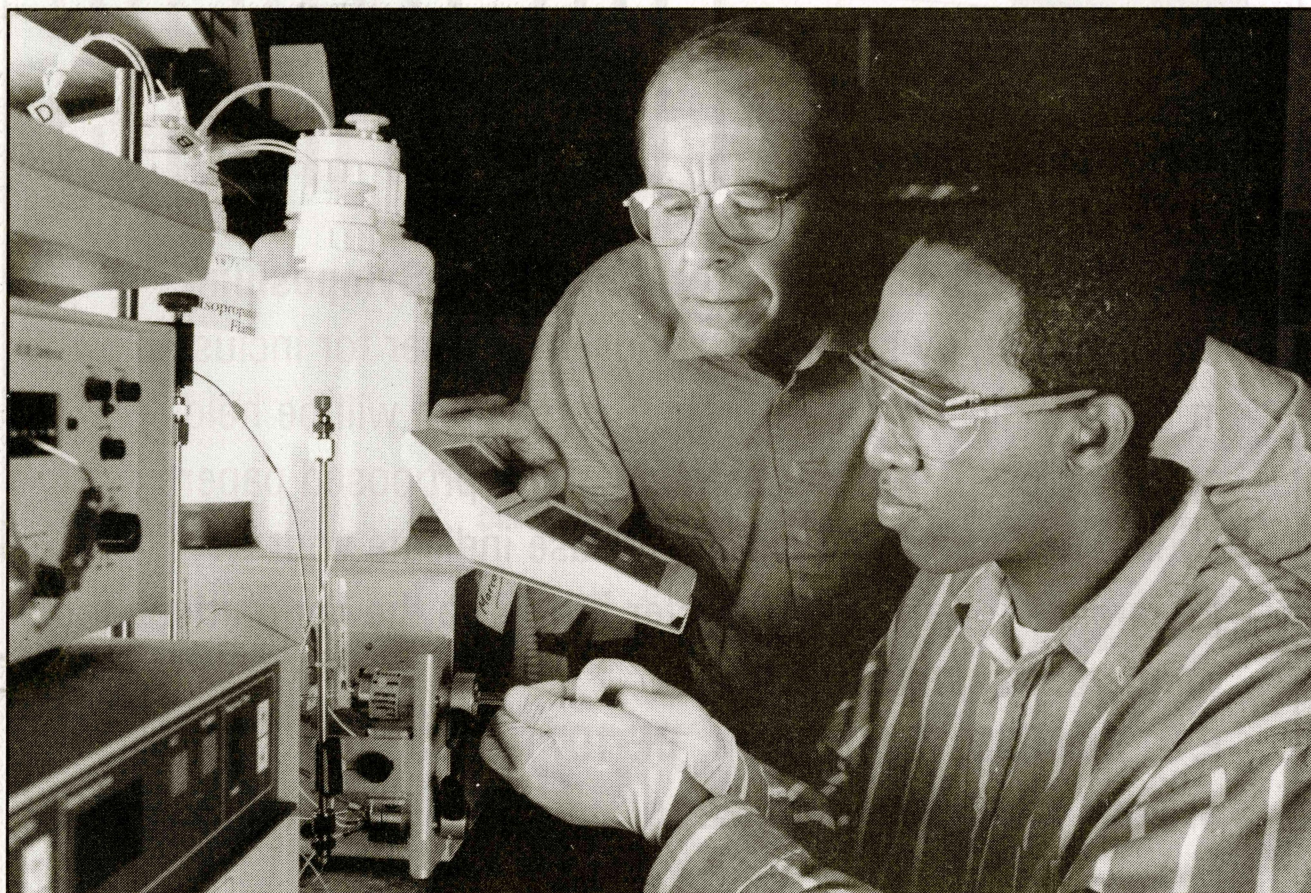


THE NUCLEUS

Centennial Year

March 1998

Vol. LXXVI, No. 7



Monthly Meeting

Richards Medal to Barry K. Sharpless

Book Review

Excel for Chemists by E. Joseph Billo

Who Was Theodore William Richards?

A biographical note

Summer Scholar Report

Reductive binding of dinitrogen by J. Christopher Thomas, et al.



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Please make the **1998 Eastern Analytical Symposium** the best ever, by submitting your own paper for inclusion in the technical program. The Symposium will be held on Nov. 15-20, 1998. Abstracts of the proposed papers should be 200 to 250 words, please indicate your preference for an oral or poster format to the committee.

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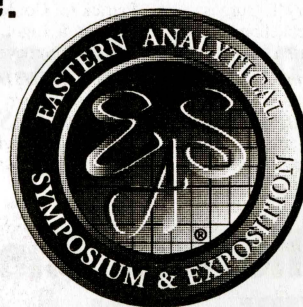
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Cover: *Prof. Sharpless and Tedros Amanios, an undergraduate research student, in the laboratory. Photo by Mark Dastrup, San Diego, Cal.*

Deadlines: *May 1998 issue: March 23, 1998*
Summer issue: June 26, 1998 (National Meeting issue)

THE NUCLEUS

The Nucleus is distributed to the members of the Northeastern Section of the American Chemical Society, to the secretaries of the Local Sections, and to editors of all local publications. Forms close for advertising on the 1st of the month of the preceding issue. Text must be received by the editor six weeks before the date of issue.

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Who was Theodore William Richards?

by M.S. Simon

Adapted from *The NUCLEUS*, 1996 (3) 4 ff.,

The presentation of the Theodore William Richards Medal to K. Barry Sharpless this month recognizes 'conspicuous achievement in the advancement of chemistry', and we can take pride not only in the choice this year, but also in the many distinguished chemists who have won this honor in past years. [See the listing in *THE NUCLEUS*, 1998 (2) 24] But as we honor Prof. Sharpless, we are also honoring the memory of Richards himself. Who was this man?

The first award of what, at that time, was known as the Theodore William Richards Gold Medal (the medal is still gold, with a silver replica for informal display) was made to Arthur Amos Noyes in 1932. The Section chairman, William Ryan, introduced the occasion with the following quotation by Henry Watterson:

*A mound of earth a little higher graded,
Perhaps upon a stone a chiselled name,
A daub of printer's ink soon blurred
and faded.*

And then—oblivion. That—that is fame.

Ryan went to point out that Watterson, as an observer in national politics, had developed a cynical attitude toward self-seeking politicians, and Ryan contrasts the impermanence of reputation of such with the seekers of truth for truth's sake for whom true fame is imperishable. With reference to Richards he said, "True fame...lives on, not merely to perpetuate the name of the individual and his accomplishments, but rather to inspire and encourage others who are serving similar ends."

But in our age, when only "fifteen minutes" of fame are allowed, it behooves us to keep alive the names

and accomplishments of our predecessors in chemistry. The Northeastern Section has many great chemists, but the earliest of the internationally renowned was Theodore William Richards. His Nobel Prize in Chemistry, awarded in 1914, was the first given an American chemist.

