B-O isotopes fractionation between borate minerals and fluids

DA-SHENG ZUO[1], HAI-ZHEN WEI[1], XIN-RAN TAN[1], MARTIN R. PALMER[2], SHAO-YONG JIANG[3] AND JUN-LIN WANG[1]

[1]School of Earth Sciences and Engineering, Nanjing University
[2]School of Ocean and Earth Sciences, University of Southampton
[3]China University of Geosciences (Wuhan)
Presenting Author: 502023290023@smail.nju.edu.cn

Most of the world's major borate deposits are formed by the evaporation of boron-rich fluid in enclosed basins in collisional tectonic settings. Boron and oxygen isotope compositions of borate minerals have shown great potentials to infer the pH of the brine and the paleotemperature for the borate deposits. To better constrain the physiochemical processes that lead to the borate deposits, we have calculated the fractionation of B-O isotopes in typical borate minerals using density functional theory.

The results show that the enrichment of heavy B isotopes decreases in the sequence of borax > ulexite > colemanite > priceite > pinnoite at 298.15K, depending on the ratio of $-BO_3$ and $-BO_4$ structures in minerals. The temperature dependent B isotope fractionation could be quantified as: $D^{11}B_{borax-water} = -0.0016T^2 +0.1375T -4.2902$, $D^{11}B_{colemanite-water} = 0.-0016T^2 + 0.1525T +-8.5653$ and $D^{11}B_{ulexite-water} = --0.0017T^2 + 0.1724T - 13.7696$. The enrichment of heavy O isotopes follows the sequence of colemanite > ulexite > borax, and the temperature dependent equilibrium O isotope fractionation between borax/colemanite/ulexite and fluids can be described by the relationships: $\Delta^{18}O_{borax-water} = 0.0004T^2 - 0.1305T + 15.869$, $\Delta^{18}O_{colemanite-water} = 0.0007T^2 - 0.2253T + 27.542$ and $\Delta^{18}O_{ulexite-water} = 0.0005T^2 - 0.1776T + 21.750$.

As the relative fraction of $B(OH)_3$ and $B(OH)_4$ vary at different pH in solution, the pH dependent boron isotope fractionation between borate minerals and fluid has been calculated. The pH-$D^{11}B_{mineral-water}$ curves indicate that the boron isotope composition of borate minerals precipitated from fluid strongly depends on the solution pH. Differ from that in neutral and acidic solution, the heavy isotope ^{11}B is more preferentially fractionated into the borate minerals than fluid in basic pH conditions, which is consistent with the experimental observation [1].

This work lays the foundation for understanding B and O isotope fractionation in the formation of borate deposits, and helps us constrain fluid sources and paleo-environmental evolution of enclosed basins where evaporate deposits formed.

[1] Oi T, Kato J, Ossaka T, Karihana H (1991) Boron isotope fractionation accompanying boron mineral formation from aqueous boric acid-sodium hydroxide solutions at 25 °C. Geochem J 25:377–385