Fig. 2. The $BCo(H_2O)W_{11}O_{39}^{6-}$ anion, $\bar{4}$ symmetry (one orientation), c-axis projection.

Kuznetsova, 1981), including the $PV_2Mo_{10}O_{40}^{5-}$ anion in its sodium salt (Sergienko, Detusheva, Yurchenko & Porai-Koshits, 1981). In the present case, our alternative model assumes that the anion has the Keggin structure, with a disordered Co atom, and has crystallographic symmetry $\bar{4}$ (Fig. 2). The $4/m$ site is then occupied by two equally weighted anions related by inversion at the B atom. The act of inversion (here equivalent to reflection in the plane $z = 0$) brings the heavy-atom set into near self-coincidence. The less strongly scattering set of O atoms is brought into rougher self-coincidence, *except* for the atoms of the BO_4 group. These coincidences generate the $4/m$ structure shown in Fig. 1. The interatomic distances which result from refinement in this model are given in Table 2(b). As usual, the lengths of M–O bonds increase with the coordination number of the O atom. The values are reasonable in view of the implicit double disorder, except for the bond to the terminal atom

O(4A) which appears to be somewhat misplaced. The possible presence of a Keggin anion in two orientations was apparently not considered in the case of $H_{3+n}[PV_nMo_{12-n}O_{40}].30–36H_2O$, or in that of $(NBu_4)_3[\gamma\text{-}PW_{12}O_{40}]$ (Fuchs, Thiele & Palm, 1982) where the anion lies at an inversion centre in space group $P\bar{1}$.

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Structure of Strontium Selenate, SrSeO4

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Abstract. $M_r = 230.58$, monoclinic, space group $P2_1/n$, $a = 6.853$ (1), $b = 7.352$ (1), $c = 7.102$ (2) Å, $\beta = 103.43$ (1)°, $V = 348.0$ (1) Å^3, $Z = 4$, $D_x = 4.401$ (1) Mg m^{-3}, $F(000) = 416$, $\lambda(Mo\,K\alpha) = 0.7107$ Å, $\mu(Mo\,K\alpha) = 25.23$ mm^{-1}, $T = 291$ K. Single crystals were obtained by hydrothermal syn-

thesis (10 MPa, 573 K). 964 unique reflections gave $wR = 0.041$. The crystal is ionic, with SeO_4^{2-} tetrahedra and Sr^{2+} ions. The mean Se—O distance in the SeO_4^{2-} ion is 1.647 (6) Å. The Sr atom is ninefold coordinated by O atoms at distances of 2.567–2.976 Å.

Introduction. In connection with studies on phase transitions of the compound $SrSeO_3$, crystal-growth experiments by hydrothermal synthesis led to the formation of single crystals of $SrSeO_3$ and $SrSeO_4$. The last compound results from the reaction:

$$SrSeO_3 + NaNO_3 \longrightarrow SrSeO_4 + NaNO_2.$$
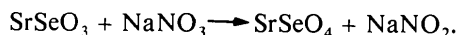
No single-crystal data being available, a structure determination has been undertaken.

Experimental. Crystals grown by hydrothermal synthesis (573 K, 10 MPa) from a mixture of SeO_2, $Sr(NO_3)_2$, NaOH and H_2O; transparent with well defined planar faces. Crystal chosen: rectangular prism, $0.09 \times 0.09 \times 0.1$ mm. Lattice parameters by least squares from the angular settings of 25 reflections measured on a Syntex $R3$ diffractometer (monochromatic Mo $K\alpha$ radiation). Data collection: θ–2θ scans, background–peak–background, $2\theta \le 65°$, hkl range from $0,0,\overline{10}$ to $10,11,10$, comprising 1260 accessible reflections in one quadrant of reciprocal space. $0kl$ and $0k\overline{l}$ reflections merged ($R_{int} = 0.022$), leaving 964 observed unique reflections with $I > 2.5\sigma(I)$. Two check reflections $(21\overline{1}, 023)$ measured at intervals of 100 reflections showed intensity variation of $\pm 4.6\%$. Empirical absorption correction (ψ scans of four reflections) and Lorentz – polarization corrections; minimum transmission 0.31 (taking maximum transmission as unity). Sr and Se atoms located by checking the results of direct methods against a Patterson synthesis, O atoms from Fourier maps. Refinement on $|F|$ with anisotropic temperature factors by cascade-matrix least squares gave $wR = 0.041$, $R = 0.042$, $w = 1/\sigma^2(F)$, and $S = 2.82$ for 55 refined parameters. Max. (mean) $\Delta/\sigma = 0.03$ (0.01), largest $\Delta\rho$ excursions $+1.17$ and -2.03 e Å^3. Calculations on a Nova 3 computer, plots on a Tektronix plotter. *SHELXTL* program system (Sheldrick, 1981), scattering factors from *International Tables for X-ray Crystallography* (1974), anomalous dispersion taken into account.

