CALCULATED PHASE EQUILIBRIA AND THERMODYNAMIC PROPERTIES IN THE Li-Na-K-Rb-Cs-Mg-Ca-Sr-Ba//F-CI SYSTEM

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Details of evaluations/optimizations of binary, ternary and multicomponent thermodynamic data (enthalpies, activities) and phase equilibria (phase diagrams, isopleths and liquidus projections) related to the Li,Na,K,Rb,Cs,Mg,Ca,Sr,Ba//F,Cl system are presented. The molten salt thermodynamic properties are represented by the modified quasichemical model in the pair/quadruplet approximation which permits the evaluation of short-range ionic ordering (first and second nearest-neighbor simultaneously) and its impact on the thermodynamic properties. A thermodynamic database with a consistent set of optimized model parameters is stored in the FACT system which permits the calculation of phase equilibra and thermodynamic properties of multicomponent systems. This database is unique, and is a powerful tool in the study of reactive metal processes.