Speciation and solubility of REE in hydrothermal aqueous fluids

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The rare earth elements (REE) have important applications in the high-tech and green technology industries. The formation of critical mineral deposits in geologic systems yields information about fractionation and enrichment mechanisms between the light and heavy REE. Thermodynamic modeling gives important insights into the chemical and mineralogical controls for REE mobilization in aqueous fluids with potential applications to separation and extraction technologies. However, the thermodynamic properties of REE-ligand aqueous complexes and the solubility of REE minerals still must be determined via multi-pronged approaches, which highlights the need of interdisciplinary collaborations covering a molecular to geologic field-scale understanding of REE. Here, we present our most recent experimental work on the speciation of REE hydroxyl, chloride, and sulfate complexes in acidic to alkaline hydrothermal aqueous solutions. A combination of data from REE mineral solubility experiments with in situ Raman spectroscopy and UV-Vis spectrophotometry, and high temperature-pressure solubility, are used to optimize the thermodynamic properties of aqueous REE complexes at sub- to supercritical conditions. The optimization program GEMSFITS permits generating internally consistent thermodynamic datasets which are implemented in the MINES thermodynamic database for geochemical modeling of hydrothermal fluid-rock reactions in geologic systems.