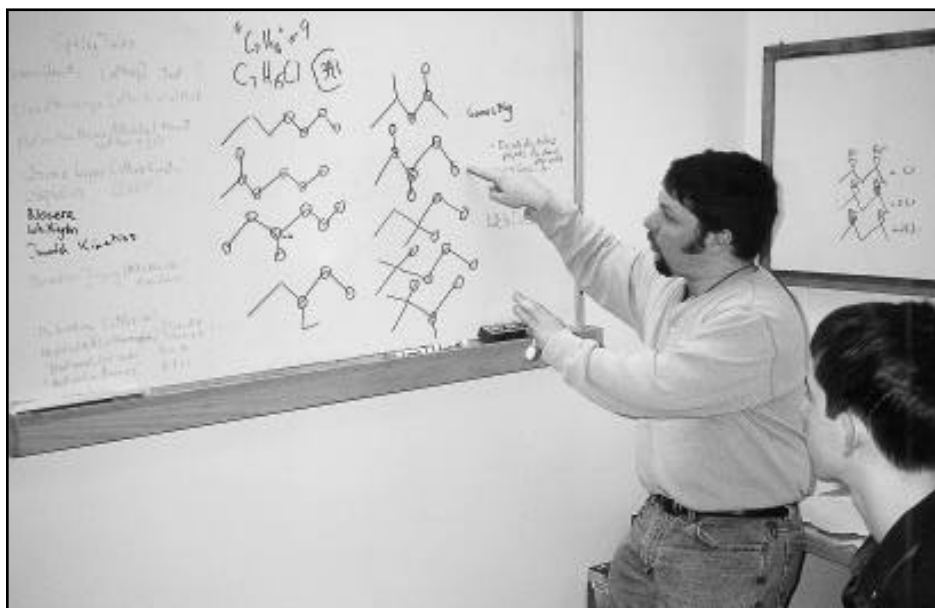


ChemNotes

FALL 1998 – SPRING 1999

The Dual Mission of Chemistry at Tufts: Education & Research



Christopher Morse explains the basic organic chemistry principles taught in Chem 12 to Scott Pherson.

One of the characteristics that distinguishes Tufts Chemistry from other academic chemistry programs is our commitment to the dual mission of teaching and research. While some universities are content merely to be "teaching schools" or "research institutes," we believe that the two endeavors are not only both necessary, but actually reinforce each other. Therefore, we are constantly seeking to advance both areas. In this issue we highlight some new developments in teaching and curriculum development in our department and report on some of the exciting new scientific developments coming from the Pearson and Michael research laboratories.

EDUCATION

The Chemistry Department has a new set of courses in its general chemistry sequence. Chem 11, taught in the fall semester, will be followed by Chem 12 in the spring. Chem 11/12 will offer a higher level alternative (with a 1.5 credit value) to the standard Chem 1/2 sequence. This year, the sequence is being taught by Dr. Christopher Morse, as his first teaching assignment at Tufts.

The students enrolling in Chem 11 are expected to have a minimum score of 3 on the Chemistry AP exam or have had very strong chemistry preparation in high school. With about fifty students in the class, half of the students are premedical and the rest a mixture of

Chair's Corner

Marc d'Alarcao

Several weeks ago I met a graduate of Tufts University who had majored in chemistry in the mid sixties. He was in the Boston area on business and decided to drop by Pearson and visit with some of the faculty he remembered warmly from his college days. I bumped into him (literally) on the first floor of Pearson just outside the large lecture hall (P-104) where so many of our students have heard their chemistry lectures over the years.

I walked with our guest to the Michael Building, which was fully refurbished two years ago. He was deeply impressed with the brand new laboratories, the research posters that hang outside almost every laboratory, and the general buzz of activity of the graduate students, postdocs, undergraduates, and faculty as they worked on the various research projects. I told him of some of the recent exciting research results coming from Tufts Chemistry (see articles elsewhere in this newsletter) and he beamed the smile of a proud alumnus. We then walked around the corner and back into the central part of the Pearson Building, where we poked our heads into some of the old labs and classrooms in the building. As we did his jaw dropped. He was struck by the dramatic difference between the new labs in the Michael Building and the older ones in some parts of the Pearson Building. He remarked that some of the Pearson rooms looked exactly as he remembered them.

This observation really struck me. Some parts of our facility have not been modernized in over thirty years! In the span of a few minutes, we had

continued on next page

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pure science or engineering majors. The initial intent for the class to foster more interest in the pure sciences has been supported by a strong showing of future scientists in the class.

