Equilibrium boron isotope fractionation related to silicate melt: A density functional theory study

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In the geological process, boron has a strong fluid mobility. The 10% mass difference between ^{10}B and ^{11}B leads to large boron isotope composition variations up to 100 ‰ in nature [1]. While advances have been made in quantifying the fractionation behavior of boron isotopes among melt, minerals, aqueous fluid, and vapor phase, boron isotope fractionation behavior in complex silicate melts is less well understood. Here, we carry out a theoretical investigation of boron isotope fractionation processes in silicate melt using a quantum mechanical calculation approach.

Boron isotope fractionation depends largely on its coordination in silicate minerals and melts. Hence, the reduced partition function ratios (RPFR, β) of silicate melts/glasses are calculated for trigonally and tetrahedrally coordinated boron. The differences in arrangements of BO_4/BO_3 units and chemical bonds strength in melt/minerals, together with the hydration effect in fluids, are found to dominate boron isotope fractionation. These processes can yield a large $\Delta^{11}B$ up to 10 ‰ between silicate melt/aqueous fluid and silicate minerals at 800 K. By comparison, there is minor boron isotope fractionation between gas and fluids (i.e. $\Delta^{11}B_{\text{gas-fluid}} = 0.4\text{-}1.0$ ‰) at temperatures of 600-1000 K. These results are consistent with experimental studies, and aid in the application of the boron isotope geo-thermometer and constrain boron isotope compositions in original silicate melts.

[1] Marschall H. R. and Foster G. L., 2018. Advances in Isotope Geochemistry: Boron Isotopes The Fifth element. Springer.