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References

AIKI, K., HUKUDA, K., KOGA, H. & KOBAYASHI, T. (1970). *J. Phys. Soc. Jpn*, **28**, 389–394.

COPPENS, P., GURU ROW, T. N., LEUNG, P., STEVENS, E. D., BECKER, P. J. & YANG, Y. W. (1979). *Acta Cryst.* A**35**, 63–72.

COPPENS, P. & HAMILTON, W. C. (1970). *Acta Cryst.* A**26**, 71–83.

CRUICKSHANK, D. W. J. (1956). *Acta Cryst.* **9**, 747–756.

GATTOW, G. (1962). *Acta Cryst.* **15**, 419.

GESI, K. & IIZUMI, M. (1979). *J. Phys. Soc. Jpn Lett.* **46**, 697–698.

GIBBS, G. V., CHIARI, G., LOUISNATHAN, S. J. & CRUICKSHANK, D. W. J. (1976). *Z. Kristallogr.* **143**, 166–176.

HOSHINO, S., VEDAM, K., OKAYA, Y. & PEPINSKY, R. (1958). *Phys. Rev.* **112**, 405–412.

IIZUMI, M., AXE, J. D., SHIRANE, G. & SHIMAOKA, K. (1977). *Phys. Rev. B*, **15**, 4392–4411.

IIZUMI, M. & GESI, K. (1977). *Solid State Commun.* **22**, 37–39.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

KALMAN, A., STEPHENS, J. S. & CRUICKSHANK, D. W. J. (1970). *Acta Cryst.* B**26**, 1451–1454.

MAKITA, Y., SAWADA, A. & TAKAGI, Y. (1976). *J. Phys. Soc. Jpn*, **41**, 167–173.

ONODERA, A., CYNSHI, O. & SHIOZAKI, Y. (1985). *J. Phys. C*, **18**, 2831–2841.

ONODERA, A. & SHIOZAKI, Y. (1981). *Ferroelectrics*, **31**, 27–36.

PAULING, L. (1960). *The Nature of the Chemical Bond*, p. 518. Ithaca, New York: Cornell Univ. Press.

SAWADA, A., MAKITA, Y. & TAKAGI, Y. (1976). *J. Phys. Soc. Jpn*, **41**, 174–180.

SHANNON, R. D. & PREWITT, C. T. (1969). *Acta Cryst.* B**25**, 925–946.

STRUKOV, B. A., SKOMOROKHOVA, T. L., KOPSTIK, V. A., BOIKO, A. A. & IZRAILENKO, A. N. (1973). *Sov. Phys. Crystallogr.* **18**, 86–88.

UNRUH, H. G. (1970). *Solid State Commun.* **8**, 1951–1954.

Acta Cryst. (1987). C**43**, 182–184

Structure of Strontium Diselenite

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Abstract. $SrSe_2O_5$, $M_r = 325{\cdot}54$, triclinic, $P\bar{1}$, $a = 6{\cdot}916\,(1)$, $b = 6{\cdot}971\,(1)$, $c = 10{\cdot}875\,(2)$ Å, $\alpha = 85{\cdot}07\,(1)$, $\beta = 81{\cdot}46\,(1)$, $\gamma = 79{\cdot}56\,(1)°$, $V = 509{\cdot}0$ Å^3, $Z = 4$, $D_x = 4{\cdot}25$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}710688$ Å, $\mu = 24{\cdot}32$ mm^{-1}, $F(000) = 584$, room temperature, $R = 0{\cdot}035$ for 3753 observed reflections up to $\sin\theta/\lambda = 0{\cdot}81$ Å^{-1}. The mean Sr—O distance for the eight-coordinated Sr(1) atom (2·604 Å) is somewhat shorter than that for the nine-coordinated Sr(2) atom (2·661 Å). The two crystallographically different diselenite groups have Se—O bond lengths to the bridging O atoms ranging from 1·822 to 1·879 Å, others from 1·645 to 1·685 Å; the Se—O—Se angles are 120·7 and 122·5°.

Introduction. Crystal structures of compounds with the general formula $M^{2+}Se_2O_5$ have been determined for M = Ca (Delage, Carpy & Goursolle, 1982), M = Mn (Koskenlinna, Niinistö & Valkonen, 1976), M = Cu (Meunier, Svensson & Carpy, 1976), and M = Zn (Meunier & Bertaud, 1974). Other diselenite groups in inorganic crystal structures were found in $VO(Se_2O_5)$ (Meunier, Bertaud & Galy, 1974), $MnH(SeO_3)(Se_2O_5)$ (Koskenlinna & Valkonen, 1977*b*), $PrH_3(SeO_3)_2(Se_2O_5)$ (Koskenlinna & Valkonen, 1977*a*), $Y(NO_3)(Se_2O_5).3H_2O$ (Valkonen & Ylinen, 1979), $(NH_4)_2(Se_2O_5)$ (Chomnilpan, 1980), $Au_2(SeO_3)_2(Se_2O_5)$ (Jones, Schwarzmann, Sheldrick & Timpe, 1981), $Ca_2(HSeO_3)_2(Se_2O_5)$ (Valkonen, 1985), and $K_2Se_2O_5$ (Rider, Sarin, Bydanov & Vinogradova, 1985). During synthesis of the monazite-type strontium selenate $SrSeO_4$ (Effenberger & Pertlik, 1986), the new compound $SrSe_2O_5$ was obtained. In connection with studies on the chemical behaviour of selenites, the crystal structure of $SrSe_2O_5$ was determined.

