

THE OCTAGON



Volume 86, No. 2, February 2003

Lehigh Valley Section of the American Chemical Society

In This Issue:

Meeting Announcement	1	Chemistry Olympiad Announcement	2
2003 Meeting Schedule	1	January Meeting Minutes	3-4
Section Officers	2	Advertising Article Policy	5
LVACS Scholarship Announced	2	This Month in the History of Chemistry	5
Editor's Message	2	Chemistry Question of the Month	5

762nd LVACS Meeting:

Date: February 20, 2003

Location: Lafayette College

Reception: 5:30 pm - Faculty Dining Room - Maquis Hall

Dinner: 6:00 pm - Faculty Dining Room - Marquis Hall

Meeting: 7:30 pm - Gagnon Hall - Hugel Science Center

Talk: At conclusion of meeting - Hugel Science Center

Menu: Slow Roasted Prime Rib of Beef, Hazelnut Crusted Salmon, or Eggplant Roulade Twice baked potato Chef's choice vegetable. Dessert - Peanut butter pie

Cost: \$20, students \$10

Contact: Debbie Bastinelli by noon on Friday, Feb. 14th. Please provide name, affiliation, choice of entree and contact information. e-mail: bastined@lafayette.edu; phone 610-330-5213

Directions: Marquis Hall is building number 21 on the campus map. Parking may be found near the area marked March Field, or on the Parking Deck (2). Hugel Science Center is building 6 on the campus map. For more information see: <http://www.lafayette.edu/community/campusmap/campmap.htm>

Speaker: Paul Bouis, Ph.D.

Paul Bouis was born in Nice, France and immigrated to the United States when he was six years old. The son of a Chemist/Perfumer he was destined to a life in chemistry. Currently Paul is Director of Research and Technology for laboratory Products at Mallinckrodt Baker. Paul holds a BS in chemistry from the Virginia Military Institute and a PhD in Physical Organic Chemistry from the University of Tennessee. Paul has authored chapters on radioactivity, chromatography and other analytical chemistry techniques. He is chair of the Reagent Chemicals Committee for the

American Chemical Society. He is once again serving as chair of the Lehigh Valley section of the ACS. He has periodically been an Adjunct Professor teaching various aspects of analytical chemistry. His research interest is in the area of purification of biopharmaceuticals and organic solvents.

Talk: "The Legacy of a Zinc City"

Abstract: Before Bethlehem Steel began its downward spiral into Chapter 11 bankruptcy another Lehigh Valley industrial giant had disappeared from the ranks of the valley's great companies. New Jersey Zinc, which settled in Palmerton, did so for many of the same reasons that Bethlehem Steel settled in Bethlehem. It disappeared for many of the same reasons Bethlehem Steel soon will.

In this talk we will reminisce about the birth, life and death of a company and an industry, which left a permanent mark on the city, citizens, and landscape of Palmerton. We will examine the chemistry involved in zinc processing and the role it played in the eventual demise of New Jersey Zinc.

So that we do not forget the part this company played in improving the way of life for all mankind we will review the many contributions zinc and its compounds have made to modern society.

2003 Spring Meeting Schedule:

(Please *pencil* these dates on your calendar)

February 20, Lafayette College
March 14, DeSales University
April 15, Moravian College
May (TBA)

LVACS Officers:

Chair: Paul Bouis

Mallinckrodt Baker Inc., Phillipsburg, NJ 08865
paul.bouis@tycohealthcare.com 908-859-9443

Chair Elect: Steve Weiner

Chemistry Department, Muhlenberg College
2400 Chew Street, Allentown, PA 18104
sweiner@muhlenberg.edu 484-664-3665

Immediate Past Chair: Joe Sherma

Lafayette College, Easton, PA 18042
shermaj@mail.lafayette.edu 610-330-5220

Secretary: Tara Baney

Merck Research Laboratories, Dept. 864,
10 Sentry Parkway, BL1-4, Blue Bell, PA 19422
tara_baney@merck.com 484-344-3346

Treasurer: John Freeman

522 Raub St., Easton PA 18042
jcf2@fast.net 610-923-358

Councilor: Roger Egolf

Penn State LV Campus, Allentown, PA 18051
rae4@psu.edu 610-285-5110

Councilor: Pamela D. Kistler (2000-2001)

