IOWA CHEMISTRY

The Newsletter of the University of Iowa Department of Chemistry, May 1998

Development Fund have also generated transition states which have led to enrichment of the educational programs in the Department. This fund has been used to finance travel of graduate students to professional meetings, scholarships for undergraduate and graduate students, and expansion of the seminar programs. We appreciate your support.

This newsletter reports many recent changes in the operations and infrastructure of the Department of Chemistry. These changes have all had transition states which have been energized by dedicated faculty, staff, postdoctoral associates, graduate students, undergraduate students, and alumni. Your interest in the Department of Chemistry is a continuing source of reward and renewed energy for those on the local scene. We all appreciate hearing from you and encourage you to communicate with us about things in your world.

A Message from the Chair

Transition state, a terminology chemists frequently use in discussions of the energetics and mechanisms of reactions, is an appropriate metaphorical reference to many of the recent past and near future situations confronting the Department of Chemistry. Our transition states have been, and will continue to be, associated with changes in faculty composition, research emphasis, space, teaching emphasis and methodologies, and funding. Numerous ideas for future initiatives continue to be evaluated and debated as we approach the new millenium. The faculty and staff of the Department have willingly and unselfishly expended the energies necessary to reach the various transition states associated with recent changes. I continually sense abundant enthusiasm for future initiatives which can further elevate the stature of our department.

Education of our students and scholarly activities which generate new information, our primary objectives, have been significantly facilitated since the completion of the most recent departmental review in 1996. This is because many new resources have come to the Department from the College of Liberal Arts and the Office of the Provost. The most noticeable of these include a large increase in the number of Teaching Assistants, now 60, competitive start-up packages and space renovation funds for new faculty hires, and new sources of non-recurring and recurring funding for instructional equipment including computers.

Recent striking and impressive increases in donations from alumni to the Department of Chemistry

A Note from the Editors

As you read this newsletter you will see many changes in our department. Some characteristics appear to remain constant such as the building, some of the faculty, services, etc; but they are also changing. This newsletter was put together to give you an idea of what is happening in our department. Unfortunately due to space and time limitations we have not included everything. You will have to wait for the next newsletter to hear more! Or for those of you that can't wait visit our web page:

http://www.uiowa.edu/~chemdept Specific details of our faculty can be seen there including publications and research interests. D.C. Tardy and D.F. Wiemer

Alumni

In this age of connectivity we want to inform you of what we are doing in the Department of Chemistry at the University of Iowa. As you read on you will see that many new technologies are being used and developed in the Department. A flavor of some of the research projects can be seen by scanning the list of PhD's (recipent, dissertation title, and advisor) that were awarded in 1996 and 1997 that appears near the end of this newsletter. New courses are being taught and new research projects initiated. We want to enlarge our range of influence and learn even more so that we will continue to grow as we enter the next millenium. We ask you to share with us what you are doing and what you believe will be important future paths for us to pursue. Please do this by dropping us a note, an email (chemdept@uiowa.edu) or fill in the 'boxes' on our web page

(http://www.uiowa.edu/~chemdept/alumni and include the following:

Your name, when you graduated, what degree you received from UI.

Where you are working, what kind of work you are doing.

What you perceive as important directions in chemistry.

What were important courses you took at Iowa

What courses do you wish you had taken (not necessarily those in the Department of Chemistry).

Opportunities at your company, i.e. summer employment for our chemistry majors.

Provide us with your email address and your web homepage.

We will enter this information in a database and include some of it in our next newsletter. We are

hopeful that your help in this endeavor will be beneficial to you and our department.

Graduate Students

Our graduate students continue to attend and present papers at regional and national professional meetings. The average enrollment in the graduate program fluctuates around 100, with spring enrollment being somewhat lower. Our PhD students are spending an average of 5 years to receive their degrees. To give you a glimpse of some of the research projects being done in the department take a look at the list of recently conferred PhD's tabulated in this newsletter.

Many of our graduates are pursuing more specialized research in terms of postdoctoral positions at prestigious academic institutions or national labs; some are working at major industrial firms or on a faculty.

Our graduating doctoral candidates have also received recognition at the national level by receiving the American Institute of Chemistry Awards. Gary **DeBoer** received the award for 1997-98, Michelle **Dreisen** for 1996-97 and Tracy **Rae** in 1995-96.

