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The crystal structure of a 3*T* lepidolite

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Abstract

A 3*T* lepidolite with composition near $K_2(Al_{2.5}R_{0.2}Li_{3.2})(Si_7Al)O_{20}(F_3OH)$, $a = 5.200$, $c = 29.76$A, space group $P3_112$, has been refined from diffractometer data using least-squares methods. Octahedral cations are ordered on three sites: *M*1 has $(Li_{0.7}Al_{0.3})$, *M*2 has $(Li_{0.9}Al_{0.1})$, and *M*3 has $(Li_{0.1}Al_{0.9})$. *M*1 is the *trans* octahedron. Significant bond-length differences also indicate tetrahedral ordering for the two independent tetrahedra. *T*1 has $(Al_{0.2}Si_{0.8})$, and *T*2 has Si only. The σ and Δ values of 7.7° and 0.36A due to tetrahedral rotation conform to the empirical relation of McCauley and Newnham (1971).

Introduction

The lepidolite micas have proved an interesting group for structural study, embodying, as they do, a number of stacking variations and ordering arrangements. These variations have helped to clarify structural relationships which are important to the mica group as a whole. This report summarizes a crystal-structure investigation of a lepidolite having a 3*T* stacking arrangement and a composition well within the polylithionite range. Malcolm Ross of the U.S. Geological Survey kindly provided this sample, U.S. National Museum specimen R4365, which is one of Stevens' (1938) samples from Coolgardie, Australia.

Content and symmetry of the unit cell

The composition of this mica as derived from Stevens' (1938, Table 1, anal. 14) analysis is: $(K_{1.69}Na_{0.22}Rb_{0.10})$ $(Al_{2.50}Mn_{0.18}Fe_{0.03}Mg_{0.02}Ti_{0.01}Li_{3.23})$ $(Si_{6.96}Al_{1.04})O_{20}[(OH)_{0.87}F_{3.07}]$. This allocation assumes the sum of the valences of all cations except hydrogen will be 44. The composition in terms of polylithionite, trilithionite, muscovite end members (Foster, 1960, p. 116) places this lepidolite closest to the polylithionite end member, with a relative ratio PL 84.8, TL 12.7, MS 2.5.

Symmetry and cell dimensions were determined on 0.5mm squares cut with a wire saw from the high-quality 0.1mm thick mica sheet. This mica is uniaxial, which suggests that the symmetry is trigonal or hexagonal. Zero and first-level *c*-axis precession photographs are identical at intervals of 120° around the dial axis and show the trigonal nature of the mica. Precession photographs of levels perpendicular to the trigonal (*c*) axis (a^*a^*) show sixfold symmetry on the zero level and threefold symmetry on upper levels. The *a* axes are chosen to be the 5.2A axes, consistent with the practice of Güven and Burnham (1967) in 3*T* muscovite. The a^*a^* zero and upper-level precession photographs show $2/m$ symmetry to be associated with the ⟨21.0⟩ directions. Reflections of type $00l$ with $l \neq 3n$ are systematically absent and indicate the presence of a threefold screw axis parallel to *c*. The above observations lead to a diffraction symbol of $\bar{3}mP3_1$ with the twofold axes normal to *a*, giving possible space groups $P3_112$ and $P3_212$. The existence of reflections with indices simultaneously following the rules $(h - k) = 0$ and $(k + l) \neq 0$ plus the agreement between calculated and observed structure factors along the $(10l)$ row indicates that the crystals are not twinned (Güven and Burnham, 1967).

The cell dimensions as measured from precession photographs are $a = 5.205$, $c = 29.77$A. Cell dimensions determined on the single-crystal diffractometer by least-squares methods are $a = 5.200$A $\pm$ 0.005 and $c = 29.76$A $\pm$ 0.01.

Experimental

Data for the refinement were recorded using monochromatized Mo$K\alpha$ radiation on a Picker single-crystal diffractometer. The data set consisted initially of 3400 observed and unobserved reflections. This triply and doubly redundant set was reduced to 705 non-equivalent reflections through the symmetry relationships in Laue group $\bar{3}$ ($\bar{3}$ was used rather than $\bar{3}m$) and

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CC/ER: 00:00:09.442 WAIT: 00:00:00.001
SUAS USED: $ 1.51 SUAS REMAINING: $ 140.42
THE ABOVE DOLLAR CHARGES FOR THIS RUN ARE APPROXIMATE;
THE ACTUAL COST WILL BE REFLECTED ON YOUR MONTHLY INVOICE.
IMAGES READ: 721 PAGES: 6
START: 17:43:13 NOV 28,1977 FIN: 17:44:12 NOV 28,1977