ThermAc: A Joint Project on Aquatic Actinide Chemistry and Thermodynamics at Elevated Temperature Conditions

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The ThermAc project aims at extending the chemical understanding and available thermodynamic database for actinides, long-lived FPs and matrix elements in aquatic systems at elevated temperatures. Such conditions are expected when storing highly active heat producing waste in a repository system over a significant period of time after starting repository operation. If early canister failure occurs, radionuclides may contact aquatic systems at higher temperatures. Scientific tools must be available to assess the related chemical effects and their impact upon safety. ThermAc approaches this challenge by evaluating the capabilities of a variety of estimation methods to obtain thermodynamic parameters (formation constants, enthalpic and entropic data) as *f*(T). This is done by intercomparison between such methods and pointwise checks with experimental results. A clear focus is on long-lived actinides in oxidation states III, V and VI, with selected fission products and important redox controlling matrix elements like Fe also receiving attention. ThermAc addresses the temperature range from ~5°C to ~90°C, focusing on systems at low or intermediate ionic strength. Only for selected cases with scientific interest, higher temperatures up to 200°C or salt brine solutions are investigated. Chemical analogs help to gain information on solid phase transformation processes. Ion-ion-interaction processes are treated with the SIT, in agreement with the NEA-TDB project. Quantum chemical calculations are used to support the interpretation of experimental findings, and establish a fundamental understanding of chemical effects on a molecular level.