The students have shown great interest in the "Frontiers in Chemistry" seminar. The class meets three days each week. Monday and Wednesday are reserved for regular class lectures, while the Thursday slot can be used for guest lectures. This seminar was the brain-child of Professor Robert Dewald and parallels the Biology Department's equivalent seminar Bio 15 which is now integrated into the standard introductory course.

The Chem 11 lectures are designed so that students with a partial general chemistry background are exposed to cutting-edge research in different areas of chemistry. Lectures this term have included our own Robert Dewald (liquid ammonia solutions), Karl Illinger (infrared properties of gases), and Christopher Morse (fullerenes). The guest lecturers have also been well received. Professor Richard Shader from the Department of Pharmacology gave an exciting lecture on the biological role of St. John's Wort and the flurry of research it has spawned. One of our own graduate students, Lieutenant JG Greg Hall, talked about the chemical aspects of pollution response from his work with the US Coast Guard.

Since the students have strong chemistry backgrounds, there is more time to get into the deeper aspects of each chemical topic, as well as having more time to discuss the real world applications. The class will do more in-depth exploration into topics such as molecular orbital theory and coordination chemistry. This should motivate them to enroll in upper level classes and prepare them more rigorously for these classes.

The Chem 1 laboratory is also being modified for Chem 11. Students are expected to develop the methodology for themselves. The labs are being altered to be more challenging and to include library research to complement understanding of the experiments. In Chem 12, there will be an introduction to more inorganic experiments to balance the physical and analytical labs.

The course has been well received by the students. Several have already decided to enter into a chemistry or



Samuel Kounaves and his graduate students have plenty of work ahead before the Mars Surveyor 2001 Lander heads for the Red Planet after the turn of the century. From left, Vladislav Tarasov, Stefan Lukow, John Birtles, Kounaves, Rosemary Feeny, Melissa Nolan, Sandie Tan and Brian Comeau.

chemistry-related major. Although the students have strong backgrounds, they are still challenged by new aspects of each general chemistry topic. This class should have a bright future as a part of the Tufts curriculum.

RESEARCH

Recent News from the Tufts Chemistry Research Laboratories

Has Life Ever Existed on Mars?

What would be the chemical signatures of such life? What is the chemistry of the Martian soil? What hazards does Martian dust pose to human explorers? These are some of the questions Prof. Samuel Kounaves and his research group are helping to answer during the ten years of planned missions to Mars and other planets in our solar system. They have been selected by NASA's Jet Propulsion Laboratory to participate in the Mars Environmental Compatibility Assessment Project (MECA) on the Mars Surveyor 2001 Lander Mission. MECA is a set of instruments on the Mars '01 Lander, which will attempt to provide answers to many long-standing questions about Mars and eventually about other planets and moons. The 2001 Lander instrument box includes a microscopy station containing optical and atomic force microscopes, an electrometer, a set of adhesion/abrasion plates, and a wet chemistry laboratory

(WCL). The WCL, fabricated by Orion Research, consists of four "chemistry cells" each containing an integrated array of electroanalytical devices, dubbed by NASA an "electronic-tongue." In addition to pH, carbon dioxide, oxygen, redox potential, and ion selective electrodes (ISE), the sensor array includes several microfabricated electrochemical sensors that have been the focus of Kounaves's research and development effort for several years, funded by EPA and NSF. These microsensors will analyze the chemistry of the soil and also determine the presence of any toxic heavy metals. Designing the sensor array, and then using it to analyze the surface material in a remote hostile environment poses a unique set of scientific and analytical challenges. In addition to fitting within a small volume and consuming a minimum of power, the sensors have to withstand temperature fluctuations ranging from -120 to 30 °C and try to anticipate any unexpected chemistry such as an alien environment may present. The Mars Surveyor 2001 is scheduled for launch mid April of 2001 and should land on Mars toward the end of January 2002. More information about this and other research can be found at the Kounaves Research Group web site:
<http://planetary.chem.tufts.edu/>

continued on page 3

Exploring "Structure Space" with Combinatorial Synthesis and Spectrometry.

Over the last three years, Prof. Clemens Richert's research group has developed techniques for finding molecules with new binding properties more efficiently than by the traditional single molecule approach. Their technique has been termed "SMOSE" for spectrometrically monitored selection experiments.¹ It uses small chemical libraries, i.e. collections of molecules synthesized in a single mixed-component reaction, as a source of molecular diversity. After synthesis, the libraries are subjected to a selection process, usually a binding event with an immobilized target molecule or an enzymatic degradation reaction. Unlike previously known assays, SMOSE allows a direct mass spectrometric visualization of the selection process. The structure-affinity relationships thus obtained are used to design the next generation of high affinity molecules. Using SMOSE, the Richert Group has found modifications to short DNA strands that make them more selective in their Watson-Crick base pairing. Another successful application of SMOSE was the elucidation of membrane incorporation effects for porphyrin mixtures that are similar to those clinically used for photodynamic therapy of tumors.