Undergraduate Students

Our number of undergraduate chemistry majors continues to grow. This February we had 16 freshmen, 19 sophomores, 27 juniors and 40 seniors for a grand total of 102. In 1997 there were 23 chemistry majors who graduated; 8 with the BA and 15 with the BS degrees. Our undergraduates enjoy their undergraduate research experience and their association with a research group. Typically at the end of the spring semester we have a poster session in which they present their results to the department. It is a time that the students gain experience in communicating their results and finding out what others are doing in the department.

This is also the time that awards to our undergraduates are announced. The UI Alumni Awards were presented to:

Seniors: Amy Voelliger (1997-98), Nathan Baker (1996-97), Laura LaBerge (1995-96) Juniors: Michael Harder (1997-98), Amy Voelliger (1996-97), Sarah Holstein (1995-96) **Sophomores**: Ali Djalali (1997-98), David Sosnowski (1996-97), Lynn Woo (1995-96)

The Merck awards for 1997-98, 1996-97 and 1995-96 were received by Michelle Verweyst, Sarah Holstein and Nathan Baker while the Simms Fellowships in 1997-98 were awarded to Amy Voelliger (senior) and John MacMillan (junior). The American Institute of Chemists awards were received by Lynn Woo (1997-98), Sarah Aeilts (1996-97) and Laura LaBerge (1995-96). John MacMillan (1997-98) and Cathy **Spolar** (1996-97) received the Analytical Chemistry Award. David **Sosnouski**, a junior working with Professor Nair received a prestigious Barry M. Goldwater Scholarship for his studies on potential inhibitors of the enzyme reverse transcriptase, which is essential to the replication of HIV.

Our REU program has attracted a variety of chemistry students from across the country (from California to Ohio and Minnesota to Louisiana) to perform research in the summer. These students gain research experience in an environment different from their undergraduate institution. Let us know if you are aware of students that would benefit from such an exposure. Our faculty to student ratio are important ingredients for these REU students to gain enthusiasm in doing chemical research.

Curriculum Revision Leads to New Courses for Chem Majors

The Chemistry Department recently completed introduction of a full four-year curriculum for undergraduate majors, by introducing new freshman and sophomore courses whose enrollment is restricted to "chemical sciences" majors. The new courses include Chemical Sciences I, II, and Laboratory (4:18, 19, and 20), all taught at the freshman level, and Basic Measurements (4:21) and Organic Chemistry I, II, and Organic Laboratory for Chemical Sciences Majors (4:123, 124, and 142) which are taught at the sophomore level.

Because enrollment in these classes is restricted to majors in chemistry, biochemistry, and chemical engineering, class size is much smaller than that in the parallel courses for non-majors. A smaller class size allows closer contact between the students and the faculty throughout the sequence. In the laboratory courses, it also

allows more challenging and open-ended experiments, designed to let students share the excitement of modern chemical research.

A key facet of these laboratory courses is their growing use of sophisticated computer technology and advanced analytical instrumentation. The Chemistry Department's undergraduate computer lab now hosts 20 modern stations (Pentium PC's or Power Macs), while 25 Pentium computers have been purchased for use in the instructional computer lab. These computers are used by students throughout the curriculum, for both specific experiments and in more general applications such as word processing, database management, and literature searches. In addition, FT-IR is now introduced in the freshman level labs, and at the sophomore level students also collect GC-MS data to analyze their experiments and process FT-NMR data to characterize their products. These course improvements should provide our undergraduates with a stronger background whether they seek employment directly upon graduation or pursue a graduate degree.

Several New Staff Join the Chemistry Department

Several new staff members have joined the Chemistry Department over the past year, including Dr. Peter **Sandusky** (NMR Specialist and Staff Scientist), Steven **Bullard** (Undergraduate Laboratory Coordinator), and Jan **Widmer** (Secretary II).

Dr. Sandusky comes to the University of Iowa from Central Michigan University where he was Director of the NMR Facility. He received his PhD from the University of Michigan for EPR studies on photosynthesis, and has done postdoctoral research on EPR at Stanford and research on solution conformations of oligonucleotides by NMR at Michigan. At the UI he will work with John Snyder to oversee both the Chemistry Department's NMR instruments and instruments that are formally part of the UI High Field NMR Facility and located in the Chemistry Building. Thus he will oversee the spectrometers we now have, ranging from 300 to 600 MHz, the new 400 MHz instrument on order, and others we hope to acquire in the future. Dr. Sandusky has taken the position formerly held by Dr. Gerald **Pearson**, who retired last year.

