This summer I studied complexes formed in solution between different metal species and tris[3-(2-pyridyl)pyrazol-1-yl] hydroborate (1). For sake of simplicity I will refer to this molecule as the ligand. This particular molecule can bind up to three metal cations and can form two known structures with equal equivalents of metal to ligand, a 1:1 and a 4:4, both of which have been crystallized out of solution previously. What I have been looking into this summer is whether or not these structures and possibly other structures are forming in solution. In order to determine this, I have been running spectrophotometric titrations where small amounts of a solution with ligand is added to a solution of metal cation and scanned using a UV vis. This data is then analyzed using a computer program written by Prof. Vander Griend and previous student call SIVVU™, which can tell the user how many species are in solution as well as other useful information.

Several good models have been determined for the interaction between the ligand and Co$^{2+}$ or Ni$^{2+}$ in solution. The ligand-Co$^{2+}$ data indicates that there are 6 or 7 species, including Co$^{2+}$, forming in solution. At this point I have tentatively determined that [Co$_3$L]$_5^+$, [CoL]$^{1+}$, and [CoL$_2$] complexes are forming during the Co$^{2+}$ titration. The other two species are a bit harder to pin down, but a list of possible candidates has been created. For the ligand-Ni$^{2+}$ system, there are primarily 6, and possibly 7 species including Ni$^{2+}$ forming in solution. I have found several good models for this data, including the best model which contains Ni$^{2+}$, [Ni$_3$L$_2$]$^{4+}$, [Ni$_3$L$_3$]$^{5+}$, [NiL]$^{1+}$, [Ni$_3$L$_4$]$^{2+}$, [Ni$_3$L$_3$]$^{1+}$, and [NiL$_2$].

There are some interesting similarities between the two systems. The systems are more complex than they initially appeared and there are many more species in solution than the 1:1 and 4:4. What is especially fascinating is that the ligand interactions between both of the metal cations appear to prefer the formation of the 1:1 configuration over the 4:4 configuration in solution even though Ni$^{2+}$ prefers the 4:4 when it has been crystallized. Because the 1:1 and the 4:4 could have similar properties that would make distinguishing them a bit tricky, a mass spec experiment would need to be conducted in order to rule the 4:4 completely out.

This summer has taught me a lot about problem solving, designing experiments, and using computer modeling to analyze the data. Each of problem and challenge forced me to analyze my techniques and determine a better ways to do things. Designing experiments helped me learn to prioritize and figure out what I really needed to do to progress onward with the analysis. One of the best learning experiences of all though was getting to meet with some of Prof. Vander Griend’s collaborators and talk to actual graduate students and learn about what they have been researching. All of these factors have helped me grow as a scientist and have gotten me to think more about what I want to do after graduating from Calvin.

---