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NESACS

THE NUCLEUS

February 2001 *Vol. LXXIX, No. 6*

Monthly Meeting

Jeffrey I. Steinfeld on the Environmental Sciences- Instrumentation link

50-Year Member Bio

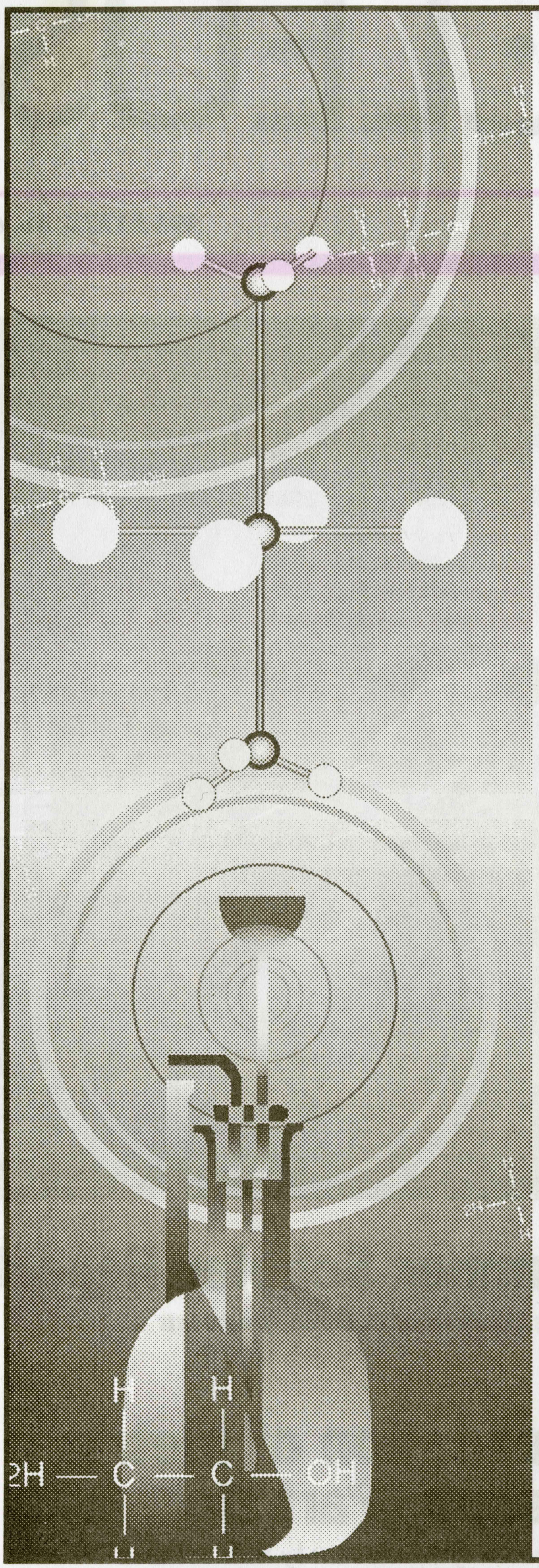
B.J. Ransil's biography and Robert S. Mulliken

Summer Scholar Report

On the synthesis of Fullerene fragments

Foundation of Metric System, Part II

Conclusion of the account by W.A. Smeaton



Call for Papers

❖ Deadline – March 31, 2001 ❖

2001 Eastern Analytical Symposium
Sept. 30 – Oct. 4, 2001
Atlantic City, NJ

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Regardless of the method of submission, please include the following information on your abstract:

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- Your preference for oral or poster format
- Approximately six keywords that can be used to categorize the subject matter of your presentation

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Cover: *Jeffrey I. Steinfeld in Wolong, Szechuan, May 1999*

Deadlines: *April 2001 issue: February 23, 2001*
May 2001 issue: March 16, 2001

THE NUCLEUS

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Editor:	Arno Heyn, 21 Alexander Rd., Newton, MA 02461, Tel: 617-969-5712, FAX: 617-527-2032; e-mail:aheyn1@juno.com
Associate Editor:	Myron S. Simon, 20 Somerset Rd., W. Newton, MA 02465, Tel: 617-332-5273
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Calendar Coordinator:	Donald O. Rickter, e-mail: 72133.3015@compuserve.com
Proofreaders:	E. Joseph Billo, Donald O. Rickter, M.S. Simon
Webpage:	Webmaster: Frank R. Gorga, fgorga@bridgew.edu Asst. Webmasters: Terry Brush, tbrush@medione.net Kurt Heinselman, heinslmn@earthlink.net

Directions

Since the MIT Lot is likely to be pretty full and on-street parking is tight, use the T, if possible.

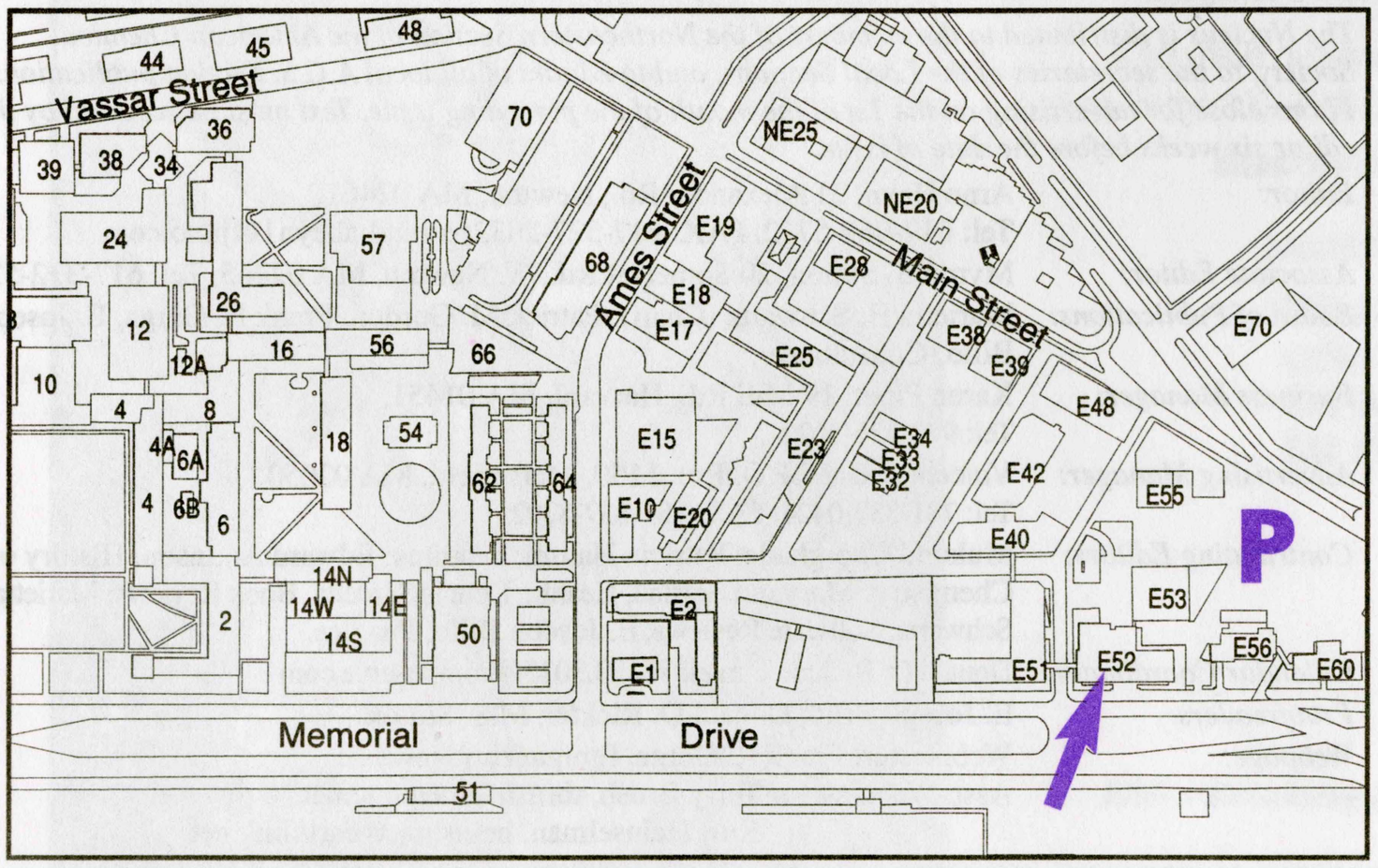
Red Line: Exit at Kendall, walk towards Boston on Main St., turn right into Wadsworth St. The large building on the left at the corner of Wadsworth and Memorial Drive is the Sloan Ctr. (less than 500 feet from the T).

Driving:

From Down-town Boston:* Cross to Cambridge on the Longfellow Bridge and at the end of the bridge take the right turns into Memorial Drive (westbound). Take the first right, into Wadsworth St. and at the end of Wadsworth Street, turn right into Main Street. The entrance to the MIT Sloan parking lot is 1/2 block on the right. Parking free after 3:30 pm.

From Back Bay, Brookline, etc.: Take Storrow Drive to the Cambridge St. Exit, stay left and cross the Charles River on Longfellow Bridge, follow * above.

