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Thermodynamic calculation of solute concentrations in fluid inclusions based on bulk element ratios and microthermometric data.

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Recent improvements in chemical analysis of fluid inclusions (using techniques such as LA-ICP-MS, PIXE, SXRF, LIBS and SIMS for individual inclusions, and crush–leach analysis for bulk samples), now permit ratios of certain solute elements to be determined with high accuracy. In order to apply these results to geochemical problems, the element ratios must be converted to concentrations in the inclusions. Approaches to this conversion problem have remained very approximate so far, and have not kept pace with the improved quality of the raw analytical data.

We have developed a thermodynamic procedure to calculate the absolute solute concentrations in multicomponent electrolyte solutions from input element ratios and microthermometric determinations of final-melting temperatures of daughter crystals such as ice and various salts. Equilibria are calculated using the algorithm of Mironenko and Polyakov (2009), which employs the Gibbs free energy minimization method and applies Pitzer's model to calculate the water activity and solute activity coefficients. The thermodynamic database of Marion (2008) is used for the system Na-K-Ca-Mg-FeCl-SO4-CO3-H-H2O over the temperature range –60 °C to 25 °C, and the database of Greenberg and Møller (1998) is used for the system Na-K-Ca-Cl-SO4-H2O for phase transitions from 25 °C to 250 °C. The model has been verified with experimentally studied systems. In addition to providing the solute concentrations, the model also predicts other melting transitions not used as input for the calculations (eutectic, peritectic, etc.), thereby allowing the results for specific fluid inclusions to be checked for consistency.