Experimental. *Synthesis.* Crystals of $SrSe_2O_5$ were synthesized hydrothermally in a steel vessel lined with Teflon. 2 g of a mixture of $SrCO_3$ and H_2SeO_3 (molar ratio 1:2) were put into the vessel with ~6 ml capacity and 1 ml H_2O_2 (Perhydrol) was added. The vessel was filled up with H_2O to about 80 vol% and was heated for 48 h at 493 (5) K. After cooling to room temperature (~12 h), crystals of $SrSe_2O_5$ were observed. The title compound forms colourless and equidimensional crystals up to a diameter of 0·5 mm.

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Crystal 0·09 × 0·12 × 0·32 mm; four-circle AED2 diffractometer (Stoe & Cie, Darmstadt, Federal Republic of Germany), graphite-monochromatized Mo $K\alpha$ radiation; lattice parameters from 75 reflections up to $2\theta = 48°$; $2\theta/\omega$ scan, minimum of 42 steps per reflection increased for (α_1,α_2) dispersion, step width 0·03°, step time 0·5 to 1·5 s per step, data collection up to $2\theta = 70°$, three standard reflections with no significant intensity variation; 4503 reflections measured (h: $-11\rightarrow11$, k: $-11\rightarrow11$, l: $-18\rightarrow0$), 4479 reflections in unique data set, 3753 reflections with $F_o > 3\sigma(F_o)$ were used for refinement; four ψ scans for absorption correction (transmission factors from 0·185 to 0·364), correction for Lorentz and polarization effects. Complex neutral-atomic scattering functions (*International Tables for X-ray Crystallography*, 1974). All calculations were performed with program system *STRUCSY* (Stoe & Cie, 1984). The Sr and Se atoms were found with direct-method strategy, O atoms in a Fourier summation. Several cycles of least-squares refinements on F with anisotropic temperature parameters for all atoms gave $R = 0{\cdot}035$ and $wR = 0{\cdot}032$, $w = 1/\sigma[(F_o)]^2$; max. $\Delta/\sigma = 0{\cdot}002$, max. and min. height in final difference Fourier map 1·13 and −2·19 e Å^{-3}. The value of g for the isotropic secondary extinction (Zachariasen, 1967) is 2·10 (7) × 10^{-5}. The final atomic coordinates and the equivalent isotropic temperature parameters are given in Table 1.* Table 2 gives some important interatomic distances and bond angles.

Discussion. The two crystallographically different Sr atoms in $SrSe_2O_5$ show the following coordinations: The Sr(1) atom has eight and the Sr(2) atom has nine neighbouring O atoms with Sr—O distances varying from 2·493 to 2·759 Å. In both cases the coordination is clear-cut. Up to 4·0 Å only around the Sr(2) atom occurs one further O atom; due to its long distance Se(2)—O(6) = 3·451 (3) Å it is excluded from discussion of coordination. In correlation with the different coordination numbers [8] and [9], the average Sr(1)—O bond length is 2·604 Å and the average Sr(2)—O bond length is 2·661 Å. The coordination figure of the Sr(1) atom can best be described as a slightly distorted tetragonal antiprism, with O(2)–O(3)–O(9)–O(5) and O(4)–O(8)–O(7)–O(10) defining the basal planes. The $Sr(2)O_9$ coordination polyhedron may be described as a distorted trigonal prism, the atoms O(1)–O(2)–O(4) and O(8)–O(5)–O(4′) building the corners of the basal planes; in addition the atoms O(9), O(3) and O(3′) are each situated above the centres of three prismatic faces.

