MINTEQ v9: A review and update to an old classic

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Geochemical databases such as MINTEQ, LNLL, PHREEQC and many others form the basis of the geochemical modelling softwares that are used for defining and modeling our geochemical reality, from laboratory experiments to the environmental impact of industrial activities. The definition of thermodynamic databases is one of the great advance of the past century.

Most of the databases in use to date evolved from earlier precurors such as SUPCRT92 [1], which emerged from the primordial soup of thermodynamic data reported in the last century (e.g. [2]). However the original data is sparse, incomplete and filled with correlations [4] while the original datapoints are often difficult or impossible to find.

An update to the main databases is required as a large number of speciation constants has been ignored or revisited in the last decade [3]. Moreover the increasing use of organic molecules in geochemistry makes their presence in geochemical codes essential. Similarly a number of complexes with REE and dissociation constants of mineral phases need to be both reviewed and implemented. The aim of this work is to compile and update the US EPA geochemical database MINTEQ.V4 into a more comprehensive database. To that end, the species and phases present in other databases (e.g. LLNL) are recalculated and corrected to fit within the Minteq database. Additionally a systematic review of published (for example [5]) and pre-existing thermodynamic properties is used to improve the predictive capability of the database.

[1] Johnson, Oelkers, & Helgeson, 1992. *C. Computers & Geosciences*, **18**

[2] Helgeson, 1969. *American Journal of Science*, **267**

[3] Schott, Mavromatis, Fujii, Pearce & Oelkers, 2016. *Chemical Geology, **accepted***

[4] Oelkers, Bénézeth, & Pokrovski, 2009. *Reviews in Mineralogy and Geochemistry*, **70**

[5] Nordstrom, Majzlan, & Königsberger, 2014. *Reviews in Mineralogy and Geochemistry*, **79**