Steven Bullard began a new post in the Chemistry Department as Undergraduate Laboratory Coordinator early in the spring semester. His responsibilities include oversight of the famous "preps room" where reagents and equipment are prepared for use in undergraduate lab courses. He comes to us from the Biology Department, where he had been involved in research in molecular genetics for several years. His scientific and chemical background, including a bachelors degree in Biochemistry from Iowa State University, will be put to good use in this new position.

Jan Widmer, formerly from Pediatrics, joined the Chemistry Department staff as a Secretary II in August of 1997. She provides support for our graduate student recruiting and admissions efforts. She also offers assistance to the Summer Undergraduate Research Fellowships (SURF) program, which provides summer research opportunities for undergraduates. Her efforts in these activities ensure that students interested in joining our department have a common contact who can answer most of their questions, or direct them to specific places for further information.

Faculty

Our faculty has undergone many changes since our last newsletter. In the 1990's our list of emeriti professors exhibited a dramatic increase; the 2 decades before the 1990's we had 3 retirements. Between 1992 and 1996 we had 4 retirements: Professors Bennett, Baenziger, **Dovle** and **Pflaum**. And most recently in 1996 and 1997 Professors Edward Buchanan, David Cater and Leodis Davis joined the list. Ed misses teaching but is enjoying his retirement in Iowa City. David is spending the majority of his time in Minnesota while Leo will be moving to Kansas City this summer. Ed, David, and Leo together have provided service to the Department and University for more than 100 years. We wish them the best in their future endeavors.

Professors Johna **Leddy** and Mark **Young** have been promoted to the rank of Associate Professors with tenure.

New Assistant Professors for the 1997-98 academic year were Edward Gillan (materials chemistry and synthesis of new electronic materials) and Jan Jensen (quantum chemistry). Ed is utilizing the advantages of molecular compounds as precursors in the growth of solidstate materials that are technologically important and difficult or impossible to produce by conventional syntheses, namely metastable or thermally unstable phases as single crystals, nanocrystals, or porous solids. Jan is developing computational tools that provide users to extract chemical information from quantum mechanical calculations. His specific interests are in problems related to intra- and inter-molecular bonding, solvation, catalysis, and molecular recognition in general and particularly where they occur in bioorganic and bioinorganic chemistry.

Sonja **Franklin** (bioinorganic and metal--DNA interactions) will join the department in the fall of 1998. She received her Bachelors degree from Carleton College and her PhD from University of California at Berkeley. She received an NIH Postdoctoral Fellowship and did her postdoctoral appointment at Cal Tech with Professor Jacqueline Barton.

Our sad news is the untimely death of Professor Kenneth **Sando** in December of 1997. In addition to his normal teaching and research activities he was also Coordinator of the Freshman Chemistry Program, an important post in our undergraduate program. He will be greatly missed and hard to replace; he was a caring colleague and a personal friend to us all.

Visiting Assistant Professors who have joined the Department in the 1996-1998 years include Professors: Chris Coretsopoulos (University of Illinois), Doris Eckey (University of Minnesota), Lisa Fields (University of Illinois), Galina Goloverda (L.V. Pisarzhevskii Institute, Kiev, Ukraine), Russell Larsen (Harvard University) and Tim Smith (University of California, Berkeley). A few of our recent PhD graduates have also filled the role of Visiting Assistant Professor. They are: Chris Brooks, Jason Burmeister, Scot Pedersen and Steven Schauer. These "visitors" have provided an important contribution to our Freshman and Sophomore level courses.

