APPLICATION CHECKLIST
Presidential Faculty/Student Collaboration and Publication Grant

Deadline February 26th

Please print and complete this checklist and attach it as the cover page of your grant application. For more information about Presidential Faculty/Student Collaboration and Publication grants, please see http://gustavus.edu/facdev/GrantOpportunities/PresidentialGrant.php.

Faculty information

Name: Stephen R. Miller   Dept: Chemistry

Email: smiller3@gustavus.edu   Rank: Assistant Professor

Student Information

Name: Garrett Stoddard   Year: Sophomore

Email: gstoddar@gustavus.edu   Major: Chemistry (Undeclared)

Checklist

Project Details

- ☐ Brief description of the proposed project including its collaborative nature
- ☐ Clear statement of anticipated outcomes
- ☐ Likely placement for publication or performances
- ☐ Anticipated research completion date

Participant Details

- ☐ Names and brief biographies of all participants
- ☐ Explanation of how this project fits into the career of the faculty
- ☐ Explanation of how this project fits into the educational trajectory of the student (include year of graduation; student eligibility is limited to full-time returning students)

- ☐ **Presidential Budget Proposal Form attached as last page of application**
- ☐ **Nine (9) copies of completed application (including this checklist) to be submitted to the John S. Kendall Center for Engaged Learning (SSC 119)**

If successful, my proposal can be used as an example to assist future faculty applications. This decision will not in any way influence the evaluation of my application.

[✓ Yes] / No (please circle one)

Presidential Faculty/Student Collaboration Grant
BUDGET INFORMATION

Faculty Stipend ($300 per week, up to $2,400)

Student Summer Stipend ($400 per week, up to $3,200)

Student Summer Campus Housing ($XXX per week, up to 8 weeks)

ITEM		**AMOUNT**
Equipment (e.g., transcription machine, camera, cassette recorder – but not to include computer hardware)		$
1:	Cost:	
2:	Cost:	
3:	Cost:	
Materials (e.g., books, printing, software, lab supplies)		$150
1: Chemicals	Cost: $100	
2: Printing	Cost: $50	
3:	Cost:	
Travel Costs (cannot include conference travel, see http://gustavus.edu/finance/travel.php for allowable travel expenses)		$
Airfare:		
Mileage: Number of miles______ @ $0.55/mile		
Lodging:		
Meals:		
Stipends & Housing		$5950
Faculty Stipend	$300 per week, up to $2,400	
Student Summer Stipend	$400 per week, up to $3,200	
Student Summer Campus Housing	$43.75 per week, up to 8 weeks, $350	
TOTAL EXPENSES		$6100
AMOUNT REQUESTED		$6100

Have you applied for, or received funding from, another source to help support this project? NO

Funding Source:

Amount:

Please explain how the Presidential will be used in addition to the other funding.

Presidential Faculty/Student Collaboration Grant Proposal
Spectroscopy and characteristics of transition metal complexes

Stephen R. Miller and Garrett Stoddard
Department of Chemistry

February 26, 2010

I. Project details

A. Project summary

The proposed project is fundamental to the establishment of an ongoing research project in my laboratory, the goal of which is to better understand fundamental interactions between metals atoms/ions and other chemical systems, especially small organic compounds.

Metal atoms/ions have long been known to bond to small organic molecules (called ligands) such as benzene to form organometallic complexes. For example, one of the better known organometallic compounds in chemistry is ferrocene [$Fe(C_5H_5)_2$], in which an iron atom binds two planar cyclopentadienyl ligands in a so-called "sandwich" complex[1] (Figure 1). The structures of organometallic complexes are often interesting and provide insight into how metals interact with elements commonly found in organic molecules. Information about bonds formed between metals and oxygen or nitrogen are especially illuminating; such bonds typically form quite readily, and understanding them often provides insight into a variety of chemical systems, including many at the leading edge of modern scientific research. For example, metalloproteins (proteins which incorporate one or more metal atoms into their structures) typically bind their requisite metal atoms through electron donor atoms such as nitrogen[1]; metal-oxygen bonds are quite common in new and novel materials, such as high temperature superconducting ceramics[2,3]; and metals are often incorporated into industrial chemical catalysts[1,3-7]. Many organometallic complexes have been studied by a variety of means in the past[1,5]. However, the number of possible complexes is virtually limitless, and continued study of organometallic systems is both useful and necessary.

