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Ba isotope fractionation during granitic magmatism and potential of $d^{138/134}Ba$ for distinguishing magmatic-hydrothermal transition

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The geochemistry of barium is commonly used to study igneous processes and fluid-melt interaction in subduction zone and granitic environments [1]. Understanding Ba isotope fractionation mechanisms is critical if this potential is to be fully realized. Hence, we have used the first-principles calculations to calculate Ba isotope fractionation during felsic magma evolution. In fluids, the reduced partition function ratio of aqueous Ba^{2+} is highly variable, depending on the coordination number of H_2O in the first hydration shell. At ambient Earth surface conditions, the temperature dependent equilibrium Ba isotope fractionation between barite/witherite and fluids can be described by the relationships: $10^3 ln\beta = -0.00009'(10^6/T^2)^2 + 0.0603'(10^6/T^2) + 0.0003$ and $10^3 ln\beta = -0.0001'(10^6/T^2)^2 + 0.0648'(10^6/T^2) + 0.0004$. In silicate minerals, the enrichment of heavy Ba isotopes decreases in the sequence of muscovite > microcline, celsian, sanbornite > barylite > phlogopite. At high temperature (>600°C), the melt phase is enriched in heavy Ba isotope relative to any coexisting aqueous fluid and minerals. During the early stages of felsic magma differentiation involving plagioclase crystallization as the main mineral, the $\delta^{138/134}Ba$ in the residual melt remain close to their initial values, but any fluid exsolved from the melt will have light $\delta^{138/134}Ba$ values. The high Ba distribution coefficient of K-feldspar means that the resultant K-feldspar granite inherits >90% of the Ba contained in the initial magma reservoir. The $\delta^{138/134}Ba$ of K-feldspar is close to the initial melt. During the final stage of magma evolution, mixing of exsolved fluids from deeper reservoir may significantly reduce the $\delta^{138/134}Ba$ of the Ba-depleted melt, and account for the low $\delta^{138/134}Ba$ values measured in highly differentiated leucogranites and pegmatites.

[1] Huang, F., Bai, R., Deng, G., Liu, X., Li, X. (2021). Science Bull., 66, 2329-2336.