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Synthesis of the N4 Tetradentate Ligand

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TOWARD A BETTER UNDERSTANDING OF...

Synthesis of the N4 Tetradentate Ligand Emily Morgan

Mentor: Liviu Mirica

In today's industry there is a high demand for the ability to synthesize large organic molecules for use as drugs or fuel sources. Metal catalysts represent one powerful method thru which two hydrocarbons are fused together via a cross-coupling reaction. Our group focuses on the catalysts for these reactions, specifically those of palladium and nickel varieties. Much work has been done on palladium catalysts in their 0 and +2 oxidation states. The +3 and +4 oxidation states of Pd and the +3 state of nickel also appear to catalyze these coupling reactions, but the mechanisms thru which they do so are poorly understood.

In order to clarify the mechanisms thru which Pd^{III-IV} and Ni^{III} catalyze these reactions we use the N4 tetradentate ligand which interacts with and stabilizes the metal ions and allows us to study their properties. This ligand is well-suited for our investigations for several reasons. The ligand is flexible and macrocyclic which allows it to stabilize the octahedral geometry of the Pd^{III}, Pd^{IV}, and Ni^{III} ions. Additionally, we are able to add various functional groups to the ligand, and by studying the effects of the addition of these functional groups we can infer certain properties of the metal complexes.

One current limitation on our research is the labor and time-intensive nature that the synthesis of the N4 ligand requires several steps. Thus, one goal is to increase the efficiency of the N4 tetradentate ligand synthesis. Additionally, we will be investigating other reactions that involve modifications of the ligand.