(1) K. Berlin, R.K. Jain, C. Tetzlaff, C. Steinbeck, C. Richert "Spectrometrically Monitored Selection Experiments: Quantitative Laser Desorption Mass Spectrometry of Small Chemical Libraries" *Chem. Biol.* 1997, 4, 63-77.

Tuning the Assembly of Ligands around Transition Metal Ions.

Prof. Elena Rybak-Akimova and her group are seeking to design selective transition metal- based catalysts for oxidation-reduction reactions. Recently, as a part of an effort to activate oxygen in this way, Rybak-Akimova and collaborators were attempting to synthesize a series of macrocyclic ligand complexes of copper or nickel. But a surprising effect was discovered. The assembly of ligands surrounding these ions was found to produce a series of complexes differing in the exact location of double bonds in the macrocycle.² This represents a new type of metal ion control over the outcome of these condensation reactions. Apparently, small changes in the spatial orientation of the double bonds in the macrocycle result in fine-tuning of the coordination sphere of the central metal ion. Beyond the potential synthetic utility, this new effect may help explain the way in which biological transamination reactions catalyzed by vitamin B₆ are controlled.

(2) E.V. Rybak-Akimova, A.Y. Nazarenko, S.S. Silchenko. "Unusual Ligand Isomerization Dictated by Coordination Requirements of the Metal Ion: a Double Bond Shift in Cu(II)-Assisted Template Condensation Between Diacetylpyridine and a Tripodal Tetramine." *Inorganic Chemistry* 1999, in press.

Tufts Analytical Chemists Coordinate a Major Environmental Study in Massachusetts.

Last year, Prof. Albert Robbat and his research group coordinated a hazardous waste site investigation at Hanscom Air Force Base in Bedford, Massachusetts.³ The project was funded as part of the Environmental Technology Initiative, President Clinton's initiative to promote the development and use of innovative environmental technologies. Robbat, working with the federal and state environmental protection agencies and the U.S. Air Force, tested the hypothesis that analytical instrumentation when used in the field to produce data quickly can save both time and money. Results of the study were completed this year. Field instrumentation and methods developed by several New England companies and Robbat's group were used to assess whether contaminated soils posed a risk to groundwater and the surrounding communities. Both metals and organic data were produced in the field to direct the sample collection activity and answer the scientific and engineering questions under investigation. All data were entered into a site visualization map to help facilitate the decision-making process.

A Nose for Land Mines.

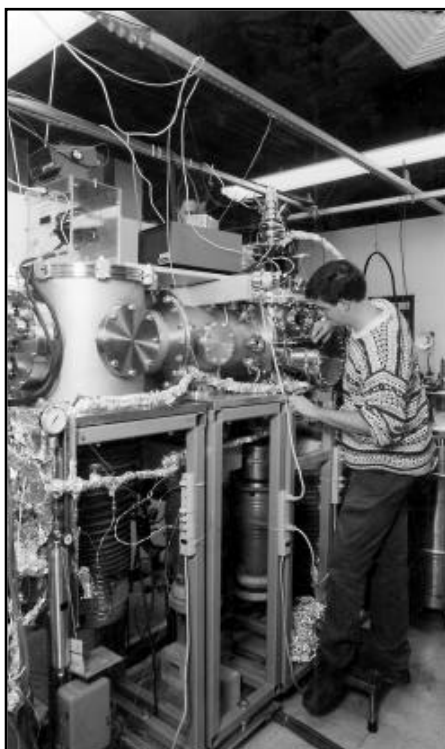
For the last several years, Professor David Walt and his research group have been developing fiber-optic micro- and nanosensors. Recently, Walt and his colleagues have been applying their cross-reactive arrays to the formidable problem of land mine detection. For this effort, work continues on the device known as the "artificial nose" in which cross-reactive sensors are employed to detect complex mixtures.⁴ For land mine detection (as well as for many other applications) the artificial nose has the great advantage over its biological counterpart that it can be attached to a robotic device and operated remotely. A major emphasis of the current work centers on trying to improve the sensitivity of the arrays so that they can achieve the low detection limits necessary to "sniff out" buried land mines.

(4) D. R. Walt *Acc. Chem. Res.* 1998, 31, 267-278.



Graduate student, Colleen Bleczynski, is collecting spectra of DNA on the MALDI-TOF mass spectrometer.

continued on page 4



Graduate student Richard Smith adjusts the alignment of the Utz group's supersonic molecular beam-surface scattering apparatus

Why is Methane so Tough to Crack?