Cedar Crest College, Allentown, PA 18104
pdkistle@cedarcrest.edu
610-437-4471 Ext 3507

Alternate-Councilor: T-Michelle Jones-Wilson

East Stroudsburg University
East Stroudsburg, PA 18301
mjwilson@po-box.esu.edu 570-422-3446

Alternate-Councilor: Carol Baker Libby

Moravian College, Allentown, PA 18018
cblibby@cs.moravian.edu 610-861-1629

recommendation and the essay guidelines will be available on the LVACS website by March 1. (www.esu.edu/lvacs). Requests for paper copies may be mailed to John Freeman 522 Raub St, Easton, PA 18042. Please include a self addressed stamped envelope.

Scholarships are supported by the general fund of the section and donations to the Lehigh Valley Foundation in Chemistry Scholarship Fund. The Scholarships are part of an ongoing effort by our section to promote the study and appreciation of chemistry in the Lehigh Valley. Donations to the Scholarship Fund may be mailed or given directly to the Treasurer or other officer of the Section. The Treasurer is currently John Freeman at 522 Raub St Easton PA 18042

Editors Message:

In the past several issues I have harangued members to subscribe to the Octagon via email. The response has been positive (40 more email subscribers for this issue) and I will discontinue the plea for this month, although gentle encouragement is still in effect.

In this month's message I would like to focus on user participation. This is your newsletter; to grow, it needs your input. Please let me know about any events concerning chemistry in the Valley from preschool to graduate school and in industry too. If you have an event or product to promote, consider advertising in the Octagon. Copy submission guidelines are on page 5 of this newsletter. We have a subscriber base of almost 1000 professional chemists and chemical engineers. Can you think of a better way to get your message or product information to your colleagues in the area? Contact information is provided on pg 5.

LVACS and the National Chemistry Olympiad

The LVACS will be participating in the U.S. National Chemistry Olympiad (USNCO). The goals of this program are to stimulate interest and achievement in chemistry among highschool students throughout the US and to provide recognition of outstanding young chemistry students, teachers and schools. Please consider participating in this program. Students competing in the USNCO are eligible to be selected as members of the US team for the International Chemistry Olympiad which will be held in Athens, Greece this summer. If you are a teacher in our secondary schools please encourage your students to participate in this academic olympiad. Deadline is February 2nd. For a complete announcement and more information contact the LVACS program coordinator:

Marion W. Smith, phone 484-664-3267, email:
msmith@muhlenberg.edu

Scholarship to Recognize Outstanding Organic Chemistry Student to be awarded at the May Meeting.

The Lehigh Valley Section of the American Chemical Society would like to invite applicants for its Organic Chemistry Scholarship. The student must be a rising junior having completed organic chemistry, attending school in the Fall of 2003 at an institution in the Lehigh Valley Section. We especially welcome applications from Jr. College transfer students. The applicant should plan to attend a morning examination in organic chemistry on Saturday the 26th of April. The application consists of a letter of recommendation from a faculty member at the student's current institution, an essay on a topic in organic chemistry, and documentation of the student's performance on the ACS organic chemistry examination. Applications, information, letters of

January Meeting Minutes:

The 761st meeting of the LVACS was called to order by Chair Dr. Paul Bouis at 7:42 PM on Wednesday, January 22, 2003. Muhlenberg College hosted the meeting on their campus. Dr. Bouis welcomed everyone to the first meeting of 2003, and introduced the LVACS Officers: Chair, Paul Bouis; Chair-Elect, Steve Weiner; Secretary, Tara Baney; Treasurer, John Freeman; Councilors, Roger Egolf and Pamela Kistler; and Alternate-Councilors: Michelle Jones-Wilson and Carol Libby. Contact information for the officers is located on our local ACS website (<http://www.esu.edu/lvacs/>) and in every issue of the Octagon. Dr. Bouis thanked Immediate Past-Chair Dr. Joe Sherma for Joe's leadership during the 2002 term. Dr. Weiner also thanked everyone for his or her vote, and noted that he will "make it your section." Carol Libby was recognized for her continued efforts as Nominating Committee Chair, and if anyone is interested in running for an office, please see her for information. Next, the Question of the month was answered: "Who coined the term protein?" There were two different answers: G.J. Mulder and Jons J. Berzelius, although both were dated 1838.* The November 2002 minutes were approved. Dr. Bouis brought the attendees up-to-speed regarding the annual report and the by-laws. He is working on the final version of the by-laws, and would like members to view the document on-line in order to volunteer comments. The complete update will be in the next issue of the Octagon. In addition, Drs. Bouis and Sherma are working on the annual report. Dr. Bouis extracted some statistics from the 2001 report, noting similarities and differences between the Lehigh Valley Section and Princeton, since both sections are equivalent in size. Memberships are down for both sections, section dues are higher in Princeton, and the average attendance at meetings is ~5-6% for both sections. Next, Dr. Bouis gave a brief Treasurer's Report, stating we have a deficit and John Freeman will present a more detailed budget report at the next meeting.

