



Release Notes

Version	2023a	Date	08.04.2024	Status	Final
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Revision of Release 2023

On 2024-02-16 new data were released from the Thermodynamic Reference Database (THEREDA).

Major changes or additions compared to the former release are:

- Systems NaOH - Mg(OH)₂ - Ca(OH)₂ - CO₂(g) - H₂O(l) (polythermal)
- Systems Mg²⁺ - Cl⁻ - OH⁻ - H₂O(l) (polythermal)
- Systems Na⁺ - Mg²⁺ - Cl⁻ - OH⁻ - H₂O(l) (polythermal)
- Systems Zn²⁺ - Na⁺ - K⁺ - Mg²⁺ - Ca²⁺ - Cl⁻ - SO₄²⁻ - OH⁻ - H₂O(l) (25°C)
- U(+IV)-Hydrolysis and -solubility: Systems U(+IV) - Na⁺ - Mg²⁺ - Ca²⁺ - H⁺ - OH⁻ - Cl⁻ - H₂O(l) (25°C)
- Systems Al(OH)₄⁻ - Si(OH)₄(aq) - Na⁺ - K⁺ - Ca²⁺ - Mg²⁺ - Cl⁻ - SO₄²⁻ - CO₃²⁻ - H₂O(l) (polythermal)
- Double salt CsCl-NaCl and solid solution (25 °C)
- Update for systems O₂(g) - Na⁺ - K⁺ - Mg²⁺ - Ca²⁺ - Cl⁻ - SO₄²⁻ - CO₃²⁻ - PO₄³⁻ - OH⁻ - H₂O(l) (polythermal except for carbonates and phosphates)

Supported codes: PHREEQC, Geochemist's Workbench. The released data are provided additionally in a generic JSON-format. Support for CHEMAPP and TOUGHREACT has been abandoned.

Released parameter files were rigorously tested. Test cases from earlier releases were re-run and new test cases for additional data added. Results with both codes are in agreement with each other and with earlier releases.

This implies that for calculations for untested systems no quantitative measure for the description quality can be given and no warranty can be accepted for computational results. However, THEREDA is applied to an increasing number of published experimental data. Results from these applications can be accessed on our homepage under "Application examples".

The responsibility for this release lies with

- Helmholtz-Zentrum Dresden-Rossendorf, Institute for Resource Ecology, Dep. for Surface Processes, Germany: F. Bok, A. Richter
- Karlsruher Institut fuer Technologie, Institute for Nuclear Waste Disposal, Germany: N. Cevirim, X. Gaona, C. Marquardt
- D. Freyer, TU Bergakademie Freiberg, Institute for Inorganic Chemistry, Germany
- D. Miron, Paul Scherrer Institut, Waste Management Laboratory, Switzerland
- H. C. Moog, Gesellschaft fuer Anlagen- und Reaktorsicherheit, Dep. for Repository Research, Germany

You are welcome to visit us under www.thereda.de/en

On 2024-04-08 the release was revised. Fixed errors:

- **Water stability line at $p(\text{H}_2) = 1 \text{ atm}$ was wrong (GWB only)**
- **Miscibility gap in solid solution $\text{SO}_4\text{-CO}_3\text{-AFt}_{\text{ss}}$ was wrong**

On behalf of the THEREDA management board

Helge C. Moog