Pittsburgh Section

The Crucible

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Volume: XCIV No.1 September 2008

Dr. Stephen G. Weber Named Recipient of the 2008 Pittsburgh Award

Dr. Stephen G. Weber of the University of Pittsburgh has been named the 2008 ACS Pittsburgh Award winner. Dr. Weber's record of accomplishment, his creative research in bioanalytical chemistry combined with his dedication to training students (he has mentored 36 M.S. or Ph.D. students) made him an outstanding candidate for the Pittsburgh Award. Stephen Weber received his B.A. degree in Biology and Chemistry from Case Western Reserve University, and his doctoral degree in Chemistry from McGill University. He is currently a professor at the Department of Chemistry at the University of Pittsburgh. In his group, analytical techniques are being developed with higher sensitivity and selectivity compared to the traditionally used methods.

Dr. Weber's group has been working on molecularly selective microextractions using artificial receptors. Powerful separations based on molecular recognition, e.g., the interaction of lanthanides with oxygen-containing molecules, have been developed. Through the improved selectivity of extraction, fewer components of analytical systems will be introduced into separation/detection systems leading to better detection limits and faster analysis. The group also uses a "green" procedure for separation based on biphasic extraction from aqueous solutions using non-volatile polymeric systems as the organic solvents. These thin films are used in a procedure called Solid-Phase Micro Extraction (SPME), which was recently combined with capillary electrophoresis. The method is very useful in the separation of drugs such as barbiturates. To analyze complex biological molecules such as peptides, Dr. Weber's group employs a combination of liquid chromatography and electrochemical detection of the peptide complexed with copper ions. The metal center in complexes with peptides composed of three or more amino acids is oxidizable (Cu(II) to Cu(III)), and it is this electrochemistry that is used for the detection. One current application that is being pursued is the hunt for acidic dipeptides in the brain. In addition to separation and detection, the group focuses on developing sampling protocols, especially for very small samples such as fluid from brain. Sampling the contents of single living cells is another challenge that is currently being addressed.

Dr. Weber's service to the chemistry community is impressive. He has served on numerous committees at the University of Pittsburgh, from the Provost to the Departmental level, and has been Director of Graduate Studies at the Chemistry Department since 2001. He has been active in professional societies such as the ACS, SSP, and SACP. He has been on the Editorial Boards of several high-impact journals, including Analytical Chemistry, and has been reviewing NIH grants and technical papers. Additionally, he has organized numerous symposia and conferences both on the national (ACS, NSF, Pittcon, Gordon Research Conference) and international level.

The Pittsburgh Award, which is presented annually, was established in 1932 to recognize outstanding leadership and distinguished service to the field of chemistry in the local and larger professional community. It is given to professionals who have been instrumental in increasing chemical knowledge, promoting the chemical industry, benefiting humanity, or advancing the Pittsburgh Section of ACS. We are delighted to recognize Dr. Weber's many accomplishments and congratulate him on this well deserved honor. The Award consists of a plaque and will be presented at a special, open to the public, dinner organized by the Pittsburgh Section of ACS. Details of the Award dinner will be published in the next issue of the Crucible.

Submitted by Nick Tsarevsky
Chair-elect, Pittsburgh Section of ACS

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SPECTROSCOPY SOCIETY OF PITTSBURGH

September Meeting

Wednesday, September 17, 2008

Duquesne University, Mellon Hall of Science

(Laura Falk Hall)

6:00 PM - Social Hour
6:30 PM - Dinner
(City View Cafe - 6th Floor)

"Application of FT-IR and Vibrational Circular Dichroism to Problems of Pharmaceutical Interest: From Proteins to Chiral Drugs"

Dr. Rina K. Dukor
BioTools, Inc.

Proteins play a vital role in the development of new biotechnology drugs and pharmaceuticals. New protein sequences and existing protein based products require rapid, cost-effective methods of characterization. Infrared spectroscopy, such as Fourier Transform Infrared (FT-IR) and vibrational circular dichroism (VCD) are ideally suited for this purpose. The main advantage of infrared techniques is that the protein sample can be studied in any state: liquid, solid, powder, fibrils or suspension. In the past decade, FT-IR and VCD techniques have been shown useful in applications such as developing formulations for stabilizing proteins, drug design, mutation studies, environmental effects and secondary structure prediction for membrane proteins and globular proteins.

