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Understanding the Interactions of Seawater Ions with Amidoxime through X-Ray Crystallography

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ABSTRACT:

We aim to understand how metal ions from seawater bind to uranium-selective amidoxime functionalized sorbents by experimentally determining the structures of metal complexes with molecules simulating the possible binding sites. Based on this new understanding, we also aim to develop a method for recovering the metals and recycling the sorbent by using hydroxylammonium salts as stripping agents which mimic the chemical character of the sorbent.

The extraction of uranium from seawater is viewed as a nearly unlimited long term source of fuel for nuclear power. The leading approach is sorption onto polymers functionalized with the amidoxime [$RC{=}NOH(NH_2)$] group but requires improvements in sorbent capacity and recyclability to be economically viable. Approaches to improving the sorbent would benefit from an understanding of how uranium *and* its competitors interact with amidoxime. It is known that amidoxime can convert into multiple forms or bind cooperatively with neighboring groups on the sorbent. Identification of the most important binding sites is uncertain because metals bound to the surface of the sorbent are difficult to characterize unambiguously, and the modes of interaction of possible binding sites are not yet known for all the different metal ions in seawater.

The proposed research will advance the understanding of how metal ions interact with amidoxime functionalized sorbents through the following objectives:

1. Crystallize and structurally characterize complexes of seawater ions with small molecule analogs of possible binding sites to develop experimentally validated models for potential absorbed species.
2. Spectroscopically characterize these metal complexes in order to identify spectral features which can be used to identify the actual absorbed species on metal-loaded sorbents.
3. Use hydroxylamine based stripping agents to remove metals from loaded amidoxime sorbents and determine if elution is correlated with the affinity of the metal ion for hydroxylamine.

Small molecules containing multiple amidoxime functional groups will be made from a variety of commercially available polynitrile precursors and used to crystallize metal complexes for structural characterization by single crystal X-ray diffraction. These complexes will act as models to aid in both fundamental understanding of the interactions and identification of actual species on the sorbents. To complement our solid state study, we will also study the stripping of metals from amidoxime-functionalized sorbents with hydroxylamine-based leaching agents, which due to their structural similarity to the coordinating moiety in amidoxime are expected to strip metals with the highest affinity for the sorbent.