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Vibrational analysis of the dioctahedral mica: $2M_1$ muscovite

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ABSTRACT

Raman spectra and lattice dynamics calculations are presented for the dioctahedral mica, muscovite. Calculated fundamental mode frequencies for the Raman-active and A_g and B_g species were fit to observed fundamentals assigned to features in the two polarized Raman spectra collected, so that unambiguous vibrational assignments could be made to most peaks in the Raman data. Calculated frequencies for the IR-active A_u and B_u modes generally fall within the frequency ranges of bands in the IR spectra for muscovite presented earlier. Factor group analysis indicates that motion from all atom types in the muscovite structure can be found in modes for all four vibrational species. Force constant values determined for muscovite are similar to equivalent values calculated for the trioctahedral mica, phlogopite. Raman and IR-active modes calculated at frequencies greater than 800 cm^{-1} are dominated by internal sheet T-O stretch and T-O-T bend motions, where T is a tetrahedral site. Modes between 800 and 360 cm^{-1} have internal tetrahedral sheet motions mixed with K and octahedral Al displacements. Modes at frequencies less than 360 cm^{-1} have lattice and OH motions. Inter-sheet bonding in the muscovite structure is strong enough to affect modes at frequencies as high as 824 cm^{-1}.