Prof. Arthur Utz and his research group have spent the past several years designing and building a sophisticated experimental apparatus for studying chemical reactivity on surfaces. This powerful apparatus is now up and running, and the Utz group is using it to study the mechanism of methane dissociation on catalytically active metal surfaces.

Methane (CH_4) is the chief component in natural gas. Its heterogeneously catalyzed conversion into carbon monoxide and hydrogen gas is the first step in the industrial production of nitrogen-based fertilizer. In a modern reactor though, only one in a trillion incident methane molecules dissociates into a methyl group (CH_3) and an H atom, both key reaction intermediates that are chemically bound to the catalyst surface. This low reaction probability arises from an activation barrier, whose mechanistic origin remains controversial. In one theory, activation energy is required to deform the tetrahedral methane molecule, expose the central carbon atom to the electron density of

the catalyst surface, and facilitate formation of the carbon-surface bond. Alternatively, that same energy has been postulated to stretch the C-H bond sufficiently for the reaction to proceed.

The Utz group is using ultrahigh vacuum surface science analytical techniques, supersonic molecular beams, and quantum-state-resolved laser excitation to resolve this controversy. Their experiments measure the reactivity of methane molecules that have been prepared (through infrared laser excitation) with a specific vibrational motion prior to their collision with the surface. In this way, the reactivity of a methane molecule containing significant C-H stretching excitation can be compared directly with that of a molecule containing significant bending excitation.

The group's experiments are the first to document the reactivity of a vibrational-state-selected polyatomic molecule in a gas-surface reaction and indicate that C-H stretching motion does not promote reactivity sufficiently to account for previously observed increases in kinetic rates for methane dissociation. Their results strongly suggest that the reaction barrier arises, at least in part, from a need to distort the methane molecule into a geometry favorable for reaction. Experiments that directly measure the reactivity of methane molecules containing bending excitation are currently underway.

Lasers as Tools for Environmental Analysis in the Field.

For some time, Prof. Jonathan Kenny and his group have been developing spectroscopic techniques for analysis of contaminated environmental sites. Recently, Kenny and his group concluded a successful field demonstration of their laser-induced fluorescence probe for in situ characterization of hazardous sites. The instrument utilizes a special laser system to deliver ten different wavelengths (colors) of laser light to the sample, each via a separate optical fiber. The fibers connect the instrument, located in the back of a 20-ton Mack truck, to the underground soil sample, which is accessed by 1.75 inch diameter rods pushed into the earth using a hydraulic press located in the truck. Depending on the types of contaminants present, the laser light is

absorbed and re-emitted as fluorescence, which is collected by a separate set of ten optical fibers and returned to the instrument for wavelength analysis. The wavelength dependence of the absorption and fluorescence by the soil contains information about the types and amounts of contaminants present. A software package developed by post-doctoral fellow Yu-Min Chen allows this information to be extracted and reported efficiently. The work was funded by US EPA and DOD, the latter through the AATDF program at Rice University. The results of field demonstrations at Hanscom Air Force Base in Bedford, Massachusetts, and Otis Air National Guard Base on Cape Cod, have recently been reported in a book.⁵

(5) Jonathan E. Kenny, Jane W. Pepper, Andrew O. Wright, Yu-Min Chen, Steven L. Schwartz, and Charles G. Shelton. "Laser-Induced Fluorescence for Subsurface Contaminant Monitoring," 1999, in press. Ann Arbor Press.



Jonathan Kenny at the portable multiwavelength laser system developed by his group for in situ detection of soil and groundwater contaminants.

Can Sugars be Used to Treat Diabetes?

Diabetes mellitus is one of the most prevalent diseases in the United States with an estimated 15 million people affected. Of these, 5-10% suffer from Type I diabetes which results from an inability to produce the hormone insulin, while the rest have type II diabetes. This latter form of the disease is not due to a deficiency of insulin, but rather to a resistance to the hormone. Type II diabetes can be considered a disease of the insulin signal transduction system.

Previous work has demonstrated that binding of insulin to the cell-surface insulin receptor results in (among other things) the release into the cell of a small inositol-containing phosphorylated oligosaccharide that serves to activate the cell. Such a substance, known as a second messenger of insulin action since it carries the insulin message from the surface of the cell into the interior, is of tremendous interest in the treatment of diabetes mellitus.



Marc d'Alarcao and graduate student Alex Kornienko discussing research.