From Cambridge: Take Main St. eastbound. The MIT Sloan parking lot is on the right shortly after the Kendall Square T-stop, just beyond Wadsworth St. Parking free after 3:30 pm. ◇



Phyllis A. Brauner 1916-2000

Phyllis Ambler Brauner died on December 23, 2000 following a heart attack and after succumbing to multiple infections.

She has been one of the prime moving forces in our Section: A member of many committees, NESACS Chairman in 1974, Henry A. Hill awardee in 1985, long time Councilor, and even from her sickbed she helped in organizing the successful November 5,2000 National Chemistry Week Event at the Museum of Science.

With her enthusiasm and ability to organize she will be sorely missed.

A more complete account will appear in the next issue. ◇

Board of Directors

Notes of Meeting of November 9, 2000

NOTE: Board Meetings are held on the monthly meeting day at 4:30 p.m. Section members are invited to attend

Officers' Reports:

Chair: T. Frigo reported for D. Lewis that the National Chemistry Week event at the Museum of Science was a huge success. After taking the chair, D. Lewis announced that the 2001 Budget Committee meeting will be on December 8, 2000, with all budget requests to be submitted to the Treasurer by that date.

2000 Annual Reports: Are to be submitted in electronic form and committee reports should be formatted accordingly.

E.A. Hopkins has submitted her resignation as Councilor effective Jan. 1, 2001..In accordance with the provisions in the Constitution, Alt. Councilor T. Light was elected to fill the vacancy until a Councilor could be elected to fill the remainder of the term, ending 12/31/2003, and D. Wierda was elected to fill the vacancy created by T. Light's move to Councilor. It was MOVED and VOTED by acclamation to send a Special Acknowledgement of the Board to Dr. Hopkins in recognition of her 30 years of service as a Councilor and her Distinguished and Exceptional Service to NESACS.

Chair-Elect: T. Frigo stated that the

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Monthly Meeting

The 822nd Meeting of the Northeastern Section of the American Chemical Society

Thursday, February 8, 2001

M.I.T. Faculty Club, 6th floor, 50 Memorial Drive, Cambridge, MA

5:30 pm Social Hour; a table of Career Services Literature and Aids will be available

6:30 pm Dinner

8:00 pm Evening Meeting, Dr. Timothy Frigo, presiding

Prof. Jeffrey I. Steinfeld, M.I.T. *Challenges in Environmental Science: Instrumentation for Measurement and Technology for Sustainability*

Dinner reservations should be made no later than noon, February 1, 2001. Please call or fax Marilou Cashman at (800) 872-2054 or e-mail at MCash0953@aol.com. Reservations not cancelled at least 24 hours in advance must be paid. Members, $25.00; Non-members, $28.00; Retirees, $15.00; Students, $ 8.00.

THE PUBLIC IS INVITED.

Anyone who needs special services or transportation, please call Marilou Cashman a few days in advance so that suitable arrangements can be made.

Free Parking: (after 3:30 pm) in the MIT lot off Main St. behind the Sloan Building. Also free meter parking (after 6:00 pm) on Memorial Drive and side streets.

Next Meeting: *March 8, 2001 at ArQule, 19 Presidential Way, Woburn, MA. Joint Meeting with the Am. Inst. of Chem. Eng. and the Int'l. Soc. for Pharmaceut. Eng.; Elliot Hillback, Genzyme, Inc., on the impact of new technologies on bioethics.*

Biography

Jeffrey R. Steinfeld

Professor of Chemistry, M.I.T. Received B.S. degree in Chemistry at M.I.T. in 1962, and Ph.D. in physical chemistry (with Prof. William Klemperer) in 1965. Postdoctoral Fellow with Sir George Porter at the University of Sheffield (U.K.), joined the M.I.T. Chemistry Department in 1966.

Research specialties include molecular spectroscopy, molecular energy transfer, and laser applications to chemistry, including optical methods for remote sensing and atmospheric monitoring. Currently ca. 180 research publications on these topics. Author of textbooks on molecular spectroscopy and chemical kinetics. Co-editor of *Spectrochimica Acta, Part A,* 1983 - 1988; member of International Advisory Board, *Progress in Natural Science: Communications from State Key Laboratories in China.*

Visiting appointments have included professorships at the University of California, Berkeley and University of Leiden, Netherlands, University of Southern California [1981], Joint Institute of Laboratory Astrophysics, Boulder, Colo. [1983], Université de Bourgogne, Dijon, France [1991], and University of Sydney, Australia [2000]. Served as Project Specialist for World Bank Chinese Provincial Universities Development Project [Hebei University, Baoding, Hebei, P.R.C., 1988]. Co-chair of "Symposium on Future Trends in Spectroscopy" at the Vatican in 1989.

Present research and teaching emphasis is on atmospheric chemistry and introducing concepts of sustainability and environmental responsibility across the curriculum. Current activities in this area include serving as co-Director of the Program on Environmental Education and Research at M.I.T. and as Chair of the American Chemical Society's Committee on Environmental Improvement. Received 1999 ACS Director's Award for Advancing ACS Public Policy in Environment, for work to encourage the use of sound science in global climate change policy. ◇

Abstract

Safeguarding the health of our environment is essential for maintaining the delicate balance of life on Earth. Our well-being is inextricably linked to the well-being of the planet's ecosystems. Mounting scientific evidence, however, is signaling significant disturbance of these systems across local, regional, and global scales. It is our responsibility as scientists to characterize the nature and extent of these critical problems, and thereby help society to formulate an appropriate set of corrective and preventive actions to alleviate the growing stress on our environment.

The ability to measure accurately a wide range of chemical and biological species, physical parameters, and trends in these quantities, is an essential requirement for understanding the environment. Communicating this understanding to the scientific community, to policymakers, and to the public is also essential if this information is to be appropriately interpreted and used. Among the challenges posed by environmental measurements are:

(i) the environment is highly undersampled, that is, data are sparse with respect to species identification, spatial coverage, and temporal continuity;

(ii) the desired information is often a small signal embedded in a high degree of natural variability;

(iii) the sample environment is not well

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Board of Directors

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December meeting will be a joint meeting with the Medicinal Chemistry Group on Wednesday, December 13 at MIT on *Mechanistic approaches to Pharmacotherapy in Oncology.* With Drs. Olivier Laverne (Institut Beaufour, Les Ulis, France), Ian Bell (Merck, West Point, PA), and Dr. Michael Su (Vertex Pharmaceuticals, Cambridge, MA)

Chair-Elect designate: M. Hoffman reported that the March 8, 2001 meeting will be held at ArQule, Inc. in Woburn, MA.

Secretary: The minutes of the October 12, 2000 meeting were APPROVED.

Treasurer: J. Piper presented the October report. The report was ACCEPTED.

Archivist: M. Simon announced that Regis College will again house the archives, to be located in a space in their library. The Regis contact is Sara Barnett, Assoc. Academic Dean.

Standing Committees:

Bd. Of Publications: J. Billo reported that the new NESACS.ORG website is up and running.

Chemistry Education: R. Tanner reported that the Connections to Chemistry event in October was a great success (report appended to minutes [and to be in the in the January 2001 *NUCLEUS, ed.*]).

Sixteen ACS Scholars will be guests at this evening's dinner meeting.

Grants in Aid have been awarded to students at Stonehill and Harvard for the 2001 San Diego ACS Meeting.

Undergraduate Day was held on November 3, 2000 at Boston University, 125 students attending.

D. Lewis expressed the Chair's and the Board's gratitude to R. Tanner and M. Hoffman for organizing these successful events.

Local Arrangements: M. Burgess stated that her goal is to have the Arrangements Table staffed by 3 people, including local graduate/undergraduate students and members of YCC.

Richards Medal: F. Greene reported that the original 12 in. plate for the medal has been obtained on loan from the Dallin family so that a mold could be made for NESACS use.

New steel dies are expected to be finished shortly. The mold is owned by NESACS, as will be the steel dies. The eventual location of the dies is under discussion.

It will be more economical to have several medals produced at the same time. Is the Board willing to approve funds for this? F. Greene will present a cost breakdown.

It was MOVED and PASSED by acclamation to express the gratitude of the Board to F. Greene for his labors on behalf of the Richards Medal.

Other Committees:

Continuing Education: A. Viola, by written report, stated that the two-day ACS Short Course *Asymmetric Synthesis* will be held Nov. 30/Dec. 1, 2000. Preregistrations assured that the course can be given. He reported orally that there are currently 14 registrants, thus the event is expected to have a positive cash balance.

Health and Safety: J. Kaufman announced that the Laboratory Safety Training Seminar for students was held November 4 at Boston University. He is looking for additional academic hosts for this seminar.

Natl. Chemistry Week: D. Lewis reported that, in order to make the Museum of Science event successful, there was a radio ad on WCRB during the Children's Concert Hour, and the Museum of Science advertised the event. P. Brauner was unable to attend, but was kept informed. The event was a joint effort of NESACS, YCC and the Museum of Science.

During the event, seven YCC members organized a Connections to Chemistry Passport program, with participants receiving Minimoles. The YCC members also identified Museum exhibits that were relevant to chemistry. Demonstrations were given throughout the day both by museum staff and H.S. teacher volunteers. These demonstrations will continue throughout November. M. Chen attended the NESACS table at the museum.

