Chemistry at The University of Kansas

Department of Chemistry
GRADUATE PROGRAM

The University of Kansas
Lawrence, Kansas

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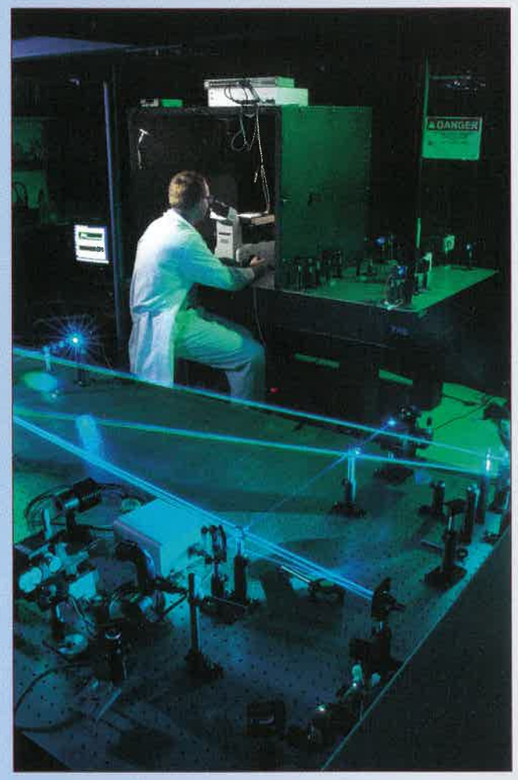

Single molecule fluorescence microscope system and laser source.

On the cover:

Above: The main campus of the University of Kansas is in Lawrence, a city of more than 80,000 in hilly, northeastern Kansas. National Geographic has called the Lawrence campus one of the nation's most attractive.

Below, from left: Preparing an atomic force microscope (AFM) for nanoscale imaging. Chemistry graduate student injecting a peptide sample for MS/MS on the Q-Tof-2 hybrid tandem mass spectrometer. Professor Malinakova and a chemistry graduate student in an organic synthesis laboratory. Chemistry graduate student at a single-molecule fluorescence microscope.

Cover photos by Doug Koch.

Photography by University Relations staff: R. Steve Dick, Kelly Heese, Doug Koch, and Aaron Paden. Produced by the KU Department of Chemistry and KU Office of University Relations, February 2003.

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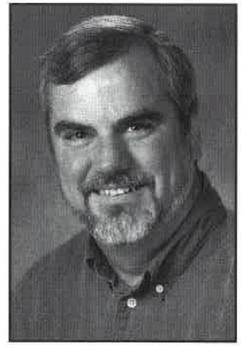
Welcome!

A message from the Chemistry Department Chair



Craig Lunte

Greetings from the Department of Chemistry at the University of Kansas. The fact that you are reading this page is an indication that you may be interested in pursuing a graduate degree in our department.

As you doubtless have realized, the selection of a graduate school is a key step in realizing your career goals. Your choice will not only determine where you will be during the next several years, but will lay the foundation for your career. Your decision to enter a particular graduate program will only be the beginning of exciting challenges and opportunities. During your first year as a graduate student you will decide on a specific area of chemistry and a research adviser. Then you will begin work on an innovative research project that will eventually become your Ph.D. dissertation or M.S. thesis.

At KU, we feel that our program provides excellent opportunities for the graduate student of today who is interested in a career in chemistry. We have a department of outstanding faculty, each of whom is dedicated to providing mentoring to both graduate and undergraduate students and to helping them achieve scientific maturity. The Department of Chemistry at the University of Kansas offers a diverse range of research programs at the leading edge of modern scientific inquiry. In addition to strong programs in the traditional areas of chemistry, we offer interdisciplinary research programs in areas such as bioanalytical, bioinorganic, bioorganic, and biophysical chemistry, chemical physics, and computational chemistry. Among the wide range of research projects available to students are studies in molecular dynamics, supramolecular chemistry, molecular recognition, drug design and development, the theory of molecular relaxation, single molecule spectroscopy, and biosensor design. In addition, programs in chemical education research are available. We maintain these programs with state-of-the-art instrumentation such as that found in the X-ray Crystallography, Instrumentation Design, Mass Spectrometry, and Nuclear Magnetic Resonance Resource Laboratories described later in this brochure.

We are proud of our tradition of excellence in research and of our many former graduate and undergraduate students who have gone on to highly successful careers in chemistry. I encourage you to visit our campus if possible and to correspond directly with either me or other faculty members whose research areas interest you. I hope you will decide that the University of Kansas is your first choice for graduate school.

Craig Lunte
Professor and Chair, Department of Chemistry

The University of Kansas Campus and Lawrence

The University of Kansas opened its doors to its first eager students in 1866 and progressed rapidly to offer full undergraduate and graduate degrees. Today, the University of Kansas is a major educational and research institution with more than 28,000 students and 2,100 faculty members. The university includes the main campus in Lawrence; the Medical Center in Kansas City, Kansas; the KU Edwards campus in Overland Park; a clinical campus of the school of medicine in Wichita; and educational and research facilities throughout the state.

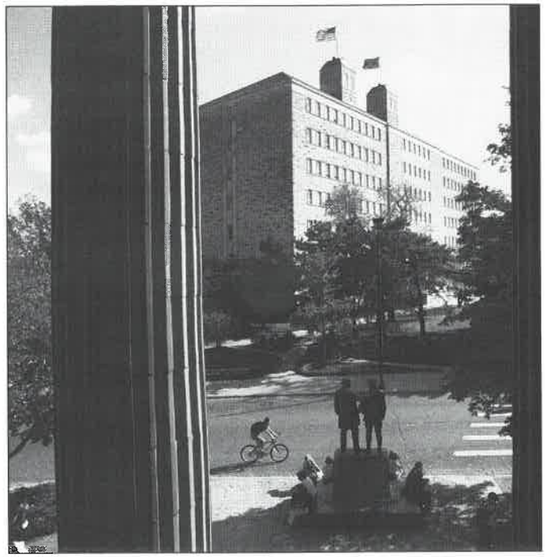
Research is an integral part of the university's educational mission. KU has more than 40 special research facilities, in addition to those in individual departments and schools. The National Science Foundation classifies KU as a major research university receiving substantial research support.

Funding for research at KU has increased rapidly, reaching a level of $243 million in 2002, a $39-million increase in one year.

KU offers a diverse array of cultural and extracurricular activities. The Lied Center, a 2,020-seat performing arts auditorium, is the setting for many cultural events, including concert and chamber music series, theatre and ballet performances, and lectures. In addition, there are classical, popular, and experimental films and special exhibitions and permanent exhibits in the Helen Foresman Spencer Museum of Art and the Natural History Museum and Biodiversity Research Center. Additional activities are organized by the more than 300 registered student organizations. There are sports for spectators and participants, including Big 12 Conference athletics, intramurals, and extensive recreational activities.

Library collections at KU contain more than 3.8 million volumes and many microforms, manuscripts, maps, and photographs. Adjacent to Malott Hall, the Anschutz Library contains more than 470,000 volumes covering chemistry, biology, geology, pharmacy, and physics. The library is equipped for computer searching (e.g., CAS online) of the important databases in the sciences.

The University of Kansas occupies a lovely campus consisting of 1,000 hilly, wooded acres surrounded by the city of Lawrence. The panoramic view of the Kaw Valley from its vantage point atop Mount Oread reflects KU's dominance of the physical surroundings and cultural events in the area.



Fraser Hall seen from the steps of Lippincott Hall on KU's Lawrence campus.

Lawrence, Kansas, lies 40 miles west of Kansas City and 25 miles east of Topeka. In 2000, its population was just over 80,000. The city is home to independent theatres, art galleries, museums, parks, bike trails, and recreation leagues. Lawrence attracts a moderate number of tourists each year because of its unique downtown: a five-block

Lawrence is the perfect blend of small town life with metropolitan amenities.

length of stores, restaurants, art galleries, and clubs that extends along Massachusetts Street, the town's original main street. Along this stretch are trees, benches, walkways and an uncommon blend of the old and new, the preserved and reborn, with many locally owned shops and restaurants.

The treasures of Kansas City are also readily available. Lawrence is a 45-minute drive from a variety of Kansas City attractions: the Country Club Plaza area, museums, galleries, shopping centers, major-league sports, restaurants, and nightclubs. The Kansas City International Airport is less than an hour away and, by using the shuttle services that run from Lawrence to the airport, traveling from Lawrence to other parts of the country is easy and convenient.

The Department of Chemistry

The Department of Chemistry at Kansas provides an environment offering personal attention and collegial interactions among faculty and students, all in a context of vigorous, cutting-edge scientific research and committed teaching. The department has played a central role in recent dramatic advances in research funding and ranking at the University of Kansas, and it is a key participant in the recently launched Life Sciences research initiative in the Kansas City area. A mix of younger faculty bringing in new areas of research and established faculty with productive research programs combines to yield an exciting array of research opportunities.

The Eleanor S. Malott Plaza and Memorial Garden adjacent to Malott Hall.

Our students can look forward to personal development in an atmosphere of interdisciplinary research, collaboration, and mentorship, leading to development as independent scientists and scholars. If this program fits your needs and plans for the future, we invite you to join us.

The Kansas tradition

The Kansas tradition in chemistry goes back 120 years. In 1883, KU was one of the first universities to offer a course in the practical applications of chemical principles to everyday life. In 1905, Professor H.P. Cady, a faculty member in the Department of Chemistry, discovered the existence of helium in natural gas, the first discovery of helium from a terrestrial source. Bailey Hall, the building where this discovery was made, was recently designated a National Historic Chemical Landmark. The tradition of excellence continues today. As the 21st century began, Daryle Busch, Distinguished Professor of Chemistry at the University of Kansas, was the President of the American Chemical Society. The seven female professors in the department — who account for 29 percent of the department's 24 faculty members — give KU the highest percentage of female faculty members among the nation's top 50 chemistry departments, according to a 2002 survey by Chemical and Engineering News.

Forward-looking research programs

The department's research programs and faculty place it at the leading edge of scientific research in areas such as nano-scale imaging, natural-product synthesis, supramolecular chemistry, biosensor design, laser spectroscopy, and enzyme catalysis. Studies in molecular dynamics, supramolecular chemistry and molecular recognition, NMR, mass spectrometry, ultrafast spectroscopy, electroanalytical chemistry, theory of molecular relaxation, and biosensor design are among the many research opportunities.

Building on a strong tradition in chemical education, analytical, inorganic, organic, and physical chemistry, we emphasize interdisciplinary programs in bioanalytical, bioinorganic, bio-organic, biophysical, theoretical, and environmental chemistry.

The chemistry department is at the center of a large community of scientists pursuing chemical research at the University of Kansas, offering many opportunities for interdisciplinary research. Graduate students in chemistry collaborate with scientists in molecular biosciences, medicinal chemistry, and pharmaceutical chemistry. These interdisciplinary teams are engaged in chemical research aimed at understanding basic health-related metabolic processes and development of new drugs.

Our invitation

We invite you to browse through this brochure to see for yourself some of the exciting research opportunities available through the graduate program of the Department of Chemistry at the University of Kansas. Further information is readily available on faculty research group home pages, accessible via the departmental Web site, *http://www.chem.ku.edu*.

The graduate program in the chemistry department offers both the M.S. and Ph.D. degrees. The Ph.D. signifies completion of a substantial project of original research and achievement as an independent scholar in the discipline. The degree prepares students for careers as mature research scientists and science educators. The master's degree provides students with expertise in chemistry with an emphasis on one of its subdisciplines.

Distribution courses

Although the graduate degree involves specialization within the broad field of chemistry, it is vital for graduate students to develop a base of competence in the broader field of chemistry. To this end, introductory graduate courses are offered in analytical, inorganic, organic, physical chemistry, and biochemistry during the fall semester. Incoming graduate students generally take courses in three of these areas. These courses lead students quickly into a productive research program in their specialty.

Joining a research group

One of the most important tasks of graduate students in the first semester is the choice of a research group. To help students make an informed decision, faculty members give short, informal presentations of their research programs early in the semester. Students then discuss research opportunities with several faculty members in their areas of interest before making a decision. Students are encouraged to join a research group by the end of the first semester, so that they will be ready to begin laboratory research the second semester.

Interdisciplinary opportunities

Chemistry graduate students participate in a variety of interdisciplinary projects. Training grants and research institutes focus research effort in challenging areas where future researchers are needed. Participation in training programs provides both a stipend and an excellent setting for interdisciplinary research. Currently traineeship programs in Dynamic Aspects of Chemical Biology, Biotechnology, and Clinical Drug Analysis of Anticancer Agents offer specific opportunities for interdisciplinary programs. KU's Center for Bioanalytical Research, Higuchi Biosciences Center, Center for Supramolecular Materials, Kansas Center for Advanced Scientific Computing, Center for Environmentally Friendly Processing, and Center for Cancer Experimental Therapeutics (a National Institutes of Health Center of Biomedical Research Excellence) bring together faculty and graduate students from chemistry, biology, physics, engineering, pharmaceutical chemistry, and medicinal chemistry, to organize interdisciplinary approaches to complex research problems.

