THEREDA – Thermodynamic Reference Database for the nuclear waste disposal in Germany

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Introduction

The disposal of nuclear waste including the assessment of long-term safety is still an open question in Germany. In addition to the pending decision about the repository host rock (salt, granite, or clay) and the associated site selection, the basic necessity of a consistent and obligatory thermodynamic reference database persists. Such a database is essential to assess potential radionuclide migration scenarios accurately and to make well-founded predictions about the long-term safety up to one million years.

Specific challenges are comprehensive datasets covering also elevated temperatures and high salinities. Concerning the required elements (actinides, fission products as well as matrix and building materials), no other thermodynamic database is available that is compatible with the expected conditions. Due to these deficiencies THEREDA [1,2], a joint project of institutions leading in the field of safety research for nuclear waste disposal in Germany and Switzerland, was started in the year 2006.

Database features

THEREDA offers evaluated thermodynamic data for many compounds (solid phases, aqueous species, or constituents of the gaseous phase) of elements relevant for a nuclear waste repository:

- actinides and their chemical analogues: Th, U, Np, Pu, Am, Cm & Nd,
- fission products: Se, Sr, Tc & Cs,
- matrix elements: Na, K, Mg, Ca, Al, Si | Cl, SO_4, CO_3, PO_4,
- cementitious phases: integration of CEMDATA18.1 [3].

THEREDA provides direct support for a number of geochemical codes:

- GEMS, ChemApp (Gibbs Energy Minimizers),
- Geochemist's Workbench, PHREEQC, ToughReact (Law-of-Mass-Action codes).

THEREDA supports various relevant activity models:

- PITZER model for the activity of hydrated ions and molecules in saline solutions [4],
- ideal and non-ideal REDLICH-KISTER solid solution models [5],

Application examples

The capabilities of THEREDA are demonstrated by comparative test calculations with experimentally determined values:

- invariant points,
- solubility,
- water activity,
- speciation.

A small selection of the more than 400 test calculations currently available on the website is shown here:

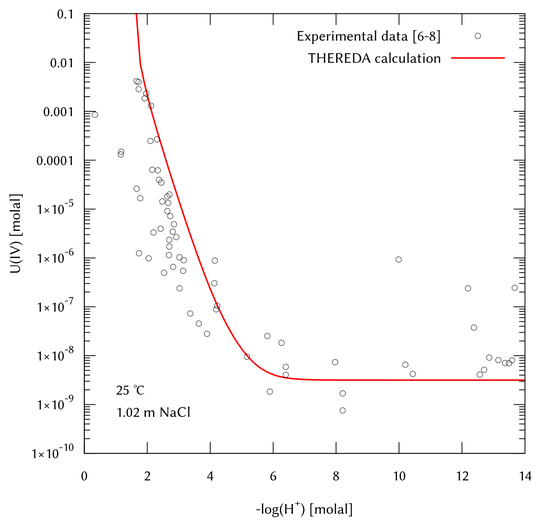

Figure 1: Solubility of amorphous uranium(IV) hydroxide in 1.02 molal NaCl solution at T = 25 °C.

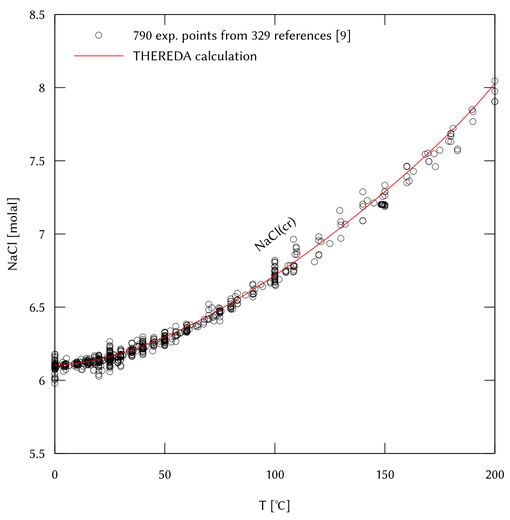

Figure 2: Temperature-dependent solubility of halite in the range of T = 0–200 °C.