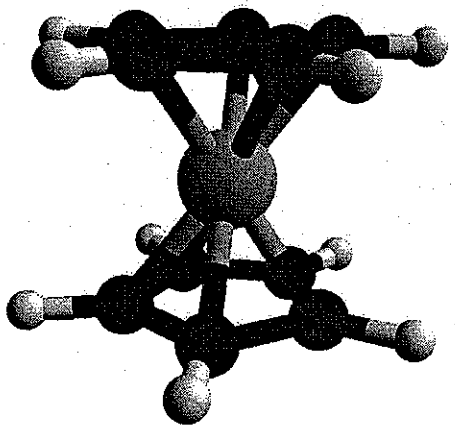

Figure 1. Ferrocene, a typical organometallic complex, in which an iron atom (gray) binds two planar cyclopentadienyl rings (black/white).

Methods

Our goal in the proposed study is to establish a systematic and widely applicable set of experiments designed to study multiple aspects of a wide range of organometallic compounds. Once determined, these techniques will then be used to begin fundamental characterization studies for a class of previously unstudied systems. Adequate instrumentation and expertise for the methods to be employed are available in the Gustavus Chemistry Department. In general, there will be three primary avenues of study:

1) Spectroscopy—a variety of spectroscopic methods (including ultraviolet-visible, infrared, and resonance-enhanced Raman) will be employed to gather experimental information about the chemical changes which accompany the formation of an organometallic species from its individual components. These data provide insight into the types, locations, and/or strengths of bonds formed in the complex. Nuclear magnetic resonance (NMR) spectroscopy may also prove a useful tool for obtaining structural information about complexes under study. As I have limited experience with NMR, use of this method would most likely involve collaborative associations with other research groups in the Chemistry Department.
2) Analytical techniques—one aspect of organometallic chemistry in which I am interested as a physical chemist is the determination of how readily organometallic complexes form; this information is obtained by measuring equilibrium constants for complex formation reactions. Equilibrium constant determination, in turn, requires the precise measurement of reactant and product concentrations in solutions. This will be a new avenue of research for me, and will require an initial investment of time and close collaboration with other research groups to determine appropriate methods. Fortunately, the Chemistry Department has several instruments (and the accompanying expertise) that promise to be useful for this type of study, especially an electrospray mass spectrometer and our recently acquired inductively-coupled plasma mass spectrometer.
3) Computational methods—another resource available in the Chemistry Department is the computational chemistry cluster, which allows us to conduct theoretical investigations of many of the same properties studied experimentally (e.g. molecular structure, energy, etc.). In fundamental research such as that proposed here, theoretical results often provide a means to better understand the experimental data; therefore, computational methods will serve as an invaluable complimentary tool to experimental techniques.

Systems for ongoing study and initial results

Some initial spectroscopic and computational studies of the sort proposed here were begun during the 2008-2009 academic year by Molly Beernink (GAC '09) and myself. The complex we investigated was that formed between copper ions (Cu^{2+}) and pyrazole (see Figure 2). An active vibrational mode at 1175 cm^{-1} appears in the resonance Raman spectrum (Figure 3) of the complex; although we have not yet positively identified the specific vibration observed, the measured frequency is almost certainly evidence of a change in the structure of the pyrazole ring which occurs when it binds to Cu^{2+}. Computational studies will be needed to identify the specific vibration, which would then provide insight into the nature of the Cu^{2+}-pyrazole bond itself.

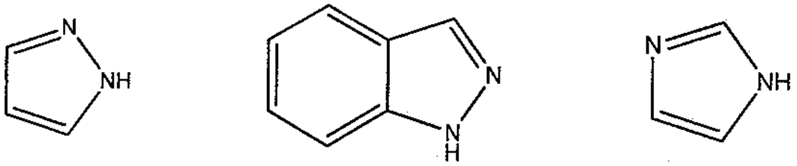

Figure 2. Ligands of interest: pyrazole (left), indazole (middle), and imidazole (right).

