

magnesian amphibole and it seems probable that a fairly wide range of compositions is present in the minverite kaersutites.

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The crystal structure of joesmithite: a preliminary note

JOESMITHITE is a new mineral from Långban, Sweden, named by the author¹ and soon to be described elsewhere. Pertinent structure cell data are: a 9.88, b 17.87, c 5.277 Å, $\beta = 105^\circ 40'$, $P2/a$, $D_{\text{obs}} = 3.83$ gm/cc. Based on a quantitative emission spectrographic analysis by Ing. Benita Rajandi at the Swedish Geological Survey, and water and iron oxidation grade determinations by Mr. A. Parwel at the Swedish Natural History Museum, the cell contents are: $(\text{Pb}_{0.62}, \text{Ca}_{0.56}, \text{Ba}_{0.14}, \text{Mn}_{0.84})_{2.16} \text{Ca}_{4.00} \text{Fe}_{2.00}^{3+} (\text{Mg}_{6.34}, \text{Fe}_{1.40}^{3+}, \text{Fe}_{0.78}^{2+})_{8.42} (\text{Si}_{13.82}, \text{Al}_{0.32}, \text{Be}_{0.18})_{14.32} \text{O}_{39.72} (\text{OH})_{14.9}$. The three-dimensional crystal structure analysis suggests $(\text{Pb,Ca,Ba})_2 \text{Ca}_4 \text{Fe}_{2}^{3+} (\text{Mg,Fe})_8 [\text{Si}_2 \text{O}_6]_4 [\text{Si}(\text{O,OH})_4]_4 (\text{OH})_8$.

Joesmithite so resembles hornblendes that it was almost overlooked as a possible new mineral. The structure cell, though dimensionally similar to the common clinoamphiboles, has different symmetry elements, which prompted complete crystal-structure analysis. Its

¹ After Prof. Joseph ('Joe') V. Smith. It has been approved by the Commission on New Minerals and New Mineral Names, International Mineralogical Association.

essential features were revealed on the c -axis projection by fitting the well-known crystal structure of cummingtonite upon the allowable symmetry elements for space group $P2/a$. The strongest scatterer, (Pb,Ca,Ba), hindered a quick crystal-structure analysis because it was

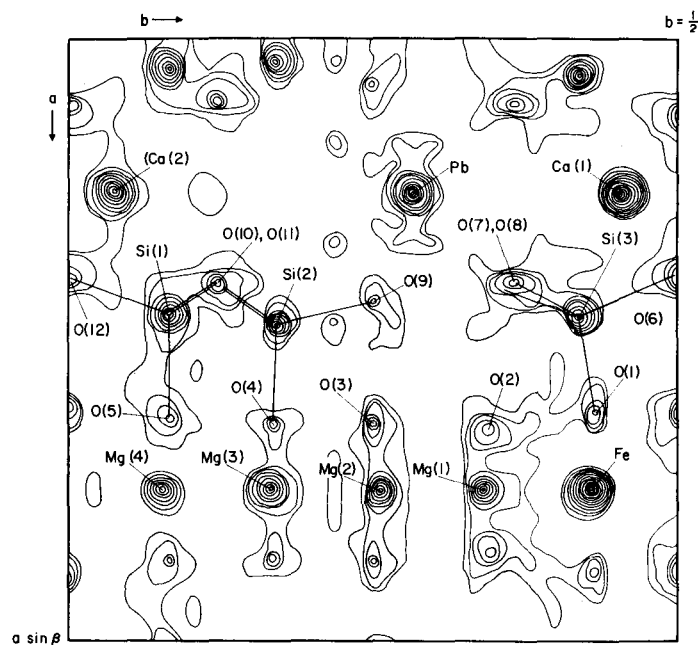


FIG. 1. Electron-density projection down the c -axis for joesmithite. The silicate units are sketched in.

first assumed to lie on the 'A' site. The Patterson projection, $P(uv)$, was needed to locate its true position.

Fig. 1 shows the principal plan of the joesmithite structure projected down the c -axis. It is an arbitrarily scaled electron density map, obtained when $R_{hk0, h0l} = 0.29$. At this stage all atom parameters in the asymmetric unit were refined as well as multipliers associated with the cations.

The most remarkable feature is the absence of one equivalent set of silicon atoms associated with the amphibole unit, evident in fig. 1. Unlike the clinoamphiboles, where the amphibole ribbon is generated by reflection and subsequent fusion of two equivalent pyroxene chains,

the entire cross-section of one ribbon is the asymmetric unit in joesmithite. However, joesmithite is not properly an amphibole or amphiboloid, since it is a hybrid structure consisting of $[\text{Si}_2\text{O}_6]_\infty$ pyroxene chains and insular $[\text{SiO}_4]$ tetrahedra.