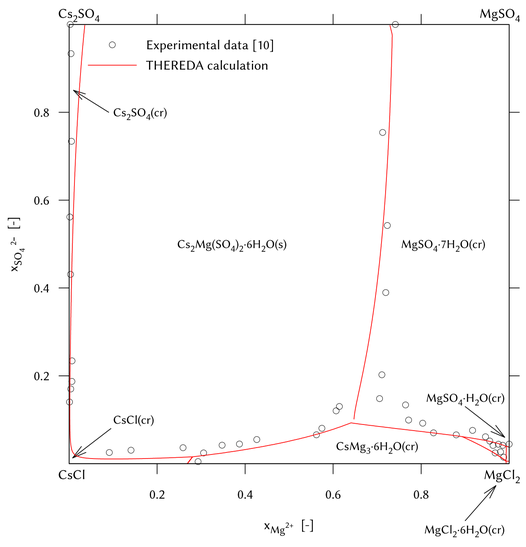

Figure 3: Phase diagram of the quaternary system CsCl-Cs_2SO_4-$MgCl_2$-$MgSO_4$-H_2O at T = 25 °C.

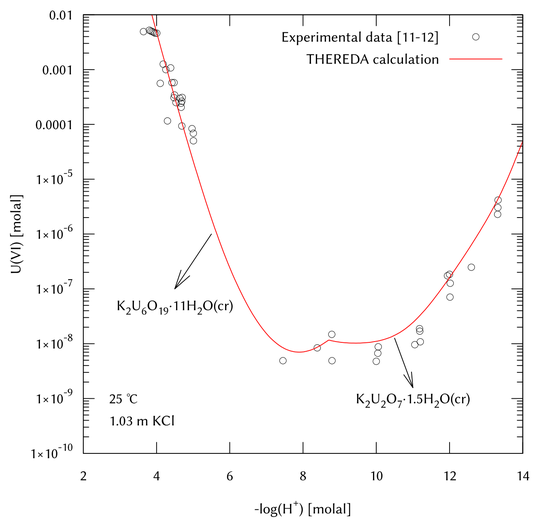

Figure 4: Solubility of $K_2U_6O_{19}·11H_2O$(cr) and $K_2U_2O_7·1.5H_2O$(cr) in 1.03 molal KCl solution at T = 25 °C.

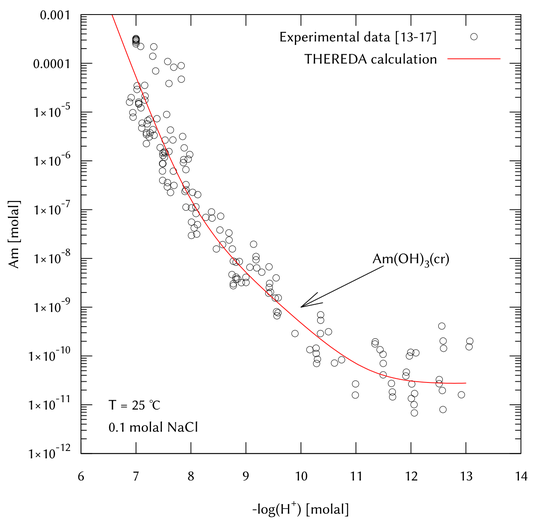

Figure 5: Solubility of $Am(OH)_3$(cr) in 0.1 molal NaCl solution at T = 25 °C.

Conclusions

After a free registration, THEREDA offers full access to the provided data via a web interface.

THEREDA allows users to view all data including their bibliographic reference on the project website. This also provides transparency regarding the results of calculations performed with THEREDA.

THEREDA offers users the opportunity to get in direct contact with team members and discuss various aspects of the data, models, and geochemical codes.

We strongly encourage your feedback!

References

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