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THE CRYSTAL STRUCTURE OF TILASITE

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ABSTRACT

The crystal structure of the mineral tilasite, $4[\text{CaMg}(\text{AsO}_4)\text{F}]$, has been determined and found to be very similar to that of sphene, as was predicted by Strunz in 1937. The structure refinement shows tilasite to be slightly noncentric, however, and its space group is *Cc*.

INTRODUCTION

Tilasite, $4[\text{CaMg}(\text{AsO}_4)\text{F}]$, was originally described by Sjögren (1895) from an occurrence at Långban, Sweden. Piezoelectric evidence (Smith and Prior, 1911) indicated tilasite to be noncentric. Based on similarity of chemical formulas, morphology, and unit cells, Strunz (1937) proposed the analogy of the structure of tilasite to that of sphene, which had been determined in the centric space group *C2/c* by Zachariassen in 1930. Williams (1970) redescribed tilasite from a new occurrence at Bisbee, Arizona, and commented on its noncentric morphology. The present study was initiated in an attempt to resolve the confusion over the inclusion of apparently noncentric tilasite in the group with centric sphene.

TABLE 1. ATOMIC PARAMETERS FOR TILASITE

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i>
As	.00000	.4293(1)	.25000	.42(1)
Ca	.4867(5)	.5817(2)	.2392(5)	.57(2)
Mg	.252(4)	.747(1)	.500(4)	.54(3)
O(1)	.012(2)	.311(2)	.076(2)	.7(2)
O(2)	.263(2)	.967(2)	.626(2)	.4(2)
O(3)	.248(2)	.537(1)	.382(2)	.7(1)
O(4)	.001(2)	.316(2)	.422(2)	.7(1)
F	.508(2)	.333(1)	.247(2)	.7(1)

EXPERIMENTAL

Fragments of tilasite from Bisbee were ground into spheres. Intensity data were collected on a 4-circle automated diffractometer with monochromatized MoK α radiation. The resulting 1199 observed intensities were corrected for absorption by linear interpolation of the spherical corrections in the *International Tables for X-Ray Crystallography*, Vol. II, pp. 302 and 303. Unit cell dimensions determined concurrently with the data collection were: $a = 6.688(2)\text{\AA}$, $b = 8.944(2)$, $c = 7.570(2)$, and $\beta = 121^\circ 10'(01')$ with standard errors in parentheses.

TABLE 3. INTERATOMIC DISTANCES AND ANGLES IN TILASITE

<i>i</i>	<i>j</i>	$d_{ij}\text{\AA}$	<i>i</i>	<i>j</i>	<i>k</i>	Angle ijk°
As	O(1)	1.72(2)	O(1)	As	O(2)	108.8(8)
As	O(2)	1.65(2)	O(1)	As	O(3)	112.1(7)
As	O(3)	1.72(1)	O(1)	As	O(4)	104.1(8)
As	O(4)	1.65(2)	O(2)	As	O(3)	111.7(7)
Average		1.684	O(2)	As	O(4)	113.9(8)
			O(3)	As	O(4)	106.1(7)
Mg	F	1.91(3)	F	Mg	F	176(1)
Mg	F	1.92(3)	F	Mg	O(1)	93(1)
Mg	O(1)	2.04(3)	F	Mg	O(1)	90(1)
Mg	O(2)	2.17(2)	F	Mg	O(2)	96(1)
Mg	O(3)	2.08(2)	F	Mg	O(2)	84(1)
Mg	O(4)	2.12(3)	F	Mg	O(3)	83(1)
Ca	F	2.22(1)	F	Mg	O(3)	97(1)
Ca	O(1)	2.44(2)	F	Mg	O(4)	87(1)
Ca	O(2)	2.45(2)	F	Mg	O(4)	89(1)
Ca	O(2)	2.73(2)	O(1)	Mg	O(2)	88(1)
Ca	O(3)	2.38(1)	O(1)	Mg	O(3)	93(1)
Ca	O(3)	2.55(1)	O(1)	Mg	O(4)	178(1)
Ca	O(4)	2.49(2)	O(2)	Mg	O(3)	179(1)
			O(2)	Mg	O(4)	90(1)
			O(3)	Mg	O(4)	89(1)

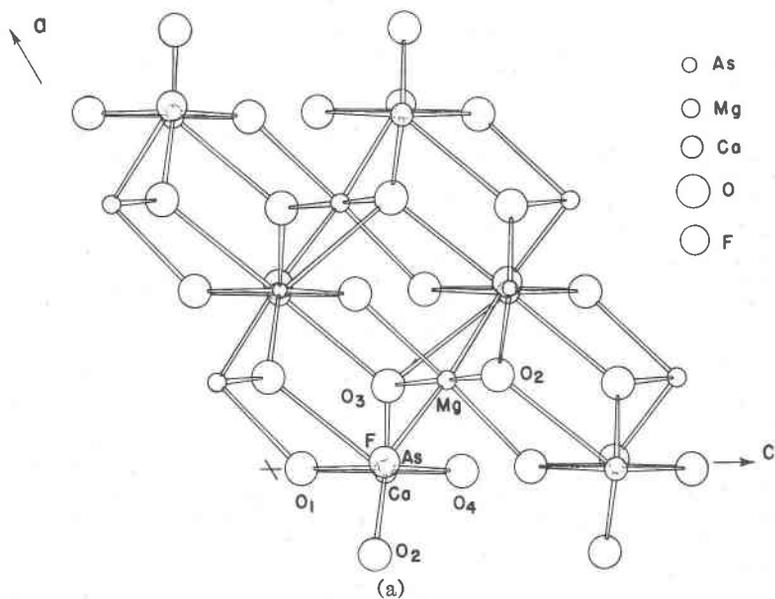


FIG. 1a. The structure of tilasite viewed in projection from the $+b$ direction showing noncentric distortions.