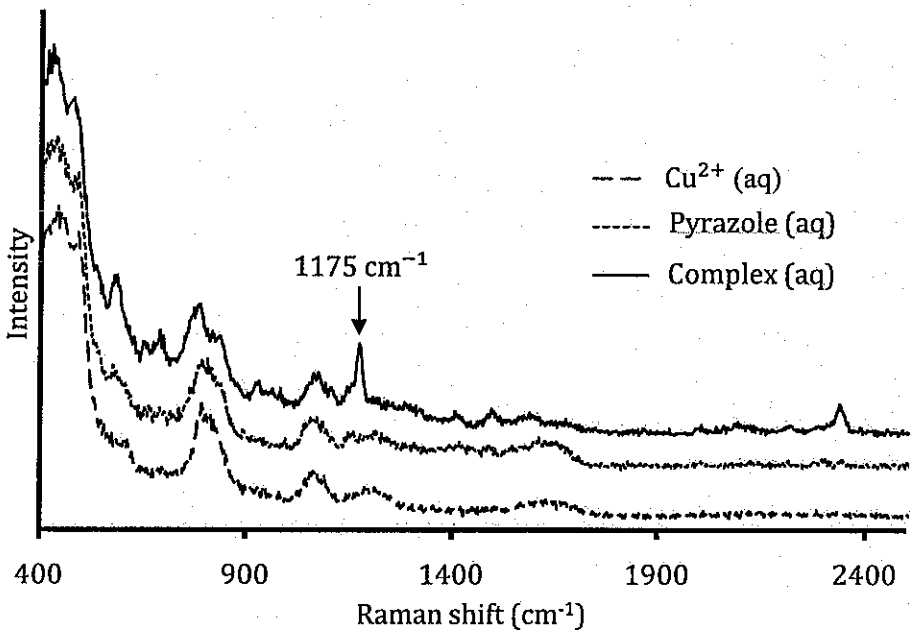

Figure 3. Resonance enhanced Raman spectra of Cu^{2+}, pyrazole, and the Cu^{2+}-pyrazole complex, all collected in water.

The proposed project will continue and build upon this previous work. The Cu^{2+}-pyrazole complex will be used as a test case for determining an adequate method for measuring equilibrium constants; theoretical calculations will continue to be employed to better understand the existing spectra of the same complex. Further work will be aimed at employing all of the methods outlined above to begin characterizing other species, including complexes between other metals (chromium, iron, cobalt, etc.) and pyrazole and/or complexes formed between metals and other ligands (such as indazole or imidazole; see Figure 2). In this way, we hope to examine similarities/differences in the way metals bind similar ligands.

B. Collaboration details

Successful advancement of this project will require that Garrett and I work closely both in and out of the laboratory. Working on this project would be Garrett's first pure research experience. All of the spectroscopic or computational techniques are very accessible to undergraduates, but he and I will have to work closely together as he learns to effectively employ these techniques in a research setting. Fortunately, Garrett will be able to learn to use the appropriate instrumentation as we together examine organometallic complexes relevant to our larger project goals (e.g. an iron-pyrazole complex); therefore, no significant time would be lost as he learns most of the basic techniques fundamental to the project as a whole. For aspects of the project which would be new to me as well (e.g. NMR and/or any analytical techniques), Garrett and I would work closely as we both learned to use the instrumentation, and then determined the best way to apply the technique(s) learned to systems of interest to us. As Garrett becomes more comfortable with the experimental methodologies, he will undoubtedly work somewhat more independently in the lab than he will initially; however, I will continue to monitor his progress (through regular, scheduled meetings) even as I allow him more freedom to demonstrate his growing independence and competence as a researcher.

A significant portion of the work necessary for this project would be accomplished outside of the laboratory. Non-laboratory work would include literature searches to find relevant background information, previously published data upon which we might build, and/or techniques which might further improve our methods; any of these literature findings would require discussion to better understand them. Perhaps the most significant activity to be completed outside of the lab is to simply understand our results. The nature of spectroscopy is such that collecting spectra is often a somewhat straightforward task, but understanding the results may not be. Garrett and I will have to regularly discuss the results we generate and what they might mean. Finally, we will work together to assemble proper dissemination materials based on our results (see below).

