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Normal and inverse ringwoodite at high pressures

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Abstract

We present a first-principles computational study of the structural properties of ringwoodite and the influence of cation exchange on these properties as well as the enthalpy differences between ringwoodite and inverse ringwoodite. Our results agree with low-temperature experiments, in that cubic ringwoodite is the stable structure up to 25 GPa. This pressure range encompasses the lower part of the mantle transition zone where ringwoodite is thought to be the most abundant phase. The equation of state as derived from experiment and theory are in good agreement. In contrast to normal ringwoodite, inverse ringwoodite compresses highly anisotropically and the compression mechanisms differ considerably for the two structures. The predicted enthalpy difference between normal and inverse ringwoodite is significantly smaller than that obtained from a simple ionic model (O'Neill and Navrotsky 1983), emphasizing the importance of including structural relaxation in models that address the energetics of order-disorder reactions, at least in the case of ringwoodite.