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## Abstract Information

### Abstract ID:

22728

### Abstract Text:

Rare Earth Elements (REE) are critical minerals (metals) for the transition from fossil fuels to renewable and clean energy. Accurate thermodynamic properties of REE minerals and other crystalline solids are crucial for geochemical modeling of the solubility, speciation, and transport of REE in ore formation, extraction, chemical processing, and recycling processes. However, the Gibbs free energies of formation ( $\Delta G_{f,REEX}^{\circ}$ ) for these solids from different sources vary by 10s kJ/mol. We applied the Sverjensky linear free energy relationship (LFER) [1] to evaluate and predict the  $\Delta G_{f,REEX}^{\circ}$  of REE solids.

By considering both the effects of ionic radii size and corresponding aqueous ion properties, the Sverjensky LFER,

$$\Delta G_{f,REEX}^{\circ} - \beta_{REEX} \cdot r_{REE^{Z+}} = \alpha_{REEX} \cdot \Delta G_{n,REE^{Z+}}^{\circ} + b_{REEX}$$

allows estimates with much accuracy and precision. Here,  $r_{REE^{Z+}}$  represents the Shannon-Prewitt ionic radii (Å) of  $REE^{Z+}$ , and  $\Delta G_{n,REE^{Z+}}^{\circ}$  denotes the non-solvation contribution to the  $\Delta G_{f,REEX}^{\circ}$  of the aqueous  $REE^{Z+}$  ion. X represents remainder of the compounds. In this study, the parameters  $\alpha_{REEX}$ ,  $b_{REEX}$ , and  $\beta_{REEX}$  were regressed from  $\Delta G_{f,REEX}^{\circ}$  compilations in the literature for 16 isostructural families.

Based on the linear relationships, we recommend a set of internally consistent  $\Delta G_{f,REEX}^{\circ}$  for 155 end-members of REE phosphates, oxides, hydroxides, chlorides, fluorides, carbonates, hydrous carbonates, and ferrites. These  $\Delta G_{f,REEX}^{\circ}$  are combined with experimental or predicted values of  $S^{\circ}$ ,  $V^{\circ}$ , and  $Cp^{\circ}$  from the literature and incorporated into a new SUPCRT database SUPCRTBL\_REE, which allows the calculations of thermodynamic properties to high  $P$ - $T$  conditions (e.g., 1000 °C and 5 kb) at <https://models.earth.indiana.edu>. The log  $K$ s of REE mineral reactions were incorporated into a modified USGS PHREEQC program for calculation of speciation, solubility, and reactive transport

up to 1000 °C and 5 kb. These thermodynamic databases will also be incorporated into the MINES database to be used together with the GEMS code package in the future. This work is part of a collaboration with NMT and LANL on experimental and theoretical geochemistry to develop a comprehensive, internally consistent, and open-source thermodynamic database for REE minerals and aqueous species.

[1] Sverjensky and Molling (1992), *Nature* 356, 231-234.

**Keywords:**

Critical minerals, REE and Thermodynamic database

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