Medicinal Chemistry: T. Frigo reported that MCG is discussing the establishment of a Medicinal Chemistry Award to recognize a scientist on the national level at every December Meeting which is held jointly with the NESACS monthly meeting. P. Gordon is chairing this MCG Award Committee. Guidelines for the award are to be established and solicitation of funds for the award is being explored.

Old Business: none

New Business: none

From the minutes of M. Singer ◇

Abstract

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controlled, but is a complex mixture of components in a highly variable matrix;

(iv) information is required not only on ambient species concentrations or populations, but on identification of sources and sinks for these species and fluxes between these reservoirs;

(v) the stakes are high, since decisions and regulatory enforcement based on the measurement results may cost – or preserve – billions of dollars, many human lives, or the continued existence of entire species.

New discoveries in instrumentation, information systems, and complex systems analysis are beginning to provide us with the tools which we need to carry out and properly interpret these measurements. At a recent NSF-sponsored Workshop on Instrumentation for Environmental Science, a number of strategies were evaluated for in situ measurement and remote sensing to achieve these objectives. Some examples of successful measurement strategies, and areas in which improvement is needed, will be described. While identifying the nature and severity of a threat to the environment is the essential first step, simply doing so is inadequate unless a suitable strategy can be developed for alleviating the problem. In this context, the emerging Green Chemistry approach offers a methodology for developing such strategies. ◇

50-year Member Biographical Sketch

Bernard J. Ransil, PhD, MD

We had asked 50-year members who were being recognized at our October 13, 2000 meeting to submit some biographic material, if they were so inclined. It also so happened, that we were publishing the manuscript of Dr. David L. Adams on Robert S. Mulliken, a Newburyport Native, in the October 2000 issue. I had laid the several biographical notes from 50-year members aside until going through them in detail for publishing some of them as I was getting material together for this issue. Imagine my surprise to come across this extensive biography of one of our 50-year members, Dr. Bernard J. Ransil, who was at the very source of the molecular orbital work being done by Robert S. Mulliken and his associates.[ed.]

Bernard J. Ransil received his initial chemistry education at Duquesne University, Pittsburgh, PA from a dedicated teaching faculty headed up by Tobias Dunkelberger, who motivated many of the students to join the ACS at an early age, hence this biosketch. Graduating Magna Cum Laude with the Chemistry Gold Medal, Dr. Ransil pursued further studies in Physical Chemistry as a Teaching and Research Assistant at The Catholic University of America, Washington, DC (having also been accepted at MIT, Wisconsin and Notre Dame) because of its exceptional depth at the time in Physical Chemistry, which included F. O. Rice (Free Radicals, Chemistry Chairman), Karl Herzfeld (Chemical Physics. Physics Chairman), Keith Laidler (Chemical Kinetics), Walter J. Moore (Physical Chemistry) and Gilbert Castellan (Physical Chemistry), the latter two being authors of widely-adopted standard texts for several decades.

He wrote his PhD thesis (1) under Virginia Griffing on "The Molecular Orbital Treatment of Simple Open-Shell Molecular Systems", specifically, the H3 linear complex, using the LCAO-MO-SCF formulation that had been published by Clemens C. J. Roothaan in 1951 (2); which he programmed for an analogue computer built by Joseph F. Mulligan SJ as a Master's thesis (long before computers were regarded as research/ teaching tools) from a design by Roothaan (a PhD student of Robert S. Mulliken at the University of Chicago) while he was Instructor in Physics (through the good-offices of Maria Mayer) under Karl Herzfeld at Catholic University, but who by this time was a member of Robert S. Mulliken's Laboratory of Molecular Structure and Spectra (LMSS), and Associate Professor of Physics at the University of Chicago.

Having completed his PhD requirements by October, 1955, and declining an invitation to head up a nascent Department of Chemistry at St. Mary's University in San Antonio, Texas, Ransil was among those awarded the first National Research Council-National Science Foundation Fellowships at the National Bureau of Standards (NBS, now The National Institute of Standards and Technology) where he worked in the Thermodynamics Section directed by Charles W. Beckett, under the mentorship of Abraham Friedman (Thermodynamics) and Irwin Oppenheim (Statistical Mechanics). At that time, the NBS was one of the few research facilities in the US boasting a digital computer (the Standards Eastern Automatic Computer, or SEAC)—a vacuum tube affair occupying a 20-room mansion, headed up by the redoubtable Milton Abramowitz and his invaluable assistant, Irene Stegun. Motivated by Dr. Beckett's futuristic wisdom and advice ("If there's one thing you should learn this year, Bernie, it's the computer."), Ransil teamed up with two SEAC staff members, programmer Phil Walsh and mathematician Emilie Haynsworth, and learned the principles of research computing, if not programming language (which in those days was machine language without compilers) by programming the H3 molecule in six-figure precision and obtaining agreement with the three-figure precision of his thesis performed on the analogue computer. Ambitious experimental and theoretical projects under Friedman's and Oppenheim's direction, extending work on the isotope effect, yielded precedence to this vital learning experience and were not completed.

At this stage, the spring of 1956, Ransil realized that a pilot model for computing the electronic structure of small molecules from first principles, using Roothaan's LCAO-MO-SCF formulation and Slater orbitals, had been achieved and successfully tested, but that it now needed to be applied to a representative range of simple molecules, for which experimental values of chemical and physical properties were available, such as the diatomic homopolars, hydrides and heteropolars of the first row of the Periodic Table. He also realized this could not be done at the Bureau or any academic chemistry department to his knowledge because it required state-of-art computing and support staff, whereas the pervasive attitude in many if not most academic departments regarding computers at the time was, as a renowned, illustriously named physicist of the time remarked one day in his most infallible manner, "If it requires a computer, Bernie, it's not chemistry or physics", an attitude that continued to prevail in many academic departments into the 70s, to the disservice of computer based science.

At the advice of his thesis director, Virginia Griffing, Ransil wrote Professor Mulliken at Chicago, informing him of these developments at the Bureau, and inquiring whether there might be any interest at Chicago in writing a computer program that would compute selected chemical and physi-

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cal properties for selected diatomic molecules of the first rows, using his MO theory, the Roothaan algorithm and Slater orbitals. There not only was such interest, Ransil learned, progress was already being made on programming the difficult 3- and 4-center integrals by several of Roothaan's students.

Mulliken invited Ransil to a luncheon meeting at the Cosmos Club in Washington, DC which established that both men were on the same wave length, not only about what ought to be done, but how it ought to be done. Ransil was quickly recruited, arriving at LMSS in the fall of 1956 to assume leadership of the Diatomic Molecule Project at LMSS, while Roothaan departed for Europe on a Guggenheim Fellowship, and Mulliken, not a computer person, continued his work on the experimental spectroscopic development of the MO theory. On Roothaan's return, the team consisted of Professors Mulliken and Roothaan, and Dr. Ransil, jocularly dubbed "Big Boss", "Little Boss" and "Straw Boss" by the remaining members, three superlative graduate students possessed of a great sense of humor as well as talent: Douglas McLean (Australian), Andrew Weiss (American) and Megumu Yoshimine (Japanese). The effort was funded by the Office of Scientific Research, Air Force Cambridge Research Center, Office of Ordnance Research, Office of Naval Research, Wright Air Development Center and the National Science Foundation, with Dr. Ransil as a Principal Investigator on one of the grants together with Mulliken and/or Roothaan. The team was given free access to off-hours computing at the Wright Patterson Air Force Base, Dayton, Ohio.

A brief history of this effort and its outcome is found in Mulliken's scientific memoirs (3). Others working in a similar vein elsewhere during that decade were Robert Nesbet at Boston University, John Slater and his group at MIT, Coulson and Barnett at Oxford, and Kotani and his group in Japan. John Pople was also active, in collaboration with Nesbet, but had not yet formed his group at Carnegie-Mellon.

Programming and debugging took approximately two and one-half years. When the three graduate students moved on to thesis work under Roothaan, Ransil was joined by Serafin Fraga y Sanchez, a Juan March Fund Fellow from Spain, to "milk the program", compile and publish the results, with the first two papers published in the Reviews of Modern Physics, one of which ultimately became a Citation Classic (4). In all, ten papers were published between 1960 and 1962, presenting wave functions, potential curves, calculated values of spectroscopic constants and other selected chemical and physical properties of selected first row diatomic molecules.

Fraga moved on to a faculty position at the University of Alberta, Edmonton, the graduate students

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earned advanced degrees and moved on to research positions at NBS and IBM. And Paul E. Cade (now at the U. of Massachusetts) was recruited from Hirschfelder's group at Wisconsin to take over the diatomic molecule project from Ransil, and implement the projected extended orbital approximation. Meanwhile, Ransil had regretfully turned down a unique joint-appointment in Chemistry and Physics at MIT, initiated by Professor John Slater, in order to attend medical school at the University of Chicago (now the Pritzker School of Medicine) and acquire the broader scientific perspective toward which the physical sciences appeared to be heading.

