THEREDA Release Notes

On 2022-03-29 new data were released from the Thermodynamic Reference Database (THEREDA). This new data release adds the following systems to earlier releases: Pb(II) - Na, K, Mq, Ca - CI, SO₄, CO₃ $- H_2O(I)$.

Valid range of temperature: 298.15K

Supported codes: CHEMAPP, PHREEQC, Geochemist's Workbench, TOUGHREACT

The new release has been rigorously tested for simple subsystems only.

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. Therefore, users are advised, to have a look on our continuously growing list of application examples on our website.

Consistency with earlier releases: with the new parameterfiles calculations from earlier releases can be reproduced.

For more information please don't hesitate to visit us: https://www.thereda.de

On behalf of the THEREDA management board Helge C. Moog 2022-03-29