bonds have $\mathrm{O} \cdots \mathrm{O}$ distances in the narrow range of 2.7252 (11) to $2.8660(11) \AA$ with $\mathrm{O}-\mathrm{H} \cdots \mathrm{O}$ angles between 157 (2) ${ }^{\circ}$ and 176 (2) ${ }^{\circ}$. The water molecules of O5w, O6w, O8w (has two symmetry equivalent H -bonds and therefore only one entry in Table 2), and O 9 w feature exclusively intra-layer hydrogen bonds. Only O 7 w and O 10 w 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 $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ layers. It reveals that the electron lone-pairs of Se 1 and Se 2 point to an open space between the layers. The shortest distance between adjacent Se atoms of two different $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ layers is $\mathrm{Se} 1 \cdots \mathrm{Se} 2(1-x, 1 / 2-y, 3 / 2-z)=3.438 \AA$ and corresponds to a mutual off-set of the
two Se by $2.152 \AA$ along [100]. This $\operatorname{Se} 1 \cdots \mathrm{Se} 2$ distance is ca $0.2 \AA$ smaller than the sum of the van der Waals radii for two Se ( $2 \times 1.80 \AA$; Rowland \& Taylor, 1996) and might indicate a weak mutual interaction.
The crystal structure of anhydrous $\mathrm{Na}_{2} \mathrm{SeO}_{3}$ 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 $\mathrm{Se}-\mathrm{O}$ bonds while two Na atoms maintain their octahedral $\mathrm{NaO}_{6}$ 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 $<\mathrm{Na}-\mathrm{O}>=2.48 \AA$ and $<\mathrm{Se}-\mathrm{O}>=1.70 \AA$. Anhydrous $\mathrm{Na}_{2} \mathrm{TeO}_{3}$ (Masse et al., 1980) is isostructural with $\mathrm{Na}_{2} \mathrm{SeO}_{3}$ but is more regular because of the larger size of Te ( $<\mathrm{Te}-\mathrm{O}>=1.88 \AA$ ) within the host lattice of the $\mathrm{NaO}_{6}$ octahedra with $<\mathrm{Na}-\mathrm{O}>=2.50 \AA$. Both salts furnish on crystallization from water pentahydrates, namely the title compound $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ and $\mathrm{Na}_{2} \mathrm{TeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$. In view of the isomorphism of the anhydrous couple it is somewhat unexpected that $\mathrm{Na}_{2} \mathrm{TeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ 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 $\mathrm{Na}_{4}\left(\mathrm{H}_{2} \mathrm{O}\right)_{10}\left(\mathrm{TeO}_{3}\right)_{2}$ containing three different kinds of Na . Two of these Na have relative regular octahedral coordination figures by water molecules and form infinite chains $\mathrm{Na}_{3}\left(\mathrm{H}_{2} \mathrm{O}\right)_{10} \equiv\left(\mathrm{H}_{2} \mathrm{O}\right)_{3} \mathrm{Na} 1\left(\mathrm{H}_{2} \mathrm{O}\right)_{3} \mathrm{Na} 2\left(\mathrm{H}_{2} \mathrm{O}\right)_{3} \mathrm{Na} 1$ with two face- and one edge-sharing links per section. A third kind of Na with a strongly deformed centrosymmetric octahedral coordination by four $\mathrm{H}_{2} \mathrm{O}$ and two O bridges the chains via four corner-sharing links and carries simultaneously two $\mathrm{TeO}_{3}$ groups bonded to it $\eta^{1}$-O-mode, i.e. via only one of their three O atoms. A reasonable alternative for the structures of $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ and $\mathrm{Na}_{2} \mathrm{TeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ could be the structure of $\mathrm{Na}_{2}\left(\mathrm{HPO}_{3}\right) .5 \mathrm{H}_{2} \mathrm{O}$, a phosphonate with a layered structure of $\mathrm{Na}\left(\mathrm{H}_{2} \mathrm{O}\right)_{5}$ square pyramids, $\mathrm{Na}\left(\mathrm{H}_{2} \mathrm{O}\right)_{5}(\mathrm{O})$ octahedra, and $\eta^{1}-$ O-bonded $\mathrm{HPO}_{3}$ 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 $\mathrm{XO}_{3}{ }^{2-}$ anions is the series $\mathrm{MgSO}_{3} .6 \mathrm{H}_{2} \mathrm{O}$ (Andersen \& Lindqvist, 1984), $\mathrm{MgSeO}_{3} .6 \mathrm{H}_{2} \mathrm{O}$ (Andersen et al., 1984), $\mathrm{MgTeO}_{3} .6 \mathrm{H}_{2} \mathrm{O}$ (Andersen et al., 1984), and $\mathrm{Mg}\left(\mathrm{HPO}_{3}\right) \cdot 6 \mathrm{H}_{2} \mathrm{O}$ (Powell et al., 1994) consisting of $\mathrm{Mg}\left(\mathrm{H}_{2} \mathrm{O}\right)_{6}$ octahedra and $\mathrm{XO}_{3}$ pyramids (disregarding the H in $\mathrm{HPO}_{3}$ ) bound together by an elastic system of hydrogen bonds into a trigonal lattice of space group $R 3$.

