Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.11920

New developments of the ThermoChimie database

ELISENDA COLÀS[1], OLGA RIBA TORT[1], JORDI RODRÍGUEZ[1], MARTA LÓPEZ-GARCÍA[1], DARÍO PÉREZ[1], JAMES D BEGG[1], LARA DURO[1], ADAM FULLER[2], WILL BOWER[3], STÉPHANE BRASSINNES[4] AND BENOIT MADÉ[5]

[1]Amphos 21 Consulting S.L.
[2]Galson Sciences Limited
[3]Nuclear Waste Services
[4]ONDRAF-NIRAS
[5]Andra

Presenting Author: eli.colas@amphos21.com

ThermoChimie (http://www.thermochimie-tdb.com/; [1]) is a thermodynamic database developed by Andra (France), Nuclear Waste Services (UK) and Ondraf/Niras (Belgium). It is intended to be used for geochemical calculations supporting radioactive waste management activities.

The ThermoChimie database is under constant revision and development. After its public release in 2014 (version 9) and further updates in 2015 (version 9b) and 2018 (version 10a), versions 10d and 11 have been released in 2021 and 2022, respectively. These new versions contain significant updates and improvements of interest in the field of radioactive waste disposal.

ThermoChimie builds upon the reviews of the NEA Thermochemical Database Project, [2] and extends the selection of the NEA to allow for a complete and consistent representation of the processes of interest. ThermoChimie version 11 contains significant updates on the thermodynamic data selection for uranium, neptunium, plutonium, americium and technetium, following the update published by the NEA-TDB [3]. Furthermore, an exhaustive and accurate review of iron thermodynamic properties has been carried out, using the NEA-TDB review [4,5] and additional literature publications.

Two new elements, beryllium and copper, have been added to the database; the selection takes into account the most recent scientific publications. In addition, an effort has been made to further extend the database application to temperatures higher than 25°C. When reliable experimental data are not available, enthalpy or entropy data in the database are estimated using different approaches.

PFLOTRAN has been recently added to the list of geochemical codes for which ThermoChimie is compatible with, the others being PhreeqC, Crunch, ToughReact, CHESS, Geochemist Workbench and Spana.

ThermoChimie will continue to be updated with new relevant scientific literature. Future actions include integrating complementary data related to zeolites, cement phases and organic molecules and an extensive benchmarking exercise with other thermodynamic databases.

[1] Giffaut et al. (2014), *Applied Geochemistry* 49, 225–236.
[2] Ragoussi et al. (2019), *J. Environ. Radioact*. 225-231.
[3] Grenthe, et al. 2020, NEA-OECD Chemical thermodynamics 14.
[4] Lemire et al. 2013, NEA-OECD Chemical thermodynamics 13a.
[5] Lemire et al. 2020, NEA-OECD Chemical thermodynamics 13b.