On completing medical school at the U. of Chicago Medical School, Dr. Ransil interned at the U. of California Torrance General Hospital during which he applied for, and was awarded, a Guggenheim Fellowship for the year 1965-66, during the spring of which he presented the results of the Diatomic Molecule Project, now including Cade's extended orbital results, to quantum chemistry centers at Oxford (Coulson), Cambridge (Longuet-Higgins), Uppsala (Lowdin and his group), Stockholm (Fischer-Hjalmars), and Paris (the Pullman and Daudel groups). He returned to the US in July, 1966 to join the Research Faculty of the Thorndike Memorial Laboratory at Boston City Hospital, at that time the US's pre-eminent clinical research center (but now a victim of Boston politics and urban renewal) under the directorship of Max Finland. In September, Mulliken was awarded the Nobel Prize in Chemistry for his seminal contributions to molecular science, including the initial postulation (with Friedrich Hund, who, he strongly felt, should have shared the prize (3)), and subsequent development of the MO theory, which provides the theoretical basis for modern chemistry; and, in its computer formulation, as developed by Roothaan for computational chemistry.

In 1967 and 1972, although by now immersed in medical research projects, Ransil published two articles with John J. Sinai (Department of Physics, U. of Louisville) on the charge density analysis of the chemical bond, which were followed in 1980 by a final paper in this field which provided a rigorous statistical analysis of the reliability of quantum-mechanically calculated observables available at that time (5). In the meantime, molecular calculations had evolved in Gaussian formulation, notably at Carnegie Mellon under John Pople, who received a Nobel Prize in 1998 for his contributions to computational chemistry. During the Diatomic Molecule Decade at LMSS, Enrico Clementi, a frequent visitor, had urged the adoption of Gaussians, but Roothaan had rejected their use in favor of the more computationally difficult Slater orbitals because of improper behavior at the cusp, a tech-

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nical flaw that was subsequently overcome with the advent of high-performance computers, permitting the large-scale molecular calculations possible today.

Ransil visited Mulliken annually in Chicago during summer vacations to provide a critical reading of Mulliken's autobiography (3), the writing of which had been suggested to him by Professor Thomas S. Kuhn, Professor Emeritus of Linguistics and Philosophy at MIT who by this time was deeply involved in the history of science. To paraphrase Kuhn's argument, as relayed to Ransil by Mulliken, "No one else knows better than you, Robert, the history of the evolution of molecular orbital theory. It is your obligation as a scientist to record it for posterity." A series of small strokes, affecting his lower extremities necessitated Mulliken's moving from his spacious lake-view apartment near the Chicago campus to live with, and be cared for by his daughter and son-in-law, Lucia and John Heard in Arlington, Virginia. By this time Ransil had assumed responsibility for editing the manuscript and finding a publisher, the latter of which proved to be a long and discouraging task. It was turned down successively by the University presses of Chicago (who had taken a loss on Mulliken's massive Festschrift) Oxford and Cambridge, and the major American publishers of trade books. In the meantime, Professor Mulliken died (October 31, 1986) and the search for a publisher continued.

One day Ransil received a long-distance call from Heidelberg; it was an editor from Springer-Verlag; he had heard about the manuscript via the grapevine and wanted to read it. It was promptly shipped Air Mail Express. Several days later, the editor called back, "We would be honored to publish Professor Mulliken's memoirs." The book was published in 1989, bringing to a close a chapter in Ransil's life that is indelibly imprinted on his protoplasm.

Although Ransil was prevented from attending because of an east coast blizzard, he was informed that, during the opening session of The 27th Quantum Chemistry Symposium at Sanibel in 1993, which was a Special Symposium on Atomic, Molecular and Condensed Matter Theory, Roothaan, Ransil and other participants comprising the Diatomic Molecule Project and LMSS were recognized and honored; and, in passing, referred to as the "Grandfathers of Computational Chemistry". (Recent attempts by BJR to document the source of this sobriquet, however, could not establish attribution.) Ransil's introductory paper presenting a brief history of that period (undelivered because lost during faxing), was published in the proceedings (6).

Having thus been relegated to honorary, if putative, "grandfatherhood" at this stage in his bachelor existence, the writer begs the reader's indulgence if he gazes somewhat dotingly (as grandfathers allegedly do) on the accomplishments of contemporary computational chemistry reported almost weekly in The C&E News, that could only be speculated upon four decades ago; while recalling, not without humor, eschewing rancor, the ups and the downs, the successes and frustrations ("And how are the number crunchers today?", "If it needs a computer, it isn't science.") that characterized its long, difficult and ridiculed gestation. Yet, who at the same time realizes: It was a glorious experience while it was happening, despite the nay sayers who later became self-proclaimed prophets of the new era; an experience of which he was grateful to be so unexpectedly and unpredictably a part, not only for what was accomplished in that decade for the first time (the first computer outputs are still extant) despite conventional wisdom, but also for the colleagueship and friendship enjoyed over those years with those markedly disparate yet complementary Giants of Science in their own right, whom the writer regards as the seminal architects and enablers of modern molecular science, Robert S. Mulliken and Clemens C. J. Roothaan; the latter of whose fundamental contribution to computational chemistry, in the writer's opinion, has yet to be universally appreciated and

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appropriately recognized. And whose contribution to computational science continues as, in his "retirement", he writes the mathematical software for the new generation of chips, the successor-to-Pentium, Hewlett-Packard/Intel's Itanium, using unprecedented vector-based algorithms of his own devising which permit a 5-fold increase in computational speed.

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Prepared by Bernard J. Ransil, PhD, MD, Associate Professor of Medicine (ret.), Department of Medicine, Harvard Medical School and the Beth Israel Hospital; Research Consultant, Department of Neurology, Beth Israel Deaconess Medical Center, Boston, Massachusetts; for the American Chemical Society on the occasion of 50 years of membership. October 6, 2000

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The Foundation of the Metric System in France in the 1790s*

Part II

By William A. Smeaton, Ely, Cambridgeshire, United Kingdom

On 22nd July 1799 the definitive standards of the metric system, the platinum meter and the platinum kilogram, were ceremonially deposited in the French National Archives (1), and on 10th December 1799 a law was passed confirming their status as the only legal standards for measuring length and mass in France (2). The accurate determination of these standards had occupied a number of outstanding French scientists for ten years, using elaborate equipment partly made from platinum by Étienne Lenoir, a skilled instrument maker. This work had been undertaken after more than a century of discussion. The events surrounding this momentous occasion which now affects all our everyday lives are described here.

In Part I the confusion of systems of measurement in the several European countries was described. By 1789 both the British Parliament and the US Congress were considering decimal systems of measurement. While the US adopted decimal units for currency, efforts by Thomas Jefferson, who was Secretary of State at the time, to also introduce decimal units for length and weight were not adopted by Congress.

In France, however, in the spirit of overthrowing the old, the French Assembly in 1790 acted to set up metric standards of length based on the length of the quadrant of the earth between the north pole and the equator along the meridian going through Paris. The 1/10,000,000 of this was to be the basis of the "meter". To measure this quadrant, the distance from Dunkirk to near Barcelona (both on the same meridian) was laboriously measured on the ground by means of establishing base lines, supplemented by triangulation. Precisely measured platinum rods (of about 12' length) were used for establishing the base lines, and, by means of astronomical observations, the length of the quadrant.

The means for correcting for temperature, etc. were described.

The New System of Measurements

Lenoir made a provisional standard meter in brass and designed a machine for the manufacture of 660 accurate copies for distribution to all parts of France. In 1794 the government published a book explaining the new system and giving conversion tables for the old and new units (19). This was reprinted in several provincial towns, in some of which conversion tables for local units were also published. It was decreed that the use of the metric units should be compulsory from August 1794, but this was not in fact achieved until many years later.

Decimal currency, introduced as part of the metric system, was accepted more rapidly, as it was based on the 'franc', a coin containing five grams of silver which was almost equal in value to the 'livre' of the old regime. Circular measurement was also included in the new system, the right angle being divided into 100 and the circle into 400 'grades', with decimal sub-divisions. Lenoir engraved this scale on three of the surveyors' repeating circles.

The division of the day into 10

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Note: Several figures have been omitted.

Metric System

Continued from page 11

hours instead of 24 received hardly any support and was soon abandoned, but the Republican calendar, with a year of 12 months, each month being made up of three 'decades' of 10 days with 5 additional days at the end (6 in leap years), remained in use until 1805.

Preparation of the definitive standards was delayed not only by wartime problems affecting the surveyors but also by political developments in Paris. In July 1793 the Academy of Sciences was suppressed, along with all other organizations that had received funds from the royal government. The eleven scientists working on the new units were allowed to continue, but they suffered a severe blow in November 1793 when Lavoisier, who had been determining the density of water in experiments conducted with the physicist René Just Haüy (1743-1822), was arrested together with all his former colleagues in the Tax Farm, the unpopular private corporation that collected certain taxes under the old regime. By government decree Lavoisier was removed from the Commission of Weights and Measures, as were Borda, Delambre and two other members with links to the old regime (20). On 8 May 1794 Lavoisier and nearly thirty other Tax Farmers were guillotined. He was one of about ten academicians who suffered violent deaths during the Revolution (21).

