Chemical Bond

Volume 55
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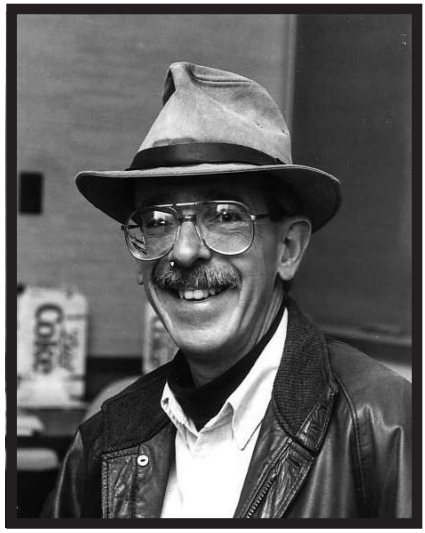
St. Louis Section, American Chemical Society



Mark S. Gordon
60th American Chemical Society
Midwest Regional Award

Member Needs Survey Results Are In !

Thank you for participating in our Member Needs Survey. I wanted to let you know that because of the input from our members, we will be creating a Pharmaceutical Discussion Group. Please let me know if you'd be interested in joining or sponsoring this group.

We have also formed a committee to look into having a picnic in the summer of 2005.

A big thank you to those of you who volunteered to be judges at the science fair and to those who volunteered to help with Kids'N Chemistry. Your names have been forwarded to the appropriate committee chairs.

Ted Gast, Chair-Elect 2004
St. Louis Local Section
American Chemical Society

2004 St. Louis Section Chemical Technician Award Call for Nominations

The St. Louis Section Chemical Technician Award will be presented to a chemical technician in the St. Louis area who has demonstrated a high degree of professionalism as a chemical technician. The award will consist of a plaque, a check for $250.00, dinner for the awardee and a guest at the Chemical Progress Week Awards Night ceremony, and nomination for the National Chemical Technician Award. The award will be presented at the Awards Night Banquet in April of 2005.

A chemical technician is a person whose training includes successful completion of an Associate or Bachelor Degree in chemistry or a chemistry-related curriculum, or the equivalent knowledge gained by experience. The primary work of a chemical technician is conducting experimentation and/or correlating information to assist in the solving of chemical problems.

Letters of nomination must be received by Sue Dudek, Pfizer Corp., mail code T2G, 700 Chesterfield Parkway West Chesterfield, MO 63017 by October 29, 2004. Nominations, including seconding letters, must not exceed six pages. The nominating letters should address each of the criteria above. A current work address, phone number and fax number must be provided for each nominee. Please include an e-mail address if one is available.

For more information contact Sue Dudek at 314-274-2464,
FAX 314-274-4426, susan.dudek@pfizer.com

Chemical Bond

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In this issue . . .

Meeting & Seminars

Board of Directors

St. Louis Section–ACS Board of Directors meets on the second Thursday of each month, at the Alumni Center, University of Missouri–St. Louis. Meetings are open to all members, and all are encouraged to attend. Elected officers and chairs of major committees have the right to vote; others in attendance have voice but no vote. If you want to attend the dinner, please contact Bijan Khazai (bkhazai@sentortech.com or 314/497-8629) at least one week prior to the meeting date. The usual cost of dinner is $15. Members wishing to become active in section activities are welcomed for their first dinner for free, compliments of the section.

Date: Oct. 14
Social hour: 5:30 pm
Dinner: 6:30 pm
Business meeting: 7:15 pm
Future meetings: Nov. 11
Dec. 9

St. Louis University

Seminars start at 3:30 pm in Room 204 Macelwane Hall, unless noted otherwise. Refreshments follow. For more information, contact Paul Jelliss, jellissp@slu.edu.

