Empowering Users as Builders: modeling aqueous complexes with the WORM Complicator

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Understanding how cations and ligands react to form complexes is key to thermodynamic modeling of the solubility, mobility, and bioavailability of elements in hydrothermal fluids. However, thermodynamic data painstakingly collected from decades of experimental research still cannot account for the sheer number of possible cations, ligands, and their combinations. How can we fill in these large gaps in our ability to accurately model aqueous complexes? Here, we introduce the Water-Organic-Rock-Microbe (WORM) Complicator, a free software tool available to the public through the open-source online WORM Portal geochemical modeling platform (http://worm-portal.asu.edu). The tool is accessible through an internet browser and does not require software downloads or installation. The purpose of this tool is to revolutionize modeling of aqueous systems by enabling WORM users to become builders of thermodynamic data.

The Complicator is designed to rapidly estimate the thermodynamic properties of aqueous multiple-ligand complexes for user-supplied lists of cations and anions. Input consists of equilibrium constants of association reactions for the complexes of interest. Standard state entropies of association can be optionally provided for more accurate estimates. The Complicator uses correlation methods that predict standard state partial molal Gibbs free energies, enthalpies, entropies, heat capacities, and volumes, as well as parameters for the revised Helgeson-Kirkham-Flowers equation of state or Deep-Earth Water model. We provide an editable template that results in thermodynamic properties for 150+ new and existing complexes. Users are guided through the processes of expanding the number and variety of complexes, which includes estimation methods applicable across the periodic table. Results are immediately compatible with other geochemical modeling tools on WORM like AqEquil for geochemical speciation and mass transfer calculations, and pyCHNOSZ for calculating reaction properties.

We invite users to perform and publish their own estimations with the WORM Complicator. As the availability of thermodynamic data grows, we hope this will enable more complete modeling of aqueous fluids in geochemical processes on Earth and elsewhere.