The standard partial molal thermodynamic properties of Nd3+ aqua ion and Nd chloride aqueous species based on calorimetric experiments from 25 to 250 °C

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Rare earth elements (REE) are important critical elements used in permanent magnets, catalysts, and electronics devices. Aqueous fluids play an important role in the formation of REE mineral deposits [1], with thermodynamic modeling providing insights into REE mobility in such magmatic-hydrothermal systems. However, a comparison of experimental studies with thermodynamic predictions [2,3] indicates that many of the REE aqueous species still need to be more accurately determined. Here, solution calorimetric experiments were carried out from 25 to 150 ºC to determine the enthalpy of solution ($\Delta_{sol}H°$) for the dissolution of Nd hydroxide and Nd chloride solids in perchloric and hydrochloric acid based aqueous solutions (with a starting pH of 2). The standard partial molal thermodynamic properties of Nd^{3+} and Nd chloride species were derived from those calorimetric $\Delta_{sol}H°$ measurements. Comparison of the experimentally derived heat capacity function with the predictions based on Shock et al. [4], reveals a good agreement between calorimetric data and the C_p values based on the Helgeson-Kirkham-Flowers (HKF) equation of state. In contrast, the enthalpy of formation ($\Delta_f H°$) values derived in this study indicate a systematic shift by 8 kJ/mol in comparison to the values derived from Shock et al. [4]. The resulting Gibbs energy of formation of Nd^{3+} ($\Delta_f G°_{298}$) was used to model the solubility of monazite, which results in excellent agreement with previous experiments by Van Hoozen et al. [5] to 250 °C. The measured $\Delta_{sol}H°$ values for Nd chloride dissolution differ by up to 25 kJ/mol from the predicted values calculated using the HKF parameters for $NdCl^{2+}$ or $NdCl_2^+$ [2]. Hence, calorimetric experiments point to a needed to revise the $\Delta_f H°$ values for REE aqueous species to allow formulating better high temperature extrapolations. This work is supported by the U.S. Department of Energy under Award DE-SC0021106.

[1] Gysi et al. (2016) *Econ. Geol.* 111, 1241–1276; [2] Migdisov et al. (2016), *Chem. Geol.* 439, 13–42; [3] Pan et al. (2024), *Chem. Geol.* 643, 121817.; [4] Shock et al. (1997), *Geochim. Cosmochim. Acta* 61, 907–950; [5] Van Hoozen et al. (2020), *Geochim. Cosmochim. Acta* 280, 302–316.