SOAR Research Proposal -- Summer 2012

Exploring the Applicability of the Dip Probe for *in situ* Spectroscopy Experiments

Faculty: **Carl Salter** Professor of Chemistry

Students: **Sean Rossiter**
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Start date: May 29 Ten weeks

Description:

Exploring the Applicability of the Dip Probe for *in situ* Spectroscopy Experiments.

The Ocean Optics dip probe (*1*) allows light absorption experiments to be carried out in a new and practical way: the probe is dropped into a solution; a light beam exits the probe, passes through the solution and then reenters the probe to go to an instrument for analysis. Rather than placing the sample into the light path, the light path is placed into the sample! This makes for a more convenient and more robust instrument, one more adaptable to a variety of situations including field work.

For this summer SOAR project I plan to have a team of three young chemistry majors explore the use of the dip probe. There are two chemical systems that we want to examine, and we want to compare the usefulness of the dip probe against the more classical, "sample in an instrument" method of spectroscopy.

The first system is the reaction of Fe(III) with thiosulfate ion, $S_2O_3^{-2}$. This project is a continuation of the project Phil Weiser and Christine McCarl started in the summer of 2009. Iron and thiosulfate are familiar, readily available chemical species: Fe(III) is commonly found in teaching labs as iron nitrate or iron chloride, and $S_2O_3^{-2}$ is obtained from sodium thiosulfate, which is the substance commonly known as photographic "hypo". As described in the *Journal of Chemical Education* (*2*), the reaction of Fe(III) with $S_2O_3^{-2}$ results in the rapid formation of a purple complex which then slowly fades away over two to four minutes as the Fe(III) is reduced to Fe(II).

$Fe^{+3} + 2\ S_2O_3^{-2} \rightarrow Fe(S_2O_3)_2^-$ fast formation of deep violet
$Fe(S_2O_3)_2^- + Fe^{+3} \rightarrow 2\ Fe^{+2} + S_4O_6^{-2}$ slow fade to colorless

During the summer of 2009, Phil and Christine were able to use traditional tube-in-instrument methods to demonstrate that the rate of decay of the purple complex was reproducible and followed second-order kinetics. However, they also noted that the rate was strongly influenced by the temperature, and it was difficult to maintain a constant temperature in the reaction mixture with the apparatus they had. The dip probe will allow us to carry out the reaction in a test tube floating in a constant temperature bath. This should improve the control we have over the experiment. In addition, we now have an opportunity to study the fast step, the formation of the purple complex. The dip probe should make it easier to follow the rapid development of the purple color in the solution without losing time during mixing. There is some question about how many thiosulfate ions participate in the purple complex with iron (III); improved temperature control will help us address this question.

The other chemical system we will examine is the measurement of zinc by formation of a colored complex with *zincon*, a commercial analytical reagent (*3*). This project is an outgrowth of last summer's work on zinc in bacteriological growth media, which is of interest because of the zinc-contaminated soil at the Lehigh Gap. We will develop a simpler procedure for the measurement of zinc in soil and in streams and in bacterial media, and we plan to use the dip probe to make the measurements easy to perform in the field. In principle, a test tube of stream water could be shaken with zincon, and then the dip probe could be dropped in to make the final measurement. Our current commercial zinc-zincon system from *Hach* uses a zincon preparation that complicates the procedure, and it requires a special light-measuring instrument into which the final solution must be inserted. Nevertheless, the *Hach* instrument does provide us with a valuable "referee" method against which to compare the simpler procedure we develop using the dip probe.

Roles:

Gabrielle Sommers is a transfer student from Pitt who is currently enrolled in Organic Chemistry and Quantitative Analysis, and she took my Research Methods class last Fall. The combination of Organic and Quant is key to working on the zinc-zincon reaction. Since Gaby has had the most chemical lab experience, and in particular Organic Chemistry, she should have a keenest understanding of the structure of zincon and how it reacts with zinc, and can work on modifying the procedure for the reaction. She received a brief introduction to the zinc-zincon analysis as a member of my Research Methods course.