Gaining expertise in chemistry

Along with course work, students gain expertise in their areas of interest through study of specific topics taken from the current scientific literature or related to fundamental areas of their specialties. This work helps students to develop the tools and skills needed in their research programs. Cumulative exams provide the opportunity to track progress. These exams are followed by the formulation of a research proposal, which is presented during the oral comprehensive examination. Upon completion of this milestone, a student's graduate career gains full stride, and the student can place full concentration on a research program.

The dissertation

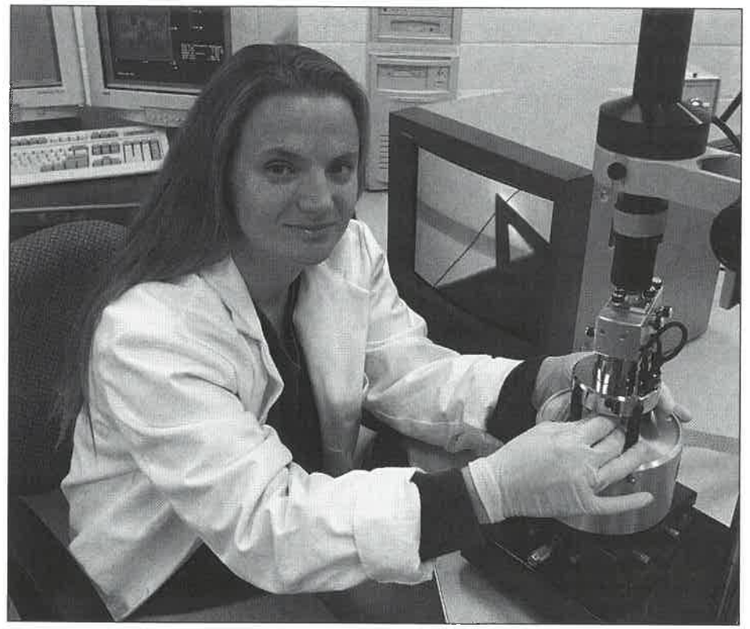
Under the direction of a faculty member or members, each student conducts an original research project. The results of the project are presented in a Ph.D. dissertation (or master's thesis for students seeking a master's degree). The work presented in the dissertation usually leads to one or more publications in scientific literature. These achievements signal the start of a student's career as a mature research scientist. Typically the graduate career, culminating in the Ph.D. dissertation, takes roughly five years.

Graduate courses

Graduate courses taught by faculty members in their areas of expertise provide the opportunity for the student to develop a thorough foundation in a specialization. Students select their course work from the following courses currently offered at the graduate level. In addition, special topics courses bring recent developments in chemical research directly into the graduate curriculum.

Analytical

CHEM 731 Fundamentals and Methods of Analytical Chemistry
CHEM 775 Chemistry of the Nervous System
PHCH 864 Pharmaceutical Analysis
CHEM 903 Electrical Methods of Analysis
CHEM 908 Spectrochemical Methods of Analysis
CHEM 959 Advanced Topics in Analytical Chemistry



A student aligns the tip of an atomic force microscope.

KU has the highest percentage of female faculty members among the nation's top 50 chemistry departments.

Anschutz Library contains most of KU's science holdings.

Chemical education

CHEM 716 Practicum in Facilitating Learning in the Chemistry Laboratory
CHEM 980 Advanced Topics in Chemical Education
CHEM 996 College Teaching Experience in Chemistry

Inorganic

CHEM 737 Coordination and Organometallic Chemistry
CHEM 767 Advanced Laboratory Techniques for the Preparation and Purification of Compounds
CHEM 902 Inorganic Preparations
CHEM 906 Advanced Topics in Inorganic Chemistry
CHEM 982 Inorganic Structure and Mechanisms
CHEM 984 Physical Methods of Inorganic Chemistry
CHEM 986 Bioinorganic and Catalytic Chemistry

Organic

CHEM 740 Principles of Organic Reactions
CHEM 742 Physical Organic Chemistry
CHEM 763 Organic Synthesis I
CHEM 766 Spectroscopic Identification of Organic Compounds
CHEM 963 Organic Synthesis II
CHEM 966 Physical Organic Chemistry II
CHEM 971 Advanced Topics in Organic Chemistry

Physical

CHEM 750 Quantum Chemistry and Spectroscopy
CHEM 752 Thermodynamics and Kinetics
CHEM 909 Statistical Thermodynamics
CHEM 913 Chemical Kinetics
CHEM 915 Intermediate Quantum Mechanics
CHEM 916 Molecular Spectroscopy
CHEM 917 Statistical Mechanics
CHEM 918 Advanced Quantum Mechanics
CHEM 919 Advanced Topics in Physical Chemistry
BIOL 952 Introduction to Molecular Modeling

Financial support

Essentially every graduate student is provided with financial support while pursuing the graduate degree. Graduate teaching assistants (GTAs) assist in the teaching mission of the department, gaining invaluable experience in teaching and scientific communication in the process. Other graduate students, appointed as graduate research assistants (GRAs), carry out grant-sponsored research.

In addition to GTA and GRA support, several opportunities exist for fellowships and traineeships. Fellowships for summer support are available in the department through contributions from various endowment and corporate sources.

Admission to Graduate Study

We invite you to explore further the graduate program at Kansas. The next step is application. The easiest way to begin the process is online, at *www.chem.ku.edu/graduate/gradprog/GradApp2*. Application materials can be downloaded (link from the same address) and sent to:

The University of Kansas
Department of Chemistry, Malott Hall
1251 Wescoe Hall Dr., Room 2010
Lawrence, KS 66045-7582
Telephone: (785) 864-4670, fax: (785) 864-5396
E-mail: *chemistry@ku.edu*, Web site: *http://www.chem.ku.edu*

If you prefer to have application materials sent to you, contact the department at the address, e-mail, telephone, or fax numbers above, and a packet will be forwarded to you.

A completed application includes (1) a Graduate School application form, (2) two transcripts, (3) GRE scores, and (4) three letters of recommendation from individuals familiar with the applicant's background. International applicants must also supply a score from the Test of English as a Foreign Language (TOEFL) exam and the Test of Spoken English (TSE). Applications should be received by April 15 for consideration for enrollment in the fall semester. Applicants should arrange for letters of recommendation and transcripts to be sent as soon as possible, because these can take the most time.

As soon as complete application materials are available, they will be reviewed, and we will be in touch with you. Admission decisions are based on academic training, research experience, and the potential of the applicant for a successful graduate career at KU. Most offers are made from January through March, with fall semester admission preferred; however, we will always consider an application from an outstanding student, regardless of the semester in which they would prefer to begin the program.

Admission requirements

Incoming students should have the equivalent of a bachelor's degree in chemistry — including two semesters of general chemistry, two semesters of organic chemistry with laboratory, one semester of analytical chemistry, and one or (preferably) two semesters of physical chemistry. Minor deficiencies may be attended to in the first year of the graduate program.

After Graduation

Students who have completed the Ph.D. program at KU are prepared to conduct vital, independent research in an academic or industrial setting and to establish careers in teaching and scholarship. Our goal and commitment is to enable students to pursue the career of their choice and to help them achieve their goals. This relationship continues as we help students evaluate available academic, government, and industrial positions or postdoctoral fellowship opportunities. Each year, a number of industrial recruiters, frequently alumni, visit for on-campus interviews. After students leave, we like to keep in touch and continue to offer whatever assistance we can.

The following list is a representative sample of the locations of KU alumni.

Some corporations with KU chemistry Ph.D. alumni

Abbott Laboratories, Amgen Inc., Bayer, BioChem-Pharma Inc., Biogen, Bristol Myers Squibb, Cypress Systems Inc., DuPont, Eastman Kodak, Eltron Research Inc., Johnson&Johnson, Metara Inc., Monsanto Corp., Pharmacia, Praxair, Procter & Gamble, Quest Diagnostics, Quintiles, Rhodia-Chirex, Sigma Chemical Co., 3M Corp., Westinghouse Nuclear, W.T. Gore Co.

Some universities and colleges with KU chemistry Ph.D. alumni

Alcorn State University, Behrend College, Bowling Green State University, California Polytechnic State University, Central Missouri State University, Colorado State University, Dickinson State University, Illinois Wesleyan University, Kansas Wesleyan University, Louisiana State University, McPherson College, Michigan State University, Pennsylvania State University, Rensselaer Polytechnic Institute, Rice University, San Jacinto College, St. Joseph's College, SUNY-Buffalo, Texas A&M at Kingsville, Truman State University, University of Iowa, University of Nebraska, University of Wisconsin at Milwaukee, University of Colombo (Sri Lanka), University of Colorado at Colorado Springs, University of Evansville, University of Maine at Machias, University of Texas of the Permian Basin, University of Wurzburg

National research laboratories/government organizations with KU chemistry Ph.D. alumni

Lawrence Livermore National Labs, Los Alamos National University, National Institute of Science and Technology, Sandia National Laboratory

Facilities

Molecular Structures Group

The Molecular Structures Group manages shared instruments and computational resources used for determining molecular structure across the KU campus. Members of the staff include specialists and technical personnel in the techniques currently represented in the group (see below). They work collaboratively with faculty and students, acquire data for users, train users to operate the instruments themselves, and help with planning experiments and interpreting the data.

Mass Spectrometry. The mass spectrometry laboratory is capable of analyzing samples with a variety of different ionization requirements. They have capabilities to acquire EI, CI, FAB, and ESI data (both low resolution and high resolution). In addition, MALDI-TOF mass spectrometry is available through the BRSL. The mass spectrometry lab routinely conducts exact mass determinations, tandem (MS/MS) experiments, and HPLC separations with MS detection. In addition to submitting samples for analysis, students may be trained to use the equipment, so they can design and run their own experiments.

NMR. The Nuclear Magnetic Resonance Laboratory is responsible for maintaining the high field NMR spectrometers; training users; providing spectra on a service basis; and assisting users with design, execution, and interpretation of NMR experiments. The facility's capabilities extend from small molecules to isotopically enriched proteins, solids, and flow samples. The NMR lab recently underwent a $1.1-million expansion, including a four-channel Varian Inova 600 MHz system suitable for two-, three-, and four-dimensional experiments, LC-NMR, and diffusion measurements. Funding has been procured for the purchase of an 800 MHz instrument. In addition, the facility has upgraded an existing 500 MHz instrument. The addition of these instruments makes the KU NMR lab one of the best-equipped and most modern NMR facilities in the region. For routine NMR on small molecules, KU also houses a Bruker DRX-400 and a 300 MHz NMR.

Loading a sample into the 600 MHz NMR.

X-ray. The Crystallography Laboratory provides X-ray diffraction facilities and services to members of the University of Kansas system. The X-ray instrumentation includes a Bruker-AXS SMART APEX CCD area detector on a D8 platform goniometer with a sealed-tube X-ray generator, a mono capillary collimator, and an Oxford Cryosystems low-temperature device and a Bruker-AXS D8 Advance powder diffractometer with a scintillation detector and a solid-state detector.

Molecular Modeling. The Molecular Graphics and Modeling Laboratory provides access to high-performance computational tools for simulation, visualization, and analysis of chemical and biomolecular processes. The lab supports and assists university research workers through consultation and training in their independent application of modeling approaches to their specific problems.

Available capabilities include molecular modeling, molecular dynamics simulations, as well as *ab initio* and semi-empirical quantum chemistry packages. The lab places four SGI workstations, two PCs, and a 16 processor Athlon cluster at researchers' disposal and supports a broad range of modeling software including most of the SYBYL suite, assorted modules from Insight II and Cerius 2, as well as programs such as AMBER, Gaussian 98, CHARMm, the Cambridge Crystallographic Database, and a broad selection of freeware.

Biochemical Research Service Laboratory

The BRSL houses resources for researchers in biochemistry and molecular biology. Some of the available services include amino acid analysis, protein sequencing, protein purification, and automated peptide synthesis, automated oligonucleotide synthesis, and DNA sequencing. Graduate students can come into the laboratory to learn specific techniques useful to their research and work in the laboratory using available equipment and facilities.

Instrumentation Design Laboratory

The IDL is an analytical resource laboratory that provides collaborative support to research scientists in the natural sciences through custom instrumentation and laboratory automation. Instrumentation and automation are often based on small computers and workstations. Instrumentation solutions to laboratory problems may be developed as "turn-key" systems in which the IDL develops all hardware and software or as a coordinated project where the IDL both consults with a member of a research group and provides hardware and software modules as needed.

