Equilibrium boron isotope fractionation between boron-bearing minerals and fluid reservoirs

Yin-Chuan Li[1], Hai-Zhen Wei [1]*, Shao-Yong Jiang [2], Martin R. Palmer [3], T. G. M. van de Ven [4]

[1]Department of Earth Sciences and Engineering, Nanjing University, Nanjing 210023, PR China (haizhenwei@nju.edu.cn)
[2]Faculty of Earth Resources, China University of Geosciences, Wuhan 430074, PR China (shyjiang@cug.edu.cn)
[3]School of Ocean and Earth Science, NOC, University of Southampton, SO14 3ZH, UK (mrp1@soton.ac.uk)
[4]Department of Chemistry, McGill University, Montreal, Quebec H3A 2A7, Canada (theo.vandeven@mcgill.ca)

The high mobility of boron in fluid-rocks interactions has made it to one of the most effective tracers for the sources of magmatic and metamorphic fluids as recorded in boron-bearing minerals (e.g. tourmaline, muscovite etc.) in magmatic rocks and metamorphic rocks. However, the efforts to quantify boron isotope fractionation between tourmaline with trigonally coordinated boron and muscovite with tetrahedrally coordinated boron and their fluid reservoirs have been largely empirical [1]. Because of the difficulty in controlling the chemical compositions of synthetic boron-bearing minerals and the unexpected disequilibrium isotope and chemical fractionation during hydrothermal experiments, quantum mechanics calculations offer an alternative approach to explore the isotope fractionation mechanisms on the atomic scale.

Here we report the theoretical understandings on equilibrium boron isotope fractionation among boron-bearing minerals and tourmaline-fluid systems. The boron isotope fractionation between tourmaline group minerals and fluid is dominated by the ambient thermodynamic conditions and other second order effects. The influence of chemical compositions on the isotope fractionation factor $\alpha_{\text{Tur-fluid}}$ becomes larger with increasing Mg/(Fe+Mg) ratios in the solid solution. The driving mechanisms of the equilibrium isotope fractionation are the B-O bond length in the trigonal planar BO_3-groups and the mass to charge ratios of total metal atoms in tourmalines. Compared with the smaller temperature-dependent equilibrium fractionation of boron isotopes between dravite and fluid (i.e. $d(1000\ln\alpha_{\text{tur-fluid}})/d(1000/T)$ of -2.37), much larger boron isotope fractionations between muscovite and fluid have been verified, such as $d(1000\ln\alpha_{\text{mica-fluid}})/d(1000/T)$ of -4.16 between muscovite and basic fluid and that of -13.07 between muscovite and acidic fluid. The boron isotope fractionation between various mica and tourmaline compositions becomes greater in the sequence of biotite, phlogopite, muscovite, boromuscovite and phengite.

[1] Palmer and Swihart. (1996) Mineral. Soc. Am. 33, 713