

CALCULATING THERMODYNAMIC PROPERTIES AND PHASE EQUILIBRIA IN MULTICOMPONENT MOLTEN SALT SYSTEMS

P. Chartrand and A. D. Pelton

Using the most recent developments of the quasichemical model, in the pair and quadruplet approximations, for short-range ordering of first and second nearest-neighbor ions, a large thermodynamic database for ionic liquids is constructed from binary and ternary evaluations/optimizations. In these optimizations, all thermodynamic data and phase equilibrium data are used to obtain a single consistent set of model parameters for all phases that best fit the available data simultaneously. The models then permit the estimation of properties of multicomponent phases from optimized model parameters of binary and ternary subsystems, and phase equilibria can then be calculated. The quasichemical model is applied to the Li,Na,K,[Rb,Cs],Mg,Ca,[Sr,Ba]//F,Cl molten salt phase and properties of solid phases are also evaluated with appropriate models. Applications of the model to other ionic liquid systems will also be presented.