Mikhail (Misha) V. Barybin

Organometallic, Coordination, and Supramolecular Chemistry

Assistant Professor

B.S., 1994, Higher College of Chemistry, Russian Academy of Sciences; Ph.D., 1999, University of Minnesota, Minneapolis; Postdoctoral Associate, 1999-2001, MIT, Cambridge, Mass.

Research interests:

Molecular design and supramolecular architecture of electron-rich organometallic and inorganic systems.

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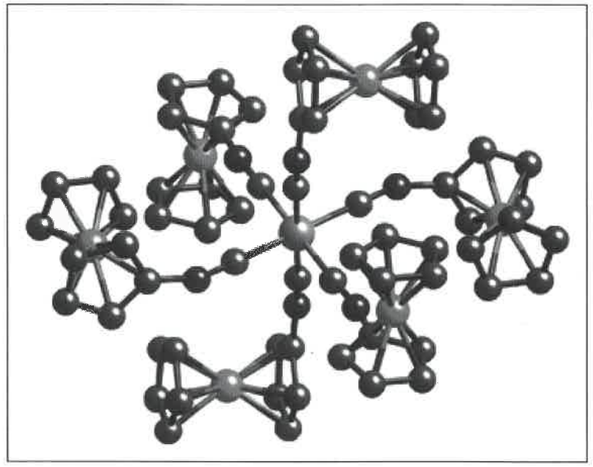
Organometallic chemistry of non-benzoid aromatic isocyanides. Isocyanide complexes of transition metals are of both fundamental and practical interest, particularly because of their valuable role in organic synthesis, catalysis, and radiological medicine. This project is focused on the chemistry of nonalternant aromatic isocyanides, which possess non-benzoid π systems and may be considered derivatives of intrinsically inaccessible $[C_5H_4NC]^-$ and $[C_7H_6NC]^+$. This research will provide new substances whose properties may be attractive for applications in materials science (e.g., non-linear optical devices).

Nano-sized metallopolygons of rare topologies. Macrocyclic compounds incorporating metal ions within their frameworks constitute distinguished examples of molecular aesthetics. Such substances may function as synthetic receptors or sensors in chemical recognition processes and as metallomesogens (liquid crystals incorporating metal ions). We are designing versatile, rigid organic ligands suitable for rational assembly of metallomacrocycles of rare topologies, which can incorporate a wide selection of transition metal ions in a variety of coordination environments and oxidation states.



Molecular wire design. Molecular electronics, a rapidly developing field of modern science, largely relies on facile synthesis of environmentally robust "molecular wires." For molecular conductors to be useful in nanoscale electronic devices, single molecular chains should be electron-rich (i.e., metal-like) and be capable of transporting substantial charge without destruction of their integrity. Taking the above considerations into account, we are establishing a new generation of organometallic molecular wire models containing low-valent metal ions bridged by multiple non-linear, conducting organic spacers.

Selected Publications

1. Barybin, M.V.; Holovics, T.C.; Deplazes, S.F.; Lushington, G.H.; Powell, D. R.; Toriyama, M. First Homoleptic Complexes of Isocyanoferrocene. J. Am. Chem. Soc., **2002**, *124*, 13668-13669.

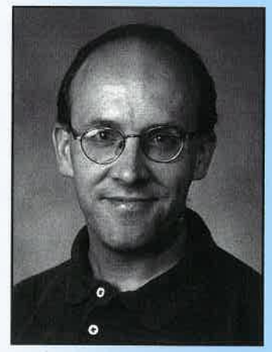
2. Barybin, M.V.; Diaconescu, P.L.; Cummins C.C. Coordination Chemistry of a Chelating Amidoximato Ligand. Inorg. Chem., **2001**, *40*, 2892-2897.

3. Barybin, M.V.; Young, V.G. Jr.; Ellis, J.E. First Paramagnetic Zerovalent Transition Metal Isocyanides. Syntheses, Structural Characterizations and Magnetic Properties of Novel Low-valent Isocyanide Complexes of Vanadium. J. Am. Chem. Soc., **2000**, *121*, 4678-4691.

4. Barybin, M.V.; Young, V.G. Jr.; Ellis, J.E. First Homoleptic Isocyanides of Niobium and Tantalum. J. Am. Chem. Soc., **1999**, *121*, 9237-9238.

David R. Benson

Bioorganic and Bioinorganic Chemistry



Associate Professor

B.S., 1985, Pennsylvania State University; Ph.D., 1990, University of California, Los Angeles; National Institutes of Health Postdoctoral Fellow, 1990-1993, University of California, Berkeley

Research interests:

The chemistry and biochemistry of heme proteins.

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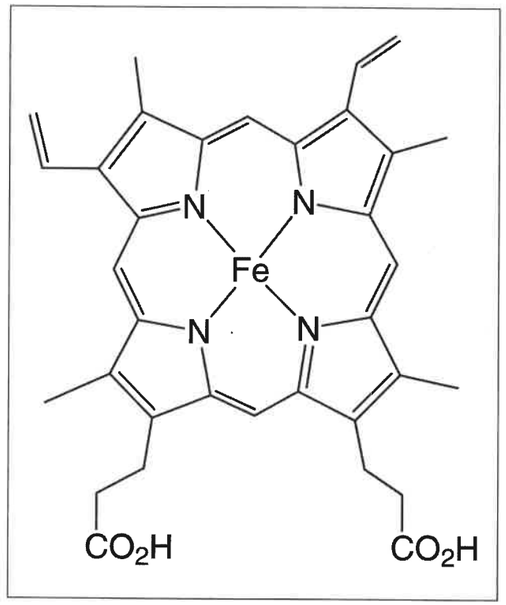
Heme is an iron-containing macrocycle that is an integral component of many proteins in bacteria, plants, and animals. It is the part of hemoglobin that gives blood its red color. Heme proteins participate in a wide array of biological processes, including transport and storage of dioxygen (hemoglobin and myoglobin, respectively), electron transport (*b* and *c* cytochromes), breakdown of hydrogen peroxide (peroxidases and catalases), and hydrocarbon oxidation (cytochrome P450). Part of our group's research effort is directed toward design and synthesis of molecules that contain structural features common to these heme proteins, but which are smaller and therefore easier to study. We have adopted a multidisciplinary chemical approach to investigate how changes introduced into these model compounds influence their structure and function, so that we may improve our understanding of how nature has fine-tuned the corresponding natural proteins to carry out their roles with remarkably high efficiency and specificity. Our studies of model heme proteins are complemented by investigations of their natural counterparts, projects that also offer students the opportunity to learn some basic techniques of biochemistry and molecular biology.



Selected Publications

1. Liu, D.; Williamson, D.A.; Kennedy, M.L.; Williams, T.D.; Morton, M.M.; Benson, D.R. Aromatic Side Chain-Porphyrin Interactions in Designed Hemoproteins. J. Am. Chem. Soc., **1999**, *121*, 11798-11812.

2. Lee, K.-H.; Kennedy, M.L.; Buchalova, M.; Benson, D.R. Thermodynamics of Carbon Monoxide Binding by Helical Hemoprotein Models: The Effect of a Competing Intramolecular Ligand. Tetrahedron **2000**, *56*, 9725-9732.

3. Kennedy, M.L.; Silchenko, S.; Houndonougbo, N.; Gibney, B.R.; Dutton, P.L.; Rodgers, K.R.; Benson, D.R. Model Hemoprotein Reduction Potentials: The Effects of Histidine to Iron Coordination Equilibrium. J. Am. Chem. Soc., **2001**, *123*, 4635-4636.

4. Altuve, A.; Silchenko, S.; Lee, K.-H.; Kuczera, K.; Terzyan, S.; Zhang, X.; Benson, D.R.; Rivera, M. Probing the Differences Between Rat Outer Mitochondrial Membrane Cytochrome b_5 and Microsomal Cytochromes b_5. Biochemistry **2001**, *40*, 9469-9483.

Cindy L. Berrie

Surface and Interfacial Chemistry

Assistant Professor

B.S., 1992, University of Nebraska-Lincoln; Ph.D., 1997, University of California, Berkeley; Postdoctoral Research Associate, 1997-2000, JILA, University of Colorado

Research interests:

Bioanalytical chemistry, protein-surface interactions, surface chemistry, scanning probe microscopy, nanoscale fabrication.

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The chemical composition and morphology of interfaces play a critical role in areas ranging from the growth of semiconductor devices to the design of successful biomedical implants. To understand the details of the molecule-surface interactions that govern these processes, we use scanning probe microscopy techniques for high resolution imaging as well as for the creation of nanoscale patterned surfaces as model substrates. Current projects include investigations of the effect of surface chemistry and structure on fibrinogen adsorption at surfaces, the mechanism by which molecular motor complexes function, and fabrication of unique nanoscale materials and investigation of their electronic properties.

50 nm

Biomolecule-surface interactions. The interaction of biomolecules with surfaces is an important problem in drug delivery, the biocompatibility of implants, and biosensor fabrication. To investigate these interactions, we create nanoscale patterns with controlled size, shape, and chemical functionality in self-assembled monolayer films that serve as the substrates for biomolecule adsorption. By using scanning probe microscopy techniques to probe the substrates, detailed information concerning the conformation of the molecules can be readily extracted under realistic physiological conditions. One specific problem of interest is the plasma protein fibrinogen that plays a role in blood coagulation (thrombosis). The figure shows individual fibrinogen molecules bound to a graphite substrate. The trinodular structure of this molecule is clearly evident. The submolecular resolution attainable with this technique allows variations in protein conformation to be observed on the single molecule level.

Nanoscale patterning of materials. We are developing approaches to nanoscale patterning that are applicable to a variety of substrates including organic thin films on semiconductor surfaces. The ability to pattern these materials on the nanometer length scale has potential applications in designing new devices with unique electronic and optical properties.

Selected Publications

1. Liu, B.; Berrie, C.L.; Kitajima, T.; Bright, J.; Leone, S.R. Atomic Force Microscopy Study of the Growth and Annealing of Germanium Islands on Si(100). J. Vac. Sci. Technol B, **2002**, *20*, 678-684.

2. Liu, B.; Berrie, C.L.; Kitajima, T.; Leone, S.R. Arsenic Induced Ge Island Morphology Changes During Molecular Beam Epitaxy Growth of Ge on Si(100). J. Cryst. Growth, **2002**, *241*, 271-276.

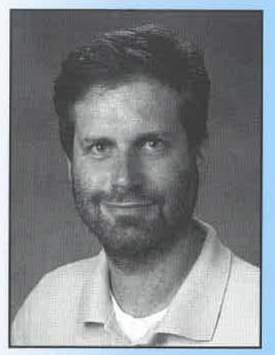
3. Berrie, C.L.; Leone, S.R. Desorption of Arsenic Species During the Surfactant Enhanced Growth of Ge on Si(100). J. Phys. Chem. B, **2002**, *106*, 6488-6493.

4. Berrie, C.L.; Liu, B.; Leone, S.R. Defect Controlled Diffusion in the Epitaxial Growth of Germanium on Si(100). Appl. Surf. Sci., **2001**, *175-176*, 69-76.

5. Berrie, C.L.; Leone, S.R. Observation of Monolayer and Bilayer Period RHEED Oscillations During the Epitaxial Growth of Ge on Ge(100). J. Cryst. Growth, **2000**, *216*, 159-170.

A.S. Borovik

Inorganic, Organic, Analytical, and Bioinorganic Chemistry; Material Science



Professor

B.S., 1981, Humboldt State University; Ph.D., 1986, The University of North Carolina, Chapel Hill; NIH Postdoctoral Fellow, 1987-1988, University of Minnesota; Postdoctoral Fellow, 1990-1992, University of California, Berkeley

Research interests:

Development of bio-inspired systems for catalysis and dispensing of drugs.

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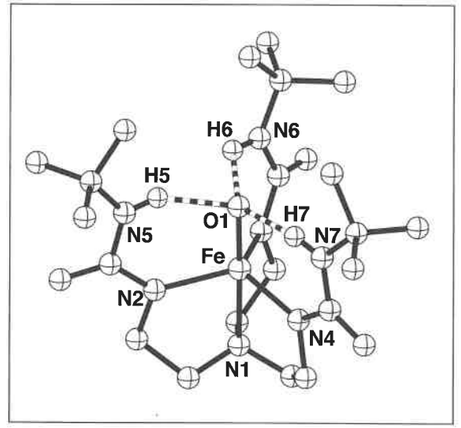
In the Borovik group, synthetic systems are developed that contain structural motifs and functional properties found in the active sites of metalloproteins. Protein active sites have unique architectural features that control the immediate environment surrounding the metal ions. These features, in turn, are instrumental in regulating the activity at the protein-bonded metal ions. The approach used combines organic, inorganic, analytical, and polymer chemistry to design, synthesize, and characterize new metal-containing species. These systems have well-defined organic structures that surround the metal ions, influencing binding and subsequent reactivity of exogenous compounds. The objectives of our research are both fundamental and applied. They include (1) developing design principles for the synthesis of metal complexes with biomimetic structural motifs; (2) examining the binding and activation of dioxygen in metalloproteins; (3) developing new synthetic heterogeneous catalysts having selectivity and rate-enhancement approaching that found in metalloproteins yet able to function under conditions where most biomolecules are unstable and inactive; and (4) fabricating materials for the storage/release and sensing of biologically important compounds. Research is currently divided into two general areas. One involves metal complexes with cavity motifs. The cavities arise from rigid organic frameworks that are appended to custom-designed tripodal ligands. A second area involves the design and fabrication of inorganic/organic hybrid materials. These materials are made from monomeric precursors and are composed of metal complexes immobilized in porous polymers.