When the Commission eventually completed its work in 1798 the length of the meter was found to be 3 feet 11.296 lines, slightly shorter than the provisional value of 3 feet 11.44 lines. The observations and calculations of the Commission were checked by a group of foreign scientists who spent several months in Paris at the invitation of the French government, as it was hoped that the new system would be universally adopted. However, Europe was still at war, so only France's allies at the time and neutral countries were represented. These were: Spain, Denmark, the Netherlands, Switzerland and several Italian states. The absentees included Great Britain, Russia, Sweden, all the German states and the United States of America. Even so, the meeting has some claim to be regarded as the first international scientific conference (22). Lenoir made the definitive meter in platinum, and the platinum kilogram (a more useful standard than the gram) was made by Nicolas Fortin, another famous instrument maker. It is pleasing to note that they both took part in the ceremony when the standards were deposited in the National Archives — public recognition of the importance of skilled craftsmen in the progress of science.

Slow Adoption of the Metric System

The foreign representatives took accurate iron copies of the standards to their own countries, but there was little enthusiasm for the metric system and its international adoption proceeded very slowly in the nineteenth and twentieth centuries. In 1791 Charles Blagden, the secretary of the Royal Society, had told Sir Joseph Banks, the then president, that in his opinion the French academicians wished 'to divert the attention of the European public from the true amount of their proposal, which in fact is that their measurement of 9 or 10 degrees of a meridian in France shall be adopted as the universal standard' (23). It is possible that Blagden's sentiment was shared by other scientists outside France.

The National institute, the successor to the Academy of Sciences, decided to permit only metric measurements in its scientific publications, but even in France there was resistance to the metric system in commerce, and the old units were still widely used. In 1812 the Napoleonic government legalized a compromise system with units such as the 'common foot' and the 'common pound', equal to a third of a meter and half a kilogram, respectively. This gave rise to confusion with the old feet and pounds, and for a time the metric system was almost abandoned. It was not until 1840 that its use became compulsory — fifty years after the reform was initiated (25).

Lenoir's platinum meter, made in 1799, remained in use until replaced in 1878 by an international standard made of iridium-platinum supplied by George Matthey of London (24). The four measuring rods, which had made

Metric System

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the accurate determination of the meter possible, were returned from the Observatory to Lenoir's workshop after being inspected by the international commission, but in 1803 they were again taken to the Observatory.

It was decided that the first platinum meter, "No,1", which had been measured by Borda, should remain in the Observatory, but the others were used in 1823 for the triangulation of Switzerland and Alsace, again for a base line near the port of Brest, and finally in 1827 for a base line in southwest France near Dax, Borda's birthplace. In Dax there is now a museum commemorating the life and work of Borda.

The fifth rod, used in the pendulum experiment, was halved in length in 1806 for pendulum measurements by Jean Baptiste Biot and François Arago (26). The 1806 experiments were combined with an extension of the meridian survey from Barcelona to the Balearic Islands, and in 1817, after the end of the Napoleonic wars, Biot carried out similar work in Scotland and extended the meridian to Shetland, publishing the results in 1821 (27). However, he did not use Lenoir's rods for the later surveys.

In 1856, the first rod was compared with one made for the Spanish cartographers, but since then it has been preserved with the others at the Paris Observatory (where they are known as 'les règles de Borda'). They are the largest and most elaborate platinum instruments made in the eighteenth century and excellent examples of the results that can be achieved by the close collaboration of scientists and skilled craftsmen.

The story does not end there, for today the meter and the kilogram are a well accepted part of the daily life of most people. 'Le Système International d'Unités' is used for measurements by scientists worldwide, with the meter and the kilogram being two of the seven base SI units. From these seven fundamental units, all other units of measurement are derived.

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The Author

William A. Smeaton is Emeritus Reader in History of Science at the University of London. He formerly lectured in chemistry at the Northern Polytechnic and in history of science at University College London. His main interest is science in 18th century France. ◇

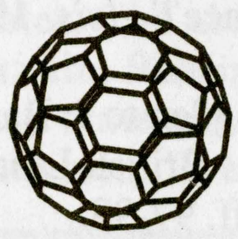
Summer Scholar Report

Synthetic Route Toward a C_{48} Fullerene Fragment

John Paul Amara* and Lawrence T. Scott, Boston College

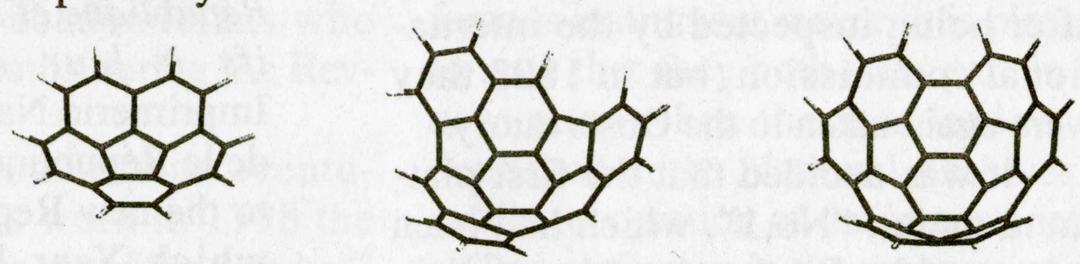
Introduction: In 1967, a large geodesic sphere, designed by the renowned architect R. Buckminster Fuller, graced the American Pavilion at the World Exposition in Montreal. Eighteen years later, H.W. Kroto, R.F. Curl, and R.E. Smalley discovered similar structures on a molecular scale.[1] The discovery of fullerenes, as these new geodesic molecules were named, was a landmark event in chemistry. Unlike the infinite lattice of tetrahedral sp^3 carbons in diamond, or the flat sheets of aromatic sp^2 carbons in graphite, fullerenes comprise finite networks of 5- and 6-membered carbon rings that form the shapes of hollow three-dimensional surfaces, closely approximating spheres. Their discovery triggered an explosion of research to find practical applications of fullerenes in the fields of medicine, fuels, and new materials, including superconductors.[2]

Buckminsterfullerene (**1**) was the first fullerene to be discovered. The molecule is comprised of sixty sp^2-hybridized carbon atoms assembled in an arrangement of fused pentagonal and hexagonal rings that form a shape identical to the seams on the surface of a soccer ball. Since the molecule is currently synthesized through the vaporization of graphite with an electric arc or a laser[2] knowledge regarding the mechanism of its formation is limited.[3] Research is underway to develop methods that would allow rational syntheses of this molecule and the higher fullerenes. The synthesis and study of bowl-shaped polyarenes that represent "fullerene fragments" serves as a proving ground for these new methods.



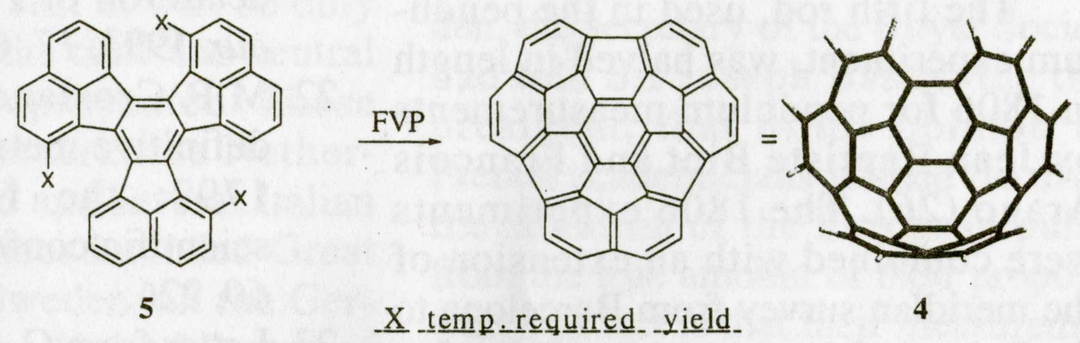
1

Through the use of flash vacuum pyrolysis (FVP), our laboratory has been successful in synthesizing a host of non-planar polycyclic aromatic hydrocarbons (PAHs) that map onto the surface of Buckminsterfullerene[4,5] In FVP, a compound is sublimed at moderate temperature and low pressure (≈0.05 mm Hg). The separated molecules then travel in the gas phase through a quartz tube inside a furnace where temperatures can reach 1250 °C.[6] Under these conditions sufficient energy is available to populate highly distorted conformations of the PAHs and to initiate radical cyclodehydrogenation reactions, which often result in the appropriate ring closures and form the desired fullerene fragments. These fullerene fragments are themselves of great interest because they possess shapes very similar to those of bowls. The insides of these "molecular bowls" could act as participants in yet to be discovered chemistry involving concave π-surfaces.[7] Fullerene fragments synthesized in our laboratory in this manner include: corannulene ($C_{20}H_{10}$, **2**)[8,9] the chiral $C_{30}H_{12}$ hemifullerene **3**,[10] and circumtrindene ($C_{36}H_{12}$, **4**).[11,12] These open geodesic polyarenes comprise 33%, 50%, and 60% of C_{60}, respectively.