To this end, Prof. Marc d'Alarcao and his group have been engaged in a program of chemical synthesis of inositol-containing oligosaccharides with the goal of producing synthetic compounds that effectively mimic the natural second messenger. This program has recently lead to the synthesis⁶ of a trisaccharide that is insulin-mimetic in an intact cell. Though this compound is not likely to be a good treatment for

type II diabetes itself (for pharmacological reasons) its synthesis represents an important step in the design of a suitable therapeutic compound for this difficult to treat disease.

(6) C. H. Jaworek, P. Calias, S. Iacobucci, and M. d'Alarcao, *M. Tetrahedron Lett.* 1999, 40, 667-670.

FACULTY & STAFF NEWS

Kimberly Hall is the most recent addition to the office staff. Prior to her employment at Tufts, she was an administrative assistant at Community Work Services in Boston. Kimberly attended Bunker Hill Community College and is interested in continuing studies to obtain a Bachelor's degree. She has already made a positive impact on the department by assuming responsibility for the data base used for graduate student payroll.

Outside interests: Researching her family history, shopping, reading and kick-boxing

Minh Nguyen, Chemistry Laboratory Services Coordinator, joined the Chemistry staff in September. He studied Biochemistry at the Massachusetts College of Pharmacy and has taken additional courses in Analytical Chemistry at the University of Massachusetts and in client/server technology at Clark University.

Minh is currently revising stockroom procedures so that accounting tasks will be completely automated and has implemented ordering on line with Fisher Scientific.

Minh is an avid sports fan and likes listening to music.

The Awards for Outstanding Achievement are given semi-annually to a teaching assistant, staff member and a faculty member for extraordinary contributions to the department. The presentations were made to the following:

SPRING 1998

Teaching Assistant: Robert Simpson

Staff: Charles Amass and Debbie D'Andrea

Faculty: Mary Jane Shultz

FALL 1998

Teaching Assistant: Mauricio Senties

Staff: Sarah Iacobucci

Faculty: Christopher Morse

FACULTY PROFILES

Krishna Kumar, who joined the Chemistry Department this fall, has come to Tufts after a two year stay as a Skaggs Research Fellow at The Scripps Research Institute in La Jolla, California. After a peripatetic childhood, Dr. Kumar studied Chemistry at St. Stephen's College in Delhi, India and graduated with a Bachelor of Science degree with honors in 1991. His undergraduate research work was in synthetic-organic chemistry. Following graduation, he entered the Chemistry Program at Brown University and did graduate work in the areas of organic and biophysical chemistry. He received a Ph.D. degree and was awarded the Sigma-Xi award by the Research Honor Society for excellence in graduate research.

In 1996, Dr. Kumar moved to the west coast for his post-doctoral research at The Scripps Research Institute where his research broadly focused upon peptide chemistry, paleobiochemistry, and the origin of life.

Of Tufts's rejuvenated graduate research program in chemistry, Dr. Kumar says, "What they've put on paper, and achieved in the last few years by refocusing their efforts in traditional university-wide strengths is incredibly exciting. Many people in my field are watching to see what happens."

Dr. Kumar brings with him considerable expertise in the diverse areas of peptide chemistry, biological autocatalysis, and physical-organic chemistry. He has taught chemistry at Brown University, contributed to a teacher training program at Scripps and was also vice-president of the Society of Fellows at Scripps. During his tenure, the society started several new projects, most notable of these are career services for postdoctoral research associates and the institution of a world-class lecture series with approximately ten speakers a year.



Krishna Kumar

In the coming year, Dr. Kumar plans to teach a course on "Bioorganic Chemistry" at Tufts, with a truly interdisciplinary perspective combining aspects of chemistry, biology, physics and computer science. Given the diverse nature of research pursued in earlier education, Dr. Kumar is an excellent candidate to develop and teach such a course.

Christopher Morse has been appointed lecturer for the Chemistry Department for the next three years. He received a Bachelor of Arts degree in 1993 from Dartmouth College, where he did honors thesis on "The Synthesis of Fluorinated Cyclopentadienyl Ligands" in the laboratory of Russell Hughes. Following that, Dr. Morse earned a Ph.D. in inorganic chemistry in the laboratory of Alan Davison at Massachusetts Institute of Technology where he completed his dissertation on "The Synthesis and Reactivity of Rhenium and Technetium Polyaryyl Complexes" as an NSF Predoctoral Fellow.

While at heart, Dr. Morse is a synthetic organometallic chemist, his real leanings and achievements are in the field of chemical education. At MIT, he taught three different versions of freshman general chemistry. His experience as a teaching assistant in the chemistry department, helped him to plan the curriculum for and teach in

Project Interphase which is a summer program designed to prepare incoming freshmen from rural and inner-city schools for the rigors of MIT course work in the sciences. At the same time, Dr. Morse served as the chemistry course coordinator for the MIT Experiment Study Group (ESG), a program for highly motivated freshmen. At MIT, he was awarded the departmental teaching award, as well as, the Goodwin Medal, a prestigious award given to the graduate student who demonstrates "conspicuously effective teaching."

