A predictive thermodynamic model for plagioclase-melt partitioning

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Partition coefficients that describe the equilibrium partitioning of trace elements between plagioclase crystals and silicate melts are widely used in geochemical modelling. We have used experimental data for plagioclase-melt partitioning of 1+, 2+ and 3+ cations in the simple system diopside-albite-anorthite (Di-Ab-An) at 1 atmosphere pressure to develop a thermodynamic model for the prediction of partition coefficients. These data were used in the original development of the lattice strain model for trace element partitioning of Blundy and Wood (1994) and measured along isotherms thereby facilitating the separation of P-T controls on partitioning from those of composition.

The general approach of the model is to use partition coefficients, K_p, of the elements Na, Ca, and La as a reference. K_p's of other 1+, 2+ and 3+ cations occupying the alkali site in plagioclase can be then predicted from the lattice strain model. From the present experimental data the two lattice strain parameters, the optimum ionic radius, r_0, and the effective Young's modulus, E, were optimized for 1+, 2+, and 3+ cations as a function of the anorthite content of plagioclase. The optimised lattice strain parameters have magnitudes and compositional and thermal dependence that are consistent with elastic data for plagioclases. For La, as for other trivalent cations occupying the alkali site, we propose incorporation as $Na_{0.5}La_{0.5}Al_2Si_2O_8$ component. Using an exchange reaction with the melt we show that K_p(La) can be expressed as a function of K_p(Na) and K_p(Ca). The respective reaction constant was calibrated from the experimental data such that K_p(La) can be estimated from K_p(Na) and K_p(Ca).

For practical purposes we propose three different strategies to predict K_p's: (i) Calculation of K_p(Na) and K_p(Ca) from a thermodynamic model of plagioclase-melt equilibria in the system Di-Ab-An; (ii) Use of directly determined K_p(Ca) and K_p(Na) from the measured albite and anorthite content in plagioclase and the glass composition; (iii) Calculation using an empirical calibration for K_p(Ca) and K_p(Na) based on plagioclase and melt compositions of 992 plagioclase-saturated melting experiments taken from the LEPR database (http://lepr.ofm-research.org). We provide an Excel spreadsheet to perform these three different types of calculations.

[1] Blundy and Wood (1994) *Nature*, **372**, 452–454.