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## CALL FOR PAPERS

This conference will explore the undergraduate research experience both from the perspective of the research advisor and the undergraduate research student. The conference will open with a virtual poster session showcasing the research accomplishments of undergraduate researchers from across the country. This session will be followed by a series of invited papers focussed on the process and educational impact of the undergraduate research experience.

## Posters

### Group A

**Mar 25** - Submit questions for any Group A poster

**Mar 26: A1** - [Studies of The Anesthetic Effect of Alcohols on Goldfish](#)

Layali Eshqaidef, Eric Williamsen, and James Sidie\*

Departments of Biology (\*) and Chemistry, Ursinus College, 601 E. Main St., Collegeville, PA 19426.

Although a wide range of compounds act as anesthetics, the anesthetic mechanism is not well understood. As part of a study of the anesthetic activity of 1-alkanols, goldfish were placed in a thermostated bath containing a known concentration of alcohol for 20 min and then allowed to recover in a bath of water for 20 min. The blood alcohol concentration was determined by gas chromatography/mass spectrometry (GC/MS) and the anesthetic activity was determined by measuring the time between initial exposure and when the fish flips on its side or on its back ("flip time"). Visual anesthetic activity was only seen for 1-heptanol through 1-dodecanol, with the most effective anesthetic activity occurring for 1-nonanol or 1-decanol, after which anesthetic activity diminished. The blood alcohol concentration followed the trend seen for anesthetic activity. The GC/MS measurements provide useful information for the anesthetic studies, as well as transport of alcohols through the fish gills to the blood.

**Mar 27: A2** - [Determination of Blood Alcohol Concentration in the Weakly Electric Fish Eigenmannia Virescens](#)

Tim D'Andrea, Eric J. Williamsen, and James Sidie, Departments of Biology (\*) and Chemistry, Ursinus College; 601 E. Main St.; Collegeville, PA 19426-1000

To better understand how alcohols act as anesthetics, the weakly electric fish *Eigenmannia virescens* has been exposed to saturated

1-alkanols. Depression in the electric organ discharge (EOD) frequency of the fish is a measure of anesthetic activity. In these studies, the fish is placed in a tank of known alcohol concentration for 20 min and then recover in a tank of distilled water for 20 min. EOD frequency measurements show that the anesthetic activity increases up to 1-decanol, after which it falls off. To determine whether the anesthetic activity is dependent on transport of the alcohol from the water to the nerves, GC/MS measurements were made to compare the amount of alcohol in the fish blood to the amount of alcohol in the bathing solution. Initial measurements show the blood concentration follows the same trend as anesthetic activity, and for higher chain alcohols the alcohol concentration in the blood is higher than the concentration in the bathing solution.

**Mar 28: A3 - [Selenium and the Great Salt Lake](#)**

Nicole Albano, Undergraduate Student, Westminster College, Salt Lake City.

Dr. P.D. Hooker, Assistant Professor, Physical Science Department, Westminster College, Salt Lake City.

Dr. Ty Harrison, Associate Professor, Biology Department, Westminster College, Salt Lake City.

Selenium is a trace element essential for life, but is also toxic at relatively low concentrations. If present in water, selenium is known to bioaccumulate in aquatic flora and fauna resulting in the decimation of fish and bird populations. The seleniferous soils of the Western deserts and anthropogenic activity, e.g., copper mining, in the vicinity of the Great Salt Lake make it a likely repository for selenium. The presence of bird sanctuaries makes it necessary to monitor the concentration of selenium in this unique environment so that potential disasters can be avoided. In this study we have analyzed for selenium in water and brine shrimp collected from the Great Salt Lake, Utah, using fluorescence spectroscopy, and investigated the role of high concentrations of NaCl and its effect on the extraction and proper quantification of Se using this analytical technique.

**Mar 29 - General Discussion for Group A**

**Group B**

**April 1 -** Submit questions for any Group B poster

**April 2: B1 - [Characterization of a Cholesteryl 10-Undecenoate Liquid Crystalline High-Performance Liquid Chromatographic Stationary Phase](#)**

Katie Shearer and Eric J. Williamsen

Department of Chemistry, Ursinus College, 601 E. Main St., Collegeville, PA 19426-1000

Liquid crystalline HPLC stationary phases have shown increased selectivity in the separation of compounds, especially those that differ only in planarity or are polyaromatic hydrocarbons (PAHs), as compared to the same separation on traditional, reversed-phase HPLC stationary phases. One promising liquid crystalline stationary phase is cholesteryl 10-undecenoate. On this stationary phase the separation of a large number of PAHs, which differ in size and planarity, was performed under conditions of controlled temperature and mobile phase composition. Changes in the enthalpy and entropy of transfer of the analyte from the mobile phase to the stationary phase were quantified through van't Hoff analysis. The same studies were performed using a traditional octadecyl stationary phase, and the results are compared. Preliminary explanations of the differences and similarities of these stationary phases are provided.

