Theoretical calculations of infrared spectra of hydrous Ringwoodite under high temperature and pressure

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Water in the Earth plays an important role in plate tectonics and the formation and evolution of the Earth. Rinwoodite is believed to be a major mineral in the Earth's transition zone at 550-660 km deep. Infrared spectroscopy (IR) is one of the main experimental tools to investigate the structural water in the minerals. However, the IR theoretical calculations under high temperatures are rare reported. In this work, the theoretical lattice dynamics calculation based on the empirical potentials was employed on the hydrous Ringwoodite to calculate its infrared absorption spectra at the temperatures of 300 – 2000 K and the pressures of 0 - 20 GPa. We have modelled three systems with water content of 0.2 wt.%, 1.6 wt.% and 3.3 wt.%, respectively. By modelling Mg vacancy mechanism [$V''_{Mg} + 2H^{\bullet}$], Mg-Si disorder mechanism [$Mg''_{Si} + 2H^{\bullet}$] and Si vacancy mechanism [$V''''_{Si} + 4H^{\bullet}$] configurations, we found that Mg vacancy hydrous mechanism [$V''_{Mg} + 2H^{\bullet}$] forms the main peak in the infrared absorption spectrum under all of our simulated temperature and pressure conditions. We can also concluded that, Mg-Si disorder mechanism [$Mg''_{Si} + 2H^{\bullet}$] is much more unstable than other mechanisms, and its infrared spectroscopy is very weak in the low water content (0.2 wt%) system. We have discussed the pressure and temperature effects on the wavenumber of the infrared absorption spectrum of the three hydrous mechanisms in Ringwoodite. Our further calculations on the water content as the functions of the temperature and pressure, indicated the water capacity in the Ringwoodite lattice will decrease under either the high temperatures or high pressure increases. The amount of water holding in the Earth's transition zone is controlled by both the water bearing mechanisms and the P-T conditions.