He was born in Germantown, Pa. in 1868, was educated at home by his mother, a poet, and his father, a marine artist. He became interested in science at the age of six when he was shown the rings of Saturn through a four inch telescope by Professor Josiah Parsons Cooke, Jr. of Harvard while the family was at Newport, R.I. At ten he was making Pharaoh's Serpents with mercuric thiocyanate and coloring flames with various salts. He obtained money to set up a chemistry laboratory when he was 13 by printing on a hand press, copywriting, and selling an edition of his mother's sonnets. He was allowed to attend chemistry lectures at the University of Pennsylvania, and at 14 entered and studied chemistry at Haverford. He received the Bachelor of Science at 17. He went to Harvard to study under Cooke and received a Bachelor of Arts and, at 20, after a year of very difficult research in which he demonstrated exceptional experimental skills in determining the atomic weight ratio of oxygen to hydrogen in water, earned the Ph.D. degree. A year in Europe on a Harvard fellowship gave him the opportunity of studying analytical techniques at Göttingen and visiting important laboratories in Germany, France, England, and Switzerland. He returned to Harvard in 1889 as an assistant and remained there for the rest of his years. When Cooke died, in 1892, Richards, already an assistant professor, was sent to Ostwald at Leipzig and Nernst at Göttingen to prepare himself to become the instructor in physical chemistry. His rise to full professorship at Harvard in

1901 came quickly, when Göttingen attempted to recruit him. His early work centered on what at the time was one of the major scientific problems, that of determining exact atomic weights. He explained his choice, "not merely because I felt more competent in that direction than in any other, but also because atomic weights seemed to be one of the primal mysteries of the universe. They are values which no man by taking thought can change. They seem to be independent of place and time. They are silent witnesses of the very beginnings of the universe, and the half-hidden, half-disclosed symmetry of the periodic system of the elements only enhances one's curiosity about them. Moreover, among the many properties possessed by an element, the atomic weight seems one of the most definite and precise. Hence in trying to satisfy a desire which had as its object the discovery of more knowledge concerning the fundamental nature of things, one

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continued on page 6

Monthly Meeting

The 796th Meeting of the Northeastern Section of the American Chemical Society

Thursday, March 12, 1998

Harvard University, Cambridge, MA Faculty Club, Quincy St.

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

6:15 Dinner.

8:15 Award Ceremony, Harvard University Science Center, 1 Oxford St.
Reflections on T.W. Richards—Dr. Steven J. Lippard, M. I. T.
Introduction of the Award Recipient—Dr. Frederick D. Greene, M. I. T.
Presentation of the Medal to Prof. Sharpless—Dr. Michael Hearn, Chair, Northeastern Section
Richards Medal Address—A Few Good Reactions—Dr. K. Barry Sharpless, Scripps Research Institute, La Jolla, Cal.

Dinner reservations should be made no later than March 5, 1998, noon. Please call or fax Marilou Cashman at (800) 872-2054. Reservations not canceled 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: At the Felton St. garage (3rd. level or higher); enter from Cambridge St.

Next Meeting: Wednesday, April 8, 1998. Gustavus J. Esselen Award to K.C. Nicolaou (Scripps Research Institute, La Jolla, Cal.). 5:30 Reception and dinner (Harvard Faculty Club), 8:15 Award meeting, Harvard Science Center

Biography

K. Barry Sharpless was born in Philadelphia, Penn. He received a B.A. at Dartmouth College and a Ph.D. at Stanford University, working under Prof. E.E. van Tamelen (organic chemistry). He held post-doctoral appointments at Stanford from 1968-70 with J.P. Collman and Harvard University, with K. Bloch, respectively. He joined the faculty at M.I.T. in 1970, advancing to Professor of Chemistry in 1975. In 1977-1980 he was on the faculty of Stanford University and rejoined M.I.T. in 1987 as Arthur C. Cope Professor of Chemistry. In 1990 he joined the Scripps Research Institute in La Jolla, Cal. as W.M. Keck Professor of Chemistry. In 1996 he became a mem-

ber of the Skaggs Institute for Chemical Biology of the Scripps Research Institute.

His current research is in diversity chemistry, in developing new homogeneous catalysts for the oxidation of organic compounds and in asymmetric catalysis involving transition metal-mediated processes.

Among many honors, he received the ACS Award for Creative Work in Organic Synthesis in 1983, was elected to membership in the National Academy of Sciences and the American Academy of Arts and Sciences. He received the Chemical Pioneer Award of the American Institute of Chemists, the Arthur C. Cope Award and the Roger Adams Award of the American Chemical Society. This year, in addition to receiving the Richards Medal

Abstract

A Few Good Reactions

Bohacek *et al.*¹ have recently estimated that there are between 10^{62} and 10^{63} discrete molecules that could be regarded as "reasonable" drug candidates. This astonishing estimate was obtained by placing two fundamental restrictions on the molecules: (1) contains ≤ 30 atoms (*i.e.* consonant with the ca. ≤ 500 M.W. cutoff for ideal drug size) and (2) use only the nine element palette currently found in drugs (*i.e.* H, C, N, O, P, S, F, Cl, and Br). The modifier "reasonable" (*vide supra*) means that the conservative choice was always favored whenever stability issues (both thermodynamic and kinetic) arose. In addition, many structures were eliminated by a drug's need to be stable in an aqueous environment.

Even using this lower estimate of 10^{62} , one realizes that the possibilities are astronomical whereas currently there are only about 10^6 representatives actually known in this special class of small molecules. This means that the ratio of known to possible "drug-like" molecules is 10^{-56} , or almost zero!

This lecture will begin with one chemist's thoughts on how realization of the "Bohacek *et al.* Number" should/could affect the future of medicinal chemistry. I will then describe our initial endeavors to make a dent in this currently sparsely populated but uniquely important region of molecular space. \diamond

¹R.S. Bohacek, C. McMartin, W.C. Guida, *Medicinal Research Reviews*, 1996, 16, 3-50

of our Section the announcement is pending of his being named an Honorary Fellow of the Royal Society of Chemistry (Great Britain).

He has received honorary doctorates from Dartmouth College, the Swedish Royal Institute of Technology, the Technische Universität München and the Université Catholique de Louvain, Belgium. \diamond

Who was Theodore William Richards?

continued from page 4

naturally assigns to the atomic weights an important place."

In the following years Richards and his students (if we include independent work of Baxter and Hönigschmid, who had been trained by him) determined the atomic weight of 55 of the 92 known elements, in many cases in parts per ten thousand, in some, parts per hundred thousand. All of the elements whose atomic weights were the basis for determining the atomic weights of other elements were determined. His work on lead from uranium and from non-radioactive sources advanced acceptance of the theory of isotopes, the only conclusive evidence until the development of the mass spectrograph.