**April 3: B2 - [Comparative Studies of Fluorinated and Nonfluorinated High-Performance Liquid Chromatographic Stationary Phases](#)**

Andrew Vincent, Jami Wilson, and Eric Williamsen

Department of Chemistry, Ursinus College, 601 E. Main St., Collegeville, PA 19426-1000.

Fluorinated HPLC stationary phases have shown promise in the separation of mixtures that are of biological, chemical, forensic, and pharmacological interest. To better understand how separations that occur using fluorinated stationary phases differ from those of structurally similar, traditional HPLC stationary phases, comparative chromatographic studies using fluorophenyl, fluoroctyl, phenyl, and octyl stationary phases have been undertaken. Under controlled temperature and mobile phase conditions, retention of polyaromatic hydrocarbon, nitrated, fluorinated, and nonaromatic compounds have been measured on all four stationary phases. As the percentage of water increased when using water/methanol mobile phases, distinct differences in retention between the four stationary phases for an individual analyte and between groups of analytes on the same stationary phase have been observed. To determine the relative importance of entropy and enthalpy changes to retention, van't Hoff analyses have been performed on the temperature-controlled data. Differences in the relative importance of entropy and enthalpy have been found. Preliminary explanations for the observed behavior will be provided.

**April 4: B3 - [Fabrication and Characterization of Ultrathin Sol-Gel Silica Films Doped with 1,1'-Bis\(triethoxysilyl\)ferrocene](#)**

Nicole M. Barrentine, Joseph W. Robertson, Jeffrey W. Anthis, and Jeanne E. Pemberton

Department of Chemistry, University of Arizona, 1306 E. University Blvd., Tucson, AZ 85721

A novel sol-gel approach has been developed for the fabrication of redox-active, ultrathin, silica-based oxides deposited onto metal substrates. The fabrication approach relies on the use of an ultra-dilute sol-gel solution of tetramethoxysilane (TMOS) modified to contain various amounts of the redox species 1,1'-bistriethoxysilylferrocene (FcTEOS) deposited onto self-assembled monolayers of (3-mercaptopropyl)trimethoxysilane on Au to produce electrochemically-active, hybrid sol-gel films. Samples were characterized by reflectance-absorbance infrared spectroscopy (RAIRS) and cyclic voltammetry. The FcTEOS is considerably more reactive than the TMOS. Therefore, the time interval between the addition of FcTEOS to the TMOS silica solution, and the deposition of the reacting solution onto the Au surface was controlled. The effect of this time interval on the resulting uniformity of FcTEOS centers throughout the film as indicated by the film electrochemistry and the relative peak heights of the silica and ferrocene components in the film as seen in RAIRS are discussed for each precursor solution ratio.

**April 5: B4 - [The Development of QSAR Models of Musk-Like Molecules Using TAE Electron Density-Derived Descriptors](#) -**

Bill Katt, Curt Breneman, Barry Lavine, Nagamani Sukumar, Matthew Sundling

A set of accurate classification models were developed using a dataset of 640 small musk-like molecules. Classifications of these molecules were performed using fifteen distinct classes that relate to biological responses, both individually and grouped as active/inactive molecules. QSAR (Quantitative Structure-Activity Relationship) models were also created for several molecular classes, including subsets based on five structural groupings within the data, as well as one subset representing the entire dataset.

Models were prepared using TAE (Transferable Atom Equivalents) descriptors that are derived from molecular electron density distributions. Molecular electron density properties were represented using TAE surface histogram descriptors, wavelet coefficient descriptors (WCDs) and hybrid shape/property (PEST) descriptors. Data used in the models was preprocessed to remove similar descriptors, and the resulting dataset was used to build models with greatly reduced numbers of descriptors (feature selection). The models presented were developed using artificial neural networks (ANN)

Abstract and reference of related work of two undergraduates from Illinois Institute of Technology:

[Rapid Detection of Bacteria from Blood Culture by an Electronic Nose](#)

