Optimization of the thermodynamic properties of the rare earth elements (REE) at hydrothermal conditions: An internally consistent thermodynamic and experimental dataset in the REE-P-O-H-Na-Cl system

RUIGUANG PAN, PHD[1], ALEXANDER GYSI[1] AND GEORGE DAN MIRON[2]

[1]New Mexico Institute of Mining and Technology
[2]Paul Scherrer Institute

Presenting Author: ruiguang.pan@nmt.edu

Over the past decades, a series of experiments have been performed to obtain the thermodynamic properties of aqueous REE species and minerals. These data include calorimetric and mineral solubility experiments and the determination of REE-ligand formation constants [1,2]. The REE phosphates (i.e., monazite, xenotime, and rhabdophane) are the most extensively studied REE minerals. However, important discrepancies were found by comparing the experimentally measured monazite and xenotime solubility with the thermodynamic modeling predictions [3,4]. The latter are commonly based on a combination of measured calorimetric data for the REE phosphates [2] and existing aqueous species for the REE hydroxyl complexes from the Supcrt92 database (slop98.dat) derived by Haas et al. [5]. Moreover, there are currently no internally consistent thermodynamic databases that have been evaluated to optimize and combine these solubility data with available experimental data for the REE chloride complexes that represent important transporting ligands in critical mineral deposits [1].

Here we present a thorough investigation of the thermodynamic properties of REE and available experimental solubility data in the REE-P-O-H-Na-Cl system to 350 °C at saturated water vapor pressure. This work builds on the previous data compilation efforts implemented in the MINES thermodynamic database (https://geoinfo.nmt.edu/mines-tdb) and aims to provide a revised dataset for the REE optimized by combining the GEMS and GEMSFITS code packages [6,7]. The preliminary results of this study and previous efforts [3,4] indicate that the parameter optimizations using GEMSFITS can be used to reconcile the observed discrepancies between the experimental and modeled REE mineral solubilities. However, new development is necessary to address some of the required optimization routines. This revised dataset improves the accuracy for modeling the transport and precipitation mechanisms of REE in hydrothermal fluids.

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