## S2. Experimental

$\mathrm{Na}_{2} \mathrm{SeO}_{3}$ (p.A. Merck) was dissolved in a small amount of deionized water. The solution was then slowly evaporated at T $\simeq 285 \mathrm{~K}$ and gave after seeding colourless prsimatic crystals of $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$, 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 MicroLoop ${ }^{\mathrm{TM}}$ 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 $\mathrm{O}-\mathrm{H}$ and similar intramolecular $\mathrm{H} \cdots \mathrm{H}$ distances using two SADI ( $\sigma=0.01 \AA$ ) restraints (Sheldrick, 2008). The isotropic $U_{\mathrm{iso}}(\mathrm{H})$ were freely refined.


Figure 1
View of a characteristic part of the crystal structure of $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$. Thermal displacement ellipsoids are shown at the $70 \%$ probability level. Symmetry operators are given on the lower right.


Figure 2
Two perspective representations of one $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ 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.


Figure 3
Projection of the structure of $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ along [100] with hydrogen bonds shown as dashed lines. Symmetry codes and the letter O for oxygen atoms have been omitted for legibility.


Figure 4
Projection of the structure of $\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ 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 $\mathrm{Na}_{2} \mathrm{SeO}_{3} .5 \mathrm{H}_{2} \mathrm{O}$ 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

$\mathrm{Na}_{2} \mathrm{SeO}_{3} \cdot 5 \mathrm{H}_{2} \mathrm{O}$
Orthorhombic, Pbcm
$M_{r}=263.02$
Hall symbol: -P 2c 2b
$a=6.5865(2) \AA$
$b=17.2263$ (6) $\AA$
$c=14.7778$ (6) $\AA$
$V=1676.70(10) \AA^{3}$
$Z=8$
$F(000)=1040$
$D_{\mathrm{x}}=2.084 \mathrm{Mg} \mathrm{m}^{-3}$

## Data collection

## Bruker SMART CCD

diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan
(SADABS; Bruker, 2003)
$T_{\min }=0.503, T_{\text {max }}=0.746$

## Refinement

Refinement on $F^{2}$
Least-squares matrix: full
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.015$
$w R\left(F^{2}\right)=0.039$
$S=1.07$
2529 reflections
150 parameters
70 restraints
Primary atom site location: structure-invariant direct methods

Mo $K \alpha$ radiation, $\lambda=0.71073 \AA$
Cell parameters from 7917 reflections
$\theta=2.4-30.0^{\circ}$
$\mu=4.58 \mathrm{~mm}^{-1}$
$T=100 \mathrm{~K}$
Prism, colourless
$0.35 \times 0.21 \times 0.14 \mathrm{~mm}$