The production of chiral pharmaceutical molecules that have known absolute configuration and enantiomeric excess is becoming increasingly important. In order to determine these properties in all types of chiral compounds, improved methods for the routine measurement of absolute configuration and enantiomeric excess are needed. In the past few years, vibrational circular dichroism (VCD) has become increasing valuable in a variety of applications of pharmaceutical interest. In cases where chromatographic separation of enantiomers is difficult or too time-consuming, VCD can be used instead since the VCD spectrum scales proportionately in size with the percent enantiomeric excess. In cases where the absolute configuration of a chiral substance is needed, and where X-ray crystallography is either impractical due to problems with crystal growth or accessibility to needed instrumentation, VCD offers an alternative for solution-state measurements. Here, the results of VCD measurements can be compared to the results of ab initio calculations for an unambiguous determination of absolute configuration. In addition, VCD spectral measurements and ab initio calculations can be used together to determine solution-state conformation of chiral molecules that can be useful as a basis for molecular modeling studies.

In this presentation, we will discuss and demonstrate the sensitivity and advantages of FT-IR and VCD spectroscopy to protein structural studies and chiral molecule analysis.

Bio
Rina Dukor is the President of BioTools, a company she co-founded with Professor Laurence Nafie in 2000.

Rina received a Ph.D. in physical chemistry from the University of Illinois, Chicago in 1991. Her thesis explored Vibrational Circular Dichroism (VCD) of biological molecules. Upon graduation, Rina joined Amoco (currently Vysis, a subsidiary of Abbott) where she established a spectroscopy laboratory focused on proteins and nucleic acids. While in industry, she pioneered the introduction of aqueous infrared spectroscopy to the biopharmaceutical industry through the development of instrumentation, sampling techniques and software for protein secondary structure determination. Her methodology, commercialized as PROTA, is now used by over 60 of the leading biopharmaceutical companies. She has pioneered the development of reflection infrared micro-spectroscopy for cancer diagnostics. And by bringing VCD to the market, Rina helped cement the use of VCD by major pharmaceutical companies for the determination of absolute configuration of chiral pharmaceuticals which has truly become one of the most-talked about techniques for chiral analysis.

Dinner Reservations: Please email Ginny Naylor at naylor@pittcon.org or call (412) 487-0915 to make dinner reservations NO LATER THAN FRIDAY, September 12, 2008. Dinner will cost $8 and checks can be made out to the SSP. If you have dietary restrictions, please let Carolyn know when you RSVP. Parking Instructions: The Duquesne University Parking Garage is located on Forbes Avenue. Upon entering the garage, receive parking ticket and drive to upper floors. Pick up a parking chit at the dinner or meeting. If any difficulties arise, contact Dr. Mitch Johnson at Duquesne University.

National Chemistry Week 2008
Poster Contest

As part of the National Chemistry Week (NCW) 2008
the American Chemical Society (ACS) is hosting a poster contest
for students in kindergarten - grade 12.

Students are invited to create a poster that celebrates the theme
"Having a Ball with Chemistry"

The poster should be fun, motivational and inspire students to discover
the connections between chemistry and sports.

Consider how science/chemistry is used in sports. For example:
•Importance of an active lifestyle for physical well-being
•Chemistry in materials used for sports
•Improvements in sporting equipment made possible through chemistry
(e.g. improve safety or allow for "extreme sports")
•Chemistry and sports nutrition

Prizes…Prizes…Prizes….Prizes…
First and second place in each of the following grade categories:
• K - 2nd • 3rd - 5th • 6th - 8th • 9th - 12th
1st Place: $50
2nd Place: $25
Plus…free admission for each winner and up to 3 guests to the Carnegie Science Center
on October 25th to celebrate National Chemistry Week!

All 1st place winners of the local contest will be entered to win the national contest.