In his spare time, Dr. Morse works on his ice hockey skills and in the off-season is a coin collector. He is an avid trivia fan and even appeared on the game show Jeopardy!

Now that Dr. Morse is at Tufts, he is teaching and creating the new course series Chem 11/12 (see article elsewhere in this issue). He said that he "hopes to get to teach all the different incarnations of general chemistry here.



Christopher Morse

I really love to teach freshmen and to get them excited about the field." In addition to working on his own classes, he will be spending a large portion of his time researching chemical education.

Chair's Corner,

continued from page 1



Marc d'Alarcao

seen in the Michael Building what dedication and generous support from the Tufts family can accomplish, and in the Pearson Building, what still needs to be done.

As I write these lines, we are about to begin Phase II of the Tufts Chemistry renovation project. In this project, we plan to complete the full renovation of the chemistry facilities that began a few years ago with the renovation of the Michael Building. This renovation is vital for both the research and teaching missions of our department. The areas to be refurbished include the second floor of Pearson, an area that will be entirely dedicated to teaching laboratories. Thus we will have new organic chemistry and analytical chemistry labs to complement the recently renovated general chemistry and physical chemistry labs on that floor. The renovation will also provide modern space for four research groups, new administrative space for the department, and a new 225 seat lecture hall.

In the next several months, I will be working with former chairman David Walt and other members of the Tufts faculty and administration to raise funds for this major project. The administration has made it clear to the department that administration support is contingent on successful external fund raising. The Chemistry alumni and other friends of the department were extremely generous and supportive as we worked through the first half of this project and I am confident we can call on our friends again now as we prepare to finish the job.

CLASS NOTES

1949 Charles R. McCrossan, now retired, began his career in 1949 as a chemist at American Smelting and Refining in Denver, Colorado. He returned to the east coast in 1951 to work at National Research Corporation in Cambridge, MA as an analytical chemist. He was made laboratory manager in 1963 and also was responsible for the electrical testing lab which fabricated a Ta capacitor. During his career, Mr. McCrossan frequently relied on the classical methodologies he learned as a student at Tufts. "If there was a dispute over a result after many repeats, I would usually drag out the old classical methods and, with a prayer to Professor Littlefield, I'd produce a result that would be believable and impeccable."

1983 Robert H. Tykot is Assistant Professor of Anthropology at University of South Florida in Tampa. After obtaining an MA in Classical Archaeology from Tufts (1984), he received an MA(1993) and PhD(1995) from Harvard University. He specializes in the elemental and isotopic analysis of archaeological materials including obsidian, marble, bone and metal and conducts field work in the Mediterranean. Two of his recent publications are in the American Chemical Society Symposium Series, volume 625(1996). You may visit his web page (<http://luna.cas.usf.edu/~rtykot/index.html>) or contact him by email (rtykot@chumal.cas.usf.edu)

1993 Michelle S. Littleton is teaching science at Carver High School in Westford, MA. She received her Master's degree in Education from University of Massachusetts in Lowell.

1994 Susan Stokes (Fox) is finishing her Ph.D. studies in organic chemistry under Daniel Rich at the University of Wisconsin-Madison. Email fox@chem.wisc.edu

1997 Susan Cobern is teaching chemistry at Wellesley High School in Massachusetts. She is planning to return to Tufts for a Master's degree in education.

1998 Tommaso Vannelli is currently pursuing a doctorate in Chemistry under Timothy Kerpshin at University of California at San Diego. He is a recent recipient of the Teddy Traylor Fellowship at UCSD and is studying porphyrin and phenanthroline photochemistry and photophysics.

Correction:

1957 Jack R. Pitman is retired and living on the Atlantic Coast of Florida.

IN MEMORIAM

1943 Olaf Knute Olsen died on December 19, 1997 following a long illness. He played on the Tufts baseball team and was a loyal Red Sox fan. He was a senior engineer at Lucent Technologies (formerly AT&T) in North Andover, MA. until his retirement.



