

## **Raman spectroscopic study of H<sub>2</sub>O in bikitaite: “One-dimensional ice”**

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### **ABSTRACT**

The zeolite bikitaite, Li<sub>2</sub>[Al<sub>2</sub>Si<sub>4</sub>O<sub>12</sub>]-2H<sub>2</sub>O, has structural channels containing infinite chains of H<sub>2</sub>O molecules running parallel to [010]. One hydrogen atom of an H<sub>2</sub>O molecule is weakly hydrogen bonded to an O atom of a neighboring molecule, while the other hydrogen atom is unbonded. The molecules are ordered and the chains they form have been called “one-dimensional ice.” Polarized Raman spectra of single crystals in the wavenumber range 40–4000 cm<sup>-1</sup> were measured from 5 to 625 K. At low temperatures, four different O-H stretching vibrations can be observed between 3330 and 3600 cm<sup>-1</sup>, as well as H<sub>2</sub>O bending vibrations at about 1640–1650 cm<sup>-1</sup>. The two lower wavenumber hydrogen-bonded O-H stretching modes increase in wavenumber with increasing temperature, while the higher wavenumber non-hydrogen-bonded OH modes decrease in wavenumber. The temperature dependence of the linewidths of the O-H stretching modes and the degree of hydrogen bonding between neighboring H<sub>2</sub>O molecules show that the main cause of line broadening is modulation of the OH potential from low-energy thermal O···O vibrations in the H<sub>2</sub>O chains. At elevated temperatures, the different O-H stretching modes become similar in energy and only a single symmetric H<sub>2</sub>O stretching band is observed above 520 K. At these temperatures the H<sub>2</sub>O molecules lose their hydrogen bonding and are only bonded to Li cations at the walls of the channels.