

Sodium selenite, Na<sub>2</sub>SeO<sub>3</sub>

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## Key indicators

Single-crystal X-ray study

T = 293 K

Mean  $\sigma(\text{Se}-\text{O}) = 0.004 \text{ \AA}$ 

R factor = 0.031

wR factor = 0.072

Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, Na<sub>2</sub>SeO<sub>3</sub>, contains two crystallographically different Na<sup>+</sup> ions, Na1 and Na2. Na1 is coordinated by four monodentate and one chelating SeO<sub>3</sub><sup>2-</sup> group, while two monodentate and two chelating selenite ions are attached to Na2. For both Na<sup>+</sup> ions, a strongly distorted octahedral coordination results. The [NaO<sub>6</sub>] octahedra are linked *via* common edges. The SeO<sub>3</sub><sup>2-</sup> ion shows a pyramidal shape, due to the lone electron pair of the Se atom.

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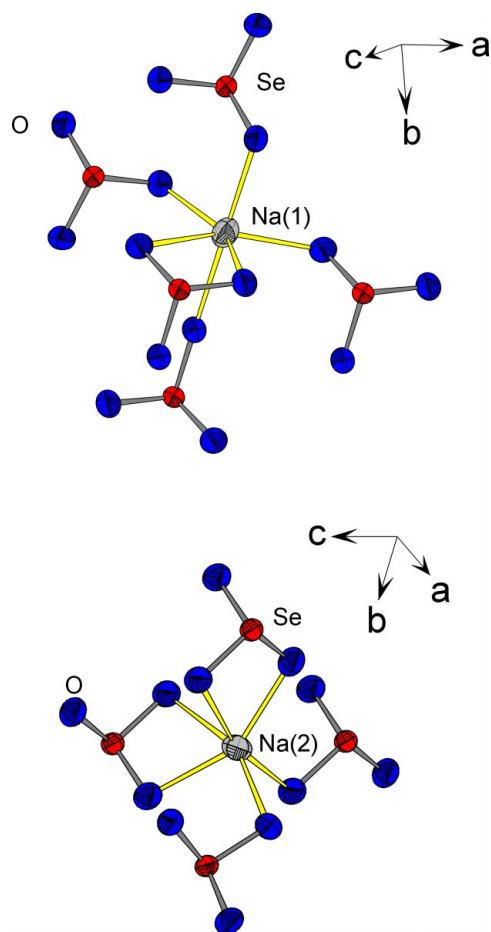
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## Comment

Recently, Helmholdt *et al.* (1999) solved the crystal structure of Na<sub>2</sub>SeO<sub>3</sub> from powder diffraction data. Although the main features of the crystal structure are correctly described, there are some unusual bond lengths reported, especially for the SeO<sub>3</sub><sup>2-</sup> ion. The Se—O distances vary from 1.676 (11) to 1.779 (14) Å, but there is no structural reason for such a large range. In order to obtain more precise results, we decided to perform a single-crystal structure investigation. It turned out that well shaped single crystals are best obtained from the reaction of Na<sub>2</sub>O and SeO<sub>2</sub>. According to the structure determination, Na<sub>2</sub>SeO<sub>3</sub> is isotypic with Ag<sub>2</sub>SeO<sub>3</sub> (Okkonen *et al.*, 1994) and contains two crystallographically different Na<sup>+</sup> ions. Na1 is surrounded by four monodentate and one chelating selenite ion (Fig. 1). Two chelating and two monodentate SeO<sub>3</sub><sup>2-</sup> groups are attached to Na2 (Fig. 1). For both Na<sup>+</sup> ions, this leads to strongly distorted octahedra as coordination polyhedra. The Na—O distances within the octahedra range from 2.346 (4) to 2.664 (4) Å (Table 1). The [NaO<sub>6</sub>] octahedra are linked *via* common edges, to form a three-dimensional network (Fig. 2). The SeO<sub>3</sub><sup>2-</sup> ion exhibits the typical pyramidal shape, due to the lone electron pair of the Se atom. The O—Se—O angles are between 100.4 (2) and 102.7 (2)°. In contrast to previously reported results, the Se—O distances are very similar, with a range from 1.685 (4) to 1.705 (4) Å. The SeO<sub>3</sub><sup>2-</sup> ion is coordinated by five Na1 and four Na2 ions.

