X-RAY STUDY OF NARSARSUKITE, $Na_2(Ti, Fe)Si_4O_{11}$

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SUMMARY

Narsarsukite $Na_2(Ti, Fe)Si_4O_{11}$, a tetragonal crystal, has been found to have cell dimensions "a"$=10.74$Å, "c"$=7.90$Å, and to contain 4 molecules per unit cell. The axial ratio is 0.735 instead of 0.5235 (Dana), and the perfect cleavage assumed by Dana to be {110} becomes {100} in terms of the new axes. The space group is one of the three possibilities S_4^2, C_4^5, C_{4h}^5, but due to complete lack of knowledge of the crystal class it has not been possible to decide between these, nor to make a complete structure determination.

INTRODUCTION

Narsarsukite is a rather rare mineral found in Greenland. According to Dana, it is tetragonal with $c=0.5235$, prominent {110} and {001} cleavages, found commonly as prisms. The specific gravity is given as 2.751 and the analysis as follows:

SiO_2	= 61.63
Al_2O_3	= 0.28
Fe_2O_3	= 6.30
TiO_2	= 14.00
MnO	= 0.47
MgO	= 0.24
Na_2O	= 16.12
F	= 0.71
H_2O	= 0.29
	100.04

UNIT CELL

The crystals used in the present investigation were cleavage fragments[1] measuring about $1\times1.5\times2$ mm. in size with what, according to Dana, were perfect {110} faces. Rotation photographs (Mo Kα) were made by rotating about the 001, 110 and 100 axes. The following primitive translations were found:

$$a_1(001) = 7.90\text{Å}$$
$$a_2(110) = 10.74\text{Å}$$
$$a_3(100) = 15.19\text{Å}$$

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[1] We are indebted to Prof. C. Palache of Harvard University for the crystals used, and to Mr. H. Berman for selecting and examining them for us.

Since $a_3 = a_2\sqrt{2}$, the true unit cell has the dimensions:

$$c = 7.90\text{Å}$$
$$a = 10.74\text{Å}$$

The cleavage faces called {110} by Dana then become in reality the {100} and {010} faces. The axial ratio 0.5235 corresponds to $7.90/15.19 = 0.520$. However the true axial ratio is $c/a = 7.90/10.74 = 0.735$.

Formula and Number of Molecules Per Cell

Since Dana gives no formula, and from the analysis alone it is somewhat difficult to arrive at a satisfactory one, the number of molecules per cell on the basis of a molecular weight of 100 was calculated.

$$n = \frac{V\rho N}{M} = \frac{912 \times 10^{-24} \times 2.751 \times 0.606 \times 10^{24}}{100} = 15.25$$

V = vol. of cell in cc.
ρ = density
N = Avogadro number
M = molecular weight

By multiplying the number of molecules of each oxide contained in a weight of 100 by this number, the number of molecules of each oxide per cell was arrived at. The cations and anions per cell could then be calculated. In this manner it was found that, if MgO, MnO, Al_2O_3, Fe_2O_3 and TiO_2 were grouped together, the cell contained approximately 16 Si atoms, 4 Ti and others, 8 Na, and 44 O, corresponding to a cell containing 4 molecules of the formula $Na_2TiSi_4O_{11}$, with the titanium partially replaced by appreciable quantities of iron and negligible amounts of magnesium, manganese, and aluminum. The fact that the number of atoms of each kind comes out almost to an exact multiple of 4, a number highly appropriate to a tetragonal crystal, makes the deduced formula very reasonable.

Space Group

A series of 15° oscillation photographs about the c axis were taken and indices assigned to about 300 reflections. It was found that no reflections appeared for which the sums of $h+k+l$ were odd.

Because of the fibrous nature of the cleavage it was found impossible to produce a satisfactory sample for a Laue pattern parallel to {001}, but a Laue pattern parallel to {100} showed no plane of symmetry parallel to the tetragonal axis. From the above data the space group is limited to one of the three possibilities S_4^2, C_4^5, C_{4h}^5. Because of complete lack of knowledge of the crystal class, it was not possible to decide between these three possible space groups, nor to make a complete structure determination.[2]

[2] Since completion of this work it has come to our attention that a similar study by Gossner and Strunz, *Zeit. Krist.*, Vol. **82,** p. 151, 1932, leads to essentially the same results.