# THEREDA, the thermodynamic reference database for a nuclear waste disposal in Germany

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The disposal of nuclear waste including the assessment of long-term safety is still an open question in Germany. In addition to the still pending decision about the repository host rock (salt, granite, or clay) the basic necessity of a consistent and obligatory thermodynamic reference database persists. Specific challenges are comprehensive datasets covering high temperatures and salinities. In response to deficiencies of other databases THEREDA, a joint project of institutions leading in the field of safety research for nuclear waste disposal in Germany and Switzerland, was started in 2006.

The core of THEREDA consists of a relational databank whose structure has been designed in a way that promotes the internal consistency of thermodynamic data. Data considered cover the needs of Gibbs Energy Minimizers and Law-of-Mass-Action programs alike. Pitzer coefficients to describe solute activity coefficients in high-saline solutions are considered. Both thermodynamic data and interaction coefficients can be described by temperature functions.

Ready-to-use parameter files are created from the databank in a variety of formats. Supported target codes are ChemApp, PHREEQC, EQ3/6, and Geochemist's Work-bench. Data can alos be downloaded in a generic JSON-type format to promote conversion for other geochemical codes Prior to their release all parameter files are submitted to internal test calculations – one essential element of the quality assurance scheme. The results are documented and provided to the users and accessible via internet through http://www.thereda.de/.

Data are currently available to describe the solubility of the following radionuclides or fission elements: U(IV/VI), Th(IV), Np(IV/V), Pu(IV) Am(III), Nd(III), Cm(III), Tc(IV/VII), Sr, Cs and the matrix elements (oceanic salt system, cement phases).

Future develpoments are thermodynamic data sets for Selenium and Oxygen in high saline solutions as well as the inclusion of low saline sorption data.