

Faculty Member Contact Information

Name: Yun Lu
 Department: Chemistry
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Description of the URCA Assistant Position(s)

Number of students requested: 2

Number of students who will be funded: **1: Only one of the two students for this position will be funded. The professor will determine which student receives funding.**

Will the student(s) earn course credit? Yes No **X** If yes, in which course?

Location of research/creative activities: **Chemistry Department**

Brief description of the nature of the research/creative activity:

The central hypothesis of the proposed research is that our recently established approach that determines the kinetics of the oxidation of alcohols via hydride transfer to organic carbocations will allow us to systematically investigate the effects of the various structures of alcohols ($R^1R^2\text{CH-OH}$) on their ability to release a hydride ion (H^-) to form the α -hydroxy-carbocations ($R^1R^2\text{C}^+\text{-OH}$). In this project, various alcohols ($R^1R^2\text{CH-OH}$) will be selected for studies of structural effects on their hydride transfer reactions to two carbocations that have very different reactivities and very different steric requirements. The focus of the overall project is to understand “quantitatively” how the hydroxyl group (-OH) of an alcohol and other structural features (R^1 and R^2) mutually effect the ionization of its α -H to form the $R^1R^2\text{C}^+\text{-OH}$. The intellectual merits of the project are to provide chemists in organic chemistry and related areas with unprecedented structure-reactivity relationship data about the ability of the alcohols to release a hydride ion and the general chemical behaviors of the $R^1R^2\text{C}^+\text{-OH}$ carbocations. The kinetic studies of the hydride transfer reactions will promote a deeper understanding of the mechanism of the general oxidations of alcohols by organic carbocations.

Brief description of student responsibilities:

Organic Chemistry Research Assistants will be involved in the organic synthesis and organic reaction mechanism investigations that include (1) performing organic reactions, (2) isolating reaction products and characterizing their structures and, (3) determining reaction kinetics employing spectroscopy techniques.

URCA assistant positions are designed to provide students with *research or creative activities* experience. As such, there should be measurable, appropriate outcome goals. What exactly should your student(s) have learned by the end of this experience?

This project centers on solving problems in both fundamental organic chemistry and biomimetic chemistry, and therefore has a broad and important education component. Undergraduate students involved in this project will learn conventional kinetic procedures, organic synthesis, mechanistic analysis techniques, enzyme-catalyzed reactions and mechanisms, and the use of modern analytical instrumentation. Students will also be trained to write lab reports and scientific papers, to prepare posters, to present seminars, and to practice proper safety procedures; and they will be encouraged to take part in national meetings. Moreover, the project is closely related to the knowledge that students learn particularly from their junior/senior classes such as Advanced Organic Chemistry, Physical Chemistry, and the corresponding labs. These include fundamental kinetic theory, spectral kinetic determinations, theoretical calculations, organic reaction mechanisms and organic carbocation chemistry related to S_N1 reactions. The project will thus reinforce these concepts and the related knowledge that students have gained from their classes and also foster their interest in research and expand their critical thinking ability. The results are expected to be incorporated as discussion topics in our Advanced Organic Chemistry and Special Topics in Organic Chemistry courses. They are closely related to S_N1 reactions and carbocation chemistry which are included in most of the Advanced Organic Chemistry textbooks. Furthermore, our work will be published in high quality journals and the results will also be disseminated through presentations at local and national chemistry conferences as well as in the SIUE's public lecture events and in seminars presented at other schools. The mastering of the knowledge and the techniques involved in this project as well as the establishment of interest in research will make students more competitive in their future career and will ensure that they will be a credit to the undergraduate education of the nation.

The following are the outcome from my previous research students including undergraduates. The undergraduate students' names are underlined. Some of them became graduate students after years of undergraduate research with the P.I.

Publications:

1. Yun Lu, Fengrui Qu, Brian Moore, Donald Endicott, William Kuester "Hydride Reduction of NAD^+ Analogues by Isopropyl Alcohol: Kinetics, Deuterium Isotope Effects and Mechanism" *J. Org. Chem. (Featured Article)* 2008, 73, 4763.
2. Yun Lu, Donald Endicott, William Kuester "Effective Oxidation of Isopropanol by an NAD^+ Model." *Tetrahedron Letters* 2007, 48, 6356.
3. Yun Lu, Jiancheng Liu, Garry Diffie, Diansheng Liu, Bo Liu "Reduction of Nitroarenes by Hydroxide Ion in Water Catalyzed by β -Cyclodextrin: Enhanced Reactivity of Hydroxide Ion." *Tetrahedron Letters* 2006, 47, 4597.

Conference poster presentations in the years of '08-'09:

1. Yun Lu*, Joshua Bradshaw, William Kuester, Brian Moore "Structure-reactivity relationship for the oxidation of alcohols via hydride-transfer to 9-phenylxanthylum ion (I): Chain-alkyl and cycloalkyl alcohols" accepted by the 237th *American Chemical Society National Meeting*, Salt Lake City, March, 2009.
2. Yu Zhao, Brian Moore, Yun Lu* "Structure-reactivity relationship for the oxidation of alcohols via hydride-transfer to 9-phenylxanthylum ion (II): Para and meta-substituted benzyl alcohols" accepted by the 237th *American Chemical Society National Meeting*, Salt Lake City, March, 2009.
3. Donald Endicott, William Kuester, Yun Lu* "Effect of Zn(II) and its complexes on the kinetics of the hydride transfer reduction of an NAD^+ model by isopropanol" Accepted by the 235th *American Chemical Society National Meeting*, New Orleans, April, 2008.
4. Yun Lu*, Fengrui Qu, Brian Moore "Kinetics of the oxidation of isopropanol by a carbocation via hydride transfer" accepted by the 235th *American Chemical Society National Meeting*, New Orleans, April, 2008.

Additional Requirements of Students

If the position(s) require students to be available at certain times each week (as opposed to them being able to set their own hours), please indicate all required days and times:

Flexible

If the location of the research/creative activities is off campus, must students provide their own transportation? Yes___ No___ N/A

Must students have taken any prerequisite classes? Please list classes and preferred grades:

Chem241a, b (with a C grade and above) and chem245 (with a B grade and above)

Other requirements:

None

Notes to applicants (i.e., any other information you'd like applicants to know about you or the position before applying):

None