SEMINAR SERIES fall 1998

August

- 26 Prof. Daryle Busch,
University of Kansas
*The Life and Times of Small Molecule
Dioxygen Carriers*

September

- 15 Prof. David Bartel, MIT/Whitehead
Institute
*Creation and Evolution of New
Ribozymes*
- 22 Prof. Patricia Mabrouk,
Northeastern University
*New Insights into Horseradish Peroxidase
Structure from Resonance Raman in
Benzene Solution*
- 29 Prof. George Ewing, Indiana University
*Thin Film Water: Its Measurement,
Properties and Chemistry*

October

- 6 Prof. William Bachovchin,
Tufts University
*Hydrogen bonds: What are they exactly,
and what are they doing in enzyme
active sites?*
- 20 Prof. Andrew Hamilton, Yale University
*The Design of Artificial Receptors for
Protein Surface Recognition*
- 27 Prof. Roma Tauler,
University of Barcelona
Multivariate Resolution in Chemistry

November

- 3 Dr. Michael Gait, MRC Laboratory
Cambridge
*Chemical Approaches to RNA Structure
and Function*
- 10 Dr. Bruce Kay, Pacific Northwest
National Laboratory
*Molecular Beam Studies of Kinetic
Processes in Nanoscale Films of
Amorphous Ice*
- 17 Dr. Mark Murcko,
Vertex Pharmaceuticals
*The Design of Amprenavir, a Potent
Inhibitor of HIV Protease*
- 24 Prof. Robert Griffin, MIT
*Solid State NMR Studies of Energy
Transduction in Bacteriorhodopsin*

SEMINAR SERIES spring 1998

January

- 26 Dr. Kai Johnsson, University of
Bochum
*Free Radical Reactions of Isoniazid;
Implications for Isoniazid Sensitivity and
Resistance in M. Tuberculosis*

February

- 2 Prof. Don Wiley, Harvard University
*X-ray Structural Studies of Viral Entry
Mechanisms in HIV-1, Influenza, and
Ebola Viruses*
- 9 Prof. Daniel Nocera, M.I.T.
*Two-Electron Mixed Valency - An
Untraveled Road in the World of Energy
Conversion Chemistry*
- 16 Prof. Theodore Cohen, University of
Pittsburgh
*Novel Synthetic Methods Using
Organosulfur and Organolithium
Chemistry*
- 23 Prof. Ingrid Fritsch, University of
Arkansas
*Time and Space in Small Electrochemical
Systems*

March

- 2 Prof. Christopher Seto,
Brown University
*Using the Electrostatic Field Effect to
Design Inhibitors and Mimics of Serine
and Cysteine Proteases*
- 9 Prof. Franz Hillenkamp,
University of Münster
*MALDI Mass Spectrometry of Nucleic
Acids with Wavelengths in the UV and IR*
- 30 Prof. Janice Hicks,
Georgetown University
*Ice Surface Chemistry Relevant to
Stratospheric Ozone Depletion Studied
by Surface Second Harmonic Generation*

April

- 6 Prof. Giacinto Scoles,
Princeton University
*Using Helium Atom Reflectivity to Study
Adsorption on Metallic Surfaces*
- 20 Prof. Gregory Verdine,
Harvard University
*The Secret Life of the Genome:
Enzymatic Processing of DNA*
- 27 Prof. Chad Mirkin,
Northwestern University
*The Programmed Assembly of Nanoscale
Building Blocks into Functional Materials*

All seminars are on Tuesdays at 4:30 PM
in Pearson Hall, Room 106, unless other-
wise noted.

Refreshments served a half hour prior to
seminars in Pearson 102.

Student Study Topics

December 3	Christy DiCologero
December 10	Tatiana Stoppe
April 8	Shannon Stitzel
April 15	Aida Herrera
April 22	Brian Comeau
April 29	Roberto Bosco



We have been updating and adding more content to the department web site. Our site provides information such as course listings, current course material, degree requirements, faculty/staff/student info, the graduate program, special events, links to other chemistry resources, an on-line historical archive, back issues of ChemNotes, and more detailed information about the exciting and ongoing research being carried out by our faculty. The hope is that this resource will provide information for prospective graduate students and alumni and will eventually contain links to many valuable chemistry resources within the department and throughout the world. Check us out and see what is currently going on in the department. You can access our site at:

<http://www.tufts.edu/departments/chemistry/>

We are still collecting information for several new areas including "Alumni Page" where we would like to list as many of you as possible. We would like to include not only names and email addresses but items of interest and WWW links to alumni pages and your areas of current employment or involvement. So please write or e-mail to us if you would like to be included. Let us know where you are and what you are doing!