National Prizes:
First and second place in each of the above grade categories:

1st Place: $250
2nd Place: $150
There are also prizes for teachers of winning students,
which will include a Periodic Table of the Elephants poster!

EDUCATORS:
Find additional resources for your classroom/students and easy ways to celebrate at www.acs.org/ncw

For additional information about the Pittsburgh contest and where to drop off your top two winning entries from your school by October 15, 2008, contact Susan Gillette Meer at 412.571.0157 or email smeer@mtlsd.net.

National Chemistry Week
Poster Contest Rules

Contest Rules:

•All entries must be original works without aid from others.

•Posters must be no larger than 14 x 22 inches.

•Entries on foam board will not be accepted.

•Entries must be hand-drawn using crayons, paint, colored pencils or markers.

•Posters must be sent to the ACS Local Section NCW Poster Contest Coordinator, Susan Meer (smeer@mtlsd.net) by October 15, 2008.

•All entries must have the following information included on the back of the poster: student's name, grade, name of school or sponsoring group (e.g. Boys and Girls Club or Scout Troop), adult contact address, contact name, contact telephone number, student/adult contact email address. Home schooled students are eligible for the contest and should include the name of any homeschool group with which they are associated.

•Entries lacking complete and legible information will be disqualified.

Other Information:
•Only two entries per school will be accepted into the local contest.
•Only one entry per category may be entered into the national contest by each NCW Coordinator.
•National winners will be announced on the ACS website and via email announcement in early November 2008.
•ACS is not responsible for lost, damaged, or delayed postal shipments.
•All posters become the property of the American Chemical Society.
•Acceptance of prizes constitutes consent to use winners' names and entries for editorial, advertising and publicity purposes.

Judging:
Entries will be evaluated based on the following:
1. Artistic Merit (use of color, quality of drawing, poster design & layout)
2. Poster Message (should be fun, motivational and promote chemistry's important role in the field of athletics)
3. Originality and Creativity (unique, clever and/or creative design)
4. Neatness (free of spelling and grammatical errors and/or stray marks)

National Chemistry Week is a program of the American Chemical Society
Office of Community Activities
800-227-5558, ext. 6097, ncw@acs.org

For additional information about the Pittsburgh contest and where to drop off your top two winning entries from your school by October 15, 2008, contact Susan Gillette Meer at 412.571.0157 or email smeer@mtlsd.net.

Spectroscopy Society of Pittsburgh

Technology forum

Duquesne University

Mellon Science Hall, Laura Falk Hall
5:30 p.m.

Wednesday
September 17, 2008

"Long Rifles of Western PA"

Richard F. Rosenberger

Richard F. Rosenberger and Charles Kaufmann have written the definitive work on the guns and gunsmiths of Allegheny & Westmoreland counties, with an emphasis on the golden age of 1785-1815. Ricks discussion will present a brief history of the longrifle, aka Kentucky rifle, and introduction to its manufacture and use in western PA. The evolution of the American longrifle, from its European ancestry, is discussed, along with its importance on the frontier and settlers and their ability to survive in the wilderness. Rick has documented western PA as an important site in the longrifle development.

Bio

Born in 1938 and grew up in Scott Twp, when it was still a rural area, Rick found the area ideal, as a youngster, for small game hunting with the bow and arrow. His love of Geometry led to employment as a Designer in the Iron, steel and glass industry and hunting led to a lifelong interest in firearms and the outdoors.

Hunting adventures peaked, in 1968, with a honeymoon trip to India for a tiger hunt. Family responsibilities put an end to hunting trips, but his interest in guns and history combined into an attraction to antique rifles. While it was know that the American longrifle (aka Kentucky rifle) was made and used in Western PA, no one had documented this industry.

In the early 70's, Rich worked from home, as an independent contractor, which afforded flexibility in pursuing his interest in history and the longrifle. His efforts included research of census, tax, deed and newspaper records.

Fellow collector C. Kaufmann and Rick accumulated and studied sufficient data to prove that an original school of long rifle design had developed in the area. The University of Pittsburgh agreed with the importance of their study and in 1993 "Longrifles of Western PA: Allegheny and Westmoreland Counties" was published.