## Experimental

A mixture of the finely powdered oxides Na<sub>2</sub>O and SeO<sub>2</sub> (molar ratio 1:1) was sealed in a gold ampoule, which was placed in a silica tube. The tube was heated to 573 K with a resistance furnace. After 24 h, the temperature was raised to 773 K, followed by slow cooling (5 K h<sup>-1</sup>) to 303 K. The slightly moisture-sensitive, colourless crystals were handled in an argon-filled glove-box, and an appropriate specimen was mounted in a glass capillary for the X-ray investigation.



**Figure 1**  
Coordination of Na1 and Na2 in the crystal structure of  $\text{Na}_2\text{SeO}_3$ . Note that some of the selenite groups act as chelating ligands. Displacement ellipsoids are drawn at the 90% probability level.

#### Crystal data

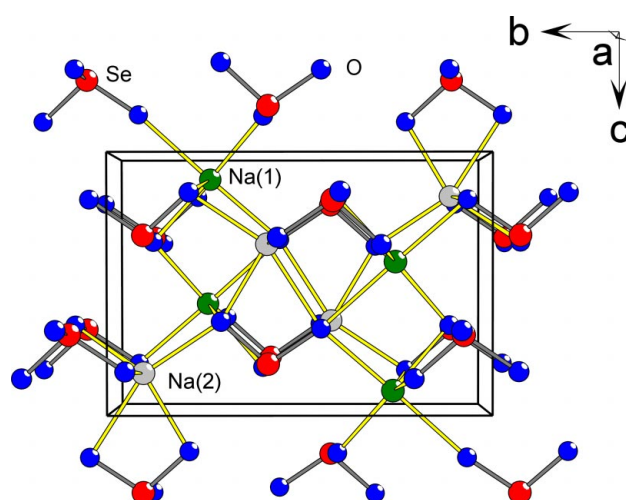
$\text{Na}_2\text{SeO}_3$	$D_x = 3.413 \text{ Mg m}^{-3}$
$M_r = 172.94$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2000 reflections
$a = 4.9089 (13) \text{ \AA}$	$\theta = 3.0\text{--}28.0^\circ$
$b = 10.0072 (15) \text{ \AA}$	$\mu = 11.22 \text{ mm}^{-1}$
$c = 6.8535 (15) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 91.11 (3)^\circ$	Column, colourless
$V = 336.61 (13) \text{ \AA}^3$	$0.25 \times 0.17 \times 0.11 \text{ mm}$
$Z = 4$	

#### Data collection

Stoe IPDS-I diffractometer	808 independent reflections
$\varphi$ scans	571 reflections with $I > 2\sigma(I)$
Absorption correction: numerical with crystal-shape optimization ( <i>X-SHAPE</i> ; Stoe & Cie, 1999)	$R_{\text{int}} = 0.069$
$T_{\text{min}} = 0.115$ , $T_{\text{max}} = 0.291$	$\theta_{\text{max}} = 28.1^\circ$
3856 measured reflections	$h = -6 \rightarrow 6$
	$k = -12 \rightarrow 13$
	$l = -9 \rightarrow 8$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.90 \text{ e \AA}^{-3}$
808 reflections	$\Delta\rho_{\text{min}} = -1.32 \text{ e \AA}^{-3}$
55 parameters	



**Figure 2**  
Perspective view of the crystal structure of  $\text{Na}_2\text{SeO}_3$  along  $[100]$ . The  $[\text{NaO}_6]$  octahedra are connected *via* common edges.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Na1—O3 <sup>i</sup>	2.347 (4)	Na2—O1 <sup>iv</sup>	2.438 (4)
Na1—O3 <sup>ii</sup>	2.373 (4)	Na2—O2 <sup>vi</sup>	2.473 (5)
Na1—O2	2.408 (4)	Na2—O1 <sup>v</sup>	2.516 (4)
Na1—O1 <sup>iii</sup>	2.518 (5)	Na2—O1	2.664 (4)
Na1—O1 <sup>iv</sup>	2.650 (4)	Se1—O3	1.685 (4)
Na1—O2 <sup>ii</sup>	2.657 (5)	Se1—O1	1.703 (4)
Na2—O3 <sup>v</sup>	2.354 (5)	Se1—O2	1.705 (4)
Na2—O2	2.391 (5)		
O3—Se1—O1	102.22 (18)	O1—Se1—O2	102.66 (18)
O3—Se1—O2	100.35 (18)		

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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