Dr. Marsha Barr, Associate Professor of Chemistry at Muhlenberg, introduced our speaker for the evening, Dr. David J. Weber, PhD (dweber@umaryland.edu). The title of Dr. Weber's talk was "Important Biochemical Advances in the Understanding of Cancer: the interaction of S100B with the tumor suppressor protein p53." Dr. Weber began by telling the audience S100B stands for 'soluble in 100% (saturated) ammonium sulfate.' The protein is found in high concentrations, and is used as a marker, in several tumor cell lines. Dr. Weber showed a listing, which included lung, bladder, kidney, cervix, breast, head, neck, larynx, lymph, and mouth. S100B exists as a dimer, while p53, which is a tumor suppressor protein, is a tetramer. Their interaction, based upon Western blot analysis, is cell cycle dependent because asynchronous Western blots were inconclusive. In addition, Western blot analysis supports S100B interaction with p53 during the GAP₁ phase (G₁) of the cell cycle; later determined that both proteins are found in the cytoplasm at the same time during the GAP₁ phase (G₁). Dr. Weber displayed a pictorial and described how p53 binds to specific DNA sequences in the cell, which activates transcription of various genes (one mentioned as p21, a cyclin-dependent kinase inhibitor). This leads to growth arrest.

The main question of his research for this presentation was posed as "does the binding interaction of S100B and p53 inhibit or activate p53?" Dr. Weber noted past experience demonstrates moieties binding to the extreme C-terminus of p53 causes activation; however, in this case the opposite proved to be true. S100B actually decreased p53 levels inside of malignant melanoma cells, either by degradation, or by lack of recognition. Dr. Weber explained to the attendees that p53 seems to have protective properties from proteins like S100B; i.e., a C-terminal negative regulatory domain. Note that S100B binds p53 in a Ca²⁺-S100B complex. This was not expected. Therefore, the research team decided it was essential to determine the 3-D structure of apo-S100B, S100B- Ca²⁺, and S100B-Ca²⁺-p53 peptide complexes. The eventual goal is to use the information for structure-based inhibitor design, leading to rationally designed therapeutics.

Dr. Weber and his group used NMR to determine the structure of the above mentioned complexes, specifically NOE-based structure design. In order to appreciate the efforts that took place, the audience was given a brief refresher on NOE, Nuclear Overhauser Effect. NOE enables the researcher to connect nuclei through space. This effect is fundamentally different, as exchange between the nuclei does not involve scalar coupling. Instead, the direct magnetic coupling (no electrons in between), termed dipolar-coupling, is involved, which usually does not have an observable effect in solution. NOE provides an indirect pathway to obtain information of this dipolar-coupling, which, in turn, can be correlated with internuclear distances (5 Å as mentioned by Dr. Weber) and molecular motion. Dr. Weber showed a diagram explaining why assigned patterns are much easier (relatively speaking) than not assigned:

Figure A

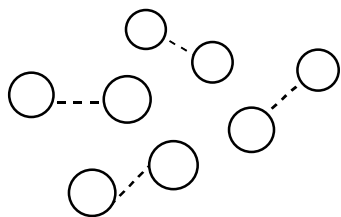
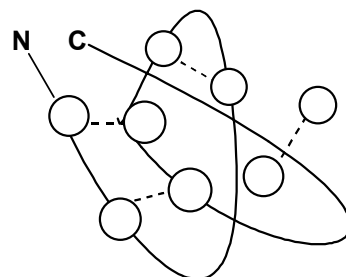


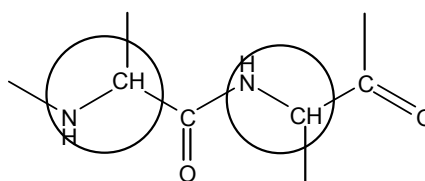
Figure A shows no assignments, while Figure B shows a protein with assignments. Basically, having assignments allows a finite number of structure possibilities.

