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Thermal behavior of vibrational phonons and hydroxyls of muscovite in dehydroxylation: In situ high-temperature infrared spectroscopic investigations

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Abstract

Temperature dependencies and thermal dynamical behavior of vibrational phonons related to different bonds/motions (e.g., K-O, Si-O, and Al-O) and O-H stretching, bending, and combinations bands, as well as those of NH_4 ions, of muscovite have been investigated in detail at high temperatures using in situ infrared spectroscopy. Phonon modes of muscovite show a complex response to heating and dehydroxylation. The mode Grüneisen parameters of muscovite are largest for low-frequency bands and some bands have negative values. Approaching dehydroxylation, bands associated with K-O stretching, Al-OH bending, and Al-O vibrations exhibit significant variations, indicating modifications of local configurations related to these ions. The O-H stretching feature near 3627 cm^{-1} shows a change in temperature dependence of the peak position near or during dehydroxylation, and this is attributed to a dramatic loss of OH and changes in local environments. The infrared spectroscopic analyses carried out in situ or on quenched samples do not record the characteristic bands of dehydroxylation-induced H_2O and these findings suggest that H_2O is unlikely to be the principal diffusing species. The results suggest that de-ammoniation or loss of NH_4 in muscovite takes place at temperatures near dehydroxylation.

Keywords: Muscovite, infrared spectroscopy, dehydroxylation, high temperature, phonon, hydroxyl