



A Modified H₃TriNO_x Ligand for Rare Earth Metal Separations

Ingemar Falcones (EAS 2019)

Advisor: Eric Schelter

The rare earth elements share many common characteristics, from exhibiting trivalent cationic behavior to having very similar ionic radii. These elements are especially important for clean energy technologies, as they are used in the permanent magnets in wind turbines and phosphors in compact fluorescent lights. However, after being mined from Earth's crust, these elements are difficult and expensive to separate. The Schelter group at the University of Pennsylvania's Chemistry Department has developed a cheap and operationally simple strategy that will contribute to a secure supply chain for the rare earth elements. Their recently developed ligand (denoted H₃TriNO_x) separates the rare earth elements based on the slight differences in ionic radii and solubility properties of the resulting rare earth monomer and dimer complexes. Throughout the summer of 2016, the goal of my project was to modify this H₃TriNO_x ligand through the addition of an electron-donating methoxy group and investigating its effect on rare earth separations.

Considering that this experience was the first time I have been exposed to a real research-based chemistry laboratory setting, I quickly developed skills relating to writing laboratory procedures and using the equipment properly. I noticed how scientists build up their research based on published content rather than starting with a completely blank slate, and I adapted to this method by working under Bren Cole, a PhD student, following his footsteps and records to assist with the experiments. However, since the molecule we aimed to create was brand new, we had to adjust the procedures slightly to make the experiments work for the unique situation. For instance, the development of the H₃TriNO_xOMe molecule required a slight change in the duration and temperature conditions at which the reaction proceeded. Chemistry reactions in research are hardly ever successful on the first try, but there are ways to analyze the reaction progress to determine if it is approaching the desired product(s). Common analytic techniques are Nuclear Magnetic Resonance (NMR) Spectroscopy and Liquid Chromatography-Mass Spectrometry (LC-MS), both of which were used to determine the amount of product relative to the reactants, and therefore the progress of the reaction.

After the synthesis of the new H₃TriNO_xOMe ligand, I learned about common crystallization

techniques so that the molecule could be analyzed and categorized through X-Ray diffraction. Personally, I found it exciting to see the crystal structures of the molecules I helped create, as such models are commonly found in published scientific papers. Although I have not taken organic or inorganic chemistry classes yet, I learned about some aspects of the subjects, from nuclear spins to oxidation/reduction electrochemistry from this research. As I progress through my undergraduate career as a Chemical & Biomolecular Engineering major with minors in Materials Science & Engineering and Chemistry, I am considering attending graduate school and would like to continue working with the Schelter group to develop my passions even further. I know I am now better equipped for my education at Penn and beyond than before this experience through PURM.