

# **Geothermobarometry revisited: towards correct and consistent transformation between natural multicomponent data and simple thermodynamic models**

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Estimation of pressure-temperature conditions and reconstruction of metamorphic paths are widespread and vital tools in geodynamic interpretations. Increasing coverage and accuracy of internally consistent thermodynamic datasets permits prediction of phase stabilities, modal and mineral composition in the phase diagram space. In numerous situations where equilibrium is not pervasive but local or partial, or additional chemical components are present, retrieval of pressure, temperature or other potentials from univariant equilibria becomes increasingly inaccurate and is non-unique. Here we discuss several alternative strategies and highlight the need for internally-consistent interaction properties.

Activity of an end-member consists of ideal and excess mixing contribution. In practice, one or both contributions have been taken from the simplified composition space (corresponding to the thermodynamic mixing model) or from the full composition space (i.e. natural composition of the phase). Magnitude of uncertainty rapidly increases with the presence and concentration of other substituents, for instance, octahedral vacancies in micas, K in amphibole, or F in hydrous silicates.

Extension of the simple configurational models to include additional components (substituents) is frequently straightforward. We have evaluated consequences of using the simple or extended excess models on end-member activity, temperature or pressure estimate. Extraction of several compositional variables from natural data for use in the simple models may lead to unacceptable temperature or pressure estimates. By contrast, different choices of end-members in extended models or extrapolation of activity coefficient from a simple excess model limits, for instance, the error on temperature estimate to 30-50 °C. As the choice of additional end-members affects the proportions of the essential end-members in the model, the consistent extension and stable extrapolation to multicomponent space will only be achieved when the microscopic interaction parameters are internally consistent or heuristically correlated.