2 **3** **4**

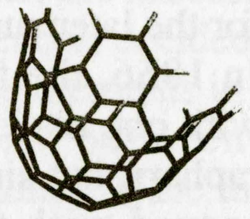
It is important to note that the yields of pyrolysis reactions involving unfunctionalized PAHs are generally extremely low, often less than 1%. The incorporation of halogen atoms (which serve as radical precursors in pyrolysis reactions), however, improves the yields of polyarene cyclizations dramatically. For example, FVP of decacyclene (**5a**, X=H) yields <1% of the desired product (**4**).[11] When X=Cl, on the other hand (**5b**), the pyrolysis yield improves to over 40% (Fig. 1).[12]



5 **4**

	X	temp. required	yield
5a	H	1200-1300 °C	0.6%
5b	Cl	1100 °C	40%

Figure 1. Cyclizations of aryl radicals generated by homolysis of carbon-halogen bonds are invariably far superior to brute force cyclodehydrogenations of unfuctionalized hydrocarbons.



6

Project Objective and First Experiments: This research project focuses on the rational synthesis of a $C_{48}H_{12}$ fullerene fragment (**6**). The synthesis of a C60 fragment containing 48 carbons would be a significant step forward in this research, since this fragment constitutes 80% of the parent fullerene.

Initial attempts to form the target $C_{48}H_{12}$ fragment were based on the FVP of tribenzodecacyclene (**7**) and its halogenated derivatives. Tribenzodecacyclene is a large PAH that I have prepared in seven steps from commercially available phenanthrene (Fig. 2). The original plan was to introduce chlorine or bromine atoms into the fjord regions of **7** by direct halogenation of the hydrocarbon. Unfortunately, these attempts proved futile, and FVP of the unfunctionalized PAH was examined as a last ditch effort to complete the synthesis. Not surprisingly, in light of previous experiences (e.g., Fig. 1), FVP of **7** failed to yield any isolable geodesic polyarenes.

A New Approach and the Latest Results: As an alternative to zipping up the 48-carbon bowl from a 48-carbon pre-

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cursor in a single pyrolysis step, "building the big bowl" from a smaller one by extending the perimeter was considered as a potentially more feasible strategy (see retrosynthetic scheme below, Fig. 3). This plan would make use of a smaller fullerene fragment as the starting material and ring annulation techniques developed in our laboratory to produce the $C_{48}H_{12}$ fragment. The Norris/Richards Undergraduate Research Scholarship directly supported this second phase of the research.

The new route utilizes the $C_{30}H_{12}$ fullerene fragment (**3**) as the starting material. This molecular bowl constitutes 50% of buckminsterfullerene and has been synthesized by our laboratory in five steps from commercially available α-tetralone and 2-naphthyl lithium (Fig. 4).[10]

The ring annulation techniques required to produce the $C_{48}H_{12}$ bowl from the smaller $C_{30}H_{12}$bowl have been successfully utilized in our laboratory for a number of related

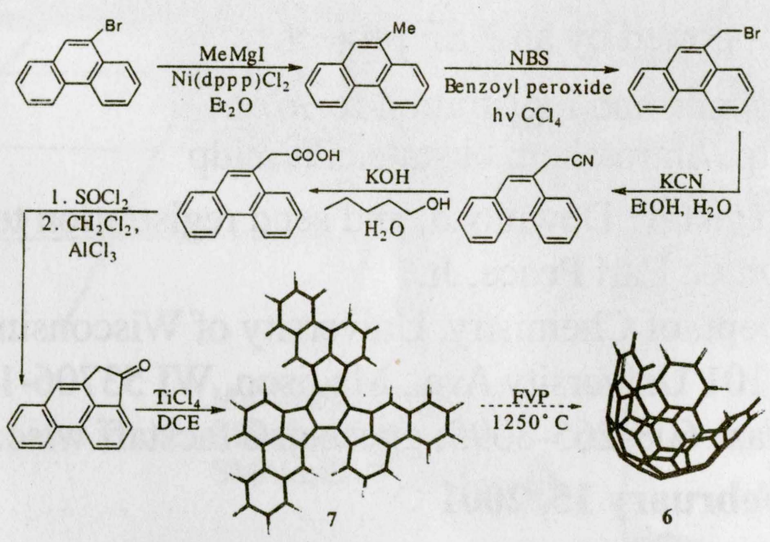

Figure 2. Synthesis of tribenzodecacyclene (**7**), a potential precursor to the $C_{48}H_{12}$ target molecule (**6**).

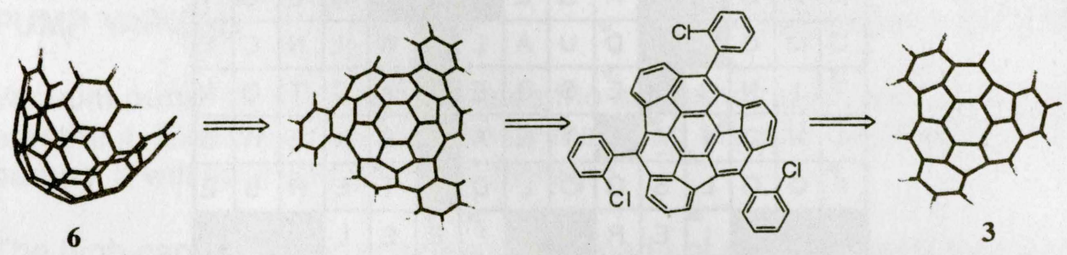

Figure 3. Retrosynthetic analysis of the $C_{48}H_{12}$ target molecule (**6**) by an annulation strategy.

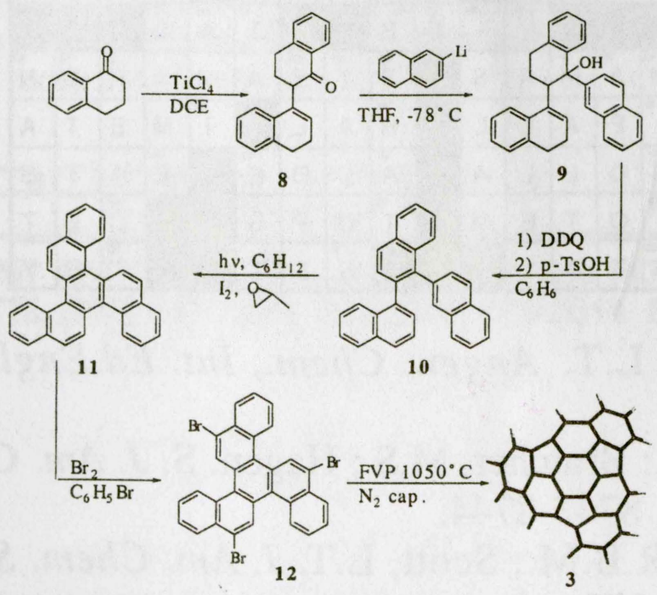

Figure 4. Synthesis of the chiral $C_{30}H_{12}$ hemifullerene (**3**).[10]

applications. The first step involves palladium-catalyzed Suzuki coupling of an aryl boronic acid to a brominated PAH. The aryl boronic acid contains a strategically placed halogen which facilitates the subsequent formation of a five membered ring by FVP. Figure 5 illustrates a successful demonstration of this ring annulation methodology to produce fluoranthene in good yield from 1-bromonaphthalene and *ortho*-chlorophenylboronic acid.

As practice for the triple annulation required to form the target $C_{48}H_{12}$ fragment (**6**),1 first focused on the attachment of one phenyl ring to the $C_{30}H_{12}$ bowl and closure to a $C_{36}H_{12}$ bowl (**15**). The route to this bowl requires initial bromination of the $C_{30}H_{12}$ bowl to give $C_{30}H_{11}Br$ (**13**), a Suzuki coupling utilizing *ortho*-chlorophenylboronic acid, and flash vacuum pyrolysis to produce the necessary ring closures (Fig. 6).

After considerable experimentation with various reagents and reaction conditions, it was found that fullerene

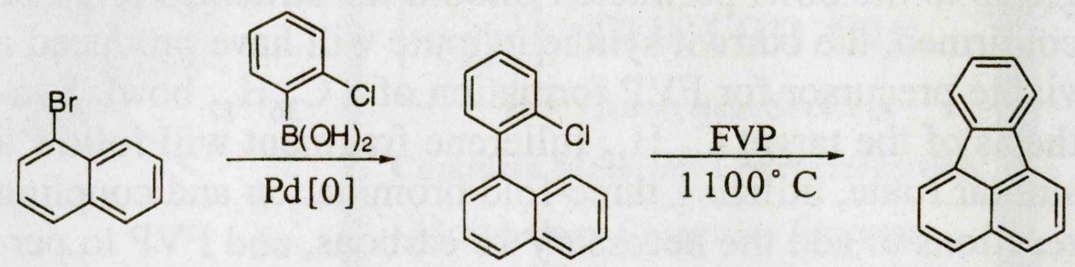

Figure 5. Synthesis of fluoranthene to test a new ring annulation technique.