Structure of the first isolated Fe(III)-0 complex, which is stabilized by intramolecular hydrogen-bonds (N-H···0).

Selected Publications

1. MacBeth, C.E.; Golombek, A.P.; Young, V.G. Jr.; Yang, C.; Kuczera, K.; Hendrich, M.P.; Borovik, A.S. O_2 Activation by Non-Heme Iron Complexes: A Monomeric Fe(III)-Oxo Complex Derived From O_2. Science **2000**, *289*, 938-941.

2. Sharma, A.; Borovik, A.S. Design, Synthesis and Characterization of Templated Metal Sites in Porous Organic Hosts: Application to Reversible Dioxygen Binding. J. Am. Chem. Soc., **2000**, *122*, 8646-8655.

3. Padden, K.M.; Krebs, J.F.; MacBeth, C.E.; Scarrow, R.C.; Borovik, A.S. Immobilized Metal Complexes in Porous Organic Hosts: Development of a Material for the Selective and Reversible Binding of Nitric Oxide. J. Am. Chem. Soc., **2001**, *123*, 1072-1079.

4. Gupta, R.; MacBeth, C.E.; Young, V.G. Jr.; Borovik, A.S. Isolation of Monomeric $Mn^{III/II}$-OH and Mn^{III}-O Complexes from Water: Evaluation of O-H Bond Dissociation Energies. J. Am. Chem. Soc., **2002**, *124*, 1136-1137.

5. Larsen, P.L.; Parolin, T.J.; Powell, D.R.; Hendrich, M.P.; Borovik, A.S. Hydrogen Bonds Around $M(\mu\text{-}O)_2M$ Rhombs: Stabilizing a $\{Co^{III}(\mu\text{-}O)_2Co^{III}\}$ Complex at Room Temperature. Angew. Chem. Int. Ed., **2003**, *42*, 85-89.

Kristin Bowman-James
Supramolecular and Biomimetic Chemistry

Professor

B.S., 1968, Temple University; Ph.D., 1974, Temple University; Postdoctoral Fellow, Ohio State University, 1974-1975

Research Interests:

Inorganic chemistry: biomimetic and supramolecular chemistry, design and synthesis of selective receptors for ions (particularly anions) of biological and environmental relevance.

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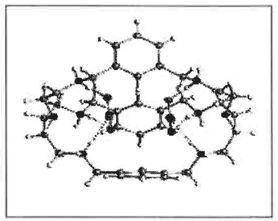
The quest for molecules capable of carrying out specific functions such as selective recognition and catalysis is being pursued in our group. Our research centers around designing molecules to achieve specific chemical goals. A significant portion of our work is targeted toward environmental remediation, for example in the selective identification and extraction of contaminants. Other research focuses on catalysis as well as biomedical areas. In all our research, we use a variety of techniques including X-ray crystallography, NMR spectroscopy, and other analytical methods including potentiometric and electrochemical measurements.

For example, achieving selective recognition of anions is a difficult analytical problem, our group is examining the chemical principles governing anion recognition and using that information to design selective anion receptors. Several different Lewis acid functional groups are being explored, and we have identified certain structural motifs that correlate well with those found in transition metal coordination complexes. These include ditopic (binuclear) complexes (the dinitrate complex **1**), "sandwiches" (the sulfate complex **2**), and "cascade" complexes (the fluoride complex **3**) with a water cascade. These studies are being applied to environmental and/or health-related areas.



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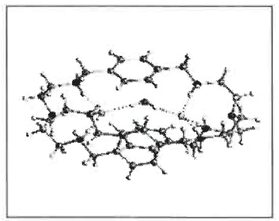

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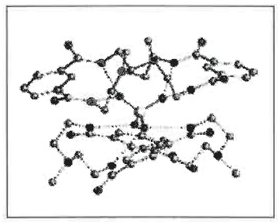


3

The transition metal chemistry of new classes of thioamide macrocycles is also being explored. These new ligands and their transition metal complexes are anticipated to have a major impact on various aspects of catalysis, including C-H and C-C bond activation. Applications in biomedical fields also are being explored, such as DNA intercalation by a novel ditopic palladacycle complex with one of the prototype thioamide macrocycles.

Selected Publications

1. Hossain, M.A.; Llinares, J.M.; Powell, D.; Bowman-James, K. Multiple Hydrogen Bond Stabilization of a Sandwich Complex of Sulfate between Two Macrocyclic Tetraamides. Inorg. Chem., **2001**, *40*, 2936-2937.

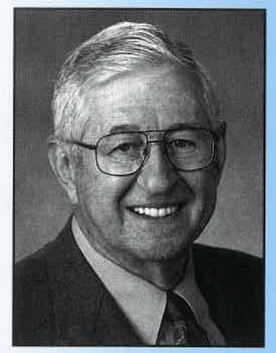
2. Clifford, T.; Danby, A.; Llinares, J.M.; Mason, S.; Alcock, N.W.; Powell, D.; Aguilar, J.A.; García-España, E.; Bowman-James, K. Anion Binding with Two Polyammonium Macrocycles of Different Dimensionality. Inorg. Chem., **2001**, *40*, 4710-4720.

3. Hossain, M.A.; Llinares, J.M.; Mason, S.; Morehouse, P.; Powell, D.; Bowman-James, K. Parallels in Cation and Anion Coordination: A New Class of Cascade Complexes. Angew. Chem. Int. Ed., **2002**, *114*, 2338-2341.

4. Hossain, M.A.; Kang, S.O.; Powell, D.; Bowman-James, K. Anion Receptors: A New Class of Mixed Amide/Quaternized Amine Macrocycles and the Chelate Effect. Inorg. Chem. **2003**, *in press*.

5. *Supramolecular Chemistry of Anions*. Bianchi, A.; Bowman-James, K.; García-España, E.; Eds.; Wiley-VCH: New York, 1997.

Daryle H. Busch
Inorganic Chemistry



Roy A. Roberts Distinguished Professor of Chemistry

B.A., 1951, Southern Illinois University; M.S., 1952, Ph.D., 1954, University of Illinois, Urbana-Champaign

Research interests:

The modern coordination chemistry, bioinorganic chemistry, supramolecular chemistry, homogeneous catalysis.

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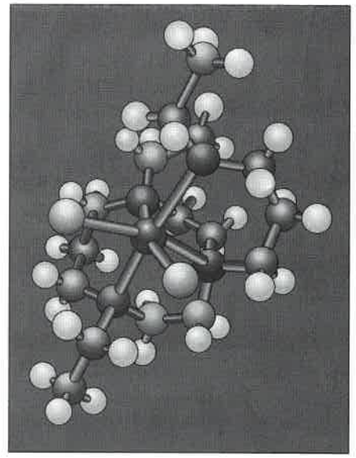
We apply the principles of modern coordination chemistry to the design of functional molecules and green chemical processes. In the area of catalysis, bioinorganic chemistry guides us to study compounds of iron, manganese, copper, and zinc, and the principles of green chemistry cause us to focus on media like water and dense phases of CO_2.We overcome the thermodynamic sink represented by the metal oxides with special ligands and make available aqueous oxidation catalysts of exceptional stability and selectivity. The structure of one of our new oxidation catalysts, a manganese complex, is shown here. Tons of that complex have been made by an industrial partner. In addition to solution and catalytic studies in aqueous media, we have isolated and characterized this catalyst with the metal ion in the +2, +3, and +4 oxidation states and studied the abilities of all of these species to attack substrates.

In collaboration with Professor Bala Subramaniam from the Department of Chemical and Petroleum Engineering, we pursue pioneering investigations into oxidation catalysis in dense phases of CO_2, including mixtures of organic solvents with CO_2, the so-called CO_2-expanded organic solvents. We are exploring the range of known oxidation catalyst types in these media and are finding that special advantages accrue to green systems; i.e., those using the greenest of oxidants, O_2, and simpler versions of a range of known catalyst types.



The federal program to clean up the contamination left by many decades of nuclear weapons production has revealed the need for new chemical tools. Applying those principles mentioned above, we have entered the field in search of ways to make the strongest-binding ligands useful in separations chemistry. It is generally true that the strongest ligands bind very slowly whereas the usual separations techniques require relatively rapid equilibration processes. In a three-pronged approach we seek to exceed the rates of equilibration processes by developing new "switch-binding" methods, and we are exploring a slow methodology that we call a soil poultice. The latter mimics the manner in which single cell organisms extract iron from the minerals in the soil.

Selected Publications

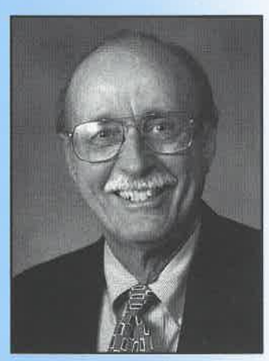
1. Zhang, X.; Busch, D.H. A Totally Synthetic Peroxynitritase Model that is a Post-functional Suicide Catalyst. J. Am. Chem. Soc., **2000**, *122*, 1229-1230.

2. Hubin, T.J.; McCormick, J.M.; Alcock, N.W.; Busch, D.H. A Topologically Constrained Manganese(III) and Iron(III) Complexes of Two Cross-Bridged Tetraazamacrocycles. Inorg. Chem., **2000**, *40*, 435-444.

3. Wei, M.; Musie, G.T.; Busch, D.H.; Subramaniam, B. CO_2-expanded Solvents: Unique and Versatile Media for Performing Homogeneous Catalytic Oxidations. J. Am. Chem. Soc., **2002**, *124*, 2513-17.

4. Clifford, T.; Abushamleh, A.; Busch, D.H. Factors Affecting the Threading of Axle Molecules Through Macrocycles: Binding Constants for Semi-Rotaxane Formation. Proceedings of the National Academy of Sciences, **2002**, *99*, 4830-4836.

Robert G. Carlson
Organic Chemistry



Professor

B.S., 1959, University of Illinois; Ph.D., 1963, Massachusetts Institute of Technology

Research interests:

Synthetic organic chemistry and the development of new synthetic methods.

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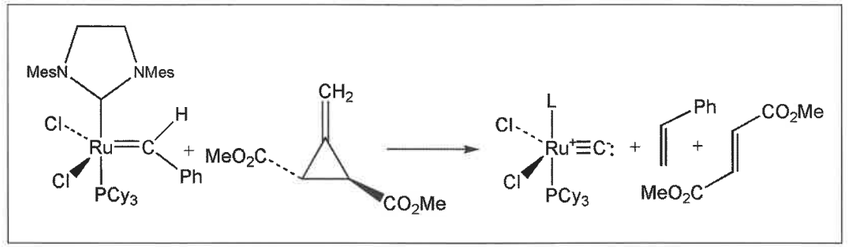
Our chief research interest is in synthetic organic chemistry and the development of new synthetic methods. Recent work has focused on the fascinating reactions of the highly strained methylenecyclopropane system. We are also interested in the design and synthesis of new reagents for the ultrasensitive analysis of bioactive molecules.



Selected Publications

1. Carlson, R.G.; Gile, M.A.; Heppert, J.A.; Mason, M.H.; Powell, D.R., Vander Velde, D. The Metathesis-Facilitated Synthesis of Terminal Ruthenium Carbide Complexes: A Unique Carbon Atom Transfer Reaction. J. Am. Chem. Soc., **2002**, *124*, 1580-1581.

2. Rose, M.J.; Lunte, S.M.; Carlson, R.G.; Stobaugh, J.F. Transformation of Analytes for Electrochemical Detection: A Review of Chemical and Physical Techniques. Advances in Chromatography, **2001**, *41*, 203-248.

3. Takusagawa, F.; Carlson, R.G.; Weaver, R.F. Anti-Leukemia Selectivity in Actinomycin Ananlogues. Biorg. Medicinal Chem., **2001**, *9*, 719-725.

4. Rose, M.J.; Lunte, S.M.; R. G. Carlson, R.G.; Stobaugh, J.F. Hydroquinone-Based Derivatization Reagents for the Quantitation of Amines Using Eletrochemical Detection. Anal. Chem., **1999**, *71*, 2221-2230.

