



Proposal title	Radionuclide Complexation with TBP and DBP: Thermodynamic Data Generation for the ThermoChimie Database
Funders	ThermoChimie Consortium (Andra-Nuclear Waste Services-ONDRAF-NIRAS)
Dates	To commence latest Q1 2023
Project Brief	
<p>The overall aim of this PhD is to design and execute a programme of experimental research to help address key data gaps in the ThermoChimie database. Whilst there has been significant work to date to assimilate thermodynamic data for radionuclide complexation with organic species into the ThermoChimie database, these data broadly cover a limited set of organic species (primarily EDTA, ISA). Very limited research into the behaviour of radioelement complexation with di- and tri-butyl phosphate (DBP & TBP) has been performed.</p> <p>As such, thermodynamic data for the complexation of TBP or DBP in aqueous systems (particularly at neutral to alkaline pH) are scarce, and no data for these systems of interest are currently present in the ThermoChimie database. As likely components of the waste inventory destined for a cementitious geological disposal facility, a deeper understanding of their behaviour, and provision of preliminary underpinning data, will aid process and system modelling.</p> <p>ThermoChimie propose a small screening study with key radioelements (e.g., Pu(IV/V), U, Th, Fe, Ni, Ca, Na, K) of interest to understand the particularities of these ligands that may be useful to derive its complexation properties. We encourage proposals which target priority radionuclides according to an institute's specialisms and do not expect all radioelements listed to be considered. A targeted experimental testing programme will fill key data gaps, as well as help to infer behavioural properties of these ligands, for comparison with other species in the existing database. This is intended to be an exploratory study; work should be kept constrained and provide an initial basis for ongoing experimental work. Proposals may wish to explore the effect of competing ions or test the hypothesis that organic ligands are assumed to be out-competed by hydrolysis at high pH.</p> <p>ThermoChimie welcomes proposals for a fully funded, maximum 4-year PhD project, commencing in Q1 2023. Proposals should be no more than 4 sides of A4 and include a robust project plan, a Gantt chart incorporating a set of milestones, and a breakdown of research costs.</p>	
Background and context of research	
<p>ThermoChimie is a high-quality thermodynamic database, established in 1995, focused on providing datasets of relevance for geochemical modelling of cementitious geological disposal facilities for radioactive waste. To date, there have been three phases of the ThermoChimie Project. As of Phase 3 (the current Phase), a tripartite consortium of ANDRA, ONDRAF/NIRAS, and Nuclear Waste Services (NWS) jointly lead in its development.</p> <p>ThermoChimie has funded several historic activities to expand the database to incorporate a broader range of organic/radionuclide interaction data. A series of literature surveys between 2017 – 2021 identified that thermodynamic data for TBP and DBP complexation with radionuclides, under conditions of relevance (pH 8-13) were scarce, and that a general understanding of the behaviour of these species in comparison to other complexants was lacking. These reports are available on request.</p>	