Discussion. Final atomic coordinates are listed in Table 1.* Selected interatomic distances are given in Table 2. The structure may be described in terms of nearly regular SeO_4^{2-} tetrahedra linked by Sr^{2+} ions. The

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38904 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

slight distortion of the SeO_4^{2-} tetrahedron [bond angles varying from 104.4 (3) to 113.3 (3)°, Table 2] is of the order of magnitude of that observed for the CrO_4^{2-} tetrahedron (Quareni & De Pieri, 1965). The mean Se—O interatomic distance of 1.647 (6) Å is in good agreement with the average value found in orthorhombic transition-metal selenates $MSeO_4$ ($M =$ Mn, Co, Ni) and confirms evidence for multiple bonds in the SeO_4^{2-} ion (Fuess & Will, 1968). However, the double-bond contribution is slightly smaller than that found for the sulfate ion (Pauling, 1960).

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å$^2 \times 10^3$)

U is defined as $U = \frac{1}{3}$ trace $\tilde{U}$, $\tilde{U}$ signifying the diagonalized U matrix.

	x	y	z	U
Sr	1015 (1)	3429 (1)	7774 (1)	8 (1)
Se	6140 (1)	3351 (1)	8054 (1)	9 (1)
O(1)	7150 (10)	2810 (8)	6227 (9)	14 (2)
O(2)	4440 (9)	4966 (8)	7519 (10)	14 (2)
O(3)	8055 (9)	3931 (9)	9800 (9)	14 (2)
O(4)	5007 (9)	1623 (8)	8835 (8)	13 (2)

Table 2. *Selected interatomic distances* (Å) *and bond angles* (°) *in the* SeO_4^{2-} *ion with e.s.d.'s in parentheses*

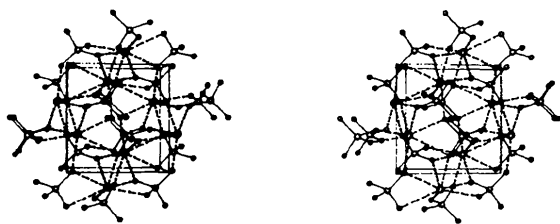| Sr—O(1)	2.771 (7)	Se—O(1)	1.655 (7)
O(2)	2.660 (6)	O(2)	1.645 (6)
O(3)	2.567 (6)	O(3)	1.639 (6)
O(4)	2.722 (6)	O(4)	1.650 (6)
O(4')	2.976 (6)	O(1)—Se—O(2)	113.3 (3)
O(1')	2.649 (7)	O(1)—Se—O(3)	104.4 (3)
O(2')	2.634 (6)	O(1)—Se—O(4)	113.2 (3)
O(3')	2.575 (6)	O(2)—Se—O(3)	112.7 (3)
O(4'')	2.562 (6)	O(2) Se—O(4)	105.7 (3)
		O(3) Se—O(4)	107.6 (3)
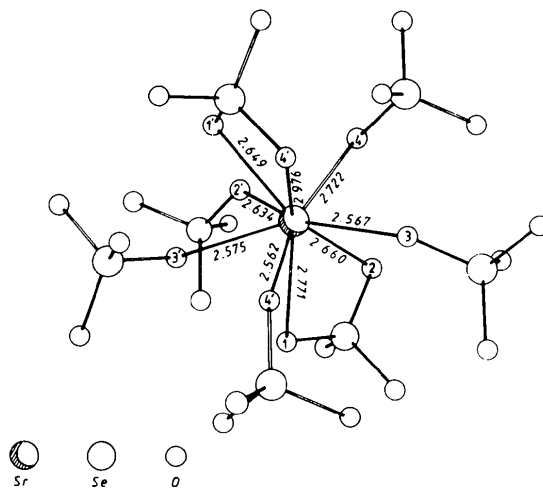
Fig. 1. The coordination of the Sr atoms. (Distances in Å.)

Fig. 2. Stereoview of SrSeO₄ structure along **c**.

The Sr atom is surrounded by nine O atoms belonging to seven different SeO_4 tetrahedra (Fig. 1), at distances ranging from 2·567 (7) to 2·976 (7) Å (Table 2). Fig. 2 shows a stereoview of the structure.

Space group $P2_1/n$ confirms that SrSeO₄ is of the monazite type as previously deduced from powder data (Pistorius & Pistorius, 1962). Cell data have been published for the other members of this important structural type including the phosphate and arsenate of the rare earths (Ln = La − Gd) (Wyckoff, 1960).

However, atomic parameters derived from single-crystal analysis have only been published for CePO₄ (Ueda, 1953; Mooney-Slater, 1962) and PbCrO₄ (Quareni & De Pieri, 1964), owing to the difficulty in obtaining single crystals from either a melt or a precipitate.

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