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Structural regularities in $2M_1$ dioctahedral micas: The structure modeling approach

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Abstract

An improved algorithm has been elaborated for computing atomic coordinates in K-dioctahedral micas-$2M_1$ from the experimental data on cation composition and unit-cell parameters. The structure modeling procedure is based on regression equations relating the structural features and chemical composition of micas that were obtained from the analysis of published data on 27 refined structures of dioctahedral micas of various compositions including 20 K-dioctahedral micas-$2M_1$, 3 paragonites-$2M_1$, 2 margarites-$2M_1$, and 2 celadonites-1*M*. The empirical relationships accurately describe the observed structural distortions in dioctahedral micas, such as tetrahedral tilt and rotation, tetrahedral elongation, octahedral flattening, hydroxyl depression, etc. The majority of the regressions have $r^2 > 0.8$ and p-values <0.05, which means that the results are statistically significant. The predicted structural parameters are used to calculate the atomic coordinates for K-dioctahedral micas-$2M_1$ with disordered distribution of tetrahedral and octahedral cations. The estimated standard deviations (e.s.d.) for modeled atomic coordinates vary for different atomic positions and range from 0.0001 to 0.003 (fractional units); the e.s.d. values for structural characteristics obtained from the calculated atomic coordinates are 0.002–0.007 Å for mean and individual tetrahedral bond and edge lengths, 0.004–0.013 Å for mean and individual octahedral bond and edge lengths, 0.013–0.015 Å for K-O distances, and 0.5° for the tetrahedral ditrigonal rotation angle. Computation of atomic coordinates for additional three dioctahedral mica-$2M_1$ structures that were not included in the derivation of the empirical structure-composition relationships used in the algorithm yielded close agreement between the modeled and observed structural characteristics.

The structure modeling algorithm can be used as an inexpensive and express method for evaluation of fine structural features in large collections of K-dioctahedral mica samples of diverse compositions.

Keywords: Crystal structure, modeling, dioctahedral mica, muscovite, phengite, aluminoceladonite