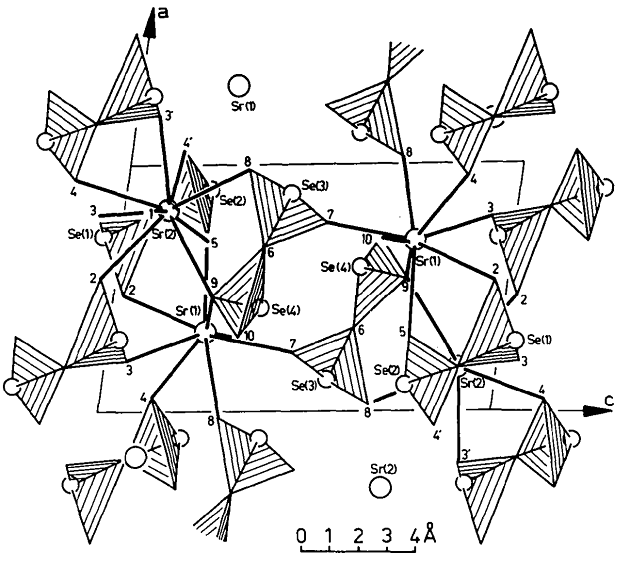

Fig. 1. Projection of the crystal structure of $SrSe_2O_5$ parallel to [010] into (010).

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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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}, λ(Cu $K\alpha$) (for unit-cell dimensions) = 1·5418, λ(Ag $K\alpha$) (for intensity measurements) = 0·56081 Å, μ(Ag $K\alpha$) = 138·36 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

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atoms are twelvefold coordinated by O atoms [Cs—O distances 3·273 (8)–3·370 (8) Å], the coordination polyhedron being a distorted cubooctahedron. Refinement of the population factor resulted in $\frac{5}{6}$ statistical occupation of the Zn position.

Introduction. The crystal structure of the title compound was determined as a contribution to the research on various new molybdenum Langbeinites $M^{I}_{2}M^{II}_{2}$-$(MoO_4)_3$ (Mueller, 1985). For the combination M^{I}=Cs and M^{II}=Zn, however, not a Langbeinite but the compound $Cs_6Zn_5(MoO_4)_8$ was found, the structure of which is presented here.

Experimental. Single crystals were prepared by melting and slow cooling of a mixture of Cs_2CO_3, 2ZnO and $3MoO_3$ at 933 K. D_m was measured with a pycnometer. The reported lattice constant was determined on a powder diffractometer (Cu $K\alpha$) using 27 reflections ($10 < \theta < 40°$).

Intensities of 761 reflections ($0 \leq h, k, l \leq 13$) with diffractometer, using graphite-monochromatized Ag $K\alpha$ radiation. The single crystal was irregularly shaped (all dimensions <0·1 mm). No absorption correction was performed.

Intensities of 761 reflections ($0 \leq h, k, l \leq 13$) with $2\theta < 40°$ were measured at room temperature with ω–2θ scans. Of these 441 were unobserved.

Three reflections ($\bar{4}44$, $32\bar{1}$, $1\bar{2}\bar{3}$) were monitored and did not show intensity variations of more than 2·6%. After averaging of symmetrically equivalent reflections 86 observations with $I > \sigma(I)$ and $R_{int} = 0{\cdot}16$ were used for the structure determination.

The structure was solved by direct methods, using *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) to locate the Cs and Mo atoms. Difference Fourier maps revealed the Zn and O positions. Refinement by full-matrix least squares on $|F|$ of positional and anisotropic thermal parameters for all atoms converged to a final $R = 0{\cdot}033$, $wR = 0{\cdot}014$ with $(\Delta/\sigma)_{max} = 0{\cdot}01$ and $S = 0{\cdot}6$ in the last cycle. The refinement of the population factors p of all atoms gave $p(Zn) = 0{\cdot}207$ (1), whereas the full population would give $p = 0{\cdot}25$. This means that the Zn position is $\frac{5}{6}$ statistically occupied.