TABLE I. Atom coordinates for joesmithite

Atom	Multiplier	x	y	z	B
Mg(1)	1.8	$\frac{3}{4}$	0.342	$\frac{1}{2}$	0.6 \AA^{-2}
Mg(2)	1.5	$\frac{3}{4}$	0.256	0	0.5
Mg(3)	1.1	$\frac{3}{4}$	0.162	$\frac{1}{2}$	0.6
Mg(4)	1.4	$\frac{3}{4}$	0.075	0	0.8
Fe	1.0	$\frac{3}{4}$	0.428	0	0.7
Ca(1)	1.0	$\frac{1}{4}$	0.459	$\frac{1}{2}$	0.6
Ca(2)	1.0	$\frac{1}{4}$	0.030	$\frac{1}{2}$	0.6
Pb, etc.	1.1	$\frac{1}{4}$	0.284	0	1.1
Si(1)	2.0	0.462	0.081	0.190	0.6
Si(2)	2.0	0.471	0.169	0.696	0.8
Si(3)	2.0	0.459	0.422	0.180	0.7
O(1)	2.0	0.632	0.425	0.625	0.7
*O(2)	2.0	0.643	0.343	-0.223	1.1
*O(3)	2.0	0.642	0.251	0.287	1.1
O(4)	2.0	0.637	0.163	-0.224	0.7
O(5)	2.0	0.632	0.080	0.273	0.6
O(6)	2.0	0.380	0.497	0.209	1.0
O(7)	2.0	0.403	0.386	-0.120	0.9
O(8)	2.0	0.412	0.363	0.377	1.2
O(9)	2.0	0.414	0.252	-0.289	1.4
O(10)	2.0	0.405	0.116	-0.117	0.9
O(11)	2.0	0.408	0.136	0.395	1.4
O(12)	2.0	0.383	0.004	0.209	1.2

* hydroxyl groups

The unoccupied tetrahedral positions appear to be a consequence of presence of the large lead cations, which, in joesmithite, have a partly covalent character. Steric accommodation of the lead is possible by the elimination of this set of silicon atoms, the lead being displaced off the 'A' site in the direction of the missing tetrahedral centres.

The marked amphibole-like character of joesmithite suggests that the octahedral bands—not the silicate units—play the predominant role. With the exception of the off-centred 'A' site, the large cation and octahedral bands are essentially the same as in the common clino-amphiboles.

The present $R_{hkl} = 0.15$ for 1774 independent F_{hkl} . Further refinement is in progress and the details of the structure will be presented

elsewhere. Joesmithite has 23 atoms in the asymmetric unit, presented in table I.

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A comparison of Grenville and Lewisian granites

It is generally agreed that for a given cycle of plutonic activity older granites tend to be rich in sodium relative to potassium, while younger ones tend to be rich in potassium relative to sodium (Read, 1949, pp. 148–149). Bowes (1967) has demonstrated a compositional trend of this kind for Lewisian granites, which he interprets in terms of Read's Granite Series.

TABLE I

	Mineralogy	Mode of occurrence	Lewisian type similar in composition
Type I*	30% quartz, 45% plagioclase (An ₁₅ -An ₃₀), 10% microcline, 10% biotite. Hornblende common.	1. Grey, well-foliated gneiss. 2. Granitic layers in migmatite. 3. Massive granite with angular xenoliths. 4. Dike.	Autochthonous
Type II	35% quartz, 30% plagioclase (An ₅ -An ₂₀), 25% microcline, 2% biotite. Perthite common.	1. Pink, well-foliated gneiss. 2. Granitic layers in migmatite. 3. Discordant lenses and phacoidal bodies. Xenolithic in places. 4. Dikes and veins.	Parautochthonous
Type III	20% quartz, 20% plagioclase (An ₀ -An ₁₀), 55% microcline. Perthite common, biotite masses in some pegmatites.	1. Dikes and veins commonly 2. Tabular sheets } pegmatitic. 3. Patches of graphic granite in type II granite.	Intrusive

* South of the Haliburton Highlands, granite of this kind occurs in the Weslemkoon and Elzevir discordant plutons, see Lumbers, 1964, fig. 7.

The Lewisian granites provide an interesting basis of comparison for Precambrian granites associated with metasedimentary and metavolcanic rocks of the Grenville province and outcropping in the Haliburton Highlands of Ontario. Salient features of the Canadian granites are shown in table I and their normative compositions in fig. 1.