Rick is past president and was a board member of the Fort Pitt Museum Associates. He is also called upon to authenticate ancient artifacts. Retired now, and relocated to Butler Co, Rick keeps busy with volunteer work and his hobbies.

Society for Analytical Chemists of Pittsburgh

September Meeting

Monday, September 8, 2008
8:00 PM
Duquesne University
Laura Falk Hall

Speaker Information: TBA

Dinner Reservations:

Please email Larry Senor, Arrangements Co-Chair at senor@pittcon.org, by Thursday, September 4, 2008 to make dinner reservations. Should you not have email, please call Larry at 724-327-4428. Dinner will cost $8 ($4 for students) and checks can to be made out to the SACP. If you have any dietary restrictions, please let Larry know when you leave message.

Parking:

Duquesne University Parking Garage entrance is on Forbes Avenue. Upon entering the garage receive parking ticket and drive to upper floors. Pick up a parking sticker at the dinner or meeting. Contact Dr. Mitch Johnson at Duquesne University if any difficulties arise.

Joint Meeting of ACS Pittsburgh Chemists Club and ACS Energy Technology Group

Tuesday September 23, 2008

Duranti's Restaurant
128 North Craig Street
Oakland Section of Pittsburgh, PA

6:00 PM Cocktail Time - Cash Bar
6:45 PM Dinner
7:55 PM Program

"Organic Solar Cells and Organic Solid State Lighting: State of the Art and Path to Commercialization"

Jessica Benson-Smith,
Plextronics, Pittsburgh, PA

Abstract
Organic solar cells and organic light emitting diodes are technologies that are developing rapidly and have the potential to significantly impact electronics markets. By using standard printing and coating methods, organic electronics can be cast from solution at room temperature – leading to products that are less expensive and more energy efficient than competing semiconductor technologies. This talk with give a brief history of the organic electronics field (specifically the history of organic light emitting diodes (OLEDs) and organic photovoltaics (OPVs)) and will discuss the pathway to commercialization of products using these technologies.

Biography:
Jessica Benson-Smith is originally from McKeesport, PA. She attended Ohio University in Athens, OH where she completed a double major in Mechanical Engineering and Physics. Jessica received a PhD in September of 2007 from Imperial College of Science and Technology, London, UK. At Imperial, she studied the spectroscopy of organic donor-acceptor systems for organic solar cell applications under the supervision of Professor Jenny Nelson. Currently, Jessica is a device scientist at Plextronics in Pittsburgh, PA.

Note
This joint meeting has been developed to introduce energy-related subjects as a more common theme into the Pittsburgh Section ACS Group meetings agenda. It will provide attendees with an opportunity to become involved with the Energy Technology Group and will enhance interaction among Groups. The Section's Coal Technology Group, founded about 1945, became the Energy Technology Group in 2002 to reflect that King Coal in Pittsburgh in the 20th Century has become King Energy in the 21st."

For Reservations, please call Ed Martin by noon Friday, September 19, 2008 at (724) 335-0904 or by e-mail at esm@icubed.com

POLYMER GROUP
Pittsburgh Section
American Chemical Society

Tuesday, September 23, 2008

Duranti's Restaurant
128 N. Craig St. Pittsburgh, PA

Social Hour (cash bar)	5:30pm
Dinner	6:30pm
Technical Presentation	7:30pm

"Organoelectronics: Small Molecules to Polymers"

Britt Minch, Ph.D.
PPG Industries Inc.

Demand for low cost energy has led researchers to explore a variety of potentially low cost alternative energy solutions, including photovoltaics. Though photovoltaics have been around since the 1950s, the commercially available photovoltaics remain expensive and have low efficiencies. Since the ground breaking work of Tang and coworkers in the 1980s, researchers have looked to organic materials to take the place of the more expensive inorganics for use in photovoltaics. Among the many materials that have been reported in the literature for use in photovoltaics, phthalocyanines have been the focus of many reports.

