

Theoretical study on lithium diffusion and fractionation in enstatite

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Abstract: Enstatite is one of the major mantle minerals in the earth, which is an important Mg end member of the orthopyroxene system. Li isotopes are important tracers of mantle geochemistry, and they are very important for studying related properties of diffusion and fractionation in the major mantle minerals (such as olivine and pyroxene). We have modelled and calculated the activation energies of Li diffusion in enstatite lattice via two different migration mechanisms (interstitial and substitutional mechanism) at atomic level and degree of isotopes fractionations on different lattice sites at different temperatures. Our calculation shows that Li isotopes are more likely to migrate through enstatite by interstitial mechanism. Moreover, ⁷Li will incorporate on interstitial sites while ⁶Li prefers to move into Mg vacancies. The temperature is one of the key factors affecting fractionation, and the corresponding results can be used to explain isotopic composition of mantle Li and isotope fractionation under cooling conditions.

Keywords: enstatite; Li isotopes; diffusion; fractionation; modelling