He was always respectful to those on whose shoulders he was standing, J.J. Berzelius and J.S. Stas, pioneers in atomic weight determination, but when his superior methods showed that the Stas values had to be revised, he took the mantle on his own shoulders. A modest man, only after searching diligently for his own possible errors would he conclude that the Stas work had to be superseded.

He was guided to success by

"his ability to foresee all sources of error and possible calamities which the average investigator would have overlooked completely",

reported his son-in-law, James B. Conant. Richards put it thus,

"Every substance must be assumed to be impure, every reaction must be assumed to be incomplete, every method of measurement must be assumed to contain some constant error, until proof to the contrary can be obtained. As little as possible must be taken for granted."

It is illuminating to consider that much of his work was conducted in Boylston Hall, where his laboratory had been a stockroom, where the iron sashes of the fume hood rained rust,

and a flood on the floor above caused the ceiling to collapse on him; where fumes from elsewhere in the building could ruin his experiments. Finally, the Wolcott Gibbs Memorial Laboratory, a gift of Dr. Morris Loeb, was built in 1912 and Richards had the facilities his work deserved.

The concentration on atomic weights suggests that Richards was solely an analytical chemist. Indeed, he was a superb analytical experimentalist, but his work in other areas of physical chemistry formed an important part of the total picture. His work began at the period when physical chemistry was aborning; van't Hoff, Arrhenius, Ostwald, Nernst were the new names and the *Zeitschrift für physikalische Chemie* was founded in 1887. Richards' first student in physical chemistry was G.N. Lewis, to whom he assigned the study of the electrochemistry and thermochemistry of amalgam cells. Richards rejected the belief of that day that atoms were incompressible, developed evidence that atomic volumes change, and, according to Lewis, very nearly discovered the third law of thermodynamics in his studies of the relationship of changes in free energy and total energy accompanying a reaction. His invention (with G.S. Forbes and L.J. Henderson) of an adiabatic calorimeter led to studies of specific heats of acids, bases and salts, heats of solution and dilution, heats of neutralization and the thermochemistry of organic compounds.

His laboratory attracted students from many other countries to learn the methods of the Harvard school. His ability to devise methods which could give superb results in the hands of students led to volumes of published research. The list of his students includes many of the most capable physical chemists of the first half of the twentieth century.

At his death in 1928 the Northeastern Section appealed for funds to set up a memorial and, with 'gratifying response', raised a sum of ten thousand dollars in a few months. The Theodore William Richards Gold Medal was designed by Cyrus Dallin,

Grants-in-Aid to Undergraduates

Grants-in-Aid of \$250 each have been awarded by the Chemistry Education Committee to four undergraduates at universities within the Northeastern Section to enable them to attend the ACS National Meeting in Dallas, Texas, and to present a paper at the Undergraduate Research Poster Session in the Division of Chemical Education on Monday, March 30, 1998. Matching funds have been committed by their institutions to support travel of the students. The awardees, their research supervisors, and the titles of the papers are as follows:

Robert Boulanger, Jr., Univ. of Massachusetts Dartmouth, (Prof. B.R. Singh), *Light Regulation of Anthocyanin and Flavonol Biosynthesis in Cranberry Plants*.

Irene Chen, Harvard University, (Prof. G. Verdine), *On the Molecular Basis for Dimerization Preferences of Nuclear Factor κ B*

Curtis Chong, Harvard University, (Prof. D. Auld), *Catalytic Chelators: Mechanism and Implication for Drug Design*.

Steven Klei, Mass. Institute of Technology (Prof. C. Cummins), *A Norbornyl Substituted Ligand for the Synthesis of Three-Coordinate Niobium (III)* ◇

a distinguished sculptor and friend of Richards. A more complete account of the career of Richards may be found in a lecture delivered by Sir Harold Hartley and recorded in the *Journal of the Chemical Society (London)*, 1930, 1930-1968, from which much of this article was taken. Other sources include the *Encyclopedia Britannica* and *The NUCLEUS*. *The Scientific Work of Theodore William Richards* is the title of a Ph.D. dissertation by Sheldon J. Kopperl, U. Wisconsin, Madison, 1970, 333-359. ◇

1998 NESACS Candidates for Election

Chair-Elect: (one to be elected)
Doris Lewis

Treasurer: (one to be elected)
James Piper

Auditor: (one to be elected)
Anthony Rosner

Trustee: (one to be elected)
Esther Hopkins, Karl Weiss

Director-at-Large (two to be elected)
Joseph Billo, Leisa Corbett, William Foye, Yigong Gao, Lloyd D. Taylor

Councilor/Alternate Councilor: (4 Councilors and 4 Alternate Councilors to be elected)
Sonja Fetela, Michael Filosa, Thomas Gilbert, Michael Hearn, Morton Hoffman, Rein Kirss, Roy Kisliuk, Patricia Mabrouk, Donald Rickter, Donald Smith, Andre Rosowsky, Michael Singer, Sophia Su

Norris Award Committee: (two to be elected)
Thomas Gilbert, Gordon Gribble, Michael Hearn, Patricia Samuel

Nominating Committee: (two to be elected)
Thomas Gilbert, Arno Heyn, James Kaufman, Truman Light

Petition Candidates: In accordance with the Northeastern Section Constitution, Article VIII, Sec. 3,

"Any group comprising 2 percent or more of the membership of the Northeastern Section may nominate candidates for any elective office provided that such nomination (accompanied by the signatures of the nominating group) shall be presented in writing to the Chair(man) of the Nominating Committee not more than ten days following the March meeting of the Northeastern Section."

Accordingly, such petitions are due March 22, 1998 and are to be sent to Marilou Cashman, 23 Cottage St., Natick, MA 01760, att.: Martin Idelson. At least 106 valid signatures are required. Preferably, the petition should be sent by certified mail. ◇

Nominating Committee: Martin Idelson (chair); Mary Burgess, John Neumeyer, Myron Simon, Alfred Viola

Undergraduate Summer Research

The James Flack Norris and Theodore William Richards Scholarships

The Northeastern Section of the American Chemical Society established the James Flack Norris and Theodore William Richards Undergraduate Summer Scholarships to honor the memories of Professors Norris and Richards by promoting research interactions between undergraduate students and faculty.

Research awards of \$3,250 will be given for the Summer of 1998. The student stipend is \$2,750 (for a minimum commitment of ten weeks of full-time research work). The remaining \$500 of the award can be spent on supplies, travel, faculty support, and other items relevant to the student project.

Institutions whose student/faculty team receive a Norris/Richards Undergraduate Summer Research Scholarship are expected to contribute toward the support of the faculty members and to waive any student fees for summer research. Academic credit may be granted to the students at the discretion of the institutions.