**Group C**

**April 8** - Submit questions for any Group C poster

**April 9: C1 - [The Study of Motion of Polyatomic Ions in Ionic Solids](#)**

Amy L. Stallman, Tim Hindbjorgen, Thomas J. Offerdahl, William P. Jensen, and Jay S. Shore  
Department of Chemistry and Biochemistry, South Dakota State University, Brookings, SD 57007

Variable temperature X-ray diffraction and solid-state  $^{17}\text{O}$ ,  $^{23}\text{Na}$ , and  $^{207}\text{Pb}$  NMR spectroscopy has been used to characterize the crystal unit cell and the dynamics of polyatomic ions as a function of temperature. The samples studied include:  $\text{Pb}(\text{NO}_3)_2$ ,  $\text{PbSO}_4$ ,  $\text{NaNO}_3$ , and  $\text{Ca}(\text{NO}_3)_2$ . For some of the materials studied, the unit cell parameters were linearly dependent on temperature. From the variable temperature  $^{17}\text{O}$  NMR spectra, the motion of nitrate and sulfate ions were characterized. Due to the low natural abundance of  $^{17}\text{O}$  (0.037%), isotopically-enriched materials were synthesized using  $\text{H}_2^{17}\text{O}(\text{l})$ . The variable temperature NMR spectroscopy of the metal ions was also informative. Potentially, the X-ray diffractions measurements coupled with ab initio calculations will yield a complete description of the energetics inside the crystal lattice. While, the NMR measurements should yield a complete description of the dynamics. With a complete characterization of the energetics and dynamics inside an ionic solid, issues related to crystal formation and crystal packing effects will be addressed.

**April 10: C2 - [Proton-Coupled Electron Transfer in ruthenium Oxime Complexes](#)**

Justina Fisher and Dr. Elisabeth T. Bell-Loncella  
Department of Chemistry, University of Pittsburgh, Johnstown, PA 15904, USA

Proton-coupled electron transfer is important in biochemical systems. Because of the complexity of the enzymes involved, smaller model systems help us to understand the PCET mechanism. Ruthenium complexes are useful as versatile models for these studies. Our ruthenium complex is cis, bis-4, 4'-dimethyl-2, 2'-dipyridyl dimethylglyoxime ruthenium (II). Reaction of cis- $[\text{Ru}(\text{mbpy})_2\text{Cl}_2]$  (mbpy = 4, 4'-dimethyl-2, 2'-dipyridyl) with silver triflate followed by dimethylglyoxime (dmgH<sub>2</sub>) yields cis- $[\text{Ru}(\text{mbpy})_2\text{dmgH}_2]^{2+}(\text{SO}_3\text{CF}_3)^{2-}$ . The cis-geometry of the compound is reflected in the  $^1\text{H}$ NMR spectra. Two acid dissociations arise from the doubly protonated dmgH<sub>2</sub> ligand ( $\text{pK}_{\text{a}1} = 5.00$ ,  $\text{pK}_{\text{a}2} = 8.40$ ). When correlated with information from the Pourbaix diagram (electrochemical potential versus pH), a two electron two proton transfer capability emerges. This pH dependence is also seen in the spectrophotometric titration data, which shows two sets of isosbestic points representing three species (fully protonated,

singly protonated, and doubly deprotonated).

**April 11: C3 - [An Investigation into Using Inorganic Methods for the Removal of Metal Cations from Aqueous Solution](#)**

Alex McAneny and Charles H. Lake

Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA 15705, USA

Macrocyclic compounds have shown to be feasible in the selective separation of metal cations from aqueous solution. Tsukube, et al has shown that these ligands can selectively remove Na<sup>+</sup> cations from a solution containing Li<sup>+</sup>, Na<sup>+</sup> and K<sup>+</sup> ions. Armed macrocyclic ligands possess a major advantage because they have functional groups located in the pendant ligand arms. These functional groups can be modified to improve the selectivity of the ligand. We are reporting derivatives of 1,4,7,10-tetraazacyclododecane, which possess carboxylic acid functional groups in pendant ligand arms. Ligands of this type are suspected to be candidates for the selective removal of harder metal cations from aqueous solution. The synthesis of 1,4,7,10-tetraazacyclododecane derivatives with pendant ligand arms of varying length will be studied. The coordination chemistry of these ligands with calcium (II) cations will be examined. These coordination complexes will be crystallographically interesting and will lead to charge density studies. Charge density studies will allow us to gain a better understanding of the bonding associated with these types of coordination complexes.

