Development of a quality-assured Thermodynamic Database for Rare Earth Elements

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New materials showing specific magnetic and/or electrooptic properties often incorporate Rare Earth Elements (REE). Due to their very specific technological application, it is necessary to separate and enrich the REE from each other. The optimization of physico-chemical conditions for the design of effective extraction and recycling processes of REE relies on accurate and reliable thermodynamic data. However, no fundamental, consolidated and internationally recognized Thermodynamic Databases (TDB) is currently available for REE.

This study aims at providing a reliable, quality-assured and internally consistent TDB for Europium. The thorough evaluation of all available primary literature sources for Eu(III) complexation constants (log β) with inorganic ligands (OH^-, Cl^-, NO_3^-, SO_4^{2-} and CO_3^{2-}) enabled identifying several critical issues: i) inconsistencies between different sources, ii) lack of accurate activity coefficient treatment in case of the formation of weak complexes, and iii) absence of independent spectroscopic validation of the stoichiometry of the proposed complexes.

Thus, several actions have been undertaken for the Eu-chloro, -nitrato and -sulfato complexes:

recalculation of the log β of weak complexes by using an hypothetical reference state (at trace ligand concentration) [1]

advanced spectroscopic techniques (e.g. Time-resolved Laser-induced Fluorescence Spectroscopy) were used to monitor on line the speciation evolution at micromolar range concentrations. This also enabled identifying the prevailing species as well as their stoichiometries. Finally, complexation constants were determined from the spectroscopic data sets.

the conditional log β were extrapolated to standard conditions (I = 0 M, T = 298.15 K) using the Specific Ion Interaction Theory.

[1] Spahiu, K. et al. (1998) Radiochim. Acta 82, 413-419.