Sean Rossiter and Caroline Bartulovich, both freshmen, have expressed interest in the iron-thiosulfate project. The nature of the kinetics experiment using computer data acquisition is that the experiments are "four-handed"—a team of two is needed to do a run. Sean and Caroline bring complementary experience to the project: Sean has done statistics and experiment design in my Research Methods course in the Fall (his AP credit meant he didn't have to take General Chemistry) and Sean, like Gaby, is currently taking Quantitative Analysis. Meanwhile Caroline, who is taking General Chemistry, has used the new laptop computers and LabPro software to measure the rate of a chemical reaction (not iron-thiosulfate of course!). I have some interest in exploring the use of the iron-

thiosulfate in our General Chemistry lab curriculum, so Caroline's involvement in the project is beneficial—neither Gaby nor Sean have seen our Gen Chem lab experiments!

1st week	Introductory readings, calibration both dip probes
2nd week	background library research
3rd week	repeat previous work (use *Hach* instrument as zinc referee)
4th week	begin modifying procedures using dip probe
9th week	compare results dip probe vs. classical methods
10th week	document procedures and results.

Discipline Contribution:

All three students show great aptitude and interest in chemistry, even though they are still early in their development as chemists. This project offers them an opportunity to do hands-on chemistry at a moment when it can really make a difference in how they view chemistry, science, and scholarship.

I will benefit because the iron-thiosulfate experiment is a project close to publication—the control of temperature is the one road block that remains. The use of the new dip probe to overcome the temperature problem will make an article in a journal such as the *Journal of Chemical Education* even more interesting to the chemical education community.

Over the longer term, the zinc-zincon analysis that we develop this summer will enhance my opportunity to work with members of our Biological Sciences department on issues related to the zinc superfund site at the Lehigh Gap.

Both the zinc-zincon analysis and aspects of the iron-thiosulfate reaction are likely to become components of our chemistry lab curriculum, either in General Chemistry or my Research Methods class. I expect Sean, Caroline, and Gaby will make presentations about their work both at Scholar's Day on campus and at large conferences such as NCUR and the national ACS meetings.

Budget:

The department already has one Ocean Optics dip probe. The demands of this project will require a second. A model with a different fiber-to-mirror distance in the tip will give us more flexibility in our experiments. Other supplies and chemicals will be purchased by the chemistry department.

T300Sleeve fiber	$290
RTP-10-20 tip	$278
Three student stipends ten weeks	$9000
Faculty stipend	$2250

Literature Cited:

1. http://www.oceanoptics.com/products/tp300transdipprobes.asp
2. R.J. Tykodi *J. Chem. Ed.* **1990,** *67,* 146-149.
3. D. G. Miller, *J. Water Pollution Control Federation*, **1979**, *51*, 2402-12.

Exploring the Applicability of the Dip Probe for *in situ* Spectroscopy Experiments

Caroline Bartulovich, Chemistry, Class of 2015
Dr. Carl Salter
Not requesting On-Campus Housing

A major reason that I choose to attend Moravian was because of the numerous opportunities they have for undergraduate research. By participating in this SOAR project I would gain much needed experience doing original scientific research. Up until this point in my scientific career I have been handed a lab manual and told step by step directions on how to accomplish something. One thing that I find incredibly exciting about participating in a SOAR project is the responsibility I will have and the fact that I will be held accountable to the findings that stem from this project. There will be no answer sheet and if something does not go as planned then we will have to work together as a group to figure it out and make the appropriate adjustments. In a meeting that I had with Dr. Salter to discuss this project he showed me the type of equipment we would be using and the basic ideas that went along with it. I was pleased to find out that I had previously used the same laptops and LabPro software that we would be using for the experiment in General Chemistry. I would be very interested in using these tools for different and more complex chemical reactions than the ones I had previously used them for. Also by participating in this SOAR project I hope to gain a clearer picture as to what I would like to do after my time at Moravian is over, whether that is going straight into the job field or possibly enrolling in graduate school for further education.