Our faculty continue to publish in major journals and give invited talks at other major universities

as well as industrial laboratories. Recognition and honors to our faculty are constantly being received. Professor **Gloer** has been appointed to the NIH Study Section in Natural Products Chemistry and Professor Grassian was recently appointed to the 1998 Panel Review of the NSF Chemistry Research Instrumentation and Facilities Programs and the Major Research Instrumentation Program. Professor **Quinn** (bioorganic chemistry, physical organic chemistry on enzymes) was asked to serve on the NIH Biophysical Chemistry Study Section and Professor Wiemer (synthetic and bioorganic chemistry) has served on the Experimental Therapeutics Study Section for the U.S. Army's Breast Cancer Research Program in both 1996 and 1997. In a University-wide competition members of our faculty (Professors Jan Jensen, Dan Quinn and Lou Messerle) received two of the three University Bioscience Research Initiative grants. Professors Mark Arnold (bioanalytical chemistry and biosensor development) and Vicki Grassian (surface science and environmental chemistry) were appointed as University of Iowa Faculty Scholars (only five faculty through the University are selected per year for this prestigious scholarship). They add to the list of five other members of our department who received the award in the recent past. Professor **Jordan** (organometallic chemistry and catalysis) was honored with a British Petroleum Lectureship and was appointed to the Editorial Advisory Board of the Journal of Molecular Catalysis; he serves as Chair of the Organometallic Subdivision of the Inorganic Division of the ACS. Professor Friedrich continues as a reviewer of proposals and programs for the Department of Energy. We are also proud to announce that Professor Gillan received a Camille and Henry Dreyfus New Faculty Award; only 11, five-year, \$25,000 awards were given nationally.

Our faculty continues its service to the University and the College by being on important committees. A few of these assignments include: Advance Research Computer Advisory Committee, Biocatalysis and Bioprocessing Executive Committee, Bioscience Advisory, College Educational Policy Committee, College Executive Committee, Committee on Honorary Degrees, Conflict of Interest Committee, Electron Microscopy Facility, Faculty Senate, Faculty Assembly, Graduate Council, OpticalScience & Technology

Center Executive Committee, CGRER Executive Committee, High Field NMR Facility Advisory Committee, High Resolution Mass SpectrometryAdvisory Committee, Patent Committee, Research Council, and the Task Force on Postdoctoral Appointments.

In spite of our faculty losses we now have a permanent faculty of 24 (not including our visitors) in the Department. This is lower than the 27 we had in the early 1990's. As you can see by the interests of many of our new hires and established research groups in the department, the traditional areas of chemical research are evolving to multidisciplinary projects. We are optimistic that more interdisciplinary positions will be filled and that the department will reach its targeted size determined by the college to be in the low 30's.

Department Instrumentation Update

The quest for first-rate instrumentation is a constant in modern chemical research and instruction. Fortunately, several sources of support have allowed significant acquisitions over the past year.

Two of our most important advances, new computers for our instructional computer lab and the chemistry computer center, have been made possible by internal UI funding. A proposal by Prof. Robert **Coffman** has generated the funds for the purchase of 25 PC's for the instructional computer lab. These Pentium PC's, all equipped with high speed CD drives, will allow discussion or lab sections to explore CD supplements to standard texts, conduct some types of molecular modeling experiments, and investigate video simulations of chemical reactions. A second internal proposal, by Professor Mark Young, secured the purchase of 10 Power Macs and 10 Pentium PC's for the Chemistry Computer Center, which is used by undergraduate majors and graduate students to address their more sophisticated computational needs.

A one time award from the College has allowed purchase of advanced instrumentation for undergraduate laboratory use, including a benchtop GC-MS system and new UV-Vis and FT-IR spectrometers. The institution of laboratory fees for undergraduate lab courses also has taken place this last year, providing a constant resource for building and maintaining

the equipment base for undergraduate instruction.

External funds have been secured from NSF for purchase of a new NMR spectrometer. This instrument, a 400 MHz unit equipped for pulsefield gradient experiments, will be located in the UI High Field NMR Facility on the ground floor of the Chemistry Building. Its acquisition also should help to alleviate the sample load placed on the four high field spectrometers already in the building (2 - 300's, 360, and 600 MHz), although needs for NMR time will inevitably continue to grow, as will needs for other type of analysis. Thus the quest for first-rate instrumentation must continue as well.

