Development of Metal-based Catalysts in Undergraduate Research and Teaching Labs

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Objective

This activity has two overarching aims: 1) to engage students in the latest field of organometallic catalysis by synthesizing molybdenum cluster catalysts that produce petrochemicals and to 2) bridge the gap between research (Chem 189/198) and undergraduate teaching labs (Chem 110L and 1B) by having a common chemistry experience that all students can participate in.

Introduction

A series of molybdenum cluster catalysts, \([\text{Mo}(\mu_3-C\text{R})(\mu_2-O)(\mu_2-O_2\text{CCH}_3)(\text{H}_2\text{O})_2]^+\) where \(\text{R} = \text{alkyl} \) group, were prepared (Figure 1). By synthesizing clusters with well-defined structures (bond angles and distances can be determined using x-ray crystallography), we are confident about the structure of the molecules and can measure reactivities directly (Figure 2). Our previous work on rhodium clusters has shown that a correlation exists between bond distances and kinetic reactivity (See J.R. Houston et al. Inorganic Chemistry 2005, 45, 7799) and it is our intention to establish a similar relationship for molybdenum clusters. This work would have a broad impact on the field of organometallic catalysis if rates of hydrocarbon formation could be predicted from structural data such as bond distances, which can be easily measured. The outcomes from this project are both scientific and pedagogical. We plan to 1) obtain high-quality kinetic data on cluster catalysts in order to establish a correlation between reactivity and structure, 2) equip students with the necessary skills to be successful in the latest scientific fields such as green energy and inorganic catalysis and 3) engage both lower and upper division students on an all-inclusive research project dedicated to inorganic chemistry concepts, methods of instrumentation, and important catalytic reactions used in industry. Our intention is to create a vibrant yet united learning community in both upper and lower division chemistry labs.

Structure and Reactivity of Mo Cluster Catalysts

![Figure 1. Structure of [Mo3(µ3-O)(µ3-CR)(µ-O2CCH3)6(H2O)3]BF4](image)

![Figure 2. Hydrocarbon formation from molybdenum cluster catalysts](image)

Objective

Student Research, Spring 2014

Chemistry major, Nick Williams synthesizing his catalyst, Feb. 2014.

Biomedical science major, John Hayes, synthesizing his catalyst, Feb. 2014.

Chemistry major, Andrew Burton presenting his research at the Northern California ACS meeting.

![Figure 3. H NMR of [Mo3(µ3-O)(µ3-CR)(µ-O2CCH3)6(H2O)3]BF4 in D2O at t= 15 mins](image)

![Figure 4. H NMR of [Mo3(µ3-O)(µ3-CR)(µ-O2CCH3)6(H2O)3]BF4 in D2O at 3 hours T=60°C for t= 2 hours](image)

![Figure 5. H NMR of [Mo3(µ3-O)(µ3-CR)(µ-O2CCH3)6(H2O)3]BF4 in D2O at T= 60°C for t= 26 hours](image)

Project Results

Research students (Chem 189, 299 and 500: Spring 2014) have worked on the synthesis, characterization, and catalytic activity of molybdenum cluster catalysts (Figures 3-5). The synthesis and characterization was successful and current measurements focus on quantifying rates of hydrocarbon formation.

Funding from PFG has 1) allowed the PI to train three new research students, 2) collect data that allowed this experiment to be included in the teaching laboratory (Chem 110L) and 3) collect data for dissemination which is already underway. Chemistry major, Andrew Burton has already presented his research at the Northern California ACS meeting and other research students are scheduled to present their work at the National American Chemical Science (ACS) meeting in San Francisco. Furthermore, graduate student, Kris Pineda, is currently writing a communication on a new molybdenum cluster to be submitted to Inorganic Chemistry Communications this summer. The PI plans to use these results to submit a proposal to the ACS-Petroleum Research Fund (October, 2014) and also submit a grant application to NSF-CAREER (this award focuses on the integration of education and research) during the Summer of 2015. A submission detailing the dissemination of the pedagogy results is planned for Journal of Chemical Education (Summer 2015). In addition to publishing our results and presenting at national meetings, students involved on this project will present or attend the Chemistry Department end-of-the-year poster session so that this unique research-teaching lab experience can be shared with colleagues.

Future work

Now that the methodology is in place, Chem 110L students (Chem 110L, students from Fall 2013 shown below) will perform the synthesis this Fall semester, 2014 (Description written for the Chem 110L lab manual is attached) and once the compounds are synthesized, they will be characterized in Chem 1B, Spring 2015.

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