Phthalocyanines are attractive due to their stability and strong molar absorbtivities. The group of Steven Forrest has been prolific in the area of vacuum deposited phthalocyanine photovoltaics. However, there is a strong desire to use materials that are solution processable. Phthalocyanines can be made solution processable by adding peripheral substituents. The addition of these substituents to the rigid disc shaped pigments provides solubility and in some cases the phthalocyanines will exhibit liquid crystalline behavior. A novel synthesis was developed to prepare a series of discotic liquid crystalline phthalocyanines.

Discotic liquid crystals tend to form columnar assemblies, which can behave like molecular wires. The properties and the stability of the liquid crystalline phases can be tuned by choice of the side chain. Furthermore, the assembly can be stabilized by a variety of methods. The use of hydrogen bonding to form supramolecular assemblies and [2+2] cycloaddtions can be used to create covalently crosslinked phthalocyanine polymers.

For dinner reservations please contact Hongying Zhou (Tel: 412-492-5284; email: zhou@ppg.com) no later than Monday, September 22, 2008. The cost of dinner is $19.00 per person; discount rate of $11.00 for retirees; no charge for students. All are welcome!

ACS Debuts Global Challenges Podcasts

ACS' Global Challenges/Chemistry Solutions, a series of podcasts describing some of the 21st Century's most daunting problems, and how cutting-edge research in chemistry matters in the quest for solutions, debuted June 25. The first podcast deals with the shortages of clean water as the basis of other global problems.

This sweeping panorama of global challenges includes dilemmas such as providing a hungry, thirsty world with ample supplies of safe food and clean water; developing alternatives to petroleum to fuel society; preserving the environment and assuring a sustainable future for our children and improving human health.

An ongoing saga of chemistry for life — chemistry that truly matters — Global Challenges continues through December. Subscribe at iTunes or listen and access other resources at www.acs.org/globalchallenges.

ACS Cut and Paste July/August 2008

Bring Together Kids & Chemistry
Share Educational Resources from ACS with Your Favorite Teacher This Fall

It's back-to-school season and teachers are gearing up for a new year. As a chemist, you are in a unique position to help teachers and students learn and love science. After all, you enjoyed learning science so much that you chose to devote your career to it! Help the teachers you know by introducing them to the outstanding resources developed by the American Chemical Society.

To help you spread the word, we've created a flyer you can give to teachers describing ACS education resources. We're also offering some of our best resources at a discount during the months of September and October. Your favorite middle school teacher might benefit from Inquiry in Action, a teacher's guide to inquiry-based investigations that teaches chemistry principles through experimentation and hands-on learning. Or, a local high school chemistry teacher in your area might benefit from a gift subscription to ChemMatters, a publication that investigates the chemistry of everyday phenomena for high school students. Other resources can be accessed for free! Consult the table below for more information on other ACS educational resources and the grade levels they serve.

In addition to sharing resources, you can improve science education by offering your time and expertise. You could volunteer to give a presentation about science in a local classroom or answer chemistry questions from a class throughout the year. Visit the Kids & Chemistry section of the ACS website for presentation ideas and sample activities that you can use to introduce chemistry to students in your community. Your gifts and time will definitely be appreciated by teachers and students alike this year and for years to come!

Ways you can help K-12 teachers with ACS resources:

•Give a teacher the flyer summarizing ACS resources
•Purchase a book or magazine subscription and give it to a teacher
•Introduce a teacher to free online resources
•Answer science questions from a class throughout the year
•Teach a science lesson
•Give a career talk
•Suggest a high school textbook
Mentor a high school chemistry club
•Sponsor a professional development workshop for local elementary and middle school teachers

ACS Cut and Paste July/August 2008

Society for Analytical Chemists of Pittsburgh

October Meeting

Monday, October 6, 2008
8:00 PM
Duquesne University
Laura Falk Hall

"Chemical Amplification of Electrical Signatures in Nanopore Sequencing of Nucleic Acid"

Henry White, Ph.D
University of Utah

No Abstract or Biography to be Published

Dinner Reservations:
Please email Larry Senor, Arrangements Co-Chair at senor@pittcon.org, by Thursday, October 2, 2008 to make dinner reservations. Should you not have email, please call Larry at 724-327-4428. Dinner will cost $8 ($4 for students) and checks can to be made out to the SACP. If you have any dietary restrictions, please let Larry know when you leave a message.

