

First-principle Calculation of Equilibrium Isotopic Fractionation for Alkali Metal-bearing Minerals

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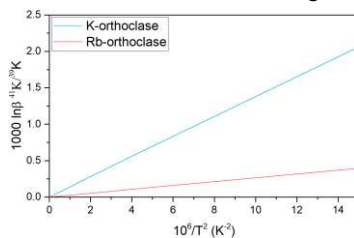
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Potassium is an important element in geochemical and cosmochemical studies but its isotope geochemistry has been largely unexplored due to analytical difficulties in K isotope measurement. Analytical developments now allow one to measure K isotopic composition with a sufficient precision to resolve naturally occurring isotopic variations^[1]. Interpretation of experimental results, however, requires a good understanding of the equilibrium isotopic fractionation factors associated with various geological processes.^[2] The experimental determination of equilibrium fractionation factors is not straightforward as experiments can suffer from kinetic isotope effects.

DFT based first-principle calculation has been proven to be a powerful tool to model various material properties, in particular isotopic fractionation under equilibrium condition.^[3] We will present theoretical results on potassium and rubidium-bearing minerals, compare those to experimentally determined values, and discuss their implications.

Our preliminary results on rubidium substituted orthoclase minerals suggested that the fractionation of rubidium is approximately 20% of that of potassium, which agreed well with the recent measurement from Pringle and coworkers.^[4]



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