October 8
Chengdi Mao
Purdue University
Self-assembly of DNA Nanostructures

October 15
Matt Fete
University of Colorado-Boulder

October 29
Masangu Shabangi
Southern Illinois University, Edwardsville
Electrochemical Investigation of Thiamin and its Phosphate Esters in Acidic Solutions

November 12
Christine Smith
Global Biologics Department
Pfizer

November 17* (Wednesday)
Charles Henry
Colorado State University
New Approaches to Proteomic and Metabolomic Analysis

University of Missouri-St. Louis

Seminars are held on Mondays at 4:00 pm in Room 451 Benton Hall unless otherwise specified. Refreshments 15 minutes prior to seminar time.

October 4
Michael Henzl
University of MO-Columbia
Rat Alpha- and Beta-Parvalbumins: Energetics of Divalent Ion Binding

October 11
Paul Duvall
University of MO-Columbia
New Coordination Environments in Uranyl Chemistry

October 18
John Enemark
University of Arizona
Variable Frequency Pulsed EPR Spectroscopy: A Beacon for Illuminating the Metal Sites of Protein

October 25
Cheng-Wei Tom Chang
Utah State University
Glycodiversification for the Development of Aminoglycoside Antibiotics

Washington University

Seminars are in McMillen 311 at 4 pm unless otherwise noted. Coffee is available 20 minutes prior to the talk, and refreshments follow. For information, contact:

Amy Walker
walker@wuchem.wustl.edu
An up-to-date list of seminars is available at:
www.chemistry.wustl.edu/~seminars/seminars.html

Seatbelts for Everyone!

by Jack Bornmann

If you drove your car into a solid, concrete wall, how many collisions would occur?

Letters & Words & More

The first collision is the one which occurs when the metal (or plastic) of the car contacts the wall. Hopefully, this collision is a continuous one (like hitting a spring) in which the contact continues instead of bouncing back. Modern cars are designed to collapse so that the kinetic energy change is absorbed in the collapse.

The second collision occurs when the driver or passenger collides with the three-point seat belt, the air bag, the steering wheel, the dashboard, the window, or some object outside the car. Hopefully it will be a collision with the seat belt and/or the airbags. In the old days, the driver might collide with the steering wheel which was often connected to the steering post by three or four spokes. When the steering wheel gave way during this secondary collision, the driver was impaled on the steering post. *Ouch! Buckle up!* We used to frequently read about passengers being ejected from the vehicle during a collision. They were not wearing the seat belt and ultimately collided with some object outside the vehicle. Collisions with the dashboard were brutal, but collisions with the front window were a bloody mess.

The third collision occurs when the inner organs of the driver or passenger collide with the bones or skin providing the outer covering of the body. The brain slams into the skull, the heart and lungs slam into the ribs, and the abdomen becomes distended. These collisions are injurious, but not necessarily fatal. But, what if the driver is a woman who is 8-months pregnant? In addition to the collisions of her brain, heart, and lung with her bony enclosures, there arise collisions of her uterus with her abdominal wall, the collision of the baby with the uterine wall, and the collision of the baby's brain, heart, and lungs with its bony enclosures. These fetal bones are elastic and should give somewhat during these collisions, but fatal damage can occur to the unborn baby. Some injuries to the baby may not be fatal, but may cause developmental problems years after the collision. How do we protect such unborn babies during collisions?

Apparently, most auto manufacturers make the economic decision that it is too costly to address problems that occur to such a small population. It is difficult to obtain reports on deaths or fetal injuries resulting from car crashes, especially if the mother survives. If the mother dies the medical examiner's post-mortem report should contain information about the fetal death. But, if the mother survives, there is no central clearing house to collect information about subsequent fetal death (miscarriage) or post-partum conditions that may have been caused by the accident. A study at the University of Pittsburgh estimated between 350 and 700 fetal deaths can be attributed to car crashes annually. Compare that with the approximately 700 deaths in car crashes for all children up to four years of age in 2001. But there is hope.

