

THE MOLECULAR WIRE CONCEPT AND DEVELOPMENT

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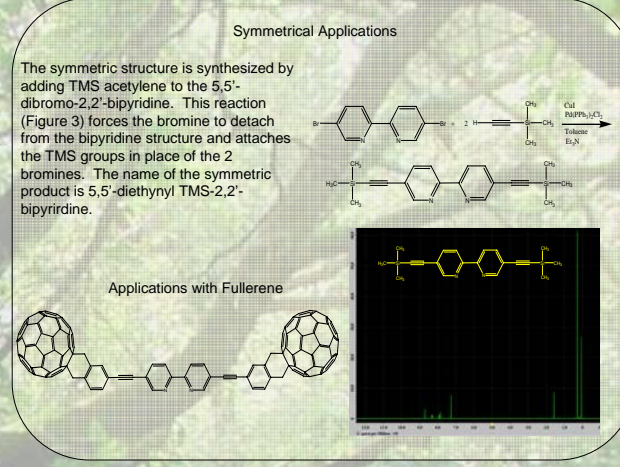
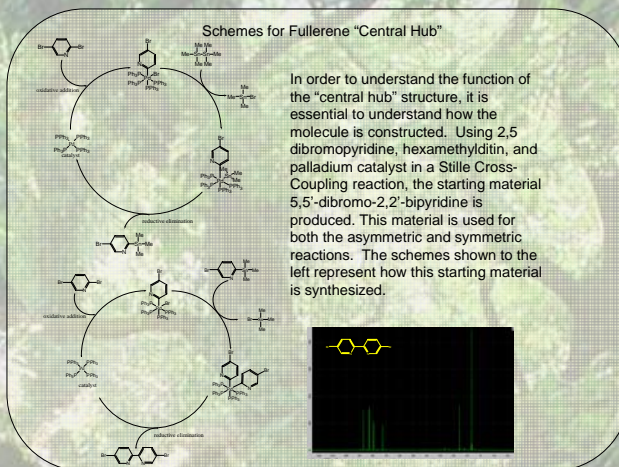
Objective:

The goal of our supramolecular research is to create a molecular wire subunit which will transfer electrons over a highly conjugated organic polymer. This unit will wrap around a metal center thus bringing the metal directly in line with the conjugated polymer backbone creating a macromolecule, a polymer incorporating metals for the purpose of transferring energy. This project first requires the synthesis of a series of ligands followed by the synthesis of the final molecular wire subunit.

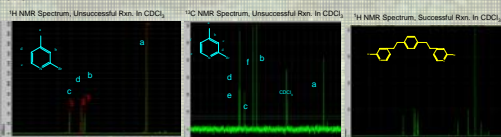
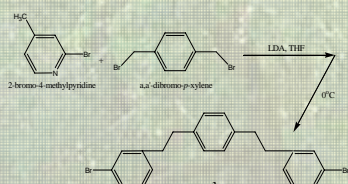
Currently, this project has been worked on from two ends. The first involves synthesizing the molecular wire ligands for the molecular wire subunit. The other project focuses on creating a "hub" molecule which will be incorporated into a fullerene complex. This highly conjugated system will be especially suited for transferring electrons over the conjugated surface. When these modular compounds are synthesized they will be attached to the fullerene and then combined in the organometallic complex.

Steps:

