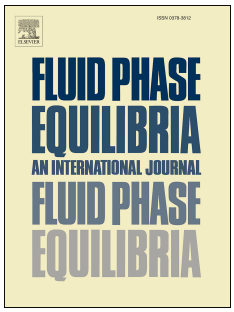

Rare-earth elements in aqueous chloride systems: Thermodynamic modeling of binary and multicomponent systems in wide concentration ranges

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Rare-earth elements in aqueous chloride systems: Thermodynamic modeling of binary and multicomponent systems in wide concentration ranges

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Abstract

A model has been developed for calculating thermodynamic properties and phase equilibria in binary and multicomponent aqueous systems containing rare earth element chlorides. Here, the rare earth elements encompass the lanthanides except promethium plus yttrium. The model is based on a comprehensive database of solid-liquid equilibria, osmotic and activity coefficients, enthalpies of dilution and heat capacities of solutions. The computational framework relies on the previously developed Mixed-Solvent Electrolyte (MSE) model. The model accurately reproduces the properties of binary rare earth chloride – water systems and of ternary mixtures that additionally include HCl, NaCl, or $CaCl_2$. Solid-liquid phase diagrams have been obtained to provide a convenient summary of the solubility of stable and metastable hydrated solid phases. Analysis of the stability of solid hydrates reveals systematic trends within the rare earth series. At ambient and elevated temperatures, the calculations show an increase in the stability range of rare earth chloride hexahydrates with decreasing cation radius, accompanied by a gradual disappearance of the heptahydrate. At low temperatures, the stable solid phases transition from the decahydrate at higher cation radii to octahydrate in an intermediate range and a combination of pentadeca- and nonahydrates at lower radii. The calculated standard-state enthalpies of formation of the hydrates agree with independently obtained values from calorimetric measurements, thus verifying the internal consistency of the model.

Keywords

Rare earth elements; Lanthanides; Electrolyte modeling; Aqueous solutions; Solid-liquid equilibria; Phase diagrams; Osmotic coefficients; Enthalpy of dilution

1. Introduction

Rare earth elements (REEs) are increasingly important in a variety of technological applications including magnets in electrical and electronic devices, battery alloys, phosphors, high-performance metal alloys, automobile and petroleum refining catalysts, polishing powders, glass additives and

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