Although this project involving Iron Thiosulfate has been worked on previously by other Moravian students, a main factor in our project is the exact effect temperature has when it comes to this reaction. This is something that the previous students who worked on this project were unable to definitively decide due to their equipment. The effect of temperature on this reaction is an incredibly crucial aspect of the experiment and with our equipment, such as the dip probe, we hope to be able to definitively answer that question. If this obstacle is overcome our results could be published in the *Journal of Chemical Education* so that other people can see and learn from the results of our experiment.

Exploring the Applicability of the Dip Probe for *in situ* Spectroscopy Experiments

Sean Rossiter, Chemistry, Class of 2015
Dr. Carl Salter
Requesting On-Campus Housing

Participation in this SOAR project would give me an opportunity to gain experience in the field of original chemical research. Previously, all of my lab experience consisted of following the procedure in the lab handout. But when investigating the reaction between Fe^{3+} and $S_2O_3^{2-}$, there will be no lab handout. My colleagues, Gabby, Caroline, and Dr. Salter, and I, would formulate our own experimental process. We would be responsible for validating our process to ensure that it works – I learned how to set up and evaluate a control experiment in Quantitative Analysis and am eager to apply it in an original setting. Though the Iron Thiosulfate project began years ago, the introduction of new lab equipment requires that it be properly calibrated to ensure both accurate and precise measurements, and thus, valid conclusions. This project would also serve as preparation and valuable independent lab experience for my future endeavors, whether it be applying for an internship at Merck next year or applying into a PhD program later down the road. But perhaps most importantly, it offers me the opportunity to collaborate with like-minded individuals on a unique and original research project.

The project will ultimately result in the identification of the effect of temperature on the rate of decomposition of the Iron Thiosulfate complex. Temperature is nearly always a factor in how quickly a compound reacts or decomposes. The previous SOAR project on Iron Thiosulfate kinetics suggested that temperature had a significant effect on the reaction, and this observation will become a fully engaging undertaking. The project may conclude with our results being published in the *Journal of Chemical Education*, a renowned journal in which several members of the Moravian Chemistry Department have published their work.

Exploring the Applicability of the Dip Probe for *in situ* Spectroscopy Experiments

Gabrielle Sommer
Major: Chemistry
Expected Graduation Date: May 2014
Faculty Mentor: Dr. Carl Salter
On-campus housing requested

The Student Opportunities for Academic Research program provides an excellent opportunity for an undergraduate student to become immersed in the research early on in the student's academic career. The program would allow me to work hands-on with an instructor and explore the ins-and-outs of the research field. Consequently, this invaluable experience would yield significant benefit regarding future research positions I may acquire, both personally, as well as enrich the institution and supervising research instructor.

The SOAR program will allow for the exploration and understanding of new material and concepts that I find particularly interesting. I believe that hands-on experience is the catalyst of comprehensive, logical understanding of any concepts. As a sophomore in college, the research experience I will gain from the SOAR program would likely provide for significant increase in my knowledge base, regarding research techniques and chemistry information. Additionally, participation in this program would potentially empower me to function independently as a research chemist. Expansion of my knowledge base in these areas would likely enhance opportunity and likelihood of similar offers in the future.

As stated above, my participation in the SOAR program will also provide subsequent benefit to the institution of Moravian College, as well as to my supervising research professor. I firmly believe that we exist in part to be of service to others. A researcher that has expanded her chemical and technical knowledge develops the ability to function more independently, and provide more quantitative and qualitative support.

I hope to maintain my initial research position through the time at which the project comes to an end. At this point, I anticipate having gained a more thorough understanding of the demographics of the research occupation. Participation in the SOAR program would be an invaluable stepping-stone as I navigate my career path, providing for the acquisition of a wealth of education and real-life experience, that would subsequently provide personal benefit, enrich the chemical research department of Moravian College, and ideally, provide benefit to the overall field of chemistry.