**April 12 - General Discussion for Group C**

## Papers

**April 15-16, 2002**

**[Academic Excellence: A Study of the Role of Research in the Natural Sciences at Undergraduate Institutions](#)**

Michael P. Doyle

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This Study was undertaken to provide a basic understanding of the environment for research in the natural sciences at predominantly undergraduate colleges and universities. These institutions have served as a national resource for a significant proportion of students who undertake professional careers in the sciences, and a primary reason cited for their output has been the research experiences of undergraduate students with faculty mentors. However, prior to the Study there was a growing perception that resources and productivity were declining. Concern over these perceived trends by five private foundations with interests in the natural sciences prompted the intensive data collection and analyses that are contained in the *SourceBook*. (More info at:

[http://www.rescorp.org/AE\\_intro.html](http://www.rescorp.org/AE_intro.html))

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**April 17-18, 2002**

**[Value and Impact of Undergraduate Research in Chemistry: Lessons Gained from 45 Years of Experience at the University of Kansas](#)**

K. Barbara Schowen

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The Department of Chemistry at the University of Kansas has a 45-year history of providing research opportunity to undergraduates via formal and informal programs. Since 1957 well over 600 students have engaged in research under the direction of its faculty. Participants have included its own undergraduates, many of them working on senior honors theses, as well as students from other colleges and universities. The combined involvement of all of these students has contributed significantly to the academic life of the department and the university. Data obtained from surveys of students and practicing chemists, directors of research and research programs, and from personal histories and anecdotes point overwhelmingly to the value of research experience for the undergraduate student during the college/university years. These data will be presented and discussed.

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**April 19-22, 2002**

**[THE NATIONAL CONFERENCES ON UNDERGRADUATE RESEARCH](#)**

Dr. Ronald L. Dotterer  
Chair, Board of Governors, National Conferences on Undergraduate Research®  
[RLDOTTERER@salisbury.edu](mailto:RLDOTTERER@salisbury.edu)

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**April 23-24, 2002**

**[The Council on Undergraduate Research: Supporting Research in the Undergraduate Environment](#)**

Kerry K. Karukstis  
Department of Chemistry, Harvey Mudd College, Claremont, CA 91711  
[Kerry\\_Karukstis@hmc.edu](mailto:Kerry_Karukstis@hmc.edu)

The Council on Undergraduate Research (CUR), founded in 1978, is a national organization of colleges, universities, and individuals that share a focus on providing undergraduate research opportunities for faculty and students at primarily undergraduate institutions. CUR members believe that education is best served by faculty\_student collaborative research and that faculty improve their teaching and contribute to society by remaining active in research. CUR provides avenues for faculty development and helps administrators to improve and assess the research environments of their institutions. CUR membership is organized in a divisional structure that includes biology, chemistry, geoscience, mathematics and computer science, physics and astronomy, psychology, social sciences, and an at-large division that serves administrators and other disciplines. The Chemistry Division is the oldest division of CUR. The programs, publications, meetings, and services of CUR will be presented, highlighting those aspects of most interest to chemists.

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**April 25-26, 2002**

**[A plan to improve undergraduate research \(UR\) and student diversity in the botany department at a large, research institution](#)**

Jeffrey Coker and Jon M. Stucky  
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We have perceived two problems in the undergraduate program in the Dept. of Botany at North Carolina State University: (1) few students participate in research; and (2) there is little racial diversity among the students. The purpose of this paper is to describe a plan that, we suspect, would improve UR experiences and the diversity among students in our department. Based on student comments, results of a survey administered by the Education Committee of the Amer. Soc. of Plant Biologists, and experiences of university faculty who have been successful in encouraging UR, problems with the department's UR course have been identified and potential solutions have been devised. We expect that these course improvements, along with efforts coordinated with campus diversity committees, will increase the amount of UR and student diversity in our program. One measure of the success of our efforts will be the results of questionnaires designed to assess changing student attitudes toward science, research, and our department that develop as a result of participation in UR.

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**April 29, 2002**

**Questions for Any Authors and General Discussion**

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## Brief Instructions

*This on-line conference has ended.* A record of the on-line discussion is available on the [CONFICHEM Majordomo archive](#) for Mar - April 2002.

The Committee on Computers in Chemical Education (CCCE) thanks George Long and Pam Mabrouk for organizing and chairing this CONFICHEM conference. We also thank the paper authors and everyone who participated in the discussion. The success of these conferences depends upon all of you.

- For future conferences see the [schedule](#) page. For past conferences see the [archives](#).
- To subscribe or unsubscribe on the CONFICHEM Majordomo please see the [instructions](#) page.
- To report broken links on this page please contact Brian Tissue ([tissue@vt.edu](mailto:tissue@vt.edu)).
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