Award winners are required to submit a report (5-7 double spaced pages, including figures, tables, and bibliog-

raphy) of their summer projects to the Education Committee by November 6, 1998, for publication in *The Nucleus*. They are also expected to participate in the NESACS Undergraduate Research Symposium in April, 1999.

Eligibility: Applications will be accepted from student/faculty teams from colleges and universities within the Northeastern Section. The undergraduate student must be a chemistry, biochemistry, chemical engineering, or molecular biology major in good standing, and have completed at least two full years of college-level chemistry by Summer, 1998.

Application: Application forms are available from departmental chairs and the NESACS office 508-653-6329 or 1-800-872-2054. Completed applications with two photocopies are to be submitted no later than March 25, 1998 to the Chair of the Selection Committee:

Professor Edwin Jahngen
Department of Chemistry
University of Massachusetts-Lowell
Lowell, MA 01854

Notification: Applicants will be notified of the results by April 24, 1998. ◇

Book Review

Excel for Chemists, by E. Joseph Billo (Wiley-VCH, 1997, 454 pp., \$49.95 softcover)

Reviewed by Kenneth Kustin
(Emeritus, Department of Chemistry,
Brandeis University)

The success of such youthful software giants as Lotus and Corel (WordPerfect) bespeak a simple fact: computers are primarily used for calculating and communicating. Facilitating calculations are spreadsheet programs, the powerful electronic equivalents of pencil, worksheet or graph paper, and handheld abacus, slide rule, or calculator. Originally intended for business offices, spreadsheets proliferated when they were adopted by scientists and engineers. Now spreadsheets, such as those from Excel, Lotus, and Quattro Pro, no longer come with comprehensive, readable manuals, and this format discourages acceptance by new users. Manufacturers provide a manual of sorts, which merely outlines useful spreadsheet applications. They rely instead on so-called "Help" files for detailed instruction, but only through the computer while the program is being used. For the first-time user or student who doesn't know how to frame the precisely correct phrase or question, the Help files are no help at all. But genuine help and instruction are available, for now we have Prof. E. Joseph Billo's book, *Excel for Chemists*, which not only teaches how to use a spreadsheet, but is a superior reference and guide to applying spreadsheets to the solution of chemical problems.

Excel for Chemists has four main parts organized into two sections, plus appendices and an accompanying diskette. The first section is a reference and teaching manual for the Excel spreadsheet. It is ordered from elementary to advanced instruction. The second section presents mathematical tools and their applications to chemical problems, and is similarly organized. Mathematical tools introduced to solve problems are both tradi-

tional and computer-oriented recursive techniques. Traditional methods, with which most of us are familiar, include solving simultaneous equations, finding roots of equations, and linear regression (linear least squares). The less familiar recursive methods such as circular reference involve guessing the value of a solution and recalculating the value until the computer converges on some n th value that differs from the previous ($n-1$) value by a predetermined inconsiderable difference; e.g. 1 part in one million. Throughout, the style of writing is lively, direct and unpedantic. In the first section, where the text could be dull, numerous chemical examples help to maintain reader interest. For example, if you are already a spreadsheet user, you may hate the appearance of conventional chemical formulas therein, but find it too time-consuming to format subscripts in each cell. Prof. Billo comes to your aid with a "macro" that converts text to chemical formulas with the click of a "button." (Macros, available on the accompanying diskette, are explained in the text.)

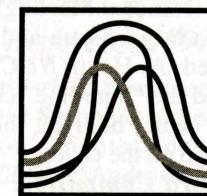
A powerful feature that has made spreadsheets so desirable for scientific work becomes apparent when handling large sets of data. How tedious it is to perform over and over again the same mathematical transformation on each data point; squaring and adding a constant or taking a logarithm, for example. With the spreadsheet, however, other options are possible. For example, in one option the transformation is performed once, then, by tracking the mouse past the data, all other data entries are properly transformed. Compare Microsoft and Prof. Billo's instructions for performing this type of operation from the viewpoint of a student or first-time spreadsheet user.

To start with, it is difficult to find the information describing one such procedure in the Microsoft manual and, once located, the instructions are presented in a very general manner. In a chapter on budgeting (!), there is a header that exhorts one to, "Consolidate the Combined Input," which wouldn't seem to point to transforming data. However, on the next page (369 in Version 7.0) the reader is instructed

how to "Copy formulas automatically." Therefore, "Once you've entered the formula to consolidate one account, you don't have to type similar formulas for the rest of the accounts." Abstract instructions for doing this then follow. In comparison with Microsoft's exhortation to "Consolidate...Input," here is Prof. Billo's header, which spells out what the student will be doing, namely, "Duplicating Values or Formulas in a Range of Cells," (and it appears near the beginning of the book, on page 26). Where Microsoft gives no further aid to the reader beyond a generalized description, Prof. Billo follows up his generalized instruction with a concrete example, "...if cell A2 contains the formula =A1+1, and **Fill Down** [another way to perform the operation] is used to copy the formula into a range of cells below cell A2, the formula copied into cell A3 will be =A2+1, and so on."

Some other highlights of Prof. Billo's book include instructions on customizing the spreadsheet for chemical purposes. The user is also shown how to prepare good charts for the graphical display of results. Among the applications are the use of the "goal-seeker" command to solve a variety of problems; for example, the use of this technique rather than the Guggenheim method to obtain rate constants for reactions where the final reading is unknown, and much more. In many of these cases, there is a comparison with far more advanced and specific commercial products such as MathCad and MathLab.

So who should use this book? It is useful for any chemist currently using spreadsheets, for anyone whose education did not include computer instruction, but who wants to get started with self-instruction. Above all, it is recommended for students who are beginning the study of chemistry. *Excel for Chemists* contains a richness of material. Once the spreadsheet is mastered, the book serves as a reference and as a source of ideas and options for problem-solving. I highly recommend this book; treat yourself to it; assign it to a class; give it as a gift. ◇



You might recognize this symbol from our ads in the *Nucleus*: It's the logo of PhaseX Corporation. Many of you are probably aware of the no-cost supercritical fluid extraction tests we've advertised, and some of you have called to take advantage of the offer. Those of you who haven't, we invite you to.

Our logo means different things to different people:

- ▶ If you're in **polymers**, it says we can take your polymer and separate it into narrow fractions (more than just three).
- ▶ If you're in **pharmaceuticals formulation**, it says we can take your pharmaceutical particles and make them smaller (by more than just a third).
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Board of Directors

Notes of the Meeting of December 11, 1997

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

Officers Reports

Treasurer: J. Piper presented the break-down of income and expenditures for the preceding month. Section funds are in good shape. The report was ACCEPTED.

Archivist: M.S. Simon invited members to provide items for inclusion in the centennial issue, such as memories of past events.

Trustees: The 1997 report of trust funds will be presented at the February 1998 meeting.