Parking:
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Business Directory

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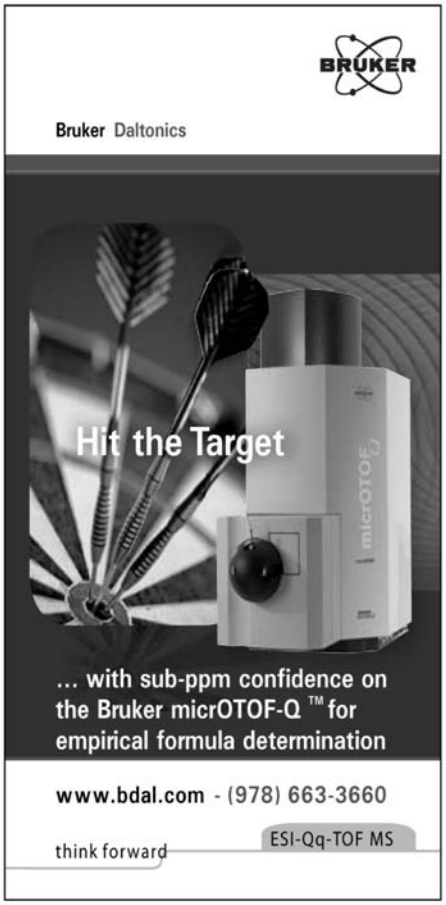
Services



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Crucible Submission Deadline

The deadline for Crucible submissions is the first of the month prior to publication. For example, all submissions for the November issue need to be to the editor by October 1st.

Business Directory

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The Crucible

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Services

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Career Opportunities

SEARCHING FOR THAT SPECIAL JOB?

There are many companies and organizations searching for chemical and biochemical personnel to fill important jobs in their organizations.

- Companies for laboratory and management positions
- Universities & Colleges for teaching positions and laboratory personnel
- Hospitals for technical and research personnel

There are several web sites that may help you search for these open positions.

- www.mboservices.net/recr_disp.php
- http://pubs.acs.org/chemjobs/

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Pittsburgh Area Calendar

September

Mon. 8 **Society for Analytical Chemists of Pittsburgh (SACP)**
Duquesne University, Laura Falk Hall
Program TBA

Wed. 17 **Spectroscopy Society of Pittsburgh Technology Forum**
Duquesne University, Mellon Hall of Science, Laura Falk Hall
"Long Rifles of Western PA"
Richard F. Rosenberger

Wed. 17 **Spectroscopy Society of Pittsburgh**
Duquesne University, Laura Falk Hall
"Application of FT-IR and Vibrational Circular Dichroism to Problems of Pharmaceutical Interest: From Proteins to Chiral Drugs"
Dr. Rina K. Dukor, BioTools, Inc.

Tues. 23 **Joint Meeting Pittsburgh Section ACS Energy Technology Group and the Pittsburgh Section ACS Chemists Club**
Duranti's Restaurant
"Organic Solar Cells and Organic Solid State Lighting: State of the Art and Path to Commercialization"
Jessica Benson-Smith, Plextronics, Pittsburgh, PA

Tues. 23 **Pittsburgh Section ACS Polymer Group**
Duranti's Restaurant
"Organoelectronics: Small Molecules to Polymers"
Britt Minch, Ph.D., PPG Industries Inc.

October

Mon. 6 **Society for Analytical Chemists of Pittsburgh (SACP)**
Duquesne University, Laura Falk Hall
"Chemical Amplification of Electrical Signatures in Nanopore Sequencing of Nucleic Acid"
Henry White, Ph.D., University of Utah

The Crucible
A newsletter of the Pittsburgh Section of the American Chemical Society
124 Moffett Run Rd.
Aliquippa, PA 15001

Change of Address

If you move, notify the American Chemical Society, 1155 Sixteenth Street, N.W., Washington, D.C. 20036.

To avoid interruption in delivery of your CRUCIBLE, please send your new address to Traci Johnsen, 124 Moffett Run Rd., Aliquippa, PA 15001. Allow two months for the change to become effective.