Towards the Synthesis and Characterization of the Planar-Chiral (PS)-1-Isocyano-2-Methylcymantrene Ligand

Prior to the work done by the University of Kansas on this project, the research concerning planar-chiral isocyanide ligand research was conducted on the organometallic complex of ferrocene. In our research project, Dr. McGinnis and I are collaborating with the University of Kansas to expand this research to the metallocene cymantrene. This will allow us to compare our cymantrene compounds with the ferrocene precedents to contrast stability, redox capabilities, and structure. These findings will determine possible applications of the planar-chiral cymantrene isocyanide ligand in a variety of situations including asymmetric catalysis, materials chemistry, and nanotechnology.

Cymantrene is an organometallic complex in the half-sandwich configuration. This structure is composed of three carbonyl groups bonded to a manganese center which is coordinated to a cyclopentadienyl ring. In the final stage of our synthesis, these complexes will be coordinated to a metal center using isocyanide ligands. These ligands exhibit planar chirality, as determined by the presence of multiple substituents on the planar ring in the compound.

Isocyanide ligands are ligands in which a carbon atom is triple-bonded to a nitrogen which is attached to some R group (in this particular case, the cymantrene complex). The carbon also possesses a lone pair of electrons which cause the carbon to be an excellent sigma donor. This allows for there to be a strong sigma bond formed between the carbon and the metal by an overlap of the carbon atom's filled sigma orbital and an empty p or d-orbital on the metal. The metal's large and diffused electron density pushes the electrons in this sigma bond back onto the ligand causing overlap with an empty pi orbital on the carbon. This phenomenon is referred to as

back-bonding and has a strong stabilizing effect on the ligand. As our final product utilizes these ligands, it is expected to be stable as well.

Our plans for further research include the following of a synthetic pathway at the UAFS and KU campuses, beginning with cymnatrene and working through ten intermediate compounds until we arrive at the desired planar-chiral isocyanide ligands. We will work to optimize the yields of this pathway and then conduct NMR characterization, optical rotation, X-ray crystallographic and cyclic voltammetric characterization on the produced ligands. The results of this synthesis and characterization will be discussed at the fall 2015 MICA conference and possibly at an ACS conference. Finally, results will be published in a peer-reviewed chemistry journal.