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Hydroxyl in $MgSiO_3$ akimotoite: A polarized and high-pressure IR study

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ABSTRACT

Hydrous $MgSiO_3$ akimotoite (ilmenite-type structure), containing 350 ppm wt H_2O as hydroxyl, was synthesized at 19 GPa and 1300 °C in a multi-anvil apparatus. Polarized Fourier-transform infrared spectra show bands at 3300 and 3320 cm^{-1} due to hydroxyl groups oriented nearly perpendicular to the *c* axis as well as a strong band at 3390 cm^{-1} caused by OH molecules aligned nearly parallel to *c*. Unpolarized infrared measurements performed up to 13.8 GPa in a diamond anvil cell show that the bands shift to lower frequencies with increasing pressure, which is consistent with hydrogen bonding. At ~9 GPa, the bands initially at 3300 and 3320 cm^{-1} merge, suggesting that these two bands represent the same type of hydroxyl group. The compression behavior of the infrared bands shows that the pressure derivative of the frequency, $d\nu/dP$, decreases with increasing initial wavenumber, ν_{io}, and this decrease is not linear. These observations are consistent with the compression mechanism of akimotoite, as previously published. The data indicate that the relative compressibility of the hydrogen bonds within a structure (i.e., the sign of $d\nu/dP$ vs. ν_{io}) is governed by a combination of the directionality of the hydrogen bonds and the anisotropy of compression, whereas the rate of compression (i.e., the slope of $d\nu/dP$ vs. ν_{io}) is a function of the bulk modulus.