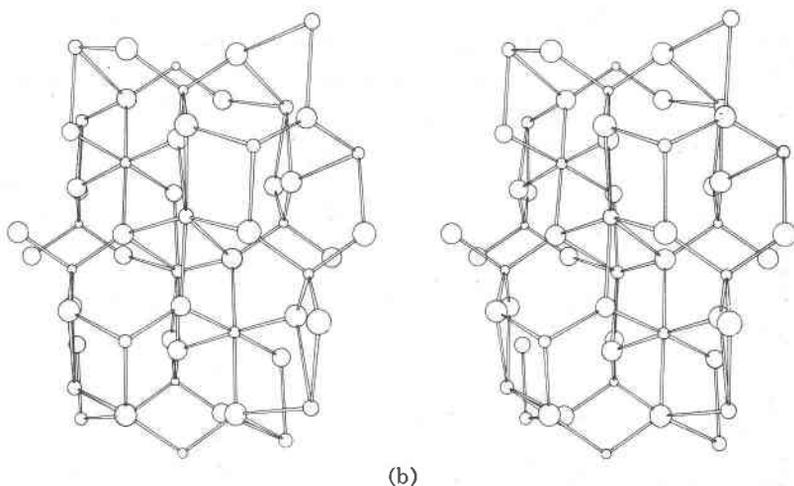


FIG. 1b. The structure of tilasite viewed in stereo from the $+a$ direction with the b axis vertical and a^* across. Atom sizes are as in Figure 1a.

STRUCTURE DETERMINATION

Intensities were reduced to structure factors and the structure was solved for As, Ca, and O atoms from a three-dimensional Patterson function. Fourier difference maps were used to locate Mg and F atoms. Least squares refinement in space group *Cc* using isotropic temperature factors reduced *R* to 0.061. Atomic parameters are given in Table 1. Observed and calculated structure factors are listed in Table 2.¹ Scattering factors used were for neutral atoms as given in the *International Tables for X-Ray Crystallography*, Vol. III, pp. 202-207.

DESCRIPTION OF THE STRUCTURE

The tilasite structure is very similar to that of sphene. The Ca atoms occupy similar sites in the two minerals and the tilasite Mg position is correlative with the octahedral Ti site in sphene. The arsenate groups are analogous to the silica tetrahedra in sphene and the fluoride ions occupy essentially the same sites as the non-tetrahedral oxygen atoms in sphene.

The structure refinement, however, indicates that tilasite is slightly, but significantly, noncentric. The As was held during refinement on the pseudo 2-fold rotor and Ca and F refined to positions slightly displaced from it, with the displacement of the Ca being many times its positional error. Slight rotation and distortion of the arsenate group also contributes to the lowered symmetry.

The arsenate group is approximately tetrahedral, with As-O distances ranging from 1.65 to 1.72Å and O-As-O angles varying from 104.1 to 113.9°. Interatomic distances and angles are detailed in Table 3. The Mg atom is coordinated by four oxygen atoms and two fluoride ions in a slightly distorted octahedron, with Mg-anion distances ranging from 1.91 to 2.17Å. Ca is seven coordinated in tilasite as in sphene. The structure of tilasite is shown in projection and in stereo in Figure 1.

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¹ To obtain a copy of Table 2, order NAPS Document #01903. The present address is National Auxiliary Publications Service of the A. S. I. S., c/o CCM Information Corporation, 866 Third Avenue, New York, N.Y. 10022; and price is \$2.00 for microfiche or \$5.00 for photocopies, payable in advance, to CCMIC-NAPS. Check a recent issue of the journal for current address and price.

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DEVELOPMENT OF (120) PRISM FACES OF NATURAL TOPAZ

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ABSTRACT

Growth hillocks observed on (120) prism faces of natural topaz crystals are illustrated. Their formation follows a sequential order: triangular, trapezium-shaped and finally semi-circular. Natural etch pits have outlines similar to the growth pyramids. The same sequential development of etch pits is established by controlled laboratory etching. From the observations of growth forms and etch pits the mechanism of development and growth of (120) prism faces of natural topaz crystals is worked out.

INTRODUCTION

Microtopographical studies of habit faces of crystals often prove useful in understanding the mechanism of development and growth of such faces in particular, and of crystals in general. In addition, if study is also made of laboratory etching on such faces, it might help to understand better the mechanism of growth. Fruitful attempts have been made by Joshi and Kotru (1968). The present paper is a report of such studies in the case of (120) faces of natural topaz crystals.

The crystal faces were thoroughly cleaned and were coated with silver films in a vacuum coating unit and were then examined under a metallurgical microscope. Occasionally, use was also made of the electron microscope.

In the present investigation, the hydrothermal etching technique exploited by Joshi and Kotru (1969), and Joshi *et al.* (1970) for quartz crystals was employed to advantage. The crystal faces under