

Hydrous ringwoodite to 5 K and 35 GPa: Multiple hydrogen bonding sites resolved with FTIR spectroscopy

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ABSTRACT

Multiple substitution mechanisms for hydrogen in γ -(Mg,Fe)₂SiO₄, ringwoodite, lead to broad, overlapping, and difficult-to-interpret FTIR spectra. Through combined low-temperature, high-pressure synchrotron-based FTIR spectroscopy, the multiple bonding sites become evident, and can be traced as a function of temperature and compression. Multiple OH stretching bands can be resolved in iron-bearing and iron-free samples with 0.79–2.5(3) wt% H₂O below 200 K at ambient pressure, with cooling to 5 K at 35 and 23 GPa resulting in the resolution of possibly as many as 5 OH stretching bands traceable at room temperature from 23 GPa down to 8 GPa. A distribution of defect mechanisms between $\square_{\text{Mg}}''+2(\text{H}^{\cdot})$ at 3100, 3270, and possibly 2654 cm⁻¹, $\square_{\text{Si}}'''+4(\text{H}^{\cdot})$ at 3640 cm⁻¹, and $\text{Mg}_{\text{Si}}''+2(\text{H}^{\cdot})$ at 2800 cm⁻¹ can then be resolved. These multiple defect mechanisms can therefore explain the higher electrical and proton conductivity in ringwoodite when compared to wadsleyite, and therefore may be applied to resolve spatial variations in water storage in the Earth's transition zone.

Keywords: Ringwoodite, FTIR, low temperature