5. Rose, M.J.; Rose, J.M.; Lunte, S.M.; Audus, K.L.; Carlson, R.G.; Stobaugh, J.F. Determination of Angiotensin II in Blood-Brain Barrier Permeability Studies Using Microbore LC with *p*-Nitrophenyl-2,5 -Dihydroxyphenylacetate bis-Tetrahydropranyl Ether as a Pre-Separation Electrochemical Labeling Reagent. Anal. Chim. Acta, **1999**, *394*, 299-308.

Shih-I Chu
Theoretical and Computational Chemistry

Our group is developing new theoretical formalisms and accurate computational techniques for in-depth *ab initio* investigation of chemical, physical, and astronomical problems. Current research interests include multiphoton and very-high-order nonlinear optical processes in intense and superintense laser fields, classical nonlinear dynamics and quantum chaos and fractals, scattering theory and reaction dynamics, complex scaling techniques for many-body resonances, time-dependent density functional theory, quantum dots, coherent control of atomic and molecular processes, quantum computing, Bose-Einstein condensation, and atomic and molecular astrophysics. A few examples are described below:

Atomic and molecular physics in strong fields. The study of the structure, spectroscopy, and multiphoton and high-order (>100th order) nonlinear optical response of atoms, molecules, and clusters in the presence of intense laser fields is a subject of contemporary importance in science and technology. Our group has undertaken a series of pioneering developments of generalized Floquet formulations as well as new time-dependent methods for nonperturbative investigation of various strong-field processes: multiphoton and above-threshold ionization or dissociation of atoms and molecules, the nature of chemical bonds in intense laser fields (bond softening and hardening), multiple high-order harmonic generation, table-top synchrotron, X-ray lasers, genetic algorithm optimization of strong-field processes, etc.

Many-body resonances. "Resonances" are metastable, quasi-bound quantum states that exist in various atomic, molecular, and cluster systems and play an essential role in chemical dynamics. These resonances possess complex energies, whose imaginary parts are related to the lifetimes of the metastable species. Our group is developing complex-scaling generalized pseudospectral techniques for accurate determination of the structure and complex energies of a number of resonance systems, including van der Waals molecules and clusters, and field-induced atomic and molecular resonances.

Time-dependent density functional theory. Professor Chu's group is developing new self-interaction-free time-dependent density functional theory (TDDFT) and associated computational techniques for accurate treatment of the structure and quantum dynamics of many-electron quantum systems (atoms, molecules, clusters, quantum dots, condensed matter). TDDFT opens a wide range of potential applications in science and technology.

Quantum computing. Recently increasing worldwide effort has been directed toward exploring the feasibility of quantum computing (QC). If QC can be realized, it can perform tasks exponentially faster than any classical supercomputer, leading to a revolution in computational technology. In quantum computing, information is manipulated not discretely, in the classical way as a series of zeros and ones (bits), but as continuous superpositions (qubits) where the number of possibilities is vastly greater. Our group is interacting with other experimental groups in exploring the feasibility of solid-state (SQUID) quantum computing technology.

Selected Publications

1. Tong, X.M.; Chu, S.I. Time-Dependent Approach to High-Resolution Spectroscopy and Quantum Dynamics of Rydberg Atoms in Crossed Magnetic and Electric Fields. Phys. Rev. A, **2000**, *61*, 031401-1 to -4 (Rapid Comm.).

2. Chu, X.; Chu, S.I. Self-Interaction-Free Time-Dependent Density Functional Theory for Molecular Processes in Strong Fields. Phys. Rev. A, **2001**, *63*, 023411-1 to -10.

3. Jiang, T.F.; Tong, X.M.; Chu, S.I. Density Functional Theoretical Study of the Electronic Structure of Quantum Dots. Phys. Rev. B, **2001**, *63*, 045317- 1 to -9.

4. Yang, Y.; Han, S.; Chu, X.; Chu, S.I.; Wang, Z. Coherent Temporal Oscillations of Macroscopic Quantum States in a Josephson Junction. Science, **2002**, *296*, 889-892.

Watkins Distinguished Professor and Director of the Kansas Center for Advanced Scientific Computing

B.S., 1965, M.S., 1968, National Taiwan Univ.; D.Sc., 1971, National Tsing Hua Univ.; Ph.D., 1974, Harvard Univ.; Research Associate, JILA (Joint Institute for Laboratory Astrophysics), Univ. of Colorado, 1974-76; J. Willard Gibbs Lecturer, Yale Univ., 1976-78; Alfred P. Sloan Fellow, 1980-84; JILA Visiting Fellow, 1985; John Simon Guggenheim Fellow, 1987-88; Fellow of American Physical Society, 1988

Research interests:

Theoretical and computational chemistry, atomic and molecular physics in intense laser fields, quantum computing.

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Heather R. Desaire

Mass Spectrometry: Bioanalytical and Physical Organic Applications

Assistant Professor

B.A., 1997, Grinnell College; Ph.D., 2001, University of California, Berkeley; Associate Scientist, 2002, Quintiles Inc., Kansas City, Mo.

Research interests:

Analytical chemistry; tandem mass spectrometry, HPLC-MS/MS, and CE-MS/MS; organic reaction mechanisms and structural determination of glycoproteins.

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Research in our group uses mass spectrometry to study a variety of molecules, from large glycoproteins to simple bi-functional organic molecules. Structural information about the molecules is obtained using *tandem* mass spectrometry. In a tandem mass spectrometry experiment, the compound of interest is isolated inside the mass spectrometer; then in a second step, it is fragmented. When the fragments are detected, a significant amount of structural information about the original compound is obtained. This technique can be used to characterize glycosylated proteins and small organic molecules, including pharmaceuticals.

Structural analysis of glycoproteins. Glycoproteins are an important class of biological compounds. For example, gonadotropins, small glycoprotein hormones, regulate the activity of the pituitary. While these molecules are important biologically, they are very difficult to study, in part because of structural ambiguity of the carbohydrate on the protein. We take a novel approach to characterizing these compounds. First, the glycoprotein is subjected to enzymatic digestion, and glycopeptides are released. The resulting glycopeptides may be separated and are used in a variety of mass spectrometry studies. Different tandem mass spectrometric methods are explored to find an approach that provides the most structural information possible about the glycopeptides. By performing tandem mass spectrometry on the glycopeptides, we may be able to learn information about the glycoprotein structure that is not accessible using traditional approaches.

Organic reaction mechanisms. Another research focus involves developing a "rule book" for the dissociation reactions observed in tandem mass spectrometry. Currently, there are no rules to explain how dissociations occur during tandem mass spectrometry. We are developing a set of rules to explain when, where, and why dissociations occur, for various types of molecules. Using the fundamental principles of physical organic chemistry, hand-selected model compounds are used to study reaction mechanisms that occur during tandem mass spectrometry. One application of this work includes using our "rule book" to develop new approaches to studying pharmaceuticals. As a long-term goal, we will demonstrate that tandem mass spectra can be as effective as NMR (and much more efficient) to characterize certain types of metabolic byproducts of drugs.

Selected Publications

1. Desaire, H.; Leavell, M. D.; Leary, J. A. Solvent Effects in Tandem Mass Spectrometry: Mechanistic Studies Indicating How a Change in Solvent Conditions and pH Can Dramatically Alter CID Spectra. J. Org. Chem., **2002**, *67(11)*, 3693-3699.

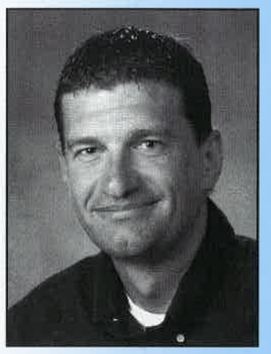
2. Desaire, H.; Beyer, M. K.; Leary, J. A. Molecular Orbital Considerations in Probing the Stereoselective Dissociations of Cobalt-Coordinated Hexosamine Monosaccharide. J. Am. Soc. Mass Spectrom., **2001**, *12*, 517-527.

3. Desaire, H.; Sirich, T.L.; Leary, J. A. Evidence of Block and Randomly Sequenced Chondroitin Polysaccharides: Sequential Enzymatic Digestion and Quantification Using Ion Trap Tandem Mass Spectrometry. Anal. Chem., **2001**, *73*, 3513-3520.

4. Desaire, H.; Leary, J.A. Multi-Component Quantification of Diastereomeric Hexosamine Monosaccharides Using Ion Trap Tandem Mass Spectrometry. Anal. Chem., **1999**, *71*, 4142-4147.

Robert C. Dunn

Bioanalytical, Biophysical, and Physical Chemistry



Associate Professor

B.S., 1988, California State University, Sacramento; M.S., 1990, University of California, San Diego; Ph.D., 1992, University of California, San Diego; Postdoctoral Fellow, Pacific Northwest Laboratory, 1993-1995

Research interests:

Single molecule spectroscopy, model membranes, protein channel dynamics, optical microscopy/spectroscopy, fiber optic sensors, development of novel microscopy techniques.

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The recent emergence of single molecule detection and spectroscopy combined with the continued development in scanning probe techniques offers unique opportunities for probing complex biological systems at the single protein level. We are currently using high resolution techniques such as confocal microscopy, atomic force microscopy (AFM), and near-field scanning optical microscopy (NSOM) to probe the structure and dynamics of membranes and membrane bound protein channels.

Pulmonary lung surfactant. Respiratory distress syndrome (RDS) is the fourth leading cause of infant mortality in the United States and arises from an insufficiently developed lung surfactant. In RDS, the absence of key proteins reduces the surfactant collapse pressure (i.e., compressibility) and the ability of the monolayer to respread during the breathing cycle, resulting in labored breathing, reduced oxygen transport, and often death in those afflicted.

Our laboratory is actively involved in using model membrane systems to understand the more complex natural biological membranes. For instance, we have recently found that the addition of surfactant protein B, one of the key proteins present in healthy surfactant, to model membranes of palmitic acid can induce critical behavior. This is interesting when one considers that large density fluctuations are associated with critical behavior, which may provide clues into how healthy lung surfactant stabilizes the large volume changes associated with breathing.

Protein channel dynamics. The nuclear pore complex (NPC) is a very large complex of proteins that forms the only known passageway across the nuclear membrane in cells. All material transported between the cytoplasm and nucleoplasm must pass through these channels, which makes understanding the mechanisms involved in transport enormously important. Currently, we are using the single molecule techniques in our laboratory to understand the origin of a large conformational change in the NPC that seems to be tied to the presence of calcium in the nuclear envelope. As an example, the figure shows an AFM image of a single NPC in the nuclear membrane. Both the symmetry of the protein channel and the presence of a mass in its center are clearly visible in this high-resolution image.

Selected Publications

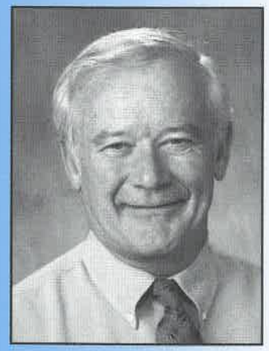
1. Moore-Nichols, D.; Arnott, A.; Dunn, R.C. Regulation of Nuclear Pore Complex Conformation by IP3 Receptor Activation. Biophys. J., **2002**, *83*, 1421-1428.

2. Flanders, B.N.; Vickery, S.A.; Dunn, R.C. Divergent Fluctuations in the Molar Area of a Model Lung Surfactant. J. Phys. Chem. B, **2002**, *106*, 3530-3533.

3. Krogmeier, J.R.; Dunn, R.C. Focussed Ion Beam Modification of Atomic Force Microscopy Tips for Near-Field Scanning Optical Microscopy. Appl. Phys. Lett., **2001**, *79*, 4494-4496.

4. Hollars, W.C.; Dunn, R.C. Probing Single Molecule Orientations in Model Lipid Membranes With Near-Field Scanning Optical Microscopy. J. Chem. Phys., **2001**, *112*, 7822-7830.

5. Vickery, S.A.; Dunn, R.C. Direct Observation of Structural Evolution in Palmitic Acid Monolayers Following Langmuir-Blodgett Deposition. Langmuir, **2001**, *17*, 8204-8209.



Professor

B.S. 1962, Marietta College; Ph.D., 1966, University of Wisconsin; NIH Postdoctoral Fellow, 1966-1967, Iowa State University

Research interests:

The discovery of new photoremovable protecting groups for rapid and efficient release of neurotransmitters, nucleotides, oligopeptides, and proteins.

