Geophysical Research Abstracts
Vol. 14, EGU2012-4272-1, 2012
EGU General Assembly 2012

The uncertainties of activity models and their effect on petrological calculations

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Comparing the uncertainties of the thermodynamic data between different research fields, surprising deficits emerge for materials relevant in the Earth sciences. The mixing properties of metallic systems, for example, have been thoroughly investigated [1]. From these studies it is well known that almost every binary alloy is characterized by significant excess entropies of mixing which play an important role when calculating phase diagrams of alloys. On the other hand, only two silicate solid solutions were investigated for this property for a long time [2, 3]. In the last few years, further calorimetric studies on the entropy-composition behavior have been performed [e.g., 4, 5]. However, there exists still need for more experimental data on the enthalpic and entropic mixing behaviour of rock-forming minerals.
The best investigated silicate solid solution is probably the ternary feldspar system. To study the impact of the experimental uncertainties on geothermometric calculations, we investigated the uncertainties of all activity-model parameters, of the mole fractions and the estimated pressure used in 2-feldspar geothermometry. Applying different methods (Gaussian error propagation, Monte Carlo methods), the precision of the 2-feldspar temperature could be obtained. We found that an uncertainty in the calculated temperatures of +/- 90 K (1 sd) must be accepted. Approximately 98% of this uncertainty came from that of the model parameters. This disappointing result is also reflected when different feldspar activity models are compared, i.e. activity models which are based on phase equilibrium experiments [e.g., 6] show large disagreement ($\sim$ 100 K) with those derived from calorimetry [7].

From the results of Monte Carlo simulations performed with the garnet-biotite geothermometer, we conclude that the uncertainty in estimating the temperature history of rocks using e.g., garnets, biotites, pyroxenes and amphiboles is similar or even larger compared to the feldspar system.

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