23979 measured reflections
2529 independent reflections
2435 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.022$
$\theta_{\text {max }}=30.0^{\circ}, \theta_{\text {min }}=2.4^{\circ}$
$h=-9 \rightarrow 9$
$k=-22 \rightarrow 24$
$l=-20 \rightarrow 16$

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

## All H-atom parameters refined

$$
w=1 /\left[\sigma^{2}\left(F_{0}^{2}\right)+(0.0224 P)^{2}+0.7143 P\right]
$$

$$
\text { where } P=\left(F_{0}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3
$$

$(\Delta / \sigma)_{\max }=0.003$
$\Delta \rho_{\text {max }}=0.64 \mathrm{e}^{\AA^{-3}}$
$\Delta \rho_{\text {min }}=-0.58$ e $\AA^{-3}$

## Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two 1.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 $w R$ 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 $F^{2}>\sigma\left(F^{2}\right)$ is used only for calculating $R$-factors $(\mathrm{gt})$ 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 ( $\AA^{2}$ )

|  | $x$ | $y$ | $z$ | $U_{\text {iso }} * / U_{\mathrm{eq}}$ |
| :--- | :--- | :--- | :--- | :--- |
| Na 1 | $0.51942(7)$ | $0.40815(3)$ | $0.62757(3)$ | $0.01543(9)$ |
| Na 2 | $0.00865(7)$ | $0.34328(2)$ | $0.49775(3)$ | $0.01121(8)$ |
| Se 1 | $0.36729(2)$ | $0.233898(8)$ | 0.7500 | $0.00946(4)$ |
| O 1 | $0.13882(15)$ | $0.28182(7)$ | 0.7500 | $0.01128(19)$ |
| O 2 | $0.48606(11)$ | $0.27444(4)$ | $0.66069(5)$ | $0.01294(14)$ |
| Se 2 | $0.30596(2)$ | $0.578291(8)$ | 0.7500 | $0.00853(4)$ |
| O 3 | $0.08542(15)$ | $0.52480(6)$ | 0.7500 | $0.01135(19)$ |
| O 4 | $0.43189(11)$ | $0.54110(4)$ | $0.66066(5)$ | $0.01209(14)$ |
| O5W | $0.7537(2)$ | $0.41001(7)$ | 0.7500 | $0.0182(2)$ |
| H 5 A | $0.840(3)$ | $0.4453(11)$ | 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 $\left(\AA^{2}\right)$

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Na1 | $0.0141(2)$ | $0.0175(2)$ | $0.0148(2)$ | $-0.00088(16)$ | $0.00163(16)$ | $0.00129(16)$ |
| Na 2 | $0.01154(18)$ | $0.01093(18)$ | $0.01114(19)$ | $0.00028(14)$ | $-0.00033(14)$ | $-0.00044(14)$ |
| Se1 | $0.00905(7)$ | $0.01022(7)$ | $0.00911(7)$ | $0.00145(4)$ | 0.000 | 0.000 |
| O1 | $0.0073(4)$ | $0.0151(5)$ | $0.0114(5)$ | $0.0017(4)$ | 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 |
| O3 | $0.0080(4)$ | $0.0127(5)$ | $0.0133(5)$ | $-0.0022(4)$ | 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 ( $A,{ }^{\circ}$ )

| Na1-O7W | 2.3266 (9) | Se2-O3 | 1.7202 (10) |
| :---: | :---: | :---: | :---: |
| Na1-06W | 2.3600 (9) | O5W-Na1 ${ }^{\text {iii }}$ | 2.3781 (10) |
| $\mathrm{Na} 1-\mathrm{O} 2$ | 2.3650 (9) | O5W—H5A | 0.831 (10) |
| Na1-O5W | 2.3781 (10) | O5W-H5B | 0.833 (10) |
| Na - O 4 | 2.4119 (9) | O6W-H6A | 0.826 (9) |
| Na2-O9W ${ }^{\text {i }}$ | 2.3458 (9) | O6W-H6B | 0.830 (9) |
| Na2-O6W | 2.3520 (9) | $\mathrm{O} 7 \mathrm{~W}-\mathrm{Na} 2^{\text {iv }}$ | 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 ${ }^{\text {ii }}$ | 2.4056 (9) | O8W-Na2 ${ }^{\text {i }}$ | 2.3930 (9) |
| Na2-O9W | 2.5108 (9) | O8W-H8AB | 0.837 (8) |
| Se1-O2 | 1.6857 (7) | $\mathrm{O} 9 \mathrm{~W}-\mathrm{Na} 2^{\text {i }}$ | 2.3457 (9) |


