



Prediction of equilibrium Li isotope fractionation between minerals and aqueous solutions at high P and T: an efficient ab initio approach

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The mass-dependent equilibrium stable isotope fractionation between different materials is an important geochemical process. Here we present an efficient method to compute the isotope fractionation between complex minerals and fluids at high pressure, P, and temperature, T, representative for the Earth's crust and mantle. The method is tested by computation of the equilibrium fractionation of lithium isotopes between aqueous fluids and various Li bearing minerals such as staurolite, spodumene and mica. We are able to correctly predict the direction of the isotope fractionation as observed in the experiments. On the quantitative level the computed fractionation factors agree within 1.0 permil with the experimental values indicating predictive power of ab initio methods. We show that with ab initio methods we are able to investigate the underlying mechanisms driving the equilibrium isotope fractionation process, such as coordination of the fractionating elements, their bond strengths to the neighboring atoms, compression of fluids and thermal expansion of solids. This gives valuable insight into the processes governing the isotope fractionation mechanisms on the atomic scale. The method is applicable to any state and does not require different treatment of crystals and fluids.

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