

Understanding and comparing calculations of partition coefficients: how P-T conditions affect the enrichment of trace elements in the crust

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To integrate partition coefficients into a numerical model, it is crucial to understand the nature of partition coefficient calculation for trace elements. Clarifying uncertainties regarding known calculation methods can help to improve numerical models dealing with mantle differentiation, which will eventually lead to a more complete model on crustal formation on early earth. In this study, the first aim is to find out how well partition coefficients can be calculated using lattice parameters. For this, resulting coefficients were compared to experimentally measured values taken from literature. In a second step the effect of pressure and temperature changes on the coefficients was investigated.

Because of its importance in mantle geochemistry, we take the radioactive element potassium (K) as an example for REE partitioning behavior. To calculate partition coefficients of K we used the partition coefficient equation of Wood and Blundy 1997. In this equation, the partition coefficients are calculated as a function of temperature, pressure, Young's modulus and ionic radii. As a calculation tool the program Matlab was used and in the resulting code, mean values for the ionic radii were applied. In this study, we focus on the partitioning behavior of K into the mantle phases clinopyroxene, garnet and majorite. As a result, we found that using this method, partition coefficients differ with varying temperature and pressure conditions. A comparison of the resulting values will clarify the accuracy of the applied method and if the results can be incorporated into a broader modelling approach.

References:

Wood, B.J., Blundy, J.D. (1997): A predictive model for rare earth element partitioning between clinopyroxene and anhydrous silicate melt, *Contrib. Mineral Petrol.*, 129, 166-181.