

High-pressure phase transitions and hydrogen incorporation into MgSiO₃ enstatite

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ABSTRACT

Hydrogen incorporation into orthoenstatite (*Pbca*), low-clinoenstatite (*P2₁/c*), and high-pressure clinoenstatite (*C2/c*) has been investigated using polarized and unpolarized infrared spectroscopy. Using shifts in OH stretching frequencies between the spectra and data from different crystal models, we test various models for hydrogen incorporation. The only significant differences between orthoenstatite and low-clinoenstatite spectra relate to anisotropy of the higher wavenumber bands, which implies a change in orientation of longer OH dipoles between the two structures. High-pressure clinoenstatite reverts to low-clinoenstatite during depressurization, but subtle differences are noted between IR spectra of samples synthesized in the high-pressure clinoenstatite and low-clinoenstatite stability fields. Differences probably relate to the splitting of oxygen sites into two sets of non-equivalent sites during transformation of high-pressure clinoenstatite. The most realistic models for hydrogen incorporation into all three polymorphs involve association of hydrogen with the underbonded O2a and O2b sites. However, changes in OH dipole orientation between the different polymorphs and the effects of phase transitions on water solubility in the system MgSiO₃ mean the effects and implications of hydrogen incorporation into the three polymorphs may differ considerably.

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