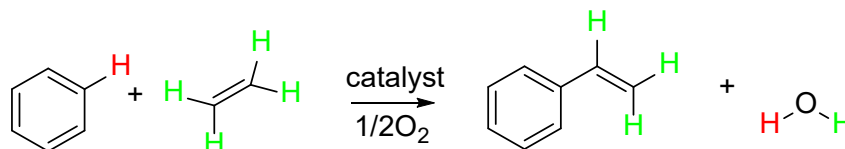


Development of Transition Metal Complexes for Breaking Unreactive Chemical Bonds

Dr. John Lee

Organometallic chemistry is a combination of inorganic and organic chemistry and is broadly defined by the presence of direct metal-carbon bond(s). The metal can be a main-group, transition, or rare earth metal, and the bond with carbon can either be a single or multiple bond. The use of organometallic transition metal complexes as catalysts in organic synthesis has been very important in recent years and has been an integral part of the development of this sub-discipline of chemistry. One area in catalysis that is currently being pursued is the selective activation and functionalization of inert chemical bonds such as the C—H bond of hydrocarbons, and an example is shown in Scheme 1.



Scheme 1

This summer we will work on the synthesis and characterization of cobalt-based homogeneous catalysts for C—H functionalization. The first complex is in collaboration with Dr. Pienkos where two different transition metals and will be in the same complex to give the heterobimetallic compound as shown in Figure 1. Each “piece” of the compound shown in Figure 1 is proposed to play an integral role in the reactivity. A second complex involving a chiral bidentate ligand represents a second potential project. An example crystal structure is shown in Figure 2, and we propose to take advantage of the removal of iodide by silver(I) acetate while utilizing both the chirality potential hydrogen-bonding of the bidentate amine ligand in C—H functionalization reactions.

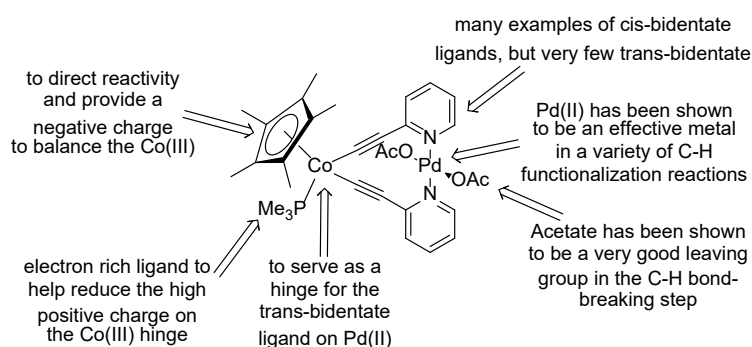


Figure 1

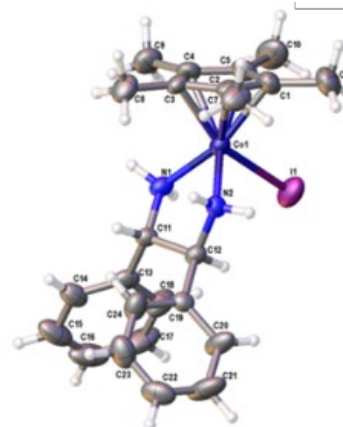


Figure 2

These proposed catalytic reactions are of interest as they represent a greener and more atom economical use of our existing fossil fuel resources. The student will learn synthetic inorganic and organometallic chemistry, which includes air-free chemistry in a nitrogen filled glove box and Schlenk techniques. A significant amount of the Department's instrumentation will be used for characterization, which includes: $^1\text{H}/^{13}\text{C}/^{31}\text{P}/^{19}\text{F}$ NMR spectroscopy, infrared and UV-vis spectroscopy, electrochemistry, and single-crystal X-ray diffraction. In addition, the student will be encouraged to present their work at the 2022 Regional American Chemical Society meeting held in Puerto Rico.