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THEREDA – Thermodynamic Reference Database

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Abstract. Part of the process to ensure the safety of radioactive waste disposal is the predictive modeling of the solubility of all relevant toxic components in a complex aqueous solution. To ensure the reliability of thermodynamic equilibrium modeling and to facilitate the comparison of such calculations done by different institutions, it is necessary to create a mutually accepted thermodynamic reference database. To meet this demand, several institutions in Germany joined efforts and created the Thermodynamic Reference Database (THEREDA; Moog et al., 2015).

THEREDA is a suite of programs at the base of which resides a relational database. Special emphasis is placed on thermodynamic data along with suitable Pitzer coefficients which allow for the calculation of solubilities in high-saline solutions. Registered users may either download a single thermodynamic datum or ready-to-use parameter files for the geochemical speciation codes PHREEQC, Geochemist's Workbench, CHEMAPP, or TOUGHREACT. Data can also be downloaded in a generic JSON format to allow for import into other codes. The database can be accessed via the world-wide web: http://www.thereda.de (last access: 13 July 2023).

Prior to release, the released part of the database is subjected to many tests. Results are compared to results from earlier releases and among the different codes. This is to ensure that, by additions of new and modifications of existing data, no adverse side-effects on calculations are caused. Furthermore, our website offers an increasing number of examples for applications, including graphical representation, which can be filtered by components of the calculated system.

References

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