SOAR Research – Faculty Proposal – Summer, 2015

Synthesis, Isolation, and Characterization of Catalytic Activity of Rhodium Complexes

Faculty: Stephen Dunham, Ph.D., and Shari U. Dunham, Ph.D., Associate Professors of Chemistry

Student: Devon Jakob

Project Start Date: June 1, 2015
Length of Project: 10 weeks

Description of the project
Synthesis, Isolation, and Characterization of Catalytic Activity of Rhodium Complexes

The Dunhams research at Moravian has primarily focused on the binding interactions of rhodium (Rh) complexes with deoxyribonucleic acid (DNA). In the process of this research, we have synthesized several new rhodium compounds that may have other interesting and useful chemical properties. An active area of research with rhodium complexes is studying catalytic reactions. A catalyst is a compound that speeds up a chemical reaction without being changed during the reaction. Rhodium catalysts are used for several chemical reactions including the formation of new bonds between carbon and hydrogen atoms, both C-H and C-C bonds. Our goals in this project are to synthesize and test several rhodium complexes to determine if they are able to carry out catalytic reactions. By developing these techniques in the Dunham lab, future rhodium compounds will be tested not only for their DNA binding and biological activity, but also for their ability to carryout catalytic chemical reactions.

Synthesis and Isolation of Rhodium Complexes
The first goal of the project is to repeat previous synthesis and isolation of the Rh complexes carried out by former SOAR and honors students (Donchez ’13 and Bartulovich ‘15). These syntheses are now becoming routine for students to complete in our laboratory.

Characterization of Catalytic Reactions
The other experimental goal for this project will be to react purified Rh complexes with various organic compounds to determine if a catalytic reaction has taken place. We will compare the activity of these new complexes to known rhodium catalysts by using standard methods of analysis available in the Chemistry department. Gas chromatography (GC) allows us to follow the progress of chemical reactions by separating compound mixtures into individual peaks that represent the amount of a compound in the mixture. GC can be used to determine if a new compound has been produced by the catalytic reaction. Any new molecules discovered during the research will be characterized by nuclear magnetic resonance (NMR) and mass (MS) spectroscopies to determine their unique structures.

Roles and responsibilities

- A project director (Shari or Stephen Dunham) will be available to train Devon on the use of instrumentation, rhodium compound synthesis, carrying out catalytic reactions, data analysis, and visual representation of results.
- Devon will prepare and present his findings at regular research meetings (~15-30 min/day) with one or both project directors (Shari and/or Stephen Dunham)
- Devon will maintain a research laboratory notebook that will include regular and complete entries. Keeping a comprehensive laboratory notebook is a fundamental part of doing research in chemistry. The notebook will have an updated table of contents at the beginning. Entries should be dated, clearly written and organized, and made at least daily with details of ideas for experiments, planning of experiments, clear reference to location and organization of electronic data for each experiment, and a summary of results from each experiment. Project directors will look at Devon's notebook periodically and provide informal feedback throughout the summer. The notebook will be submitted to the project directors upon completion of the Summer Research.
- Throughout the summer, Devon will prepare summary figures for each set of experiments (with detailed figure caption!) to clearly illustrate the results of each experiment. These summary figures will be submitted electronically to the project directors before completion of the Summer Research.
- Devon may consider continuing this research as an independent study during the 2015-2016 academic year, so a final report/poster may not be required at the end of the summer but instead by the end of his research experience and in time for the Annual Student Scholarship and Creative Endeavors Day in spring of 2016.

Project Timetable

- Weeks 1-3: Setup rhodium synthesis reactions and learn to operate various instruments: HPLC for rhodium isomer isolation, NMR, and MALDI-MS for rhodium compound characterization. GC and GC/MS for characterization of organic compounds produced from catalytic reactions.
- Weeks 4-10: Carry out catalytic reactions of purified rhodium compounds and known rhodium catalysts with organic reagents to determine if catalytic transformations occurred.

Summary of benefits

Student engagement in discipline-appropriate scholarly research. Devon will be engaged in synthetic organometallic research that includes reading and summarizing primary literature, planning and performing experiments that require the use of several new instrumental methods, and collecting/analyzing/organizing significant amounts of electronic data. In addition, he will prepare and receive feedback on various visual representations of experimental results (preparing figures in a format appropriate for publication in a Chemistry journal). The Drs. Dunham will work with Devon to prepare a scientific poster for presentation of this work for the Annual Student Scholarship and Creative Endeavors Day, and possibly at another local or national research conference.