Committee Reports:

Board of Publications: D. Lewis reported that the centennial issue in

February 1998 will be an expanded issue and more copies will be printed. The Summer (National Meeting) issue will also be a larger issue and extra copies ordered. A. Heyn, *NUCLEUS* Editor showed the "blue-line" copy of the January issue, bearing the new Centennial logo on the cover.

Esselen Award Committee: M.S. Simon reported that about \$1800 was left over from the 1997 award, making a balance of \$2585 in the account. R. Handrick recommended that the fund be left until the total reaches about \$5000 for investment in a long-term bond. H. Brown reported that the selection of the 1998 awardee is on schedule.

Chemical Education: M.Z. Hoffman reported on the successful Undergraduate Chemistry Day, held at Boston University, with about 150 participants. Speakers were Prof. S. Lippard, J. Fourkas and M. Henschman. The undergraduate group is planning for its participation at the August National ACS Meeting in Boston.

Four \$250 grants were given to four undergraduates who will report on their work at the poster session at the Chemistry Education Division Poster Session in Dallas in March. The Suffolk University Student Affiliate Chapter has received honorable mention for its activities and will receive a plaque in Dallas. Drs. Doris Lewis and George Patterson are the faculty advisors. M. Hearn stated that 200 chemistry educators participated in the ACS satellite TV program at the U.Mass Lowell.

Continuing Education: A. Viola reported that the Laboratory Health and Safety Workshop was given by J. Kaufman. It was financially successful. There were 29 registrants, including 9 ACS members. This program was for staff members, lab managers, safety officers, not for students.

Other Committees:

Public Affairs: A new chair, Mukund S. Chorghade was introduced.

Health and Safety: J. Kaufman reported that the student lab safety

Board of Directors

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training session at the U.Mass Dartmouth went well, with 35-40 undergraduates and graduates attending. A similar session is scheduled for Framingham State College on January 31.

Old Business: M. Strem thanked members for their support of his candidacy for the position of ACS Director for Region I, to which he was elected.

Tax-exempt status of the Section: J. Piper reported that the law firm of Hale & Dorr (recommended by the National ACS office) concluded that the Northeastern Section is tax exempt under a section of the tax code which is different from that under which the parent society claims its exemption. This information is being provided to the National ACS.

New Business: Councilor/Alternate Councilor positions: A. Heyn pointed out that by interpreting M.Z. Hoffman's term to include 1998, an Alter-

Board of Publications

Annual Report for 1997

The Board of Publications of the Northeastern Section is responsible for the Section's monthly publication, *THE NUCLEUS*. Additionally, a section directory is published periodically, and the Board of Publications oversees the content of the Section's home page, produced by webmasters Arthur Obermayer and Betty Solbjor. The

alternate Councilor slot is open. Under our usual procedure, the runner-up for that position, Wilmon B. Chipman, would thus be asked to fill the position of Alternate Councilor for the year.

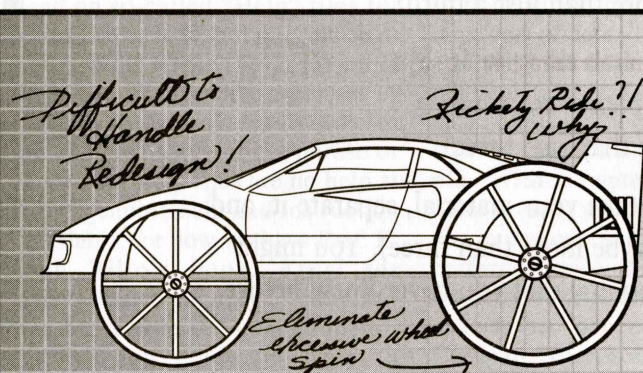
Centennial Meeting: Although originally scheduled for the April 24-25 dates, the actual date is in doubt because of the difficulty in scheduling invited speakers. ◇

From the minutes taken by M.S. Simon, Secretary pro tem.

Board is composed of three members who serve three-year terms, with a new member appointed by the Section Chair each year. In 1997 the members were Doris Lewis (chair), E. Joseph Billo, and Joseph Lima. The Board of Publications meets monthly September through June. Meetings are attended by the three voting board members, and by the editor (Arno Heyn), associate editor (Myron Simon), business manager (Karen Piper), and advertising manager (Vincent Gale).

Advertising revenue has continued to increase, following a trend observed over the past two years. For 1997 advertising revenue was approximately \$33,114, as compared with the budgeted amount of \$29,000; 1996 advertising sales were \$27,300 and the budgeted amount \$24,300. This increase in revenue has made possible an increase in

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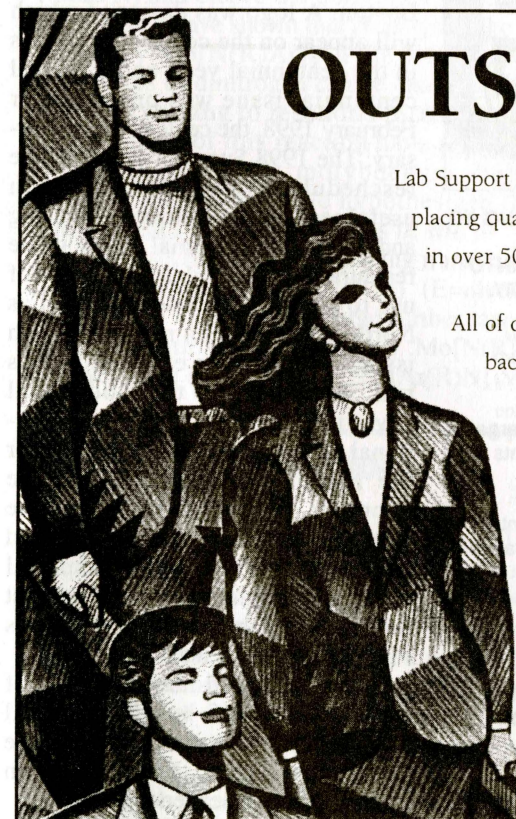
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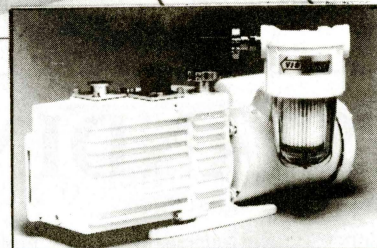
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Board of Publications

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the total number of pages published, at a decreasing cost per page and hence a diminished operating deficit. Hence the cost to the Section continued to decrease as the size of its publication grows. The 1997 operating deficit, budgeted at \$20,835, will actually be about \$12,805.

A concern of the Board over the past two years has been the obtaining of sufficient feature material of high quality in the expanded publication made possible by increased advertising. In 1987, however, a regular book review column, along with other contributed articles, has resulted in a supply of high-quality copy that has been more than adequate in quantity and has been a welcome addition to *THE NUCLEUS*.