Ms. Laura Thackray, a mechanical engineer, wants to do something about this problem. She has been developing a computer model of

a pregnant crash dummy. Whereas the auto manufacturers in the U.S. rejected her applications for employment, Volvo in Sweden encouraged her to do graduate work at Chalmers University of Technology in Sweden and, subsequently, hired her. She is now actively and gainfully employed in research that will lead to a Volvo which protects pregnant women. With Volvo leading the way, the American manufacturers will soon follow. Ford will probably be the first, because it owns Volvo.

The St. Louis Section of the American Chemical Society is pleased to announce the

Battle of the Burets

This contest for high school chemistry students will match teams from local high schools against one another in a test of titration speed and accuracy. Teams will be run in heats with the winner of each heat advancing to the next round. Trophies will be awarded to the heat winners and the winning school.

The contest will be held on:
Wednesday, October 27, 2003
at St. Louis Community College - Florissant Valley.

The first heat will commence promptly at **6:00 PM**.

For more information on how to enter a team from your high school contact:

Bruce Ritts
314-290-4744
bruce_ritts@steris.com

Nominees for Office - 2005
St. Louis Section-ACS

The Nominating Committee presents the following candidates for office to the St.Louis Section-ACS for 2005. All members of the St. Louis Section are eligible to vote. Please mark the enclosed ballot, following the instructions printed on the reverse side, and return no later than October 31, 2004. Ballots postmarked after that date will not be counted.

Chair-Elect (vote for one)

Alexa Serfis: Associate Professor of Chemistry at St. Louis University, faculty advisor for the ACS Student Affiliate group which earned national recognition for their activities. Section activities include: National Chemistry Week Coordinator 1995, 2001, 2002; Alternate councilor 1997-2000; Director ACS Board 2003; Awards Committee Chair 2002-2004; Undergraduarte Research Symposium Chair 1999, 2003; Undergraduate Programming, Midwest Regional Meeting Chair 2000; Science Fair Awards Chair 2001; ACS Peer Mentoring Workshop, Washington D.C., 2000.

Secretary (vote for one)

Keith J. Stine: Associate Professor of Chemistry and Biochemistry, University of Missouri-St. Louis. Section activities include Midwest Award 1993; Surface Science Discussion Group 1993-1999; Materials Chemistry Discussion Group 2000; Saint Louis Award 1998-2000; Alternate Councilor 1997-1999; Director 2001; Career Day 2001-2003; Secretary 2002, 2003; Program Chair - 35th ACS Midwest Regional Meeting.

Treasurer (vote for one)

Lisa Balbes: Balbes Consultants. Current activities at the section include Webmaster; Immediate Past Chair and Career Resource Coordinator for St Louis Section; Webmaster for COMP Division; Career Committee for CINF Division; and Career Consultant and Presentor for ACS/Career Services; PR chair and Computational Chemistry Discussion Group chair; PR chair and NCW Committee for Columbus OH section.

Director (vote for three)

Sue Dudek: Research Technician, Pfizer (formerly Pharmacia). Section activities includeTechnician Affiliate Group Chair 1993; Alternate Coucilor 1994, 1997; Director 1995, 1998-1999; St. Louis Technicial Award Chair 1998- ;Career Awareness Fair booth Chair 1993-2002; Battle of the Burets co-chair 2000, Section Chair 2001. She has also served as National Technician Award Chair 2001.

Hal Harris: Professor of Chemistry at University of MO, St. Louis. Section activities include St. Louis Section Chair, 1994; Director, numerous years. Hal is interested in bringing a better public understanding and appreciation of chemistry through responses to distortions in the media, and has for several years headed a committee for that purpose in the section.

Shelley Minteer: Assistant Professor of Chemistry at St. Louis University; numerous section activities.

Eric Ressner: Technical Cummunications Scientist, Sigma-Aldrich Corporation; Section activities include Chemical Bond Editor 1996-2003; Director 2003, 2004.

Bruce Ritts: Senior Scientist, Steris Corporation 2002-2003. Section activities include Treaurer 2002-2003; Director 2001; Publicity and Public Relations; Committee chair 2000; Chemical Progress Week 1997-1999, 2001-2002; Program Committee chair 1996; Education Committee chair 1994, 1995; National Chemistry Week coordinator 1993; Donation Committee chair 1992.