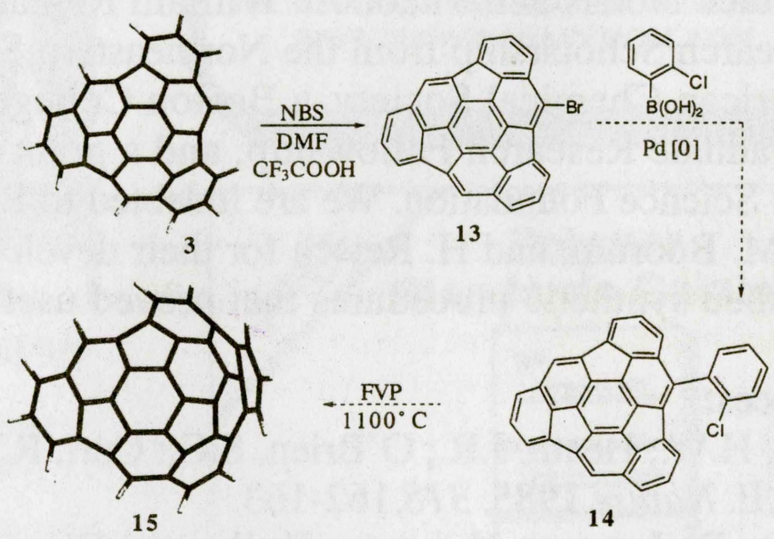

Figure 6. Synthetic route to the abbreviated target molecule (**15**).

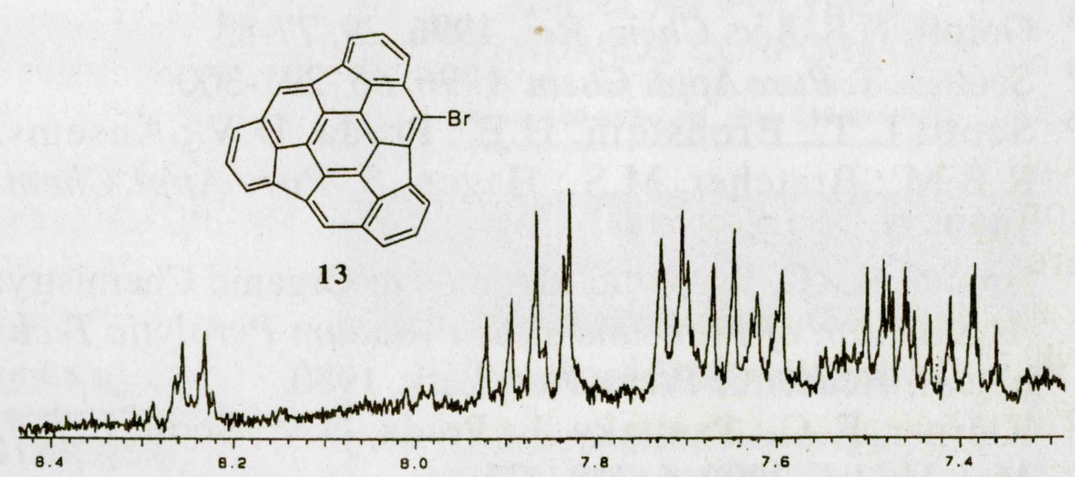

Figure 7. Spectroscopic properties of the $C_{30}H_{11}Br$ intermediate (**13**): ^1H NMR (300 MHz, $CDC1_3$, 25°C): 8.25 (d, J = 7.0 Hz, 1H), 7.91 (d, J = 7.8 Hz, 1H), 7.87 (s, 1H), 7.84 (s, 1H), 7.72 (d, J = 7.0 Hz, 2H),7.66 (d,J=7.0 Hz,1H) ,7.61 (d,J=7.8 Hz,1H),7.48(dd,J=7.8, 7.0 Hz,1H),7.46 (dd,J=7.8, 7.0 Hz, 1H), 7.36 (dd, J = 7.8, 7.0 Hz, 1H). HRMS: calcd. 450.0044, found 450.0037.

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fragment 3 could be cleanly brominated with NBS in DMF in the absence of light to produce the desired monobromoarene $C_{30}H_{11}Br$ (13). ^1H NMR and high-resolution mass spectrometry confirm the structure of the product (Fig. 7).

Through the use of a palladium catalyst in a Suzuki coupling reaction, compound **13** was arylated with *ortho*-chlorophenylboronic acid to give the product **14**. Preliminary mass spectrometry data (MALDI) indicate that the desired product was formed, although neither a ^1H NMR spectrum nor a high-resolution mass spectrum of the reaction product **14** was available at the time of this publication.

Conclusion: The research was successful in selectively functionalizing the chiral $C_{30}H_{12}$ hemifullerene **3**. Coupling reactions were performed to add an *ortho*-chlorophenyl group to the bowl perimeter. Should the structure of **14** be confirmed, the current synthetic route will have produced a viable precursor for FVP formation of a $C_{36}H_{12}$ bowl. Synthesis of the target $C_{48}H_{12}$ fullerene fragment will follow a similar route, utilizing three-fold bromination and coupling reactions to add the necessary 18 carbons, and FVP to perform the necessary ring closures.

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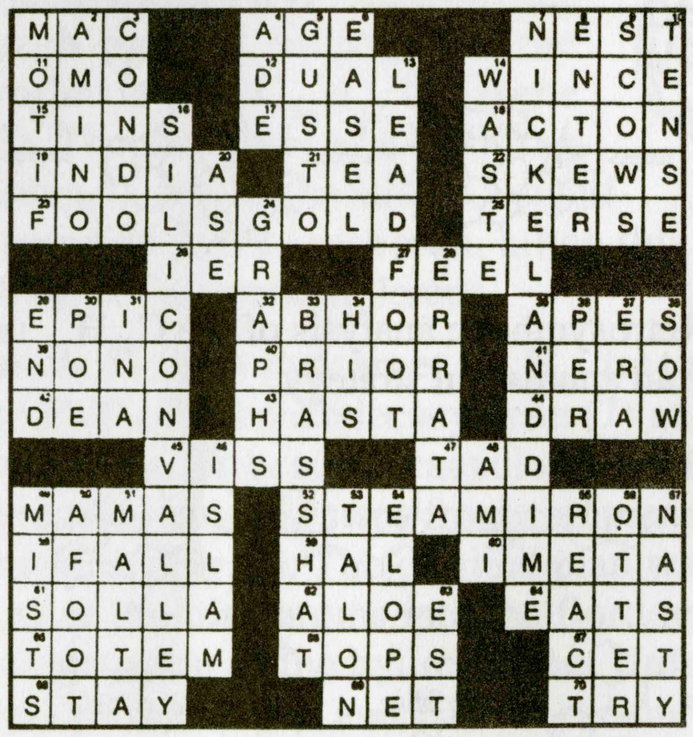
Solution of the Puzzle in January 2001 Issue



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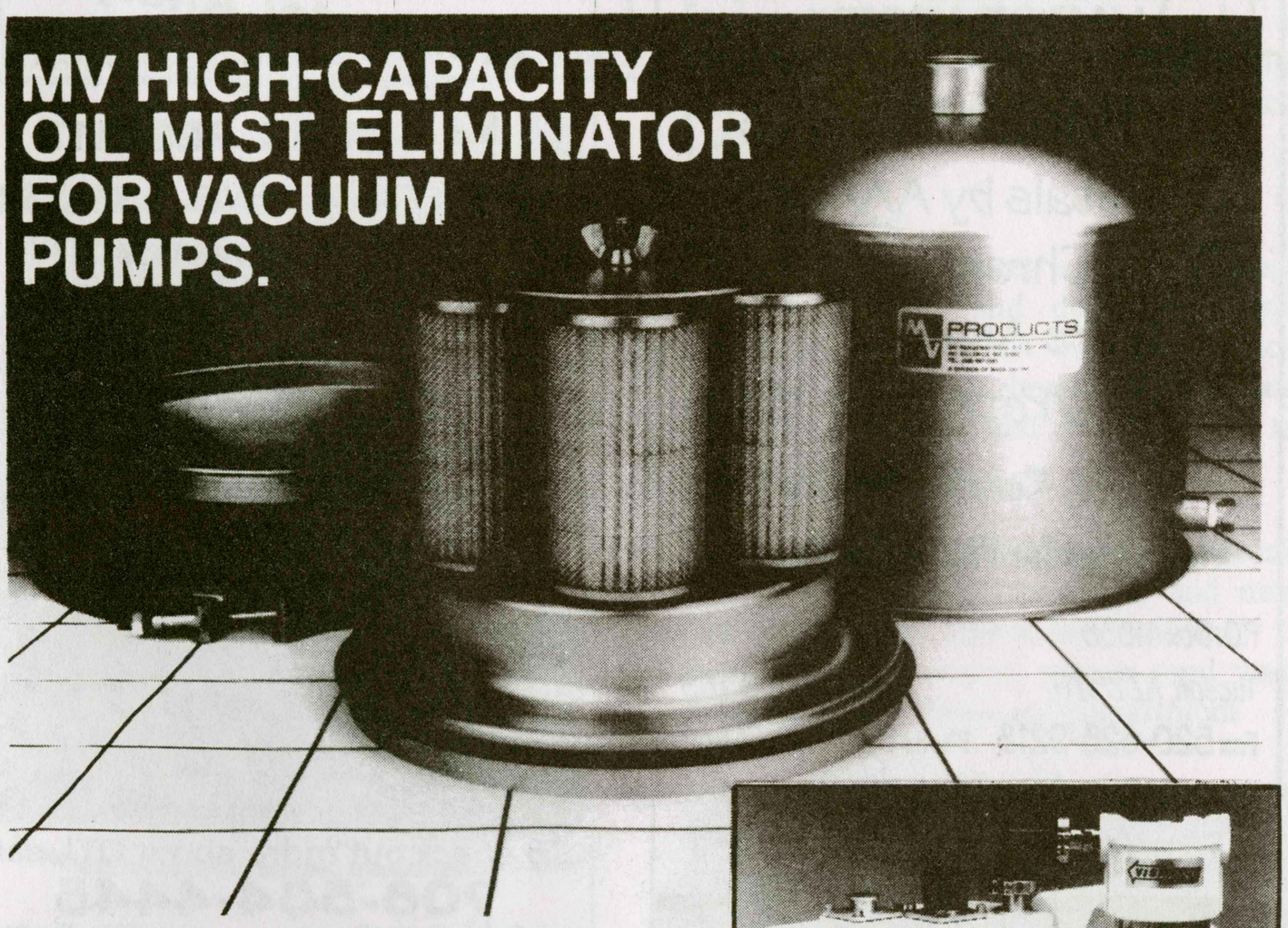

