

Vibrational properties of hydrous ringwoodite, first principles investigation

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Wadsleyite and ringwoodite are primary constituent minerals in the Earth's transition zone. These phases can contain up to a few wt% H₂O in the crystal structure and are thought to be the most important water reservoirs in the Earth. We have investigated the high pressure protonation sites in hydrous wadsleyite using first principles calculation and found that the oxygen O₁ site is the most favorable for protonation in wadsleyite because of the electric imbalance of this site. On the other hand, the crystal structure of ringwoodite does not have such peculiar protonation sites and the reason of such high retention of water in ringwoodite has been unclear so far. In present study, I have calculated the vibrational properties of hydrous ringwoodite under pressure with various protonation models by first principles. Comparing with the IR and Raman measurements, I will discuss the protonation sites in hydrous ringwoodite.

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