

## **Raman spectra and vibrational analysis of the trioctahedral mica phlogopite**

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### **ABSTRACT**

Raman spectra were measured and normal mode calculations were performed for phlogopite. Calculated fundamental mode frequencies were fit to observed frequencies assigned to features in the two polarized Raman spectra collected, so that unambiguous assignment of eigenmodes could be made to nearly all Raman spectral features. Average force constant values determined for Si-O and O-Si-O environments as well as for the non-silicate environments in cyclosilicates and gillespite provided an excellent starting point for the phlogopite calculations that quickly converged to a best fit of theoretical mode frequencies to the observed Raman fundamental mode frequencies. Final values of the force constants for T-O stretch and O-T-O bend are within the range of force constant values determined for Si-O and O-Si-O environments in cyclosilicates and gillespite. The force constant similarities extend to the K-O, M(1,2)-O bond stretch and M(1,2)-O-T bond bend environments. Raman-active modes at frequencies greater than 850 cm<sup>-1</sup> are localized intra-sheet modes dominated by T-O stretch and O-T-O bend motions. Raman-active modes between 350 and 850 cm<sup>-1</sup> are dominated by mixtures of internal sheet modes with displacements from the M2 sites. Raman-active lattice modes are calculated at frequencies less than 350 cm<sup>-1</sup>. Calculated frequencies for the IR-active A<sub>u</sub> and B<sub>u</sub> modes generally fall within the frequency ranges of broad bands in the IR spectra for phlogopite presented elsewhere. Eigenmodes calculated for phlogopite are generally unique to that mica structure and differ from those determined for the cyclosilicates and gillespite. The few eigenmodes calculated for phlogopite that resemble those calculated for the cyclosilicates are the most localized T-O stretch motions and are assigned to the highest frequency modes.