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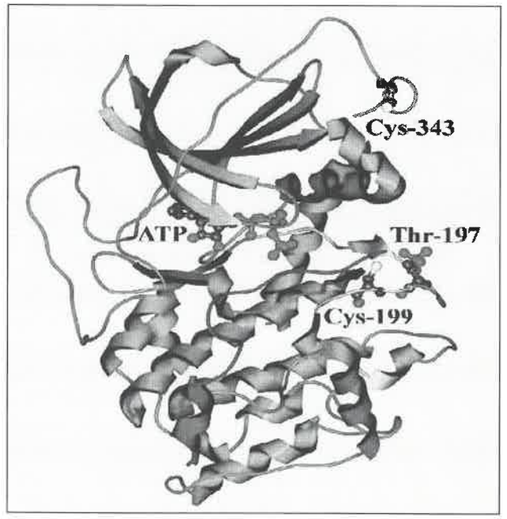
Richard S. Givens

Organic Chemistry

Applications of Organic Photochemistry to Biology and Chemistry

Several new, inherently rapid photofragmentation reactions from the organic chromophore, *p*-hydroxyphenacyl (pHP), are employed to good advantage for the controlled release of bioactive substrates in biological environments. For example, the active site of PKA is switched off by reaction with *p*-hydroxyphenacyl bromide and switched back on by photolysis.

Protected or "caged" substrates such as the *p*-hydroxyphenacyl derivatives of ATP, bradykinin, the active site of the C subunit of protein kinase A (seen here) and the neurotransmitters _-glutamic acid and GABA have been employed for the controlled release of each of these substrates. Photolysis releases the nucleotide or protein with high efficiency and at rates that exceed $10^6 s^{-1}$ up to as high as $10^8 s^{-1}$, much faster than any of the previously known caging derivatives. Greater experimental control of the temporal, spatial, and concentration variables is now afforded for biologists, biochemists, and physiologists who wish to study these bioactive substrates at their target sites.



The C subunit of PKA

A second major thrust is the design and development of a new photoactivated cross-linking agent for lysine rich proteins. Tethered 1,n-diazo- and polyazopyruvates serve as the protein cross linkers that upon irradiation at 350 nm, undergoing Arndt-Eisert rearrangements to ketoketenes that react with lysine to form malonylamide cross linkers. Two diazapyruvates tethered by a polyether were photoactivated to crosslink the lysine rich proteins of Type I collagen in rabbit Achilles tendon and cornea.

Selected Publications

1. Givens, R.S.; Timberlake, G.; Conrad, P.G. II; Weber, J.J.W.; Amslinger, S. A New Photoactivated Crosslinking Agent for Proteins: Applications to Tissue Welding of Type I Collagen. Photochem. Photobiol., **2002**, *76*, 33-39.

2. Zou, K.; Cheley, S.; Givens, R.S.; Bayley, H. Catalytic Subunit of Protein Kinase A Caged at the Activating Phosphothreonine. J. Am. Chem. Soc., **2002**, *124(28)*, 8220-8229.

3. Conrad, P.G. II; Givens, R.S.; Weber, J.F.W.; Kandler, K. New Phototriggers: Extending the *p*-Hydroxyphenacyl π-π^* Absorption Range. Organic Letters, **2000**, *2(11)*, 1545-1547.

4. Conrad, P.G. II; Givens, R.S.; Hellrung, B.; Rajesh, C.S.; Ramseier, M.; Wirz, J. *p*-Hydroxyphenacyl Phototriggers: The Reactive Excited State of Phosphate Photorelease. J. Am. Chem. Soc., **2000**, *122(38)*, 9346-9347.

5. Givens, R.S.; Weber, J.F.; Jung, A.H.; Park, C.H. New photoprotecting groups: desyl and *p*-hydroxyphenacyl phosphate and carboxylate esters. Methods in Enzymology, **1998**, *291*, 1-29.

Associate Professor

B.A., 1985, Luther College; Ph.D., 1993, University of Minnesota; National Institutes of Health Postdoctoral Fellow, 1993-1996, Stanford University

Research interests:

New methods to phosphorus- and sulfur-containing heterocycles; asymmetric methodology; natural product synthesis; and the development of functional polymers as tools for organic synthesis, combinatorial chemistry, and biological delivery.

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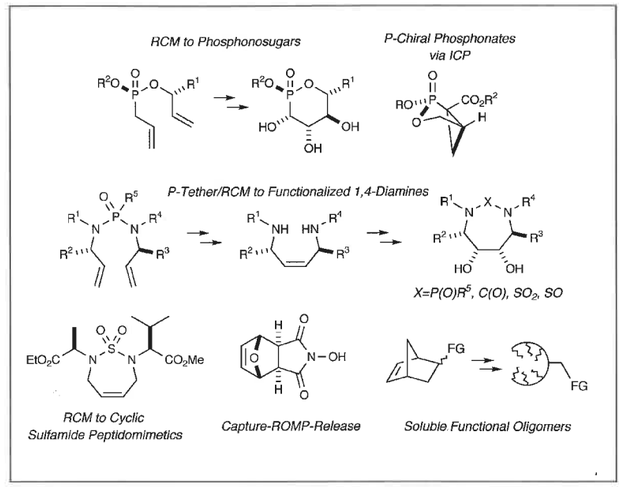
Paul R. Hanson

Synthetic Organic Chemistry, Transition Metal-Mediated Methods, Asymmetric Synthesis, and Functional Polymers

The major goal of our research program is the development of new synthetic routes to structurally diverse phosphorus- and sulfur-containing small molecules and polymers that will serve as pharmaceutical and chemical agents. Our program focuses on the use of transition-metal catalyzed processes to generate an array of novel compounds. In particular, we have focused our attention on ring-closing metathesis (RCM), and intramolecular cyclopropanation (ICP) reactions as a means to produce *P*- and *S*-heterocycles exhibiting both biological and synthetic utility. Central to these methods is the generation of *P*-chiral motifs via desymmetrization processes and/or the use of temporary phosphorus tethers (*P*-tethers). Many of the small molecules are being evaluated for their ability to inhibit several enzymes implicated in cancer, arthritis, acquired immune deficiency syndrome (AIDS), osteoporosis and other disease processes present in humans and in plants.



The other facet of our program is aimed at using ring-opening metathesis polymerization (ROMP) en route to functionalized oligomers as tools for organic synthesis, norbornenyl-tagged reagents for phase-trafficking in combinatorial purification strategies, and biological vehicles for gene and drug delivery. Fundamental to this effort is the development of ROMP technologies such as capture-ROMP-release, scavenge-ROMP-filter, ROMP-scavenge-filter, and soluble ROMP supports.

Selected Publications

1. Dougherty, J.M.; Hanson, P.R.; Klein, T.A.; Moore, J.D.; Probst, D.A.; Robinson, R.E.; Snelgrove, K.A. Ring-Closing Metathesis Strategy to Cyclic Sulfamide Peptidomimetics. Tetrahedron, **2000**, *56*, 9781-9790.

2. Stoianova, D.S.; Hanson, P.R. A Ring-Closing Metathesis Strategy to Phosphonosugars. Org. Lett., **2001**, *3*, 3285-3288.

3. Moore, J.D.; Sprott, K.T.; Wrobleski, A.D.; Hanson, P.R. Double Diastereoselective Intramolecular Cyclopropanation to *P*-Chiral [3.1.0]-Bicyclic Phosphonates. Org. Lett., **2002**, *4*, 2357-2360.

4. McReynolds, M.D.; Sprott, K.T.; Hanson, P.R. A Concise Route to Structurally Diverse DMP 323 Analogs via Highly Functionalized 1,4-Diamines. Org. Lett., **2002**, *4*, 4673-4676.

5. Harned, A.M.; Hanson, P.R. Capture-ROMP-Release: Application to the Synthesis of *O*-Alkylhydroxylamines. Org. Lett., **2002**, *4*, 1007-1110.

6. Harned, A.M.; Mukherjee, S.; Flynn, D.L.; Hanson, P.R. Ring-Opening Metathesis Phase-Trafficking (ROMpt) Synthesis: Multistep Synthesis on Soluble ROM Supports. Org. Lett., **2003**, *5*, 15-18.

Professor and Director of the Center for Science Education

B.S., 1978, San Jose State University; Ph.D., 1982, University of Wisconsin, Madison; Postdoctoral Fellow, Indiana University, 1983-1985

Research interests:

Inorganic chemistry: catalysis, methathesis, polymers, stereospecific reactions, hydrogen bonding, liquid crystals, inorganic/organic hybrid materials.

Science education: Effects of inquiry in science laboratory instruction, effect of research effectiveness of K-12 science instruction, attrition at the university/community college transition.

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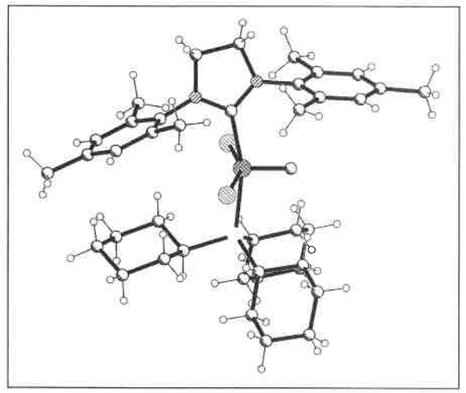
Joseph A. Heppert

Organometallic, Coordination, and Supramolecular Chemistry

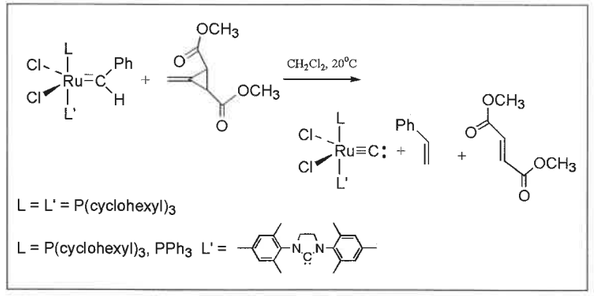
Stable ruthenium carbides. Transition metal carbides are important intermediates in the production of synthetic hydrocarbons through the Fischer-Tropsch process. Fischer-Tropsch synthesis employs group 8 metal catalysts at high temperature to dissociate carbon monoxide in an initial step, forming surface-bound carbide (C) units. Homogeneous models of most of the intermediates in this process have been known and studied for some time, with a noteworthy exception being terminal transition metal carbide complexes. Only within the last four years, the Cummins and Templeton groups have identified anionic group 6 terminal carbides that appear to be strong Brønsted bases.



Our group has isolated and characterized the first class of stable neutral terminal metal carbides. These compounds, which could be an important link in understanding the Fischer-Tropsch process, exhibit an extensive chemistry beyond Brønsted basicity. We are currently investigating the mechanism of formation and reactivity of these compounds.

Terminal ruthenium carbides are formed through metathesis reactions involving ruthenium alkylidenes and methylene cyclopropenes. The ruthenium carbon triple bond is a characteristically short 1.66 Å. Our group has prepared several classes of terminal carbides, including systems with two phosphine ligands and systems bearing one phosphine unit and a dihydroimidazol ligand.

Systems bearing pyridine ligands do not react with methylene cyclopropenes to produce carbide complexes. Instead, we have isolated ruthenium vinylidenes that result from the isomerization of one of the intermediates in the cyclopropylidene cleavage reaction.



The carbide complexes can also form coordination complexes. $RuCl_2(Cy_3P)_2(C:)$ reacts with copper triflate to generate a Cu_2Cl_2 bridged ruthenium dimer. This is the first synthesis of a molecular copper carbide complex and represents one of the few rational routes for the preparation of binary transition metal carbides. We are continuing to study the coordination chemistry of the carbide complexes.

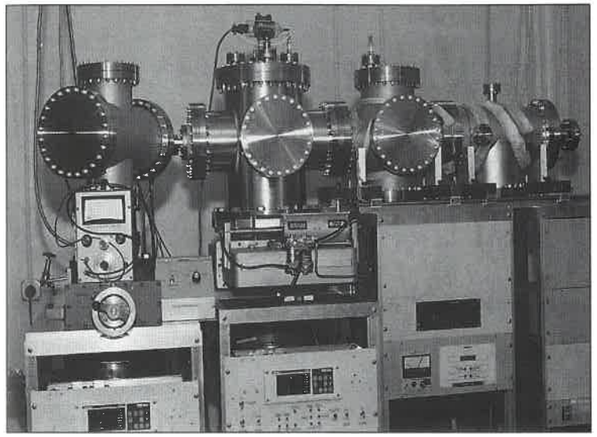
Selected Publication

Carlson, R.G.; Gile, M.A.; Heppert, J.A.; Mason, M.H.; Powell, D.R.; Vander Velde, D.; Vilain, J.M. The Metathesis Facilitated Synthesis of Terminal Ruthenium Carbide Complexes: A Unique Carbon Atom Transfer Reaction. J. Am. Chem. Soc., **2002**, *in press*.

