



Graduate Students Seminar

Department of Energy Engineering

Tuesday, June 27th, 2023

Time 14:00

Bldg. 43 Room 015

Gev Dovrat

Under the supervision of Prof. Armand Bettelheim, Prof. Israel Zilbermann and Prof. Yaniv Gelbstein

Macrocyclic Chelates of f-block Metals in Aqueous Solutions – Chemical Reactivity Tuning via Ligand Functionalization

The increasing prevalence of modern technology in everyday life and the everlasting demand for affordable and clean electrical energy has led to an increased reliance on the efficient harness of f-block metals' exquisite chemical and physical properties. The management of these elements, from mining to disposal or reuse, presents significant challenges, particularly in the context of the Nuclear Fuel Cycle and its idealized envisioned closure. These challenges call for the development of new methodologies for the safe and efficient chemical handling of these elements. One promising approach involves the utilization of macrocyclic cyclen-derived ligands, which have shown promise for their selective binding and stability of their different metal cation chelates, and of the lanthanides specifically. Though such methodologies have matured into multiple bio-technological applications, equivalent progress has not been recorded for the utilization of these substances to the actinide elements. This markedly underexplored affinity could theoretically provide a perfect match between a diverse set of chemical encapsulation tools to some of the worst poisonous elements found on earth.



Therefore, a systematic study of the aqueous properties of tetravalent uranium cations complexes and their comparison to trivalent and tetravalent cerium cations counterparts was conducted using analogue macrocyclic ligands. Simple variations of the functional coordinating moieties of the cyclen-derived macrocyclic ligands were investigated to determine their effect on the complex formation mechanism, reactivity in solution, and relative stability of the cation redox transitions. The collected data from a wide range of analytical techniques was scrutinized and revealed novel structural and solution coordination dynamics trends, which challenge the common prevalent conceptions for the kinetic properties of these elegant chemical species. These findings will be presented along with a discussion regarding their possible implications for the development of new methods and approaches for the safe and efficient handling of the f-block cations in aqueous solutions.



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