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Temperature dependence of IR absorption of hydrous/hydroxyl species in minerals and synthetic materials

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Abstract

We report on temperature dependencies of infrared (IR) fundamental, combination, and overtone vibrations of hydroxyl species (OH) in nominally anhydrous minerals (e.g., titanite), ferroelectric crystals ($KTa_{1-x}Nb_xO_3$, KTN), layer silicates (talc, mica, and pyrophyllite), and hydrous minerals such as apatite and synthetic hydrous/deuterated garnets [$Ca_3Al_2(O_4H_4)_3$ and $Ca_3Al_2(O_4D_4)_3$] for the temperature range of 20–300 K. Data obtained by high-resolution FTIR spectroscopy show that increasing temperature generally leads to a decrease in the band height and band area of fundamental vibrations of hydroxyl species, whereas the combination and first-overtone bands commonly show different temperature dependencies. The results show that in the investigated temperature range, the variations of the band height and area for different OH bands (especially for combinations and overtones) on cooling or heating do not reflect changes in OH concentrations in the materials, but relate to temperature-dependent absorption coefficients. The observations imply that absorption coefficients calibrated at room temperature cannot necessarily be used for the determination of hydroxyl contents at other temperatures.

Keywords: Infrared spectroscopy, low temperature, apatite, hydrous garnet, pyrophyllite, talc, sericite, titanite