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Multiple-reaction geobarometry for olivine-bearing igneous rocks

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Supplementary Material 4

Uncertainties on compositional variables for the experimental dataset

Following standard practice, the studies in our experimental database (Supplementary Material 1) report uncertainties on their compositional variables in the form of a standard deviation on the mean value of a measured oxide. They do not provide a complete set of individual microprobe analyses, each with its own uncertainties. However, the former approach allows only for partial error propagation, which is known to produce errant uncertainties for multi-valent and multi-site cations (Giaramita and Day 1990). The tests of Giaramita and Day (1990) on analyses of natural rocks showed that partial error propagation can overestimate errors by up to 25% relative if only relatively small analytical errors are considered and analyses producing mineral formula with unsatisfactory stoichiometry are excluded. In the case of experimental mineral assemblages, the standard deviations of the measured oxides are often large, reflecting actual compositional heterogeneities due to incomplete equilibrium, and obtaining analyses that produce good stoichiometric results is often difficult (e.g., contamination of analyses due to very small grain size). The impact of using partial error propagation for experimental samples is therefore difficult to predict. A test on some experimental samples for which the complete set of microprobe analyses was provided to the authors (Stamper et al. 2014a; Melekhova et al. 2015; Melekhova, personal communication) showed that partial error propagation can overestimate the uncertainties on clinopyroxene and spinel compositional variables by as much as 300%, and no systematic deviation is identifiable.