| $\mathrm{Se} 1-\mathrm{O} 2^{\text {iii }}$ | 1.6857 (7) |
| :---: | :---: |
| $\mathrm{Se} 1-\mathrm{O} 1$ | 1.7164 (10) |
| Se2-O4 | 1.6856 (7) |
| $\mathrm{Se} 2-\mathrm{O} 4{ }^{\text {iii }}$ | 1.6856 (7) |
| O7W-Na1-O6W | 126.90 (3) |
| O7W-Na1-O2 | 114.03 (3) |
| O6W-Na1-O2 | 82.02 (3) |
| O7W-Na1-O5W | 101.06 (4) |
| O6W-Na1-O5W | 131.46 (4) |
| O2-Na1-O5W | 85.18 (4) |
| $\mathrm{O} 7 \mathrm{~W}-\mathrm{Na} 1-\mathrm{O} 4$ | 96.58 (3) |
| O6W-Na1-O4 | 79.24 (3) |
| O2-Na1-O4 | 149.39 (3) |
| $\mathrm{O} 5 \mathrm{~W}-\mathrm{Na} 1-\mathrm{O} 4$ | 89.32 (4) |
| O9W ${ }^{\text {i }}$ - $\mathrm{Na} 2-06 \mathrm{~W}$ | 164.81 (3) |
| O9W ${ }^{\text {i }}$ - $\mathrm{Na} 2-\mathrm{O} 10 \mathrm{~W}$ | 97.56 (3) |
| O6W-Na2-O10W | 93.79 (3) |
| O9W ${ }^{\text {i }}$ - $\mathrm{Na} 2-\mathrm{O} 8 \mathrm{~W}$ | 81.60 (3) |
| O6W-Na2-O8W | 87.49 (3) |
| O10W-Na2-O8W | 94.49 (3) |
| O9W ${ }^{\text {i }}$ - $\mathrm{Na} 2-\mathrm{O} 7 \mathrm{~W}^{\text {ii }}$ | 99.97 (3) |
| O6W-Na2-O7W ${ }^{\text {ii }}$ | 90.29 (3) |
| $\mathrm{O} 10 \mathrm{~W}-\mathrm{Na} 2-\mathrm{O} 7 \mathrm{~W}^{\text {ii }}$ | 88.88 (3) |
| O8W-Na2-O7W ${ }^{\text {ii }}$ | 176.07 (3) |
| O9W ${ }^{\text {i }}$ - $\mathrm{Na} 2-\mathrm{O} 9 \mathrm{~W}$ | 82.01 (3) |
| O6W-Na2-O9W | 85.46 (3) |
| O10W-Na2-O9W | 172.76 (3) |
| O8W-Na2-O9W | 78.28 (3) |
| O7W ${ }^{\text {iil }}$ - $\mathrm{Na} 2-\mathrm{O} 9 \mathrm{~W}$ | 98.32 (3) |
| $\mathrm{O} 2{ }^{\text {iii }}-\mathrm{Se} 1-\mathrm{O} 2$ | 103.06 (5) |
| $\mathrm{O} 2{ }^{\text {iii }}$ - $\mathrm{Se} 1-\mathrm{O} 1$ | 101.98 (3) |
| $\mathrm{O} 2-\mathrm{Se} 1-\mathrm{O} 1$ | 101.98 (3) |
| $\mathrm{Se} 1-\mathrm{O} 2-\mathrm{Na} 1$ | 127.49 (4) |
| O4iii- ${ }^{\text {iii }}$ - $2-04$ | 103.11 (5) |
| $\mathrm{O} 4{ }^{\text {iii }}-\mathrm{Se} 2-\mathrm{O} 3$ | 102.24 (3) |
| O4-Se2-O3 | 102.24 (3) |
| $\mathrm{Se} 2-\mathrm{O} 4-\mathrm{Na} 1$ | 129.59 (4) |


