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**A note on the structure of Na<sub>2</sub>SeO<sub>4</sub>.** By A. KÁLMÁN\* and D. W. J. CRUICKSHANK, *Department of Chemistry, University of Manchester Institute of Science and Technology, Manchester M60 1QD, England*

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Improved coordinates for Na<sub>2</sub>SeO<sub>4</sub> are given. The SeO<sub>4</sub> tetrahedron is almost regular; the Se–O distance is 1.654 ± 0.021 Å.

The crystal structure of sodium selenate was determined by Náray-Szabó & Argay (1963) using the fact that it is isomorphous with Na<sub>2</sub>SO<sub>4</sub> (V-thenardite). The space group is *Fddd* (no. 70) with  $a = 6.099 \pm 0.006$ ,  $b = 12.590 \pm 0.016$ ,  $c = 10.163 \pm 0.012$  Å,  $Z = 8$ . The structure consists of sodium cations occupying the  $(\frac{1}{2}, \frac{1}{2}, z)$  16-fold position and isolated SeO<sub>4</sub><sup>2-</sup> tetrahedra which have the selenium atom at one of the eightfold positions  $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ .

The  $z$  parameter for sodium and the  $x$ ,  $y$ , and  $z$  parameters for oxygen were determined by a Fourier synthesis for the *OkI* projection and a difference Fourier section at the height of  $x/a = -0.03$ . The final residual  $R$  was 14.3%. As the atoms were assumed to have the same common isotropic vibration parameter and as no standard deviations were given, it appeared worth while to attempt to refine the structure for comparison with other orthoselenates.

The data used in the refinement were the 127 non-zero  $|F_o|$  obtained from the original intensities, which were kindly offered by Náray-Szabó & Argay. The reflexions on the layers  $h = 0, 1, 2, 3$  were on independent scales. The parameters varied were the four scale factors, coordinates, an isotropic vibrational parameter for selenium and anisotropic parameters for sodium and oxygen. The form factors for neutral atoms were taken from *International Tables for X-ray Crystallography* (1962). Five cycles of full-matrix least-squares refinement reduced  $R$  to 11.0%. Owing to the small number of reflexions, and because the maximum value of the index  $h$  was only 3, no better weighting scheme than  $w = \text{const.}$  could be used. The effect of the low  $h_{\text{max}}$  is apparent in the high estimated standard deviation for the oxygen  $x$  coordinate which is shown together with the other coordinates in Table 1 (for comparison,  $k_{\text{max}} = 16$ ,  $l_{\text{max}} = 12$ ). Table 2 gives the bond lengths and angles with their e.s.d.'s. The sodium–oxygen distances are given in Table 3.

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Table 1. *Coordinates with their e.s.d.'s*

	$x/a$	$y/b$	$z/c$
Se	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
Na	$\frac{1}{2}$	$\frac{1}{2}$	0.4410 (15)
O	-0.0316 (43)	0.0509 (13)	0.2211 (17)

Table 3. *Sodium–oxygen interatomic distances*

Na( $x, y, z$ )...O( $x, y, z$ )	2.60 Å
O( $\frac{1}{4} - x, \frac{1}{4} - y, z$ )	2.60
O( $-x, \frac{1}{4} + y, \frac{1}{4} + z$ )	2.31
O( $\frac{1}{4} + x, -y, \frac{1}{4} + z$ )	2.31
O( $\frac{1}{2} + x, \frac{1}{4} - y, \frac{3}{4} - z$ )	2.46
O( $-\frac{1}{4} - x, y, \frac{3}{4} - z$ )	2.46

The SeO<sub>4</sub><sup>2-</sup> anion has crystallographic 222 symmetry but is a regular tetrahedron within experimental error. The uncorrected value of the Se–O bond length, 1.654 ± 0.021 Å, is similar to the vibrationally corrected Se–O mean distances 1.643 ± 0.008 Å in Cu(NH<sub>3</sub>)<sub>2</sub>SeO<sub>4</sub> [derived from Morosin (1969)] and 1.644 ± 0.010 Å in K<sub>2</sub>SeO<sub>4</sub> (Kálmán, Stephens & Cruickshank, 1969).

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Table 2. *Interatomic distances and angles with their e.s.d.'s*

Se–O	1.654 (21) Å	O(1)–Se–O(2)	109.5 (1.2)°
O(1)···O(2)	2.701 (24)	O(1)–Se–O(3)	111.4 (0.9)
O(1)···O(3)	2.732 (31)	O(1)–Se–O(4)	107.6 (0.9)
O(1)···O(4)	2.669 (31)		