Councilor (vote for two)

Lawrence Barton: Professor of Chemistry, University of MO, St. Louis. Section activities include: **Service in ACS National Offices**: Elected to ACS Committee on Committees, 2005-2007, Committee on Local Section Activities, 1998 – 04; Committee on Membership Affairs, 1992 – 1997; Committee Associate, 1991. **Service in ACS Offices**: Member ACS since 1966. *St. Louis Section*, Councilor, 1990 – 04; Alternate Councilor, 1987-89, 1979-81; Chair, 1980, High School Career Day Organizer, 1993 – 1998, 2000; Board of Directors, 1981-89, 1977-79, 1993-date; Steering Committee member, 1980-81, 1996-98; Midwest Award Jury, 1983-89, 1992-date; Continuing Education Committee, 1972-74; Education Committee Chair 1973-75; St. Louis Award Jury (appointed) 1975; High School Chemistry Contest Organizer 1976, 1977; Member Special Committee to Review the Midwest Award 1987; St. Louis Award Symposium Chairman, 1983. Section Historian, 2000-date. **Member**: Royal Society of Chemistry, Chemistry and Physics on Stamps Study Unit; *ACS Divisions*, Chemical Education, History of Chemistry and Inorganic Chemistry.

Greg Wall: 24 year member of ACS and a 19 year member of the St. Louis Section. He is actively involved in promoting chemical literacy through public outreach programs. He has served as Chairman (1996), General Topics Chair, National Chemistry Week Chair, Program Committee Chair, and Public Outreach Chair. He remains active in the Section as the General Topics and Public Outreach Chair, Alternate Councilor, and Director.

Tom Layloff: Prinicpal Program Associate in the Center for Pharmaceutical Management, Management Sciences for Health. Section activities include: Councilor 1987-2001; Midwest Award Jury 1980-1983, 1987-2001; Alternate Councilor 1978-1986; ACS National Meeting Organizing Committee 1984; Director 1974-1976, 1978-1979, 1981-1984; 75th Anniversary Program Chair 1982; Nominating Committee 1978, 1980, 1981; Centennial Committee Chair 1975-1976; Section Chair 1973; Professional Activities Committee Chair 1971; Crime Lab Advisory Committee Chair 1969-1971; Community Relations Committee Chair 1970; Program Committee Chair 1969; General Program Chair 1968; Education Committee Long Range Planning Group 1967; Regional Meeting Steering Committee 1977-1994; Local Arrangements Committee Chair 1971; General Chair 1979,1989.

The St. Louis Section is having a special event on **Tuesday, November 16th at 7:30 pm**. Dr. Ariel Fenster (McGill University) will present "The Love and Lore of Chocolate" at the Center of Clayton meeting rooms B&C. This talk will be followed by a chocolate dessert buffet. YUM! For more information contact Leah O'Brien (314) 757-3179 or lobrien@siue.edu.

Pick up

rotating

Mass-Vac ad

from p. 5 of April 2004

The Research of Carl and Gerty Cori designated a National Historic Chemical Landmark

Gerty Cori and her husband Carl Cori in the laboratory at Washington University School of Medicine, St. Louis, 1947

On September 21, 2004 the American Chemical Society presented a plaque designating the research of Carl and Gerty Cori as a National Historic Chemical Landmark. The presentation was followed with a lecture given by Dr. Arthur Kornberg entitled "The Ten Commandments of Enzymology and the Importance of Inorganic Polyphosphate". The Cori's, who came to Washington University School of Medicine in 1931, were instrumental in the development of the field of biochemistry with interests that spanned areas from the isolation and purification of enzymes of glycolysis to the role of hormones such as insulin. As a consequence of their work, the Cori's won the Nobel Prize in 1947.

Dr. Arthur Kornberg, Professor Emeritus, Stanford University, also a recipient of the Nobel Prize, worked in the Cori laboratory in 1947 and returned to Washington University School of Medicine in 1953 to become Chair of the Department of Microbiology. He remained in that position until 1959 when he moved to Stanford.