Peter M. Hierl

Physical Chemistry

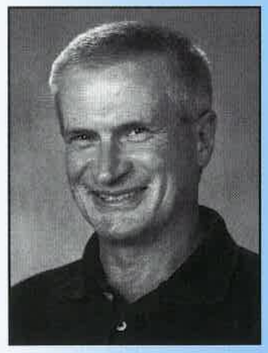
Gas-phase reactions between ions and neutral molecules play a key role in a wide variety of chemical processes, such as flames, explosions, radiation chemistry, plasmas, and upper-atmosphere phenomena. They are, moreover, ideal for investigating topics of fundamental importance in chemical kinetics, such as the effects of reactant solvation and reactant translational energy upon rate constants, reaction mechanisms, and product branching ratios.



Beam techniques, using a recently constructed tandem mass spectrometer containing ocotpole ion guides, are used to measure the intensities and velocity distributions of reactively scattered product ions as functions of the reactant ion solvation and translational energy and of the neutral reactant temperature. The results of these studies provide valuable information for the evaluation of modern theories of chemical kinetics, and enable one to better understand the often complex behavior in a variety of chemical processes.

Selected Publications

1. Hierl, P.M.; Henchman, M.J.; Paulson, J.F. Translational Energy Dependence of Cross Sections for the Reactions of $OH^-(H_2O)_n$ with CH_3Br and CH_3Cl. J. Phys. Chem., **1995**, *99*, 15655-15661.
2. Viggiano, A.A.; Arnold, S.T.; Morris, R.A.; Ahrens, A.F.; Hierl, P.M. Temperature Dependences of the Rate Constants and Branching Ratios for the Reactions of $OH^-(H_2O)_{0-4} + CH_3Br$. J. Phys. Chem., **1996**, *100*, 14397-14402.
3. Hierl, P.M.; Dotan, I.; Seeley, J.V.; Van Doren, J.M.; Morris, R.A.; Viggiano, A.A. Rate Constants for the Reactions of O^+ with N_2 and O_2, as a Function of Temperature (300-1800 K). J. Chem. Phys., **1997**, *106*, 3540-3544.
4. Dotan, I.; Hierl, P.M.; Morris, R.A.; Viggiano, A.A. Rate Constants for the Reactions of N^+ and N_2+ with O_2 as a Function of Temperature (300-1800 K). Int. J. Mass Spectrom. Ion Processes **1997**, *167/168*, 223-230.
5. Hierl, P.M.; Morris, R.A.; Viggiano, A.A. Rate Coefficients for the Endothermic Reactions $C^+(^2P) + H_2(D_2) \rightarrow (CH^+(CD^+) + H(D)$ as Functions of Temperature from 400-1300 K. J. Chem. Phys., **1997**, *106*, 10145-10152.



Professor

B.S., 1963, Massachusetts Institute of Technology; Ph.D., 1967, Rice University; Postdoctoral Fellow, 1967, Yale University; Postdoctoral Fellow, 1967-1969, University of Colorado

Research interests:

Dynamics of gas-phase ion-molecule reactions at hyperthermal energies.

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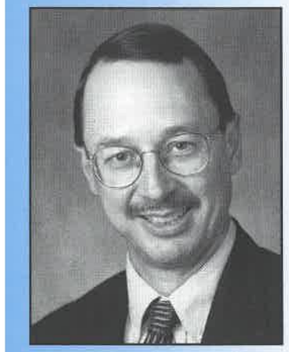
Carey K. Johnson

Laser Spectroscopy of Biomolecules, Physical and Biophysical Chemistry



Associate Professor

B.A., 1973, Tabor College; Ph.D., 1981, Iowa State University; National Institutes of Health Postdoctoral Fellow, 1982-1984, University of Pennsylvania

Research interests:

Single-molecule and time-resolved laser spectroscopic studies of dynamics in condensed phases and biological systems.

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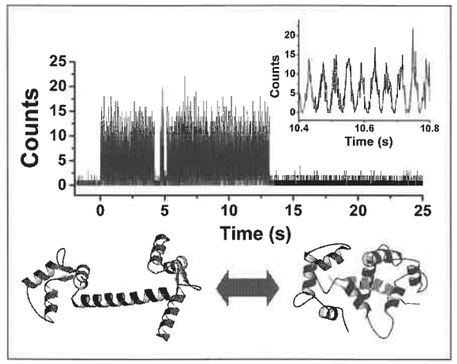
Our research focuses the formidable power of single-molecule and time-resolved laser spectroscopy on chemical events on time scales ranging from the picosecond (10^{-12} s) to the second time regimes. Aspects of molecular behavior that we are investigating include (1) the function of single protein molecules; (2) fast orientational and intramolecular motions of peptides and organic molecules in solution; and (3) ultrafast electronic relaxation in chromophores of biological importance, such as retinal.

Single-molecule investigation of target binding and activation. In single-molecule spectroscopy, fluorescence photons from a single molecule are recorded and analyzed to obtain detailed information about the dynamics of the molecule. Examination of single molecules allows us to study a distribution of molecular behaviors, rather than merely the average. This project focuses on the calcium signaling protein, calmodulin (CaM). Studying these molecules one at a time provides unique information that will help to unravel the mechanism by which proteins like CaM activate target enzymes in response to a calcium signal. One of these target enzymes is a calcium pump, the plasma-membrane calcium ATPase. Single-molecule methods promise to unveil important aspects of the mechanism of activation of this enzyme. The figure shows a fluorescence image of single fluorescence labeled CaM molecules.



Orientational dynamics in solution. Our study of orientational dynamics is aimed at understanding the conformational motions of biologically important peptides. Time-resolved fluorescence depolarization measurements track reorientational dynamics directly on the time scales on which they occur. Our goal is to uncover the time scales, amplitudes, and coupling to solvent of internal and overall motions of peptides. An example is our study of intramolecular dynamics in biologically active peptides such as enkephalin to learn about the range of intramolecular motions and conformational changes in the peptide. Time-resolved fluorescence depolarization signals are typically obtained from native amino acids such as tyrosine. The group has also introduced the non-native fluorophore, indoline carboxylic acid, which can take the place of proline residues and report reorientations of the peptide backbone.

Selected Publications

1. Harms, G.S.; Freund, W.L.; Johnson, C.K. Time-Resolved Fluorescence Study of Conformational Dynamics in Opioid Peptides. J. Phys. Chem. B **1998**, *102*, 5004-5010.

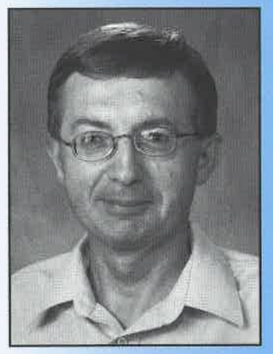
2. Jas, G.S.; Larson, E.J.; Johnson, C.K.; Kuczera, K. Microscopic Details of Rotational Diffusion of Perylene in Organic Solvents: Molecular Dynamics Simulation and Experiment vs. Debye-Stokes-Einstein Theory. J. Phys. Chem. A., **2000**, *104*, 9841-9852.

3. Larson, E.J.; Pyszczynski, S.J.; Johnson, C.K. Solvent Dependence of Electronic Relaxation in All-Trans Retinal Studied by One- and Two-Photon Induced Transient Absorption. J. Phys. Chem. A., **2001**, *105*, 8136-8144.

4. Bothwell, T.G.; Unruh;, J.R.; Johnson, C.K. Tyrosine and Peptide Reorientational Mobility in Polymer Solutions. Time-Dependent Fluorescence Anisotropy Measurements. Biopolymers, **2003**, *in press*.

Krzysztof Kuczera

Computer Simulations of Biomolecular Structure, Dynamics and Thermodynamics



Associate Professor

M.S., 1980, Warsaw University; Ph.D., 1985, Institute of Physics, Polish Academy of Sciences; Postdoctoral Fellow and Research Associate, Harvard University, 1986-1991

Research interests:

Physical and theoretical chemistry: molecular dynamics simulations, statistical mechanics, quantum chemistry of biological molecules.

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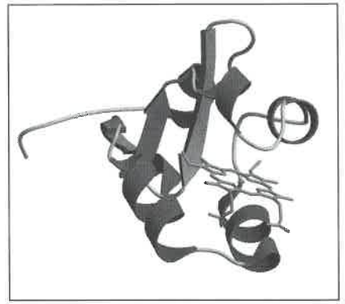
Studies of fundamental properties of complex biological and organic molecules have profound implications for many areas of science, as well as practical applications in curing disease, protecting the environment, improving industrial processes, and designing new materials. Although experimental investigations remain the main source of information on large molecular systems, their theoretical and computational studies are gaining importance. This is due to great increases in computer power and development of efficient computational algorithms and to the growing understanding that simulations provide unprecedented detail of information, which can be fruitfully employed to uncover the microscopic mechanisms of observable, macroscopic properties of molecular systems.

Our research focuses on the use of methods of modern computational chemistry to study structure, dynamics, and thermodynamics of complex molecular systems. The methods involve mainly molecular dynamics simulations and quantum chemistry. The overall goal is to relate the detailed microscopic information provided by the simulations to observable, macroscopic physical, chemical, and biological properties. Besides providing a basic understanding of important classes of molecules, the simulation results provide predictions on how to manipulate the properties for practical purposes. The work involves using existing simulation programs, development of new methods and algorithms for molecular modeling, and collaborations with experimental groups on specific systems.



Recent projects include analysis of the large-scale conformational transitions in the methyl-cycle enzyme S-adenosylhomocysteine hydrolase aimed at understanding its catalytic mechanism; study of properties of the oxidatively damaged protein calmodulin, related to modeling the processes of aging and/or development of cancer; evaluation of free energy differences between different conformations of small peptides, which are models for the more complex protein folding process; simulations of the conformational flexibility of surface loops in variants of cytochrome b5, which may be related to changes in physical properties such as stability and reduction potential; simulations of receptors that will efficiently and specifically bind cationic ligands, which can be used for environmental waste remediation; study of influence of solvent type and shape and size of a fluorescent probe on the observed reorientation dynamics of aromatic molecules in solution.

Selected Publications

1. Kuczera, K. Molecular Modeling in Peptide and Protein Analysis, *Encyclopedia of Analytical Chemistry*. R.A. Meyers, Ed.; John Wiley & Sons, Ltd.: Chichester, 2000, pp. 5894-5930.

2. Mahadevan, J.; Lee, K.H.; Kuczera, K. Conformational Free Energy Surfaces of Ala10 and Aib10 Peptide Helices in Solution. J. Chem. Phys. B, **2001**, *105*, 1863-1876.

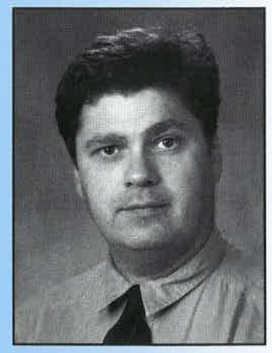
3. Altuve, A.; Silchenko, S.; Lee, K.H.; Kuczera, K.; Terzyan, S.; Zhang, X.; Benson, D.R.; Rivera, M. Probing the Differences between Rat Liver Outer Mitochondrial Membrane Cytochrome b5 and Microsomal Cytochromes b5. Biochemistry, **2001**, *40*, 9469-9483.

4. Hu, Y.; Yang, X.; Yin, D.H.; Mahadevan, J.; Kuczera, K.; Schowen, R.L.; Borchardt, R.T. Computational Characterization of Substrate Binding and Catalysis in S-adenosylhomocysteine Hydrolase. Biochemistry, **2001**, *40*, 15143-15152.

5. Jas, G.S.; Kuczera, K. Free Energy Simulations of the Oxidation of C-terminal Methionines in Calmodulin. Proteins, **2002**, *48*, 257-268.

Brian B. Laird

Computational Materials Science and Applied Statistical Mechanics



Associate Professor and Associate Chair, Graduate Programs

B.S. Chemistry, B.S. Mathematics, 1982, University of Texas at Austin; Ph.D., Chemistry, 1987, University of California, Berkeley; NATO Postdoctoral Fellow 1989-1990, Forschungszentrum Jülich, Germany

Research interests:

Theoretical and computational chemistry, phase transitions, interfacial and amorphous systems, general liquid state theory, inhomogeneous fluids, computer simulation of materials, molecular simulation algorithms.

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The ultimate goal of materials chemistry is the understanding of the macroscopic properties of materials in terms of the microscopic molecular interactions. This is a common theme in all of the natural sciences. The differences between the various scientific disciplines (chemistry, biology, physics, materials sciences, etc.) often disappear as the traditional macroscopic phenomenology is replaced by a more molecular approach. At present, most of what is known about the chemical and physical properties of materials is still largely empirical, especially in the case of amorphous, macromolecular or interfacial systems. The development of a microscopic theoretical description for a variety of such complex systems is the primary focus of our research. Several representative projects are listed below. They are all projects in which great advantage will be gained by exploiting the natural symbiosis between analytical and computer-simulation techniques.

