What’s in the Solution? An Investigation of Triazolophane Complexes
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The behavior of chemical solutions can be complicated, and scientists and non-scientists alike are often looking for ways to determine exactly what is happening when two solutions are mixed together. Our lab has taken on the challenge of investigating these complicated solutions. In order to do this, we perform spectrophotometric titrations in which a titrant solution is added to an analyte solution in very small increments and the absorbance of the analyte solution is measured at each addition (Figure 1). We attempt to answer three research questions by analyzing the data from these titrations. First, we try to ascertain how many different species are forming in solution as the titrant is added to the analyte. Second, we seek to identify the spectroscopic signature of these individual species. Finally, we try to determine the equilibrium constants and thermodynamic parameters associated with the equilibrium reactions between the species.

This approach can be applied to a variety of systems where molecules are interacting in solution. One of the systems that I studied this summer involves the interaction of triazolophane molecules and halides ions. Triazolophane is a macrocycle synthesized in the lab of Dr. Amar Flood at Indiana University. Triazolophane molecules are unique because they have a cavity lined with carbon-hydrogen bonds which form hydrogen bonds with halide anions in solution (Figure 2). Because the cavity is a specific size, the triazolophane molecule binds to different halides with varying affinities [1]. Therefore, there is relative competition between the halides, and this selectivity could potentially be harnessed in a variety of ways. One application of triazolophane system involves its use as a halide selective ionophore [2].

My research project took a new approach to the triazolophane system. The binding constants for this system had already been studied [3], but I expanded on this by collecting titration data at multiple temperatures. Temperature dependent studies allow us to gain insight into the enthalpic and entropic drivers of this specific system. Once I collected the absorbance spectra, I used an analysis program called Sivvu™ to break down the absorbance data into molar absorptivity curves and equilibrium concentrations. Sivvu™ uses matrix algebra to do this for each chemical species in solution in accordance with Beer’s Law. In doing so, it provides the information to characterize each absorbing chemical species in solution as well as identify how these species interact with each other. This summer we were able to identify four absorbing species, including triazolophane, and three complexes (1:1, 2:1, 1:2 triazolophane:halide). Using this model we were able to determine binding constants for the system at four different temperatures.

This summer of research was a really great experience for me. Even though the research process could be challenging at times, there were always new questions to investigate. This summer I also learned to more fully appreciate the power of collaboration within a lab. Our group often came across seemingly large problems, but together we were able to solve them. Despite the challenges that we’ve faced throughout the summer, I’ve really grown to appreciate working with others in order to tackle these larger research questions.