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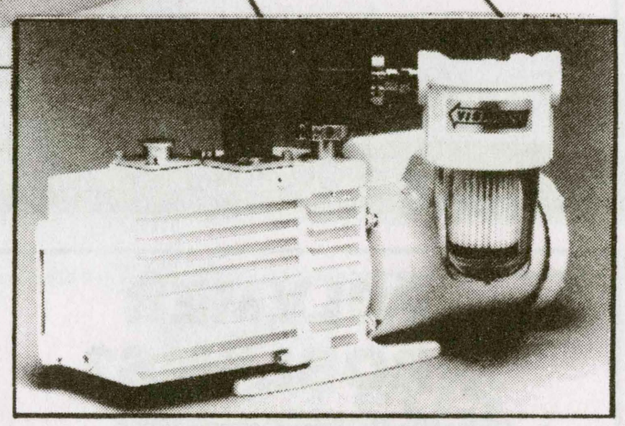

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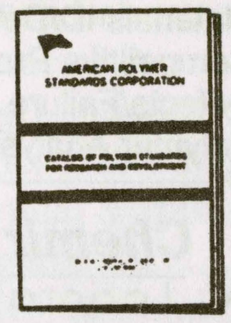

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R.J. P. Williams and J.J.R. Fausto de Silva, "Bringing Chemistry To Life. From Matter To Man," Oxford University Press (2000)

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Check the NESACS Homepage for late additions: http://www.NESACS.org

Jan 23
Prof. Sergiu Gorun (Brown Univ.)
"Artificial Enzymes: From Reversible Dioxygen Binding to Bioinspired Catalysis and Cancer Therapy"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

Jan 29
Dr. Mikael Kubista (Chalmers Institute)
"The Light-Up Probe"
Boston Univ., Science Center Auditorium, SCI 107, 4 pm

Jan 30
Prof. Catherine Drennan (Massachusetts Institute of Technology)
"B12-Dependent Ribonucleotide Reductas

Feb 1
Prof. Gregory L. Hillhouse (Univ. of Chicago)
"Reactions Involving Nickel-Nitrogen Bonds"
Boston College, Merkert 127, 4:00 pm

Prof. Daniel Herschlag (Stanford Univ.)
TBA (MIT Biochemistry Series)
MIT, Room 6-120 at 4:00 pm

Feb 5
Prof. Hilary Arnold Godwin (Northwestern Univ.)
"Why is lead toxic? Unraveling the molecular mechanism(s) of lead poisoning"
Boston College, Merkert 124, 4:00 pm

Prof. James Leighton (Columbia Univ.)
"New Olefin Carbonylation Reactions for Organic Synthesis"
Boston Univ., Science Center Auditorium, SCI 107, 4 pm

Feb 6
Prof. Monte Pettitt (Univ. of Houston)
TBA (Physical Chemistry Seminar Series)
MIT, Room 2-105 at 4:00 pm

Prof. Lincoln Lauhon (Harvard Univ.)
"Excitation and Chemical Manipulation of Single Hydrogen Atoms with a STM"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

Feb 7
Prof. Alan Heyduk (MIT/Nocera Group)
TBA (Inorganic Chemistry Seminar Series)
MIT, Room 6-120 at 4:00 pm

Dr. Marko Pregel (Genzyme Corporation)
"High-Throughput Screening for the Discovery of New Drug Candidates for Cystic Fibrosis."
UMass Dartmouth, Science & Engineering Building (Group II), Room 305, 4:00 pm

Prof. George King (Joslin-Harvard Medical School)
Title TBA
Boston Glycobiology Discussion Group
MIT Faculty Club, 6 PM
Call (781) 642-0025 for dinner reservations

Feb 8
Prof. Julie Stenken (RPI)
"Microdialysis Sampling - Overcoming Challenges and Creating Opportunities"
Univ. of New Hampshire, Iddles L103, 11:10 am

Prof. Tom Mallouk (Pennsylvania State Univ.)
"Searching the Periodic Table for Better Catalysts and Electrocatalysts"
Boston College, Merkert 127, 4:00 pm

Feb12
Prof. Wenbin Lin (Brandeis University)
"Supramolecular Approaches to Novel Materials"
Boston College, Merkert 124, 4:00 pm

Prof. James Penner-Hahn (Univ. of Michigan)
"Zn Catalysed Alkyl-transfer Reactions:
A New Class of Biological Zn Sites"
Boston Univ., Science Center Auditorium, SCI 107, 4 pm

Prof. Jeffrey D. Winkler (Univ. of Pennsylvania)
TBA (Bristol-Myers Squibb Lectures in Organic Synthesis)
MIT, Room 6-120 at 4:00 pm

Feb 13
Prof. Alanna Schepartz (Yale Univ.)
"Functional Miniature Proteins"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

Feb 14
Prof. Christina Rudzinski (MIT/Nocera Group)
"Photophysics and Applications of Chemical and Physical Sensors"
(Inorganic Chemistry Seminar Series)
MIT, Room 6-120 at 4:00 pm

Dr. Stacey M Loyland-Asbury (U. S. Department of Energy)
"Sequential Extraction and Environmental Remediation"
UMass Dartmouth, Science & Engineering Building (Group II), Room 305, 4:00 pm

Feb 15
Prof. David Budil (Northeastern)
"Probing Protein Dynamics and Electrostatics by High-Field EPR of Nitroxide Labels"
Univ. of New Hampshire, Iddles L103, 11:10 am

Prof. Kevin Lehmann (Princeton Univ.)
Topic: TBA (Physical Chemistry Lecture Series)
Harvard Univ., Mb-23 Pfizer Lecture Hall, 12 Oxford St., 5:00 pm

Feb 16
Prof. Dr. Hans-Joachim Galla (Univ. of Munster)
"The Alveolar Surfactant: Only Half a Membrane but Indispensable for the Breathing Process"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

Feb 19
Prof. Dr. Francois Diederich (ETH, Zurich)
TBA (Novartis Lecture)
Boston College, Merkert 127, 4:00 pm

Feb 20
Prof. Mario Molina (MIT)
"From Local to Global Pollution: The Impact of Human Activities on Atmospheric Ozone"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford,
Room 106, 5:00 pm (Note change of time.)

Feb 21
Prof. Roger Alberto (Univ. of Zurich)
"Classical Aqueous Coordination Chemistry with Non-classical Technetium Complexes as New Entries to Radiopharmacy" (Harvard/MIT Inorganic Colloquia)
MIT, Room 6-120 at 4:00 pm

TBA
UMass Dartmouth, Science & Engineering Building (Group II), Room 305, 4:00 pm

Feb 22
Prof. William E. Moerner (Stanford Univ.)
TBA
Boston College, Merkert 127, 4:00 pm

Prof. Gerard Meijer (Univ. of Nijmegen, The Netherlands)
Topic: TBA
Harvard Univ., Mb-23 Pfizer Lecture Hall, 12 Oxford St., 5:00 pm

Prof. Ed Yeung (Ames Lab., Iowa State Univ., Ames)
"Imaging Single Molecules: Fundamental and Chemical Implications" Northeastern University, Hurtig Hall, 4:00 pm

Feb 26
TBA
Boston Univ., Science Center Auditorium, SCI 107, 4 pm

Feb 27
Prof. Tom Muir (Rockefeller Univ.)
"Protein Ligation: Linking Chemistry and Biology one Peptide Bond at a Time"
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

Feb 28
Prof. Kenneth Suslick (Univ. of Illinois at Urbana-Champaign)
"Smell-seeing and Molecular Recognition by Metalloporphyrins"
(MIT Inorganic Chemistry Seminar)
MIT, Room 6-120 at 4:00 pm

Prof. Eric Block (SUNY-Albany)
"Chemistry in a Salad Bowl: the Organosulfur and Organoselenium Chemistry of Garlic and Onion."
UMass Dartmouth, Science & Engineering Building (Group II), Room 305, 4:00 pm