Weight function used: $w = 1/\sigma^2(F)$, based on counting statistics. The final difference Fourier map shows maximum and minimum heights of 0·8 and −0·9 e Å^{-3}.

All calculations were carried out using the *SDP* (B. A. Frenz & Associates Inc., 1983) system of programs, except for distance and bond-angle calculations, which were performed with *XRAY*72 (Stewart, Kruger, Ammon, Dickinson & Hall, 1972).

Discussion. The final atomic coordinates, equivalent isotropic thermal parameters, r.m.s. amplitudes of thermal vibrations, bond lengths and bond angles are given in Tables 1 and 2.* Fig. 1 shows a part of the framework of the Zn and Mo tetrahedra, Fig. 2 the whole unit cell.

Table 1. *Final atomic coordinates, equivalent isotropic thermal parameters and r.m.s. amplitudes with e.s.d.'s in parentheses*

$$B = \tfrac{4}{3}a^2[B(1,1) + B(2,2) + B(3,3)].$$

		x	y	z	B(Å^2)
Cs	12 (*b*)	0·875	0·000	0·250	4·49 (4)
Zn	12 (*a*)	0·375	0·000	0·250	1·79 (6)
Mo	16 (*c*)	0·3988 (1)	0·3988 (1)	0·3988 (1)	1·44 (1)
O(1)	16 (*c*)	0·3190 (7)	0·3190 (7)	0·3190 (7)	2·2 (1)
O(2)	48 (*e*)	0·3394 (6)	0·4709 (7)	0·0936 (7)	1·8 (2)

R.m.s. amplitudes (Å)

	Min.	Intermediate	Max.
Cs	0·161	0·269	0·269
Zn	0·141	0·155	0·155
Mo	0·132	0·132	0·142
O(1)	0·019	0·205	0·205
O(2)	0·118	0·147	0·181

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

Mo—O(1)	1·694 (9)	O(1)—Mo—O(2) (3×)	108·4 (4)
—O(2) (3×)	1·758 (9)	O(2)—Mo—O(2) (3×)	110·5 (5)
Mean	1·742	Mean	109·5
Zn—O(2) (4×)	1·975 (8)	O(2)—Zn—O(2) (2×)	106·9 (3)
		O(2)—Zn—O(2) (4×)	110·8 (3)
		Mean	109·4
Cs—O(2) (4×)	3·273 (8)	Mo—O(2)—Zn	143·3 (5)
—O(2′) (4×)	3·361 (9)		
—O(1) (4×)	3·370 (8)		
Mean	3·335		
Next O at 4·29			

The average dimensions of the molybdate and zincate groups are consistent with those observed in other structures.

Eight-membered rings of alternating ZnO_4 and MoO_4 tetrahedra (tetrahedra 1 to 8 in Fig. 1) are the characteristic feature of the framework. Cs atoms are located in the centers of the rings and the ring normals coincide with the $\bar{4}$ axes along [100], [010] and [001]. Each Zn tetrahedron connects two rings, whereas each Mo tetrahedron is common to three rings, thus building up the three-dimensional framework. All vertices of a Zn tetrahedron are connected to Mo tetrahedra, whereas only three vertices of an Mo tetrahedron are linked to Zn tetrahedra, the fourth O [O(1)] being 'non-bridging'.

Every eight-membered ring forms part of a cage of six Zn and eight Mo tetrahedra around the Cs atoms.

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* Lists of structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43425 (2 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The Cs atoms are 12-coordinated with an average Cs—O distance of 3·35 Å, the next largest Cs—O distance being 4·3 Å. The coordination polyhedron (Fig. 3) is a distorted cubooctahedron, in which all square planes are degenerated into two faces of triangular shape.