Figure B



Dr. Weber noted that 1-D NMR makes analysis virtually impossible; therefore, this type of analysis required the collection of heteronuclear multidimensional (2-D, 3-D, & 4-D) NMR data for the structure determination of the complexes. This makes use of heteronuclear species, such as H, N, & C, to analyze chemical shifts in the protein backbone. A schematic structure of a protein backbone is as shown:

The circles show the heteronuclear participants in H ^{15}N $^{13}\text{C}^\alpha$ A NMR analysis. Another method, called H ^{15}NCO $^{13}\text{C}^\alpha$ A, takes the -CH-CO-N portion of the backbone as the analysis template. The spin system is used to



Dr. Weber showed NMR data from the negative regulatory domain of p53, and also explained that this type of analysis can show where a drug might bind, and where H-bonding could occur. In addition to NOE experiments, the team also performed NOESY experiments, which incorporates spectroscopy into the analysis. Data displayed showed what was near in space relative to a desired point. Greater than 2400 NOE data was correlated to get a high resolution structure; however, the C-terminus of S100B was not well defined. One reason for this could be human error, or the C-terminus could be dynamic in nature. After additional experimentation, using 4-D NOESY and the overall rotational diffusion, the researchers found the C-terminus to indeed be a dynamic structure. In addition, this area of the S100B protein is precisely where p53 binds. With all this information in hand, Dr. Weber and his group developed a pictorial summary of what was occurring between S100B and p53. S100B and Ca^{2+} bind in a way that opens the complex sufficiently to allow p53 to fit (rather high affinity). This action reduces levels of p53, thereby inhibiting p53 transcription activation. S100B sterically blocks sites of phosphorylation and acetylation on p53 that are important for transcription activation. However, there is a classic feedback loop that is activated when S100B levels are elevated. This aspect requires additional research, but Dr. Weber did note that S100B- Ca^{2+} -p53 complex is highly regulated. Regulation depends on phosphorylation, cell-cycle, and Ca^{2+} -dependent structural conformational effects.

In summary, Dr. Weber noted future research projects, including additional multidimensional NMR studies, and therapeutic binding analysis. After his talk, Dr. Weber acknowledged his research team and financial sponsors, answered many questions. The meeting was adjourned at 8:55 PM. Respectfully Submitted, Tara S. Baney, Secretary, LVACS, 25-January-2003

*Post-meeting Secretary's note: I found some helpful information from the National Academy Press text Protein and Amino Acids, dated 1999. Use at your own discretion. Viewing chapter 5, "The Energy Costs of Protein Metabolism: Lean and Mean on Uncle Sam's Team" by Dennis M. Bier (pages 109-119), Dr. Bier writes: "How protein got its name is an interesting story (Hartley, 1951). The traditional credit for coining the word "protein" goes to the Dutch chemist Gerardus Johannes Mulder, who in an article published in *the Bulletin des Sciences Physiques et Naturelles en Neerlande* on July 30, 1838, stated (in French) that this material was the essential general principle of all of the constituents of the animal body and defined it by the Greek word "proteus," which he translated in Latin to "primarius," that is, the primary constituent of the body (Hartley, 1951). The interesting part of the story is that Mulder appears to have taken the term directly from Swedish chemist Jac Berzelius, who, on July 10, sent Mulder a letter in which Berzelius suggested the name "protein." Besides the apparent use of the new term without proper attribution, was the situation of a Dutch chemist, writing in a Dutch journal, defining a new word in French that was derived from Greek, and then qualifying its meaning in Latin! Further, considering that this episode took place 160 years ago, not only was the mail a lot faster, but also the publication time was substantially shorter than it is today, since the entire story took place in a period of about 3 weeks!"