C. Anticipated completion date

The work described here represents, by its very nature, the beginning stages of what will likely be a rather large and ongoing research project. Furthermore, this type of project frequently proceeds in unforeseen and unexpected directions based on the results of specific experiments. It is therefore difficult to define, let alone predict a timeframe for, completion of the project. Garrett and I will begin work in June, 2010, for a period of 8-10 weeks. He also intends to continue pursuing research during the 2010-11 academic year, which will undoubtedly be an extension of this summer project. By that time, we should have some tangible results to report; these are expected to include a standard method for determination of equilibrium constants and publication quality experimental results for one or more new complexes. I will therefore plan to submit an up-to-date follow-up report outlining our results to the Dean of Faculty no later than May, 2011.

D. Anticipated outcomes

I expect that there will be two significant outcomes from this project. First, as we delve into the study of organometallic complexes, Garrett and I will be expanding the horizon of chemical knowledge at a fundamental level; the data obtained from this project (and future directions based on it) will eventually be presented to the larger scientific community through presentations and/or peer reviewed publications. This should contribute to an ever-growing understanding of organometallic interactions among chemists in general. Second, participation in this research project will provide Garrett with an invaluable opportunity to learn and develop new laboratory skills; gain insight into the nature of fundamental, academic research; take part in the generation and dissemination of scientific knowledge; and to mature as a student and a scientist. His experience will undoubtedly be of inestimable importance as he continues in his studies and decides on the post-graduation career trajectory he wishes to pursue.

E. Placement for publication

The results of this work will largely be preliminary and exploratory in nature, and immediate publication is not anticipated. However, I do expect that the results will be combined with similar future results and contribute to later publication(s) in a peer reviewed source such as the *Journal of Physical Chemistry* or *Organometallics*. Results appropriate for poster/oral presentations are expected in the short term. Such presentations will be made at GAC venues (e.g. the Summer

Research Symposium in September and/or the Celebration of Creative Inquiry in May); we also intend to present at one or more regional/national professional meetings, such as an upcoming American Chemical Society Midwest Regional meeting or the International Symposium on Molecular Spectroscopy at the Ohio State University.

II. Participant details

A. Biographies

Garrett Stoddard

I am a sophomore chemistry major at GAC, with academic interests in chemistry and biology. I am one of four brothers from Lake Elmo, Minnesota. It is there that my interest for chemistry began. My father is a dentist in St. Paul, Minnesota. He graduated from St. Olaf College with a degree in chemistry, and, after completing his Master's degree in organic chemistry, earned a Doctorate of Dental Science from the University of Minnesota. Because of him, I have grown up with a general interest in science, and specifically in chemistry. When I took chemistry in high school, I truly fell in love with the subject. Now at Gustavus, I have completed General Chemistry and the Organic Chemistry I/II sequence, and am currently enrolled in Inorganic Chemistry I. I was also a teaching assistant (TA) for General Chemistry during Fall Semester, 2009, and am currently a TA for Organic Chemistry I. These opportunities have allowed me to share my passion for chemistry and possibly spark an interest in others. I thoroughly enjoy working as a TA because it allows me to be help people through the same learning process I underwent and allows me to delve deeper into chemistry.

Following graduation, I intend to go to graduate school, dental school, or pursue chemical engineering. I have had a glimpse of the life of a medical professional from my father, and I would like to preview what it would be like to do graduate level research. This summer research would allow me to complete the necessary preview of each field I need to make an informed decision about my career goals. Whichever option I do end up choosing, this experience would help me tremendously. It would allow me to acquire new skills and improve those I already have, which would help me if I do pursue graduate school later.

Steve Miller

I earned a Bachelor of Science degree from the University of Minnesota Duluth (UMD) in May, 2000 with a double major of Chemistry and Biochemistry/Molecular Biology (BMB). I began my collegiate career as a BMB major with plans to enter an M.D./Ph.D. program upon graduation. Midway through my undergraduate career, I discovered that my true passion was in fact for physical inorganic chemistry. I also had my first experience as an instructor when I worked as an undergraduate teaching assistant in the UMD chemistry department. By the time of my graduation, I realized that I wanted to be a faculty member at a small liberal arts college, where I would have the opportunity to teach and engage undergraduates in academic research. After graduation, I remained at UMD to earn a Master of Science degree in Chemistry in August, 2002. My research was conducted under the tutelage of Dr. Paul Kiprof in the field of computational chemistry. I then enrolled in the Ph.D. program at the University of Minnesota. I joined the research group of Dr.