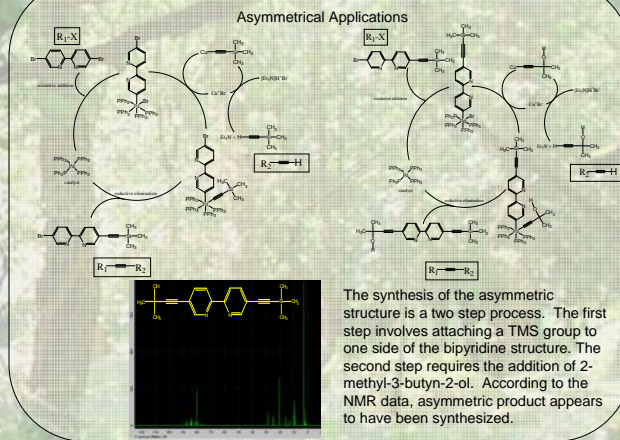
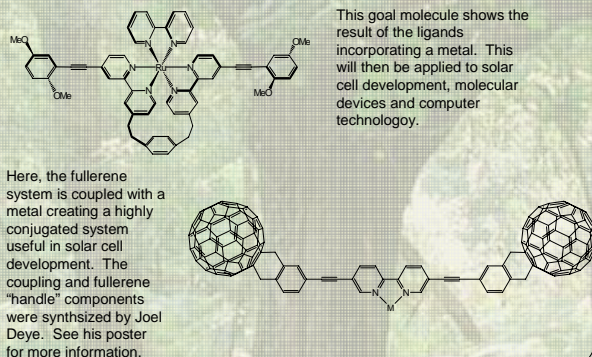
- Construct ligands through synthesis
- Form the linear multimetallic system by incorporating a transition metal into the backbone of the ligand
- Utilize the supramolecule in solar cell development, in molecular devices and in computer technology



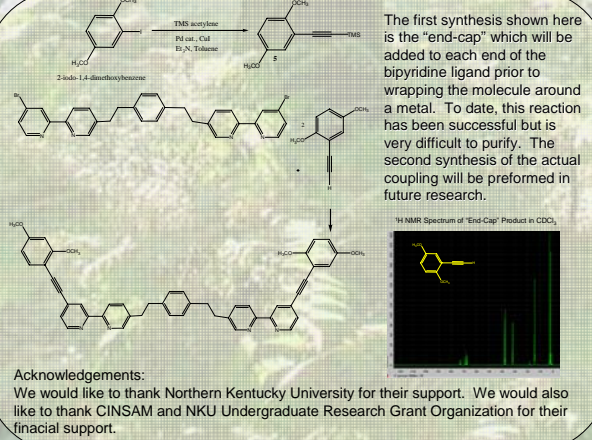
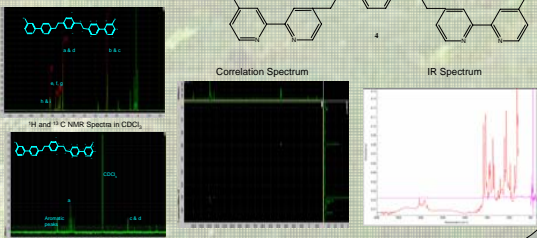
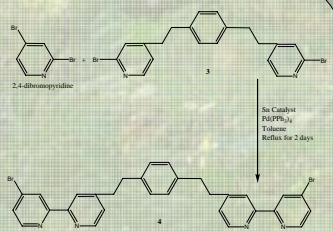
The reaction to synthesize product 3, the ligand precursor, is very sensitive to the LDA which is made from n-BuLi. A significant amount of the time spent on this reaction was finding satisfactory proportions and using fresh n-BuLi. The reaction is also very sensitive to temperature and the atmosphere. So far, one attempt of this reaction was successful. NMR spectra are shown of both the unsuccessful and successful reactions to show the starting material remaining and also trace amounts of it in the successful reaction.



The Goal Molecules



This reaction utilizes the ligand precursor (3) to synthesize the bipyrindine ligand (4). After the reaction is performed purification includes filtering through a frit and column chromatography. Although this reaction has been successful, the product is difficult to purify completely due to the various other substitutions that are created in the process.



Future Steps:

- For the Fullerene Applications:
 - Separate asymmetric product from previously synthesized product (shown above in NMR)
 - Attach a fullerene to one side of the asymmetric product and attach the other side to a system capable of transferring charge into the fullerene.
- For the Molecular Wire Applications:
 - Refine the synthesis and purification of the ligand precursor and bipyrindine ligands
 - Couple the bipyrindine ligand to the "end-caps"
 - Wrap around the metal to create the supramolecular system for solar cell development

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