The major activities of the Board in 1997 have been the preparations for special issues for the 1998 Northeastern Section Centennial and for the Fall 1998 ACS National Meeting in Boston. A logo was designed which will appear on the cover of all issues in the centennial year, and a special centennial issue was prepared for February 1998, the centennial anniversary. The 1998 Summer Issue will be rescheduled slightly for maximum usefulness for the National Meeting and will include material (for example restaurant reviews) designed to be of use to meeting attendees as well as Northeastern Section members. Both issues will have an expanded press run. We anticipate that additional advertising revenue will cover additional costs for the expanded run for the National Meeting. Since the February issue commemorating the Centennial will have both an extended run, additional pages, and a special cover, funding for the additional cost has been sought from the Section's Publication Trust Fund.

The planned distribution of *THE NUCLEUS* to the Central Massachusetts Section has not gone forward due to lack of interest shown by that Section's leadership.

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Summer Scholar Report

Reductive Binding of Dinitrogen by a Three-Coordinate Molybdenum (III) Complex and Partial Functionalization with Electrophiles

J. Christopher Thomas and Christopher C. Cummins
Department of Chemistry,
Massachusetts Institute of Technology

Abstract

The synthesis and characterization of the complexes $[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}=\text{NSi}(\text{CH}_3)_3]$, $[(\text{Ar}(\text{R})\text{N})_3\text{Mo}(\text{N}-\text{N}[\text{CH}_3]_2)]^+[\text{OTf}]^-$, and $[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}=\text{NCH}_3]$ are described. The reduction of $[(\text{Ar}(\text{R})\text{N})_3\text{Mo}(\text{N}-\text{N}[\text{CH}_3]_2)]^+[\text{OTf}]^-$ shows the formation of $[\text{Ar}(\text{R})\text{N}]_3\text{MoN}$ and $\text{HN}(\text{CH}_3)_2$. The single crystal X-ray diffraction structure of $[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}=\text{NSi}(\text{CH}_3)_3]$ is reported.

Introduction

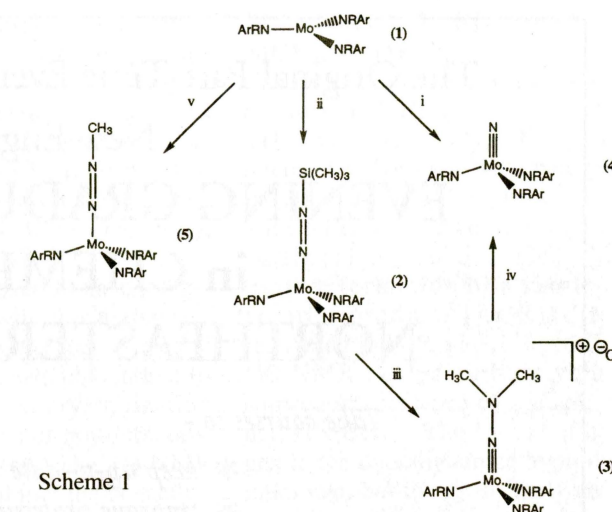
A challenging goal in the field of inorganic chemistry has been the functionalization of atmospheric dinitrogen into potentially useful organo-nitrogen compounds¹. Towards this end, the three coordinate molybdenum complex, $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$ ($\text{R}=\text{t-Bu}$, $\text{Ar}=3,5\text{-dimethylphenyl}$), has been shown to be a potentially useful system², due to its ability to bind N_2 and cleave the dinitrogen triple bond. Peters and Cummins³ have shown that cleavage of the dinitrogen triple bond by $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$ in the presence of atmospheric pressures of dinitrogen can be catalyzed by sodium amalgam, according to reaction i (Scheme 1). Studies of the mechanism of this reaction have revealed an isolatable intermediate, the molybdenum-dinitrogen anion, $[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}_2]^{-3}$. We hypothesized that this species might react with electrophiles *in situ* to "trap" the anion, providing a dinitrogen-containing transition metal complex of the form $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3(\text{N}_2\text{E})$ ($\text{E}=\text{electrophile}$). These complexes might then undergo further reaction to functionalize the nitrogen. Thus far, two $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3(\text{N}_2\text{E})$ complexes have been synthesized, $[\text{Ar}(\text{R})\text{N}]_3\text{MoN}=\text{NSi}(\text{CH}_3)_3$

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Board of Publications

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The Board of Publications is grateful to webmasters Arthur Obermayer and Betty Solbjor for producing the Section home page (<http://www.tiac.net/users/obermayr/nesacs>), and for Arthur Obermayer for hosting the page on his own web site. Nevertheless, we look forward to having the option of using ACS facilities rather than relying on the hospitality of a private site. We need to continue to seek ways to provide more and better material for the home page, both from the pages of *THE NUCLEUS* and from links to other sources, to recruit more volunteers to help



Scheme 1

Reagents and Conditions: i, Na/Hg, N_2 , THF, 25°C; ii, 7 equiv $(\text{CH}_3)_3\text{SiCl}$, Na/Hg, N_2 , THF, 25°C; iii, 7 equiv CH_3OTf , pentane, 25°C; iv, Na/Hg, THF, 25°C; v, 10 equiv CH_3OTf , Na/Hg, N_2 , THF, 25°C

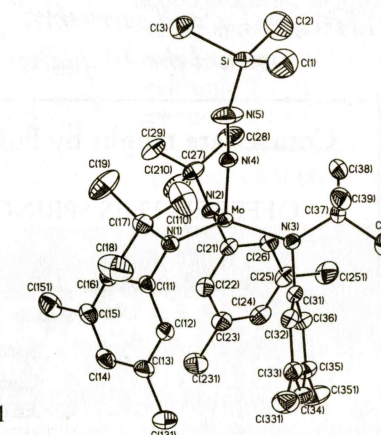


Figure 1

Structural diagram of $[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}=\text{NSi}(\text{CH}_3)_3]$. Selected bond lengths (Å) and angles (°): Mo-N(1) 1.977(2), Mo-N(2) 1.970(2), Mo-N(3) 1.970(2), Mo-N(4) 1.753(2), N(4)-N(5) 1.221(3), N(5)-Si 1.678(3), N(4)-Mo-N(av.) 99.91, Mo-N(4)-N(5) 173.7(2), N(4)-N(5)-Si 157.0(3).

with ideas for the home page, and to maintain good communications between web volunteers and the Board of Publications. On the suggestion of Dr. Obermayer, we are investigating the possibility of using a list server to link members of the Section with common interests; however, it remains to be seen whether this service would be appropriately housed under the oversight of the Board of Publications.

The chair thanks and commends the members of the Board of Publications and particularly the Editor, Associate Editor, Advertising Manager and Business Manager for their efforts in a particularly busy and successful year.

