

Single-crystal IR spectroscopy of very strong hydrogen bonds in pectolite, $\text{NaCa}_2[\text{Si}_3\text{O}_8(\text{OH})]$, and serandite, $\text{NaMn}_2[\text{Si}_3\text{O}_8(\text{OH})]$

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ABSTRACT

Polarized infrared absorption spectra of thin, oriented single-crystal slabs of pectolite and serandite were recorded between 4000 and 350 cm^{-1} at 298 and 83 K. The spectra of both minerals show a broad absorption region parallel to the silicate chains (*b* direction) that is centered around 1000 cm^{-1} , which is interrupted by a transmission window, and which is superimposed by sharp silicate, lattice, and overtone modes. This band is assigned to the OH stretching mode consistent with the alignment of the O-H ··· O hydrogen bond parallel to *b* and the short O ··· O distance of 2.45–2.48 Å that was found in previous X-ray structure refinements. At 1396 cm^{-1} (pectolite) and 1386 cm^{-1} (serandite) an OH bending mode is observed in the IR spectra parallel to *c*. At low temperatures, this mode shifts up to higher frequencies (1403 cm^{-1} at 83 K in pectolite), whereas the down-shift of the OH stretching mode cannot be observed due to the extremely broad band width. The slightly higher energy of the bending mode in pectolite indicates a slightly stronger hydrogen bond with respect to serandite. However, the bond length in serandite is slightly shorter than that in pectolite. An asymmetric O-H ··· O bond is confirmed in pectolite and serandite through comparison with different materials with similar, very strong hydrogen bonds and low-energy OH stretching modes.