

## Theoretical understanding on boron isotope fractionation during serpentinization

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Serpentinites entering subduction zones show selective enrichment in trace elements and are the most important carriers of B in this setting [1]. The evolving B isotopic composition ( $\delta^{11}\text{B}$ ) of serpentinite is used in studying mantle-crust material exchange in subduction zones, but we lack full understanding of the processes controlling B isotope fractionation during serpentinization that would allow this tracer to be better utilized. Boron isotope fractionation between lizardite/ forsterite/diopside and aqueous fluids is investigated here using quantum mechanics (density functional theory, DFT) and *ab initio* molecular dynamics simulation (AIMD).

At 0-500 MPa and 0-1000 K, the best fit curves for the reduced isotopic partition function ratio ( $\beta$ -factor) of aqueous  $\text{B}(\text{OH})_3$  and  $\text{B}(\text{OH})_4^-$  are  $1000\ln\beta_{\text{B}(\text{OH})_3} = -20.1 + 37.07(1000/T) + 8.2(1000/T)^2$  and  $1000\ln\beta_{\text{B}(\text{OH})_4^-} = -13.94 + 24.43(1000/T) + 9.12(1000/T)^2$  (T in Kelvin). The  $^{11}\text{B}$  enrichment sequence follows the order forsterite > clinopyroxene (diopside) > white mica > phlogopite > lizardite. Lizardite differs from phlogopite and white mica, in that the B/Si orderings do not influence its  $\delta^{11}\text{B}$ . Using the B speciation of serpentinite fluids [2], this theoretical approach gives an equilibrium B isotope fractionation of  $\Delta^{11}\text{B}_{\text{lizardite-fluid}} = 15.89 - 22.88(1000/T) - 0.19(1000/T)^2$  between lizardite and serpentinized fluid in the temperature range from 25 to 400 °C.

[1] Kodolányi, J. et al. (2012). *J. Petrol.* 53, 235-270.

[2] Hansen, C.T. et al. (2017). *Geochim Cosmochim Acta* 217, 51-79.