Redetermination of the Lepidolite-2M_1 Structure

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Abstract: The structure of a lepidolite-2M_1 from Biskupice, Czechoslovakia, has been redetermined. Violations of systematic extinctions and of monoclinic equivalences plus the results of a second harmonic generation test indicate that the true symmetry most likely is $C\bar{1}$. The deviation of the data set from $C2/c$ symmetry, however, proved to be too small to permit a statistically significant refinement in $C\bar{1}$. Refinement in $C2/c$ symmetry indicated no ordering of tetrahedral cations but ordering of octahedral cations so that M(1) = $Li_{0.93}R^{2+}_{0.06}Fe^{3+}_{0.01}$ and M(2) = $Al_{0.58}Li_{0.35}\square_{0.07}$. The tetrahedra are elongated to form trigonal pyramids with a rotation angle of 6.2° . The anomalous orientation of the thermal ellipsoid for the F,OH anion plus the large equivalent isotropic B value of 2.58 for F,OH and of 1.74 for the interlayer K cation, whose position is partly restricted in $C2/c$ symmetry, suggest a lower symmetry than $C2/c$.

The compositions of this sample and of a second lepidolite-2M_1 from Western Australia fall outside the stability field of lepidolite-2M_1 in the synthetic system. Structural control of the stacking sequence is discounted on the basis of the structural similarity of the lepidolite unit layers. Crystallization parameters are considered more important than composition or the structure of the unit layer in determining the stability and occurrence of different layer-stacking sequences in lepidolite.

Key Words: Crystal structure • Lepidolite • Lithium • Mica

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