Doris Lewis, Chair, Board of Publications ◇

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Summer Scholar Report

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(2) and $[\text{Ar}(\text{R})\text{N}]_3\text{MoN}=\text{NCH}_3$ (5), and complex 2 reacts further with additional methyl triflate (CH_3OTf) as shown in reaction iii (Scheme 1). All reactions were carried out under a dinitrogen atmosphere using standard Schlenk and dry-box techniques.

Synthesis of

$[\text{Ar}(\text{R})\text{N}]_3\text{MoN}=\text{NSi}(\text{CH}_3)_3$ (2):

Solid orange-red $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$ was dissolved in THF at room temperature and reduced by sodium amalgam in the presence of trimethylsilyl chloride, $(\text{CH}_3)_3\text{SiCl}$ (reaction ii, Scheme 1). Over six hours, the solution changed from red to brown-yellow in color. Filtration and removal of volatiles *in vacuo* provided a mixture of yellow and brown solids. ^1H and ^2H NMR indicated clean formation of a single diamagnetic product. X-ray quality crystals were obtained by cooling a concentrated pentane solution to -35°C , providing orange parallelepipeds in 79% yield. The crystals were further characterized by NMR and IR spectroscopy, and elemental analysis. Salient features of the spectroscopic data include strong $\text{N}=\text{N}$ stretches in the IR at 1644 cm^{-1} (s), 1650 cm^{-1} (s) and 1655 cm^{-1} (sh), and a distinct trimethylsilyl peak in the ^1H NMR spectrum at $\delta=0.49$ ppm. The geometry of 2 is C_{3v} around the molybdenum center on the NMR time scale. The X-ray structure (Figure 1) shows an $\text{N}(4)-\text{N}(5)$ bond length of $1.221(3)\text{ \AA}$, which is within the range for azo compounds. The $\text{Mo}-\text{N}(4)-\text{N}(5)$ and $\text{N}(4)-\text{N}(5)-\text{Si}$ bond angles of 173.7° and 157.0° respectively, suggest that complex 2 is best described as a singly bent diazenido complex⁴. Other notable features of this structure include a short $\text{Mo}-\text{N}(4)$ bond length of $1.753(2)\text{ \AA}$ and a short $\text{N}(5)-\text{Si}$ bond length $1.678(3)\text{ \AA}$.

Synthesis of $[(\text{Ar}[\text{R}]\text{N})_3\text{Mo}(\text{N}-\text{N}[\text{CH}_3]_2)]^+[\text{OTf}]^-$ (3):

Crystalline orange 2 and CH_3OTf were combined in solution in pentane at room temperature and allowed to stir (reaction iii, Scheme 1). The initially

golden solution formed a red-orange precipitate over six hours. The precipitate was purified by washing with pentane. Spectral data of the solid precipitate showed a single clean diamagnetic product (3), recovered in 79.1% yield. The solid was characterized by NMR and IR spectroscopy, and elemental analysis.

Complex 3 proved to have a typical solubility for a salt: it is highly soluble in ethereal solvents such as diethyl ether and THF, and insoluble in hydrocarbons. Attempts at crystallization resulted in formation of powders, oils, or crystalline clusters. The ^1H NMR spectrum of 3 exhibited the N-methyl hydrogen resonances at $\delta=3.73$ ppm, typical of a dimethyl-hydrazido species. A ^{19}F NMR spectrum showed a single fluorine resonance indicative of the triflate counter ion. No $\text{N}=\text{N}$ stretch was visible in the IR spectrum, so the proposed structure of 3 contains a Mo^{VI} species with an $\text{Mo}-\text{N}$ bond order between 2 and 3, and an $\text{N}-\text{N}$ bond order of 1. Attempts to further elucidate the structure, e.g. X-ray diffraction, are in progress.

Reduction of $[(\text{Ar}[\text{R}]\text{N})_3\text{Mo}(\text{N}-\text{N}[\text{CH}_3]_2)]^+[\text{OTf}]^-$:

Complex 3 was added to a stirring mixture of Na/Hg in either C_6D_6 or THF, causing a color change from intense yellow-red to very pale yellow in 20 minutes. The mixture was allowed to stir for an hour total. The Na/Hg reduction of 3 resulted in quantitative formation of a single non-volatile product, $[\text{Ar}(\text{R})\text{N}]_3\text{MoN}$, recovered in 90% yield. ^1H NMR and ^{13}C NMR analysis of the volatiles showed the presence of a single product, $\text{HN}(\text{CH}_3)_2$. The source of hydrogen in the dimethylamine byproduct is unknown, but the most likely sources are either solvent or ligand protons.

Synthesis of

$[\text{Ar}(\text{R})\text{N}]_3\text{Mo}[\text{N}=\text{NCH}_3]$ (5):

$\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$ was dissolved in THF, added dropwise to a stirring mixture of Na/Hg and CH_3OTf in THF and subsequently stirred for several hours. The resulting tan-yellow solution was an opaque suspension that did not noticeably settle upon standing. Filtration of the reaction mixture provided a clear

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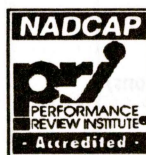
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Summer Scholar Report

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brown-yellow solution. Concentration and addition of pentane resulted in the precipitation of unreacted CH_3OTs . This mixture was filtered, and the solvent was removed *in vacuo*, providing brown-yellow micro crystalline material. By ^1H NMR, the product was a mixture of **4**, $\text{HN}(\text{R})\text{Ar}$, and a new diamagnetic product, **5**. Efforts to completely separate this mixture have been unsuccessful, so far, as the mixture has proven to be highly soluble in many solvents, even at low temperatures (-35°C). Solid samples of the mixture left exposed to dry-box atmosphere at room temperature have exhibited decomposition within 2 days.

Spectral data support the formation of the methyl diazenido complex, **5**. ^1H NMR supports the proposed product (versus **3**), as there is no evidence of a tosylate anion. The chemical shift of the ligand t-Bu hydrogens is significantly shifted from those of the dimethyl species (**3**), and the integration of a peak at $\delta=3.75$ ppm is

consistent with three hydrogens instead of six. IR spectra taken over the course of the reaction show stretches growing in at 1531 cm^{-1} (m) and 1547 cm^{-1} (sh), which may be due to an $\text{N}=\text{N}$ stretch. If so, the $\text{N}-\text{N}$ bond in **4** is more activated than the corresponding bond in **2**.

Conclusion

The $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$ system has proven to be a beneficial system for the exploration of dinitrogen fixation. At this point, functionalization of one-half of the dinitrogen molecule has been achieved through a series of three simple reactions. If compound **5** can be isolated in good yield, it is expected to demonstrate enhanced reactivity through a combination of decreased steric hindrance and higher activation of the $\text{N}-\text{N}$ bond. These reactions demonstrate the ability to add electrons to the $\text{Mo}-\text{N}_2$ system. Extended Hückel calculations on complexes **2** and **5** suggest the distinct possibility of oxidation of these species. Toward this end, it has been shown that **2** is readily oxidized by $[\text{Cp}_2\text{Fe}]^+[\text{OTf}]^-$.