The r.m.s. amplitudes of the thermal vibrations indicate for Zn and Mo nearly isotropic thermal motions, for Cs, O(2) and O(2′) moderate anisotropy and for O(1) a marked anisotropy, which is of less physical meaning.

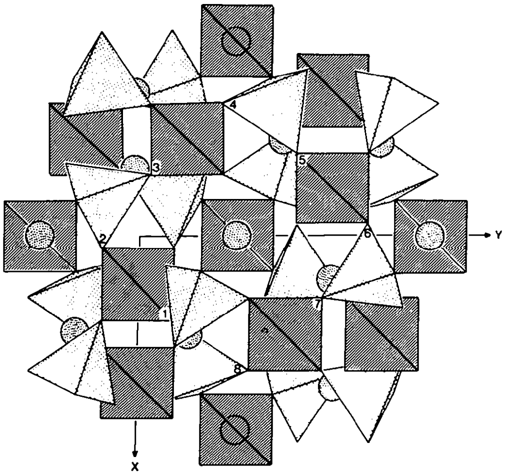

Fig. 1. A part of the tetrahedral framework viewed along **c**. Hatched tetrahedra: ZnO_4, dotted tetrahedra: MoO_4, dotted circles: Cs. Tetrahedra 1 to 8: eight-membered ring.

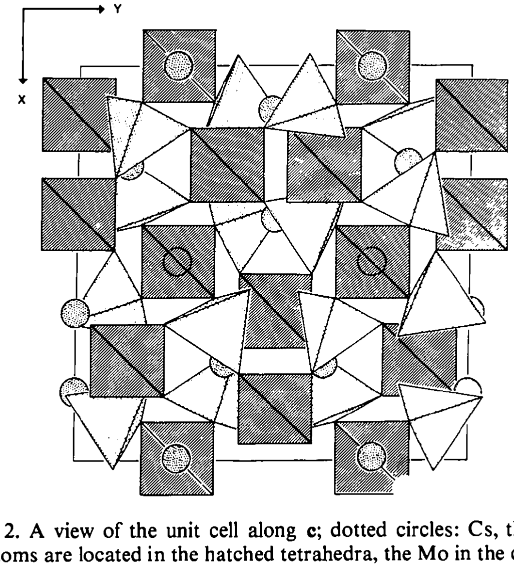

Fig. 2. A view of the unit cell along **c**; dotted circles: Cs, the Zn atoms are located in the hatched tetrahedra, the Mo in the dotted tetrahedra.

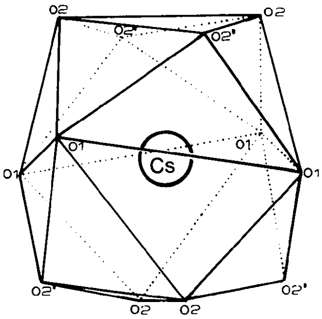

Fig. 3. Coordination polyhedron around Cs.

The tetrahedral frameworks of the title compound and of two related cement compounds are isomorphous. All three have space group $I\bar{4}3d$ and framework sharing coefficient, as defined by Zoltai (1966), 1·857 (reduced to 1·769 in the title compound if the Zn defects are taken into account):

$Cs_6[Mo_8O_{20}/Zn_5\square_1O_{12}]$ (this paper)
$Ca_{12}O_1[Al_8O_{20}/Al_6\quad O_{12}] =$ $12CaO.7Al_2O_3$ (Bartl & Scheller, 1970)
$Ca_{12}F_2[Al_8O_{20}/Al_6\quad O_{12}] =$ $11CaO.7Al_2O_3.CaF_2$ (Williams, 1973).

In the first compound the 12-coordinated sites are occupied completely by Cs^+, in the two other compounds partially by O^{2-} or F^-. There is, however, one significant difference: The 'non-bridging' vertices of the Mo tetrahedra in the title compound and of the corresponding Al tetrahedra in the two aluminates point in opposite [111] directions, in the first case away from the positive Cs ions, in the two other cases towards the negative O or F ions.

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