Doreen Leopold and performed spectroscopic and computational research to study the structure of small metal clusters. I also served as an adjunct instructor at North Hennepin Community College (Brooklyn Park, MN) and Northwestern College (Roseville, MN) during my time as a doctoral student. After receiving a Ph.D. in Chemistry in October, 2007, I accepted a postdoctoral research assistantship at the Institute for Shock Physics at Washington State University. While there, I studied anisotropy in the initiation mechanism of high explosive materials under shocked conditions. I then accepted a Visiting Assistant Professor position at GAC for the 2008-2010 academic years; I have since been hired for a tenure-track position in the GAC Chemistry Department, to begin Fall Semester, 2010. My research efforts have led to five publications in peer reviewed journals to date, with at least four more manuscripts in preparation for publication.

B. Career statements

Garrett Stoddard

The opportunity to participate in Dr. Miller's research this summer would be beneficial to my career as a scientist, as it would give me a chance to immerse myself in the real world of chemistry. I am a hard worker and eager to learn. All of my previous lab experience is based on course related lab work. The Presidential Faculty/Student Collaboration Grant would allow me to take part in research in a true research setting. I plan to work hard in Dr. Miller's lab to help him further his research while expanding my own lab skills and generally maturing as a scientist in preparation for graduate school, health sciences, or chemical engineering. Participating in this research project would enhance my quantitative and qualitative lab skills while helping me find my own niche as a scientist. I also hope to contribute to the scientific community by doing organometallic research. The skills and knowledge acquired as part of a research project will help me to a great extent, no matter which career path I choose. This research will prove to be a pivotal point in my life, and it will allow me to make a better decision on what type of career I wish to pursue. I would like very much to see this project through from the beginning to the end. Seeing the whole process would help me to more fully understand the process and thinking involved in a graduate school-like research project. This is the time in my academic career to engage in these opportunities and gain such valuable research experience. I truly look forward to being part of this project this summer and beyond.

Steve Miller

The proposed project, with Garrett's help, promises to be of great benefit to me personally as I begin my own professional activities as a member of the GAC faculty. I envision that the groundwork and initial results I expect Garrett and I would generate this summer would be beneficial in multiple ways. First, starting a new line of research is usually a somewhat slow process; getting underway this summer will enable me to start generating publishable results as early as possible. Second, the initial results I expect we will obtain should greatly enhance my ability to secure external funding to further equip my laboratory and fund future research students; granting agencies are typically more willing to fund projects which have already demonstrated an ability to produce useful results. Third, engaging a research student like Garrett now should help me recruit additional students in the future, as they are often more likely to join active groups that are known to generate results.

I feel very strongly that research-based collaboration with undergraduates is both an integral part of my scholarly activities and the highest form of education I can provide to a student. Being a scientist requires a person to be inquisitive, confident, rational, and creative. Part of my role as an educator is to pass on and/or foster these qualities in future professional scientists, and the research laboratory is the single best venue to demonstrate what it means to be a practicing scientist. Furthermore, I have limited personal experience mentoring undergraduate researchers, and working with Garrett would present a wonderful opportunity for me to further refine my abilities and expectations as a research mentor.

The opportunity to work full time with Garrett this summer, afforded by the Presidential Faculty/Student Collaboration Grant, is an exciting prospect for both of us. Garrett and I have known one another since he was a student in my General Chemistry class Fall Semester, 2008; he is also one of my Organic I TAs this spring. He is an honest, intelligent, hard-working, realistic, and respectful student who desires to become a professional scientist himself one day. My familiarity with him will allow our collaboration to be mutually beneficial in the short and long terms: he will gain invaluable experience and insight into the process of scientific research, while I will further my ability to be a productive member of the Gustavus and larger scientific communities.

III. References

[1]Crabtree, R.H. The Organometallic Chemistry of the Transition Metals (5th Ed.). 2009, Hoboken: John Wiley and Sons.

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[7]Adams, R.D.; Cotton, F.A. (eds.). Catalysis by Di- and Polynuclear Metal Cluster Complexes. 1998, New York: Wiley-VCH.