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The Medicinal Chemistry Group is looking forward to another active year serving the Northeastern Section. Watch *THE NUCLEUS* for announcements of our upcoming symposium. If you would like to receive symposia announcements via e-mail, forward your request to msinger@arqule.com. Anyone interested in becoming actively involved in the MCG should contact any of the group's officers. \diamond

Summer Scholar Report

continued from page 16

Efforts to elucidate the nature of the oxidation product are underway. Ultimately, the question to be answered is: can alpha nitrogen be functionalized as well? Based on the stability of **4** and the ease of reducing the $\text{N}-\text{N}$ bond order, it may be a difficult goal to achieve.

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Mar. 3

Prof. Roger Miller (Univ. N. Carolina, Chapel Hill)
"State-to-State Vibrational Dynamics of Polyatomic Molecules Scattered from Surfaces"
Tufts Univ.
Pearson Hall, Rm 106, at 4:30 PM

Mar. 4

Mr. Bill Warren (Waters, Inc.)
"Analysis of Bio-Molecules Using Capillary Electrophoresis"
Univ. Mass, Dartmouth
Science & Eng. Bldg, Rm 305, at 4:00 PM

Mar. 5

Prof. Jeffrey Koberstein (Univ. Connecticut)
"The Molecular Design of Smart Polymer Surfaces"
Univ. Mass, Lowell
Olney Hall, Rm 428, at 3:30 PM

Mar. 8

Prof. Stephen Hanessian (Univ. Montreal)
"Designing Reagents and Reactions for Asymmetric Processes"
Tufts Univ.
Pearson Hall, Rm 106, at 4:30 PM

Mar. 10

Prof. Michael Ward (Univ. Minnesota)
"Nanoporous Solid State Hydrogen Bonded Networks: Molecular Clathrates with Adjustable Properties"
Brandeis Univ.
Gerstenzang, Rm 122, at 4:00 PM

Prof. Anatol Zhabotinsky (Brandeis Univ.)
"Chemical Oscillations, Waves and Patterns"
Tufts Univ.
Pearson Hall, Rm 106, at 4:30 PM

Mar. 11

Prof. Richard Johnson (Univ. New Hampshire)
"Pericyclic Routes to High Energy Molecules"
Boston College
Merkert Chemistry Ctr., Rm. 127, at 4:00 PM
Prof. Gary Epling (Univ. Connecticut)
"Pollution Prevention by Synthetic Design - Development of Nontoxic Alternative Reactions"
Univ. Mass, Dartmouth
Science & Eng. Bldg, Rm 305, at 4:00 PM

Mar. 12

Prof. Alanna Schepartz (Yale Univ.)
"Protein-Protein Interactions in the Control of Protein-DNA Specificity"
Boston College
Merkert Chemistry Ctr., Rm. 127, at 4:00 PM
Prof. Sze Yang (Univ. Rhode Island)
"Double Strand Conducting Polymers: Synthesis and Properties"
Univ. Mass, Lowell
Olney Hall, Rm 428, at 3:30 PM

Mar. 17

Prof. Kathlyn Parker (Brown Univ.)
"Novel Approaches to the Aryl C-Glycoside Antitumor Antibiotics"
Boston College
Merkert Chemistry Ctr., Rm. 127, at 4:00 PM
Prof. Cynthia Friend (Harvard Univ.)
"The Surface Chemistry of Oxidation Catalysis"
Brandeis Univ.
Gerstenzang, Rm 122, at 4:00 PM

Mar. 18

Prof. Adele Wolfson (Wellesley College)
"Chemical Education at the Chemistry/Biology Interface"
Univ. Mass, Dartmouth
Science & Eng. Bldg, Rm 305, at 4:00 PM

Mar. 19

Research Symposium on Advances in Organic Synthesis Methodology
Prof. Peter Beak (Univ. Illinois)
Prof. Gregory C. Fu (M. I. T.)
Prof. Eric N. Jacobsen (Harvard Univ.)
Mass. Inst. Tech.
Room/time TBA

Mar. 20

Dr. Frank H. Stillinger (AT&T Bell Laboratories)
"Living in a Metastable World: A Theoretical Perspective"
Boston College
Merkert Chem. Ctr., Room 127, at 4:00 PM

Mar. 24

Prof. Toyochi Tanaka (Mass. Inst. Tech.)
"TBA"
Brandeis Univ.
Gerstenzang, Rm 122, at 4:00 PM
Zbigniew Jwitzak (Univ. Connecticut)
"Synthetic Analogs of Cell Surface Carbohydrates and Antigens as Potential Anticancer Agents: Dreams or Reality"

Mass. Inst. Tech.
Faculty Club, Glycobiology Dinner Meeting at 6:30 PM
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Prof. Harry Anderson (Univ. Oxford)
"Using Non-Covalent Interactions to Control the Properties of Conjugated Organic Materials"
Tufts Univ.
Pearson Hall, Rm 106, at 4:30 PM

Mar. 25

Prof. Robert McMahon (Univ. Wisconsin, Madison)
"Structure and Spectroscopy of Organic Reactive Intermediates: Relevance to the Organic Chemistry of the Interstellar Medium"
Boston College
Merkert Chemistry Ctr., Rm. 127, at 4:00 PM

Mar. 26

Prof. Marsha Lester (Univ. Pennsylvania)
"Infrared Spectroscopy and Reaction Dynamics of 'Activated' Entrance Channel Complexes"
Boston College
Merkert Chemistry Ctr., Rm. 127, at 4:00 PM
Dr. Richard Schwartzstein (Beth Israel Hospital)
"Cardiac Markers and Length of Stay in the Emergency Department"
NEACC dinner meeting
DoubleTree Guest Suites Hotel, Waltham at 6:00 PM
RSVP Dr. David Drum (617-732-6987, page 11161, e-mail: dedrum@bics.bwh.harvard.edu)

Prof. Alex Jen (Northeastern Univ.)
"Recent Advancement of High Performance Electrooptic Materials for Device Applications"
Univ. Mass, Lowell
Olney Hall, Rm 428, at 3:30 PM

Mar. 31

Prof. Daniel Romo (Texas A&M Univ.)
"Small Heterocycles Doing Big Jobs: Asymmetric Synthesis and Utilization of B-Lactones and B-Lactams in Bioactive Natural Products Synthesis"
Brandeis Univ.
Gerstenzang, Rm 122, at 4:00 PM

Prof. David E. Cane (Brown Univ.)
"Specificity and Versatility in Erythromycin Biosynthesis. From Natural to 'Unnatural' Natural Products"
Tufts Univ.
Pearson Hall, Rm 106, at 4:30 PM

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Centennial Meeting

Because of symposium speakers' prior commitments the Centennial Meeting will be held sometime in the fall, not in April, as previously announced.