National Chemistry Week's

Day at the Science Center

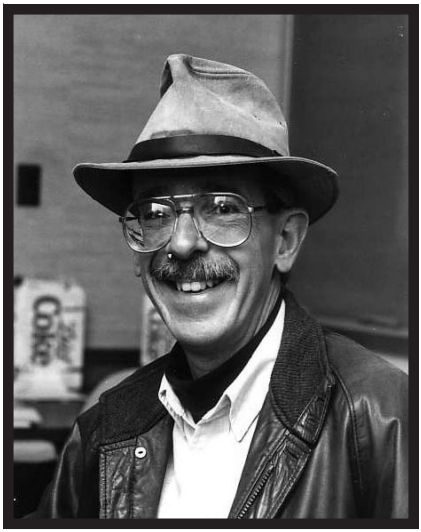
will be on October 16th from 9:00 am to 4:00 pm.

There will be an academic/industrial exposition, with displays and hands-on activities for children. This year's theme is **Health and Wellness**. In the past we have had many volunteers who have given their time to man tables, do demonstrations, set up displays, and chat with visitors to the Science Center.

Anyone interested in volunteering should contact:
Mike Shaw
michsha@siue.edu
or Eric Malina
emailina@siue.edu

Midwest Award 2004

Prof. Mark S. Gordon



Mark S. Gordon, the recipient of this year's Midwest Award of the American Chemical Society, grew up in and around New York City, received his B.S., Ph.D. and postdoctoral education at Rensselaer Polytechnic Institute, Carnegie-Mellon University (w. J.A. Pople) and Iowa State University (w. K. Ruedenberg). For 12 years on the chemistry faculty of North Dakota State University, he rose to Distinguished Professor and Department Chair. During his subsequent 12 years at Iowa State University, he has become Distinguished Professor, has been the associate Department Chair and is currently Director of the Applied Mathematics Program in the Ames Laboratory USDOE. He has been a visiting scientist at the University of California-Irvine, the Minnesota Supercomputing Institute, the National Science Foundation, the Molecular Science Institute in Okazaki (Japan), the University of Tokyo and the Australian National University. He has been the Chair of the Theoretical Chemistry Subdivision of the Am. Chem. Soc., and the Secretary-Treasurer of its Phys. Chem. Division. He is a Fellow of the Am. Phys. Soc. and a Fulbright Senior Scholar. He is on the editorial board of several journals.

Gordon's over 380 publications in quantum chemistry have had significant impact and won worldwide recognition, among "real" chemists as well as theorists, for his unique blend of systematic elucidations of important bonding and reaction mechanistic problems on the one hand and effective ab-initio method developments on the other hand. The objects of his studies typically are potential energy surfaces, reaction paths, activation energies of transition states and reaction mechanisms.

Gordon has developed MCSCF centered methods, the Effective Fragment Method for solutions and liquids, a Molecular Orbital/Molecular Mechanics method for clusters on surfaces, and several spin-orbit coupling methods. His localized analyses of electronic wavefunctions extract chemical meanings from complex computations, especially for the benefit of the non-theoretical chemists. To pursue this comprehensive program, he has developed, maintains and continues to expand the premier open quantum chemistry program system GAMESS, which is used by several thousand scientists worldwide.

Gordon's contributions cover many regions of the periodic table, notably carbon chemistry, silicon chemistry, organometallic chemistry and transition metal chemistry. He is

particularly famous as a pioneer in elucidating how and why silicon chemistry differs from carbon chemistry. He discovered the near-isoergicity between silylenes and silenes; the small barriers for silylene insertion reactions; the pi-bonds of silicon with itself as well as carbon, nitrogen, oxygen, phosphorus and sulfur, including triple bonds; silicon's participation in aromatic systems; structure and strain of small rings and clusters containing silicon; geometric and electronic structures of molecules containing pentavalent silicon; reaction paths of pseudorotational isomerizations between axial and equatorial atoms. He has extended this work to germanium, tin and titanium.