The Se—O bond lengths correlate with the environments of the O atoms. The shortest Se—O bonds in $SrSe_2O_5$ are to the atoms O(7) and O(10). Both of these O atoms are [2]-coordinated to one Sr and one Se atom (Sr—O—Se = 117·5 and 148·2° respectively). The atoms O(2), O(5), O(8) and O(9) are flat pyramidal [3]-coordinated by two Sr atoms and one Se atom (sums of angles at the O atoms range from 348·7 to 359·6°). The atoms O(3) and O(4) are [4]-coordinated (distorted tetrahedra) to three Sr atoms and one Se atom (Sr—O—Sr varies from 85·4 to 101·4° and Sr—O—Se from 97·4 to 138·1°). The atoms O(1) and O(6) are the bridging O atoms which link each of the two selenite groups to Se_2O_5 groups. In agreement with

Table 1. *Atomic fractional coordinates and equivalent isotropic temperature parameters* (Å²) *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Sr(1)	0·31794 (6)	0·38902 (6)	0·24384 (3)	0·0109
Sr(2)	0·80497 (6)	0·64238 (6)	0·10875 (4)	0·0110
Se(1)	0·70035 (6)	0·16070 (6)	−0·04011 (4)	0·0103
Se(2)	0·88351 (6)	0·16318 (6)	0·21456 (4)	0·0110
Se(3)	0·87344 (7)	0·73071 (7)	0·43229 (4)	0·0135
Se(4)	0·41867 (7)	0·83277 (6)	0·38000 (4)	0·0120
O(1)	0·8169 (5)	0·0282 (5)	0·0956 (3)	0·014
O(2)	0·4694 (5)	0·2248 (5)	0·0273 (3)	0·015
O(3)	0·7936 (5)	0·3678 (5)	−0·0536 (3)	0·014
O(4)	1·0523 (5)	0·2870 (5)	0·1317 (3)	0·013
O(5)	0·6857 (5)	0·3364 (5)	0·2359 (3)	0·016
O(6)	0·6629 (5)	0·8994 (5)	0·3741 (3)	0·020
O(7)	0·7590 (6)	0·5684 (5)	0·5185 (3)	0·020
O(8)	0·9721 (5)	0·6309 (6)	0·2986 (3)	0·021
O(9)	0·4605 (5)	0·7089 (5)	0·2506 (3)	0·017
O(10)	0·3002 (5)	1·0493 (5)	0·3378 (3)	0·020

Table 2. *Interatomic distances* (Å) *and bond angles* (°)

The e.s.d.'s are 0·003 Å for Sr—O and Se—O, 0·005 Å for O···O and 0·2° for O—Se—O.

Sr(1)—O(5)	2·493	Sr(2)—O(8)	2·501
Sr(1)—O(10)	2·514	Sr(2)—O(2)	2·571
Sr(1)—O(4)	2·580	Sr(2)—O(9)	2·627
Sr(1)—O(7)	2·592	Sr(2)—O(5)	2·633
Sr(1)—O(9)	2·607	Sr(2)—O(4)	2·691
Sr(1)—O(3)	2·673	Sr(2)—O(1)	2·697
Sr(1)—O(8)	2·684	Sr(2)—O(3)	2·732
Sr(1)—O(2)	2·692	Sr(2)—O(3′)	2·741
		Sr(2)—O(4′)	2·759

				O···O	O—Se—O
Se(1)—O(1)	1·879	O(1)	O(2)	2·714	100·2
Se(1)—O(2)	1·655	O(1)	O(3)	2·746	101·2
Se(1)—O(3)	1·672	O(2)	O(3)	2·621	104·0
Se(2)—O(1)	1·820	O(1)	O(4)	2·727	102·1
Se(2)—O(4)	1·685	O(1)	O(5)	2·685	101·1
Se(2)—O(5)	1·655	O(4)	O(5)	2·594	101·9
Se(3)—O(6)	1·852	O(6)	O(7)	2·714	101·6
Se(3)—O(7)	1·645	O(6)	O(8)	2·654	97·9
Se(3)—O(8)	1·665	O(7)	O(8)	2·662	107·1
Se(4)—O(6)	1·822	O(6)	O(9)	2·658	98·9
Se(4)—O(9)	1·675	O(6)	O(10)	2·610	97·5
Se(4)—O(10)	1·645	O(9)	O(10)	2·623	104·4

Se(1)—O(1)—Se(2)	120·7 (1)	Se(3)—O(6)—Se(4)	122·5 (1)

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43349 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

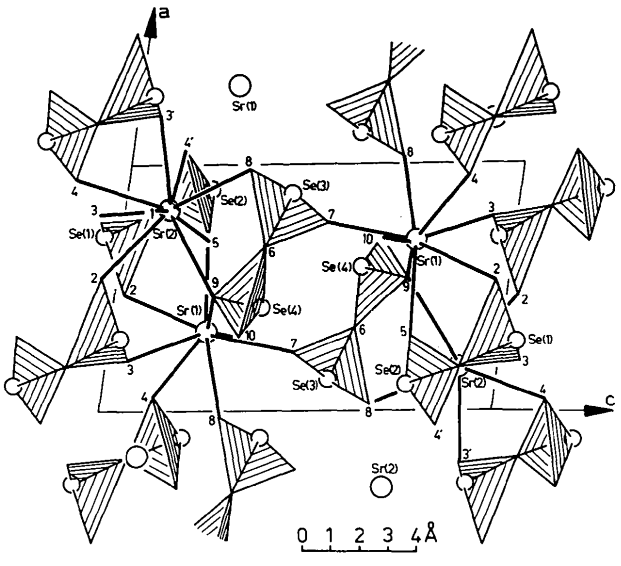

Fig. 1. Projection of the crystal structure of $SrSe_2O_5$ parallel to [010] into (010).

