

ANNOUNCEMENT – THIRD RELEASE OF DATA TO THE PUBLIC (2012-02-21)

On the 21st of February new data are released from the Thermodynamic Reference Database (THEREDA). This release is denoted as third release (R-03). The new release of data from the THEREDA database comes with parameter files for the system Na, Mg, Ca, K - Cl, SO₄ - HCO₃/CO₂(g) - H₂O.

Valid range of temperature: 298.15 K

Supported codes: CHEMAPP, PHREEQC, Geochemist's Workbench, EQ3/6 (Version 8.0a)

The data have been rigorously tested for simple, ternary subsystems only, as described in the respective benchmark document. This implies that for calculations in higher component systems no quantitative measure for the description quality can be given and no warranty can be accepted for computational results.

Although no example is given in the benchmark document which contains MgCl₂ or MgSO₄, agreement between our results and those obtained with the HMW84 database was verified for the solubility of CO₂(g) or Nesquehonite in MgCl₂ and MgSO₄ solutions.

Consistency with earlier releases: the released data are consistent with those for the system of oceanic salts (R1), calculated for 298.15 K. Thus, with the new parameter files, calculations from the first release (R1) for 298.15 K can be reproduced.

As to interactions between Am, Cm, and Nd (R-02) and SO₄ or carbonate, data are available but still subject of internal control in the THEREDA-team and can therefore not be released yet.

The responsibility of the data in R-03 lies with W. Voigt from TUBAF.

If any questions arise as to the new data, please don't hesitate to initiate a thread in our discussion forum:

<http://www.thereda.de> > Forum

The interested user is also referred to new issues of Technical Papers, available in the download section of <http://www.thereda.de>. For your convenience we give a complete record of the new issues below:

- Technical Paper "Calculation of Fugacities for H₂O(g)", Rev. 1.0 as of December 23, 2011
- Technical Paper "H₂O Formation Data", Rev. 1.0 as of December 23, 2011

On behalf of the THEREDA management board

Helge C. Moog

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