The web site was created and is maintained by Professor Samuel Kounaves (skounave@at.tufts.edu).

undergraduates

CHEMISTRY MAJOR AWARDS PRESENTED FOR ACADEMIC YEAR 1997 - 1998

The Karapetoff Cobb Award
Divya Agrawal
Kimberly Volkman
Beth Yagielski

The Durkee Angell Award
Mei Zhu Peng

The Durkee Scholarship
Greg Beutner

The Max Tishler Prize Scholarship
Matt Simon

The Victor Prather Prize
Joshua Steinberg

The Marshall Hochhauser Prize
Joshua Steinberg

**American Chemical Society,
Northeast Section, Norris/Richards
Award for Undergraduate Research**
Matthew Simon

BACHELOR'S DEGREES AWARDED 1997-98

Paul Bamba
Gregory Beutner
Beth Birnbaum
Tamaki Hiratsuka
Vanessa Hodgkinson
Zainab Jabur
Mark Jedrychowski
Dwight Kim
Edward Lee
John Moquin
Justin Nelson
Mei-Zhu Peng
John Purviance
Thomas Romano
Marcus Rosencrantz
Steven Schwartz
Conor Shea
Adam Smith
Joshua Stein
Joshua Steinberg
Ruth Wiseman
Dov Yoran

graduates

DOCTORAL DEGREES AWARDED 1998

Steve Baldelli (Shultz) "Sum Frequency Generation of Hydrogen-Bonding Liquid Surfaces"

Sean Hart (Kenny) "Applications of Laser Induced Fluorescence Excitation Emission Matrix Spectroscopy for the Analysis of PAHs"

Sam Mathew (Kenny) "Fluorescence Excitation-Emission Matrix Measurement and Analysis of Groundwater Contaminants"

Stephanie Tai (Illinger) "Vibrational Spectra, Infrared Radiative properties and Transition-State Analysis of CFC Substitutes"

MASTER'S DEGREES AWARDED 1997-98

Hemant Gupta
Lori Martioski
Todd Pagano

more news

Todd Pagano was awarded a fellowship by the U.S. Environmental Protection Agency.

I N S T R U M E N T A T I O N

Written by Clemens Richert for the Instrumentation Committee

Last summer, a new NMR spectrometer was installed in the Chemistry Department. This was made possible through generous support from several institutions and diligent work of several individuals. First, a junior faculty instrumentation grant for an upgrade of the existing Bruker AM-300 spectrometer was funded by the National Science Foundation. This grant was matched by Tufts administration, allowing, in principle, for a replacement of the entire frequency-generating and data processing electronics of the old spectrometer. During the planning phase of this upgrade, Prof. Robert Gonsalves from the Electrical Engineering Department was able to secure the donation of four high-field magnets from Analogic Corporation (Peabody, MA) for Tufts. A committee chaired by Peter Cerundolo from Tufts Development assigned these magnets to individual departments. One was assigned to the Chemistry Department and one to Prof. Bachovchin at Tufts Biochemistry Department. During the summer of 1998, the magnet donated to the Chemistry Department was carefully rebuilt by Charles Amass, the departmental instrument specialist. After several weeks of intense and careful work, which was supported by Larry Aulenback, the manager of the electronics shop, Charles was able to present a magnet that met all specifications of a new superconducting 300 MHz magnet. With some additional matching funds to boost the NSF grant, the stage was set for installation of the second high-field spectrometer in the NMR room in the basement of the Michael Building. The upgrade was converted into the purchase of a new AVANCE 300 console from Bruker Instruments (Billerica, MA) and minor renovations prepared the room for the installation.



Charles Amass, Instrument Specialist, at the new NMR console. At left is the magnet donated by Analogic Corporation.

Besides an inverse probe, digital lock, and digital filter capabilities, the new instrument features the computational capabilities required for modern two-dimensional NMR. Spin-locked experiments can now be acquired routinely, the acquisition of one- and two-dimensional spectra in aqueous solution (90% H₂O, 10 % D₂O) is feasible, and heteronuclear two-dimensional experiments are in the repertoire. With two high-field spectrometers, standard "synthetic" samples can be measured on the older AM-300, leaving longer uninterrupted time blocks for more sophisticated experiments on the new instrument. In addition, faculty can access spectrometers at the Tufts Biochemistry Department and the Francis Bitter Labs at the MIT, an NIH-funded regional facility. The new AVANCE 300 console allows processing of 600 MHz

spectra acquired at the Bitter Labs "at home", as was recently shown for a series of experiments with modified DNA-duplexes, whose processing was performed entirely at Tufts.

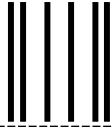
With one three-dimensional structure of a non-Watson-Crick RNA duplex solved (J. Am. Chem. Soc. 1998, 120, 11576-11580. and the structure of an aminoacylated DNA duplex in the refinement phase, the visibility of biomolecular NMR at the Chemistry Department is increasing. With the new instrument and more NMR-intensive research in the department, this trend is expected to continue.

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