general crystal chemical experience in $SrSe_2O_5$ the bond lengths to the bridging O atoms are longer by ~0·18 Å than the other Se—O distances. The angles Se(1)—O(1)—Se(2) = 120·7 (1)° and Se(3)—O(6)—Se(4) = 122·5 (1)° compare well with those found in other diselenite groups reported in the literature. Each of the two diselenite groups has one shorter (1·820 and 1·822 Å) and one longer (1·879 and 1·852 Å) Se—O bond to a bridging O atom. This is not an appreciable behaviour of diselenite groups, but it has been reported, *e.g.* in $CaSe_2O_5$ (Delage *et al.*, 1982), $VOSe_2O_5$ (Meunier, Bertaud & Galy, 1974), and $(NH_4)_2(Se_2O_5)$ (Chomnilpan, 1980).

A projection of the crystal structure of $SrSe_2O_5$ parallel to [010] is given in Fig. 1. The $Sr(1)O_8$ and $Sr(2)O_9$ coordination polyhedra are connected to each other by sharing common O—O edges and O-atom corners. The diselenite groups are involved in this framework *via* O-atom corners; only the $Se(2)O_3$ group shares the O(4)—O(5) edge with the $Sr(2)O_9$ polyhedron. This edge of 2·594 Å is the shortest one within all the coordination polyhedra of the Sr and Se atoms.

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References

Chomnilpan, S. (1980). *Acta Cryst.* B**36**, 675–677.
Delage, C., Carpy, A. & Goursolle, M. (1982). *Acta Cryst.* B**38**, 1278–1280.
Effenberger, H. & Pertlik, F. (1986). *Z. Kristallogr.* In the press.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
Jones, P. G., Schwarzmann, E., Sheldrick, G. M. & Timpe, H. (1981). *Z. Naturforsch. Teil B*, **36**, 1050–1051.
Koskenlinna, M., Niinistö, L. & Valkonen, J. (1976). *Acta Chem. Scand. Ser. A*, **30**, 836–837.
Koskenlinna, M. & Valkonen, J. (1977*a*). *Acta Chem. Scand Ser. A*, **31**, 457–460.
Koskenlinna, M. & Valkonen, J. (1977*b*). *Acta Chem. Scand. Ser. A*, **31**, 638–640.
Meunier, G. & Bertaud, M. (1974). *Acta Cryst.* B**30**, 2840–2843.
Meunier, G., Bertaud, M. & Galy, J. (1974). *Acta Cryst.* B**30**, 2834–2839.
Meunier, G., Svensson, C. & Carpy, A. (1976). *Acta Cryst.* B**32**, 2664–2667.
Rider, E. E., Sarin, V. A., Bydanov, N. N. & Vinogradova, I. S. (1985). *Sov. Phys.-Crystallogr.* **30**, 587–588.
Stoe & Cie (1984). Structure system program package. Stoe: Darmstadt.
Valkonen, J. (1985). Abstr. Ninth Eur. Crystallogr. Meet., Torino, Vol. I, p. 125.
Valkonen, J. & Ylinen, P. (1979). *Acta Cryst.* B**35**, 2378–2380.
Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.

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Structure of $Cs_6Zn_5(MoO_4)_8$

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Abstract. $M_r = 2403{\cdot}83$, cubic, $I\bar{4}3d$ (unambiguously determined by X-ray diffraction), $a = 12{\cdot}259\,(1)$ Å, $V = 1842{\cdot}32$ Å^3, $Z = 2$, $D_m = 4{\cdot}48$, $D_x = 4{\cdot}3327$ g cm^{-3}, $\lambda(\mathrm{Cu}\,K\alpha)$ (for unit-cell dimensions) = 1·5418, $\lambda(\mathrm{Ag}\,K\alpha)$ (for intensity measurements) = 0·56081 Å, $\mu(\mathrm{Ag}\,K\alpha) = 138{\cdot}36$ cm^{-1}, $F(000) = 2144$, $T = 293$ K, final $R = 0{\cdot}033$ for 86 observed reflections. The Mo and Zn atoms form a three-dimensional tetrahedral framework [Mo—O distances 1·694 (9)–1·758 (9) Å, Zn—O distances 1·975 (8) Å] and the Cs