This Month in the History of Chemistry:¹

February 2: *Leaded gasoline first marketed in the US in Dayton, OH, 1923. Thomas Midgley, Jr., of General Motors Research labs added tetraethyllead to gasoline.

February 4: *Joseph Goldberger begins the experiment that demonstrates that pellagra is a dietary disease, 1915.

*John Jacob Livingood made radium E (210Bi) by bombarding common bismuth with deuterons, 1936, the first synthesis of a radioactive substance in the US.

February 6: *Clemens Winkler, in the course of analyzing a mineral, discovered element (germanium, Ge, element 32) in 1886, consistent with predictions by J. A. R. Newlands and Dmitrii Mendeleev.

February 8: *Robert Holton announces total synthesis of taxol, an important cancer drug, 1994.

February 9: *Californium (Cf, element 98) discovered by (left to right) Kenneth Street, Jr., Stanley G. Thompson, Glenn T. Seaborg, and Albert Ghiorso using ion-exchange chromatography at University of California, Berkeley, 1950.

February 11: *Alwin Mittasch and Christian Schneider filed US patent (1914) application for catalytic production of methanol from carbon monoxide and hydrogen.

February 14: *Lawrencium (Lr, element 103) was produced in 1961 by Torbjorn Sikkeland, Albert Ghiorso, and Almon Larsh and Robert Latimer, at University of California, Berkeley.

*Dennis Searle and E. M. Skillings found borax and other soluble salts at San Bernardino, CA, 1873.

February 16: *Synthesis of diamond by F. P. Bundy, H. T. Hall, H. M. Strong and R. H. Wentoff at General Electric Research Laboratories announced in 1955.

February 18: *Frederick Soddy introduced the term "isotopic" (meaning "same place") for elements which share the same place in the periodic table in 1913.

February 19: *One atom of mendelevium (Md, element 101) was produced by Gregory R. Choppin, Glenn Seaborg, Bernard G. Harvey, and Albert Ghiorso in 1955 by bombarding a billion atoms of ²⁵³Es with helium.

February 21: *Edwin Land demonstrates Polaroid camera to optical society meeting, 1947.

February 22: *Friedrich Wöhler wrote a letter to J. J. Berzelius that he had synthesized urea, an early synthesis of an organic compound from inorganic materials, 1828.

February 23: *First organizational meeting of the Chemical Society of London, 1841.

*Charles Hall first produced electrolytic aluminum in 1886.

*Thomas Midgley, Jr., received US patent number 1,573,846 for tetraethyllead as an anti-knock agent in gasoline, 1926.

*Glenn Theodore Seaborg and coworkers chemically identified plutonium (Pu, element 94) at Univ. Cal., Berkeley, 1941.

February 24: *First atom of element 107, eventually named Bohrium (Bh) was observed at GSI Laboratories, Darmstadt,

Germany in 1981.

February 27: *James Chadwick's note announcing the possible discovery of the neutron published in Nature, 1932.

February 28: *Edward Goodrich Acheson receives US patent number 492,767 for production of artificial silicon carbide("Carborundum"), 1893.

Advertising/Article Policy

All articles of interest to LVACS members including local news and meeting details will be printed on a priority basis over ad copy. All ads for job openings and seminars with free admission of interest to LVACS members will be printed free as space is available. All ads for goods or services available at a cost will be printed for a fee. Please contact the editor for the fee structure. The editor reserves the right to reject inappropriate copy. All article copy must be submitted 5 weeks prior to the meeting date. Electronic format (ms word, word perfect email or simple text) is preferred but not required. Information can be emailed, posted or faxed to the editor. Images can be submitted electronically in either gif, jpg, tiff, or bmp format. Images submitted as hardcopy may be scanned and compressed for insertion. The editor reserves the right to make minor changes to copy in the interest of space prior to publication. Significant changes will be communicated to the author before print.

Article/Copy Submission Guidelines:

Please address all correspondence concerning this publication to the editor.

T. Michelle Jones-Wilson
East Stroudsburg University
Dept. of Chemistry
200 Prospect Street
East Stroudsburg, PA 18301
Phone: 570-422-3446
Email: mjwilson@po-box.esu.edu
Fax: 570-422-3908

Question of the Month

Who was the first woman chemistry professor at Harvard?

Come to the February Meeting for the Answer