Impact on faculty, campus community, and discipline. Devon's work on this project will contribute to the discipline of organometallic chemistry by characterizing the potential catalytic activity of several new Rh compounds. None of the compounds that he will test for catalytic activity have been published. This project will benefit the Drs. Dunham by building upon work of three former research students (Donchez & Kuperavage Summer 2011, Donchez Honors '12-'13, and Bartulovich Summer 2014, '14-'15). Devon's results will be an important part of building the future capacity of the Dunham group to study catalytic activity of rhodium compounds and may lead to a future publication of these compounds in a peer reviewed Chemistry journal. By presenting his research during the summer to the SOAR group, and as a poster at Moravian Scholarship and Performance Day in April 2016, Devon's work will impact the campus community at Moravian by exposing others to interesting and complex nature of organometallic chemistry research.

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• The body of the proposal should contain an itemized list of equipment, supplies and/or travel expenses for the project. For each item, describe why it is necessary for the successful completion of the summer project, and if relevant, how the item supports a long-term project.
• Explain why each requested material item is not available through existing on-campus resources (e.g. CIT or Inter-library loan) or why the available item is insufficient for the project. Note that SOAR has a standing agreement with CIT to make laptops available for the 10 weeks of the summer program.

Budget Items

- $500.00 to offset part of the costs for reagents required for synthesis and characterization of rhodium catalysts.

o dirhodium trifluoroacetate	$ 358
o dirhodium catalyst	$ 200
Total	**$ 558**

- Remaining equipment and reagent expenses will be covered by the Department of Chemistry.

Dirhodium trifluoroacetate is a commercial starting material required for the synthesis of potential dirhodium catalysts. It is a consumable reagent so there are no standard supplies of this compound available at Moravian.

Dirhodium catalyst is a commercially available catalyst that will be used as a control to compare to the catalytic activity of compounds synthesized by Devon. This is a consumable reagent that is not available at Moravian.

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Devon Jakob

Chemistry, Class of 2016

Dr. Stephen and Shari Dunham

On Campus Housing: Requested

Ever since I was young, I possessed a true passion for science. Lab manuals, research journals, among other scientific literature, were commonplace in my home. I remember looking through them, trying to amass as much understanding as I possibly could, even at such a young age. Upon graduating from high school, I knew I wanted to attend Moravian College from the moment I first stepped into the Hall of Science a few years ago. Just thinking about the countless academic opportunities that would await me in a small college convinced me beyond a doubt that Moravian was the school for me. Three years later, as a junior, I look back upon my college experience thus far and find myself amazed by how far I have come. However, I still want to extend my experience further with an independent research project, which is something I have not yet had the chance for.

In retrospect to how I perceived the science community three years ago, my view of the world and the universe has changed drastically. This view empowers me with an honest sense of humility and realism. The human brain has evolved in order to survive in the wild, but it is also able to contemplate vastly complex fields such as chemistry and physics. That thought alone fills me with much excitement and fuels my desire to contribute to the scientific community. I find it exhilarating and elevating to wake up every day and learn something new about our universe in my classes. I call this the "joy of discovery". Through a SOAR project, I would be working closely with Drs. Stephen and Shari Dunham in hope of discovering something that nobody has known before in organometallic chemistry.

My interest in organometallic chemistry first manifested when I started working a weekend job in an aluminium complex laboratory as a quality analyst about a year and a half ago. It piqued my interest and subsequent desire to understand just how these organometallic compounds behave and react with other compounds. My goal in life is to earn a doctorate of chemistry. Dr. Dunham told me that the experience gained through working on this project would undoubtedly benefit me in pursuing a graduate school education and prepare me for entering the field of research, since I would be directly working with organometallic compounds. Independent research is also something that is not offered in the aluminium complex laboratory, and would benefit me both inside and outside my weekend job. The results of this project could, if all goes well, be published in a major research journal. Moreover, having an original publication attached to my name would surely help in my pursuit of further education.