Gordon has furthermore complemented his gas phase investigations by realistic studies of reactions in solution as well as on solid surfaces. His solvation theory has accurately produced metalloenzyme UV shifts, chemical reactions, protein pK_as, and electrolyte dissociation dependence on solvation coordination. His surface model has yielded correct structures of Si surfaces and revealed mechanisms for reactions on this surface including oxidation, etching and addition of various substrates.

Notwithstanding the many complex mathematical and computational aspects of his investigations, it is the chemistry that drives all of Professor Gordon's work.

CEPA and Globalization

Globalization, offshoring, outsourcing, insourcing, jobless recovery... You have all heard these terms. The ACS Committee on Economic and Professional Affairs (CEPA) has formed an active Task Force on Globalization Issues to "monitor, communicate, coordinate, and cooperate" with others on globalization and how it relates to employment in the chemical industry. The task force includes liaisons from Corporation Associates, Committee on International Activities, Committee on Science, Divisions of Professional Relations, Business Development and Management, Small Chemical Businesses, and other interested parties. At the ACS meeting in Philadelphia, CEPA hosted a successful first Open Forum for all ACS members to voice their views on globalization issues, and different perspectives were shared.

Please visit the CEPA website at:

http://www.chemistry.org/committees\cepa\index.html

for more details on the activities of this task force, a bibliography with abstracts of pertinent publications on globalization, CEPA symposia and presentations related to globalization, and a new Message Board (coming soon) where you are invited to enter your opinions and comments on globalization issues, especially as it relates to your job and career!

Boy Scout Chemistry Merit Badge Clinic

The Boy Scout Chemistry Merit Badge Clinic on Sept 4th went off quite well. A total of 19 boys from 3 different troops participated. They met for an introductory session - "What is Chemistry?", presented by Dr. Alexa Serfis. Following that, they were split up into 4 groups of 5 boys, and rotated through 4 stations, for 45 minutes each. Each station had a mixture of lecture, demos, and hands-on activities.

The stations were:
Biochemistry - Dr. Greg Wall
Physical Chemistry - Dr. Vic Lewchecko
Organic Chemistry - Ted Gast
Careers and Tour of manufacturing plant - John Gleason

All boys who participated finished 8 of the 9 requirements, and received materials to complete the 9th requirement at home. One boy completed that requirement at home in advance and brought in the rusted nail to prove it, so he earned the entire badge.

"To my knowledge we had no major incidents or calls for first aid, so I'm calling it a success. We even got one boy to say it was 'really cool!'"

-Lisa Balbes

Nominate a Colleague for the St. Louis Award

The St. Louis Award, sponsored by the Monsanto Company, is presented to an individual who had made outstanding contributions to the profession of chemistry and demonstated potential to further the advancement of the chemical profession. The award, consisting of a $1,500 honorarium and a plaque, is presented at the St. Louis Award Banquet, the final event of Chemical Progress Week in April.

Please help the Awards Committee identify outstanding chemists in the St. Louis Section by submitting your nominations to the St. Louis Award Chair. The nominations should include a nominating letter, two or more seconding letters from individuals who have had a close professional affiliation with the nominee, a brief biography, a description of the nominee's accomplishments, and a list of publication and patents.

At the time of the nomination, the nominee must not have previously received the Midwest Award or any national ACS-sponsored award. The nominee must be a member or affiliate of the St. Louis Section of the ACS. The deadline for nomination packets to be received is December 10, 2004. Please send nominations and inquires to:

Dr. Joseph Ackerman
St. Louis Award Chariman
Department of Chemistry
Campus Box 1134
Washinton University
1 Brookings Drive
St. Louis, MO 63130-4899
Phone: 1-314-935-6593
FAX: 1-314-935-4481
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St. Louis Section
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Rush-Dated Material Inside

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Sigma ad

from back cover

of previous issue