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The Error of Our Ways: Analytical Uncertainty in Trace Element Partitioning Experiments

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Developing predictive models of trace element partitioning behavior requires a calibration dataset of experiments conducted over the pressure, temperature, and composition of the systems we hope to model. Analytical and experimental uncertainty have always been a concern in the design and analysis of experiments. Understanding the magnitude of the individual sources of uncertainty is complicated by the fact that they are not independent of one another and the information required to quantify the magnitude of each is often not published. Three of the primary sources of uncertainty include 1) instrument precision/sensitivity, 2) the degree to which equilibrium has been achieved (e.g., extent of zoning), and 3) multiphase analyses (e.g., inclusion of glass in mineral analysis).

Instrument sensitivity can be quantified to the first order by the analysis of standard materials. The degree to which an experiment has achieved equilibrium may be evaluated in terms of the homogeneity of the phases in reference to the standard analyses. Identifying/quantifying the uncertainty related to the presence of more than one phase in the analytical volume or systematic differences in the precision of different analytical tools using the current database is problematic due to the fact that the experimental data is normally published as averages and the uncertainty is presented as the 1s on the average. In our examination of the trace element partitioning database, the cited uncertainty of the averaged analyses from studies based on Laser Ablation Inductively Coupled Plasma Mass Spectroscopy (LA-ICP-MS) are significantly higher compared to those based on Secondary Ion Mass Spectroscopy (SIMS). The degree of difference in cited uncertainty is correlated to the partition coefficient of the specific element, with greater differences between the results from LA-ICP-MS and SIMS observed in the most incompatible elements. This is consistent with the predicted impact of contamination of the mineral analyses with glass for the analytical tool with the larger analytical volume. This represents a significant source of bias in the database that will impact any model calibrated using the existing experimental data for any mineral/melt system. Resolution of this problem requires access to the individual analyses included in the published averages.