| O9W—H9A | $0.825(9)$ |
| :--- | :--- |
| O9W—H9B | $0.826(9)$ |
| O10W—H10A | $0.828(9)$ |
| O10W—H10B | $0.829(9)$ |

99.06 (5)
116.9 (10)
116.9 (10)
109.6 (13)
109.6 (13)
104.6 (15)
117.62 (4)
99.2 (11)
97.2 (12)
135.6 (12)
95.9 (13)
104.8 (12)
111.55 (3)
119.0 (12)
112.8 (12)
99.9 (12)
106.4 (12)
105.4 (12)
115.7 (11)
118.9 (12)
84.39 (4)
103.5 (14)
118.9 (12)
115.7 (11)
82.82 (3)
113.2 (12)
104.5 (12)
127.4 (12)
120.6 (13)
105.5 (12)
132.5 (12)
111.7 (12)
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 (A, ${ }^{\circ}$ )

| $D-\mathrm{H} \cdots A$ | D-H | $\mathrm{H} \cdots \mathrm{A}$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{O} 5 W-\mathrm{H} 5 A \cdots \mathrm{O} 3^{\text {iv }}$ | 0.83 (1) | 2.12 (1) | 2.9468 (16) | 173 (3) |
| $\mathrm{O} 5 W-\mathrm{H} 5 B \cdots \mathrm{O} 1^{\text {iv }}$ | 0.83 (1) | 2.58 (2) | 3.3631 (17) | 158 (3) |
| O6 $W$ - $\mathrm{H} 6 A \cdots \mathrm{O} 1$ | 0.83 (1) | 1.95 (1) | 2.7704 (12) | 176 (2) |
| $\mathrm{O} 6 W-\mathrm{H} 6 B^{\cdots} \mathrm{O} 3$ | 0.83 (1) | 2.05 (1) | 2.8660 (11) | 169 (2) |


| $\mathrm{O} 7 W-\mathrm{H} 7 A \cdots \mathrm{O} 4^{\text {v }}$ | 0.83 (1) | 1.89 (1) | 2.7252 (11) | 176 (2) |
| :---: | :---: | :---: | :---: | :---: |
| $\mathrm{O} 7 W-\mathrm{H} 7 B \cdots \mathrm{O} 10 W^{\sim}$ | 0.83 (1) | 2.09 (1) | 2.8740 (12) | 157 (2) |
| $\mathrm{O} 8 W-\mathrm{H} 8 A B \cdots \mathrm{O} 2$ | 0.84 (1) | 1.96 (1) | 2.7744 (9) | 166 (1) |
| $\mathrm{O} 9 W-\mathrm{H} 9 A \cdots \mathrm{O} 1$ | 0.83 (1) | 1.99 (1) | 2.8027 (11) | 168 (2) |
| $\mathrm{O} 9 W-\mathrm{H} 9 B \cdots \mathrm{O} 2^{\mathrm{ii}}$ | 0.83 (1) | 1.91 (1) | 2.7259 (11) | 168 (2) |
| $\mathrm{O} 10 W-\mathrm{H} 10 A \cdots \mathrm{O} 4^{\text {v }}$ | 0.83 (1) | 1.96 (1) | 2.7672 (11) | 164 (2) |
| $\mathrm{O} 10 W-\mathrm{H} 10 B^{\cdots} \mathrm{O}^{\text {vi }}$ | 0.83 (1) | 2.01 (1) | 2.8374 (11) | 174 (2) |

[^0]
[^0]:    Symmetry codes: (ii) $x-1, y, z$; (iv) $x+1, y, z$; (v) $-x+1,-y+1,-z+1$; (vi) $-x,-y+1,-z+1$.