NSF Grant Supports Remodeling of 5th Floor SE

The National Science Foundation recently awarded the University of Iowa a grant for \$480,000 as part of its ARI program. This grant, together with matching UI funds, will allow remodeling of the 5th floor southeast wing of the Chemistry Building. Detailed plans have been prepared and construction is set to begin late this spring. Approximately 6,600 square feet of laboratories and support areas will be converted to modern research space for organic chemistry. Darrell Eyman, department chair and principal investigator on this grant, said "This NSF award is wonderful news for our department. It encourages the UI to address some of our space needs immediately by multiplying the effect of internal expenditures, and provides substantial amounts of new research space appropriate for organic research."

This remodeling project will complement work done in the west wing of the Chemistry Building in 1988-1990, and has been designed to interface with the planned remodeling of the NE wing of the building which is projected once construction of the new Biology building is complete. Two research groups, headed by Profs. Gloer and Wiemer will occupy the renovated space. Together their groups currently have 3 postdoctoral scientists, 21 graduate students, and 6 undergraduates. As Dr. Gloer stated, "It has been nice to have a chance to participate in the planning of this project, because it has enabled the students and faculty who will work there to help tailor the space to fit its intended use."

To make way for this renovation, Prof. Leddy will move her research group to the Iowa Advanced Technology Laboratory late this spring. She will lead the fourth chemistry research group in IATL space, joining Profs. Arnold, Simeonsson, and Grassian in this modern facility.

Speaker Programs Continue to Thrive

A number of notable scientists have visited our Department since our last Newsletter, as part of our efforts to introduce our students to the vigor and variety of modern chemical research. Speakers are brought to campus through several mechanisms, including named lectureships such as the university-wide Ida Beam Program and the Department's Wawzonek Lectureship, the Research Frontiers Program, and traditional departmental colloquia and seminars.

Nobel Laureate Mario Molina (MIT) was brought to campus as an Ida Beam Lecturer in the spring of 1997. He presented lectures describing his studies of atmospheric chemistry and the chemical reactions that have led to depletion of the ozone layer. In the fall of 1997, Prof. Albert Meyers (Colorado State University) came to campus to give the eighth Wawzonek Lecture, a series held in honor of the late Prof. Stan Wawzonek and supported by an endowment created by his family, friends, and students. The Research Frontiers in Chemistry program continues to bring noted chemists to campus as visiting professors to present three lectures over a period of several days. These extended visits allow time for meaningful contact between the visitors and our students and faculty. During the 1996-98 school years this series included:

Prof. Fred E. Regnier Purdue University
Prof. F. Albert Cotton Texas A & M
Prof. Richard Schrock MIT
Prof. Alexander Pines University of
California, Berkeley

Prof. Mark Ratner Northwestern

Prof. James Marshall University of Virginia

Finally, our traditional colloquium program continues with a presentation nearly every Friday afternoon, and other speakers are brought to campus for divisional seminars held during the week. While this list of speakers is too extensive to incorporate here, any of our alumni who would like to be informed of talks given in the Chemistry Department should just let us know,

and they will be added to our mailing list. Alumni are always welcome at these presentations. For the 1998-99 academic year, the following Frontiers speakers have been scheduled:

Prof. Stephen Leone
University of Colorado, Sept. 22-24
Prof. David Hercules
Vanderbilt University, Oct. 5-7
Prof. Alan Marshall
Florida State University, Oct. 28-30
Prof. Robin Hochstrasser
University of Pennsylvania, Spring, 1999
Prof. Kendall Houk
UCLA, Mar. 29-31
Prof. Stephen Lippard
MIT, Apr. 26-28

Visiting Research Scientists

Our Department and faculty continue to attract scientists from near and far away. Visitors from Japan, Korea, Taiwan, China, Australia, Russia, and the United States worked on a variety of projects. The title of these projects and sponsoring faculty members follows:

Chemistry of Fluorine-Containing Pyrroles (Burton), Fluorinated Phosphonate Chemistry (Burton), Single Molecule Detection (Geng), Bioactive Natural Products from Chaetomium spp (Gloer), Iron Porphyrin Organometallic Complexes (Goff), Photooxidation of Acetone on TiO₂ (Grassian), Cationic Titanium Alkyl Compounds (Jordan), Palladium Catalysts for Olefin Polymerization (Jordan), Early Metal Carborane Chemistry (Jordan), Magnetically Modified Ion Exchange Polymer Composites (Leddy), Organodiplatinum Chemistry (Messerle). Nucleoside and Nucleotide Synthesis-Inhibitors of HIV Replication (Nair), Laser Enhanced Ionization Studies of Arsenic, Selenium and Osmium (Simeonsson).

Postdoctoral Research

Recent PhD's gain new experiences and broaden their scientific achievements with a postdoctoral position. Postdoctoral associates in our department have not only a diversity in scientific backgrounds but also in the country in which they received the PhD. A list of postdocs that have been associated with the Department, their research projects and collaborating professors follows:

Barry Hu, Near-Infrared Spectroscopic Monitors for Optimizing Protein Crystallization (Arnold); Mark Riley, Near-**Infrared Spectroscopic Monitor for Insect** Cell Cultivations (Arnold); Long Lu, Novel **Chemistry of Fluorinated Vinyl Stannanes** (Burton); Navamoney Arulsamy, Synthesis of Iron(II) Complexes with Vacant Coordination Sites (Goff); Arezki Boudif, **Synthesis of Novel Porphyrin Compounds** (Goff); Andrew Hansen, Magnetic Resonance **Spectroscopy of Heme Peroxidase Enzymes** (Goff); Tracey Rae, Heme Structures of **Mammalian Peroxidase Enzymes (Goff)**; Kari Myli, Selective Photooxidation Reactions in Zeolites (Grassian); Grant Underwood, **Heterogeneous Atmospheric Chemistry of** HNO₃ and O₃ on Mineral Oxide Particles (Grassian); Yan Xiang, Selective Photooxidation Reactions In Zeolites (Grassian and Larsen); J-Francois Carpentier, Organometallic Chemistry Related to Olefin **Polymerization Mineral Oxide Particles** (Jordan); Osvaldo Casagrande, Single-Site Olefin Polymerization Catalysts Based on Trispyrazoyl-Borate Ligands (Jordan); Martyn Coles, Cationic Aluminum Alkyl Compounds (Jordan); Eiji Ihara, Studies on Cationic Group 13 Organometallic Complexes (Jordan); Vladimir Maryin, Synthesis and Dynamic **Properties of d⁰ Metal Olefin Complexes** (Jordan); Catherine Radzewich, Development of New Olefin Polymerization Catalysts (Jordan): Lisa Rosenberg, Metallocene Synthesis (Jordan); Kevin Ross, Metallocene Synthesis (Jordan): B. Thiyagarajan. Chemistry of Aluminum Indenyl Compounds (Jordan); Xomgwamg Zhang, Metallocene Synthesis (Jordan); Jianjun Wu, Solid State NMR Studies of Environmental Catalysts (Larsen); Sudath Amarasinghe, Magnetically Modified Ion Exchange Polymer Composites (Leddy); Gandara Amarasinghe, Cyclooligomerization **Studies of N-aralkylaziridines** (Messerle): Vladimir Kolesnichenko, Early Transition Metal Cluster Chemistry (Messerle); Snajib Bera, Nucleoside Chemistry - Synthesis of Novel Inhibitors of HIV Replication (Nair); Qi Chao, Nucleoside and Nucleotide Chemistry -New Bicyclic Nucleosides as Potential Antiviral Agents (Nair); Paula Francom, Nucleoside Bioconjugate Chemistry (Nair); Erik Larsen, Nucleoside Synthesis - Modified

Antiviral Nucleosides(Nair); Chris Mathe, Synthesis of Novel Nucleosides Targeted at HIV Integrase (Nair); Naozumi Nishizono, Novel Carbohydrate Inhibitors of HIV Replication (Nair); Suresh Pal, Enzyme-Mediated Synthesis of Nucleosides and Nucleotides (Nair); Lea Pickering, Novel Nucleosides as Potential Anti-HIV Agents (Nair); Michael Taktakishvili, Oligonucleotide Chemistry - Novel DNA Models (Nair); Serge Van Calenbergh, Inhibitors of HIV Replication - Nucleoside Bioconjugates (Nair); Thomas Wenzel, Synthesis and Structural Studies of Novel DNA Model Systems (Nair); Deqi Chen, Use of Dihydropyrones as Dienophiles in the Diels Alder Reaction (Totah); Debasis Patra, Transannular Reactions of Macrocyclic Acyliminium Salts (Totah); Junquan Wang, Synthesis of Novel Dihydropyrone Derivatives (Totah)