Crystal-melt interfaces of complex systems. The structure and dynamics of an interface between a crystal and its melt are of paramount importance in studies of crystal growth and nucleation. Experimental study is difficult as such an interface lies sandwiched between two dense phases, and experimental data is lacking, increasing the value of computer simulations to the study of such systems. Most previous studies have involved simple, one-component model systems. Using molecular-dynamics computer simulations and classical density-functional theories, we are currently concentrating on more complex systems such as multicomponent systems (e.g., alloys) and systems with realistic interactions, such as metals.

Algorithms for molecular modeling. Molecular-dynamics computer simulation has become an invaluable tool in chemistry, chemical engineering, physics, materials science, and biology. However, its uses are still limited by the relatively small system sizes and short time scales that can be simulated at present. Progress in this area therefore comes from advances in computer technology and in the development of efficient and stable algorithms. The latter is the goal of an ongoing multidisciplinary project in collaboration with Professor Ben Leimkuhler, an applied mathematician at the University of Leicester.

Dynamics in amorphous materials. The thermodynamic and dynamical properties of glasses are dramatically different from those of crystals of the same materials. The experimental evidence suggests that many of these differences are due to the presence of localized low-energy motions in the glass that are not found in the corresponding crystal. Such modes profoundly affect the thermodynamic, reactive, and spectroscopic properties of glasses, especially at low temperature, but surprisingly little is known about their structural origin. Using a combination of computer simulation and normal mode techniques, we have been able to demonstrate the existence of these localized modes in model glasses (such as SiO_2) and to connect them with details of the glass structure. In a related project, we are investigating the kinetics of peptide degradation in amorphous polymers as part of a joint project with researchers in the Department of Pharmacuetical Chemistry.

Selected Publications

1. Houndonougbo, Y.A.; Laird, B.B. Constant Temperature Molecular-Dynamics Algorithms for Mixed Hard-Core/Continuous Potentials. J. Chem. Phys., **2002**, *117*, 1001.
2. Sibug-Aga, R.; Laird, B.B. Structure and Dynamics of a Crystal-Melt Interface of a Binary Hard-Sphere Fluid in Coexistence with a One Component Crystal. J. Chem. Phys., **2002**, *116*, 3410.
3. Laird, B.B. The Crystal-Melt Interfacial Free Energy of Close-packed Metals: Hard Spheres and the Turnbull Coefficient. J. Chem. Phys., **2001**, *115*, 2887.
4. Bembenek, S.D.; Laird, B.B. Instantaneous Normal Mode Analysis of Amorphous and Supercooled Silca. J. Chem. Phys., **2001**, *114*, 2340.
5. Davidchack, R.L.; Laird, B.B. Direct Calculation of the Hard-Sphere Crystal/Melt Interfacial Free Energy. Phys. Rev. Lett., **2000**, *85*, 4751.

Cynthia K. Larive

Bioanalytical and Environmental Analytical Chemistry

Associate Professor

B.S., 1980, South Dakota State University; M.S., 1982, Purdue University; Ph.D., 1992, University of California, Riverside

Research interests:

Microcoil NMR probes, NMR diffusion measurements, structure elucidation using LC/NMR, cITP/NMR and LC/MS/MS.

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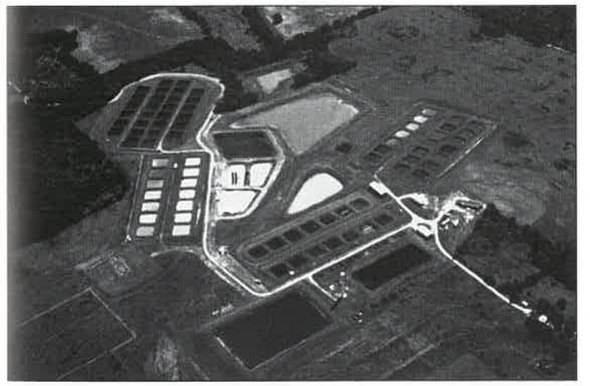
NMR diffusion measurements are a useful way to study ligand-protein binding. We have developed NMR experiments that provide improved spectral selectivity in ligand binding studies by manipulation of NMR pulse sequences to reduce the protein background or enhance specificity. In addition to providing information about the strength of the interaction, the build-up of transferred-NOEs during the diffusion experiment can provide insight into the nature of ligand-protein binding. Because limited amounts of protein are often available, we are extending these measurements to small volumes using specially constructed microcoil NMR probes capable of measuring volumes of 1 µL or less. Microcoil probes can greatly improve the mass sensitivity of NMR measurements and facilitate coupling with online capillary separation techniques such as capillary isotachophoresis or capillary HPLC. Our group is using these separation methods coupled with NMR detection to study a number of problems related to structure elucidation, such as the structural and functional group diversity of humic substances isolated from water and soils. Our group is also using LC-NMR along with LC-MS to study the diverse secondary metabolites produced by myxobacteria. Many of the natural products produced by these bacteria, such as the epothilones, are potential therapeutic agents for the treatment of cancer. We are also using LC-NMR and LC-MS-MS to study the pathways and processes by which environmental contaminants, like fluoroquinolone antibiotics, are degraded in aquatic ecosystems. The structure elucidation and quantification of the degradation products of pollutants in aquatic ecosystems presents a significant analytical challenge. An important and unique aspect of our environmental research involves field experiments conducted with collaborators at the university's Nelson Environmental Studies Area, shown here, one of largest ecological research stations in the world.

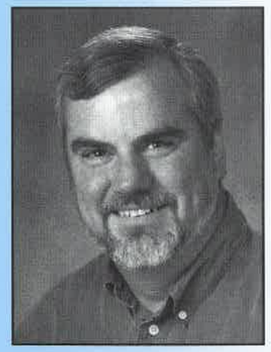


Selected Publications

1. Wolters, A.M.; Jayawickrama, D.A.; Larive, C.K.; Sweedler, J.V. Capillary Isotachophoresis/NMR: Extension to Trace Impurity Analysis and Improved Instrumental Coupling. Anal. Chem., **2002**, *74*, 2306-2313.
2. Derrick, T.S.; McCord, E.F.; Larive, C.K. Analysis of Protein/Ligand Interactions with NMR Diffusion Measurements: The Importance of Eliminating the Protein Background. J. Magn. Reson., **2002**, *155*, 217-225.
3. Otto, W.H.; Carper, W.R.; Larive, C.K. Measurement of Cadmium(II) and Calcium(II) Complexation by Fulvic Acids Using ^{113}Cd NMR. Environ. Sci. Technol., **2001**, *35*, 1463-1468.

Craig Lunte

Monitoring Chemistry in Living Organisms



Professor and Chair

B.S., 1979, University of Missouri, Rolla; Ph.D., 1984, Purdue University; Postdoctoral Fellow, University of Cincinnati, 1986-1987

Research interests:

Analytical chemistry: monitoring living systems, micro-separation techniques, electrochemistry, electrochemical detection in liquid chromatography and capillary electrophoresis, drug transport, pharmacokinetics, anticancer drugs, oxidative stress.

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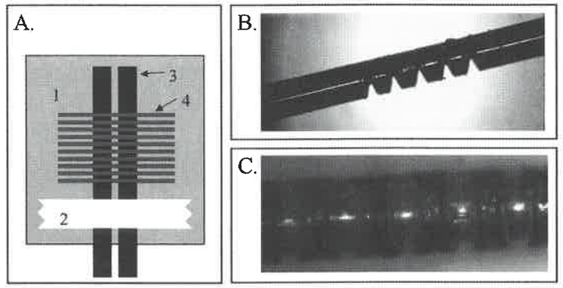
Research is focused on the development of new methods for the study of drug metabolism and disposition. All aspects of the bioanalytical problem of drug disposition studies are being addressed, from sampling of living organisms to analysis of minute biological samples. A major focus is the development of microdialysis sampling *in vivo*. The research group has provided both novel applications of microdialysis sampling and fundamental studies of the technique. Several novel microdialysis probes have been developed for sampling from peripheral tissue in conscious animals. Studies of drug transport effects on the microdialysis process *in vivo* have led to greater insight into the use of this technique.



Research also involves the development of microanalytical techniques based on separations. On-column sample concentration methods, electrochemical detectors, and mass spectrometer interfaces for capillary electrophoresis (CE) are being developed. These microanalytical techniques are being directly coupled to microdialysis sampling to provide separation-based *in vivo* sensors. These systems provide near real-time monitoring of multiple chemical species in the tissues of awake, freely moving animals.

These new bioanalytical tools are being applied to several important problems in drug metabolism and disposition studies. Some current projects include studying the tissue levels in comparison to the systemic concentrations of a local anesthetic administered in a slow release formulation, a study on the transplacental transport of pharmaceuticals and drugs of abuse, an investigation of the transdermal delivery of therapeutic agents, and the effect of antiarrhythmic drugs on catecholamine levels in the heart. The group recently embarked on a new project to develop analytical methods to detect biomarkers for oxidative DNA damage and lipid peroxidation occurring as a result of oxidative stress during heart attack and stroke. These methods will then be used with microdialysis sampling in the heart and brain to study the effects of oxidative stress during heart attack and stroke.

Selected Publications

1. Gilinsky, M.A.; Faibushevich, A.A.; Lunte, C.E. Determination of Myocardial Norephinephrine in Freely Moving Rats Using *In Vivo* Microdialysis Sampling and Liquid Chromatography with Dual-Electrode Amperometric Detection. J. Pharm. Biomed. Anal., **2000**, *24*, 929-935.

2. Weiss, D.J.; Saunders, K.; Lunte, C.E. pH-Mediated Field-Amplification Sample Stacking of Pharmaceutical Cations. Electrophor., **2001**, *22*, 59-65.

3. Osbourn, D.M.; Lunte, C.E. Cellulose Acetate Decoupler for On-Column Electrochemical Detection in Capillary Electrophoresis. Anal. Chem., **2001**, *73*, 5961-5964.

4. Backofen, U.; Matysik, F.-M.; Lunte, C.E. Determination of Cannabinoids in Hair Using High pH* Non-Aqueous Electrolytes and Electrochemical Detection: Some Aspects of Sensitivity and Selectivity. J. Chromatogr. A, **2002**, *942*, 259-269.

5. Backofen, U.; Matysik, F.-M.; Lunte, C.E. A Chip-based Electrophoresis System with Electrochemical Detection and Hydrodynamic Injection. Anal. Chem., **2002**, *74*, 4054-4059.

Helena C. Malinakova

Synthetic Organic Chemistry and Transition Metal-Mediated Asymmetric Reactions

Assistant Professor

B.S./M.S., 1989, Institute of Chemical Technology, Prague; Ph.D., 1998, Illinois Institute of Technology; Postdoctoral Fellow, Emory University, 1999-2000

Research interests:

Synthetic organic chemistry: development of methodology for total synthesis of natural products, transition metal mediated C-C bond formation, asymmetric synthesis, cascade reactions, metal-induced C-H bond activation.

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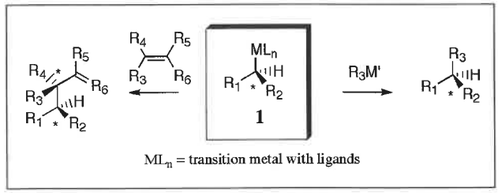
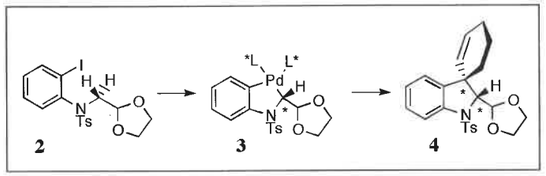
In recent years, transition metal complexes became recognized as powerful synthetic tools capable of creating new carbon-carbon bonds under impressively mild conditions in a highly selective manner. The principal aim of our research is to develop new synthetic methods using transition metal-based reagents, for example organopalladium complexes. We will investigate the chemistry of compounds with a chiral carbon directly attached to a transition metal (**1**). Our group will explore the preparation of such reagents and intermediates in an enantiomerically pure form, then use these to construct complex organic molecules with significant biological activities.

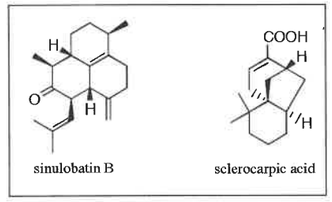


Directed asymmetric palladation. In this project, we will be preparing palladacycles (**3**). Enantiopure ligands (L*) attached to palladium will ensure that the palladium metal inserts selectively into one of the two enantiotopic C-H bonds in substrate (**2**). The palladacycles will then be converted to enantiopure organic products represented by the spirocyclic structure (**4**).



In the next stage of the project, we will apply the new method to the synthesis of natural products and molecules with interesting biological properties. Thus, in addition to expertise in the chemistry of transition metal-based reagents, researchers in our group will gain experience with a broad range of traditional synthetic reactions.

Cascade sequences for asymmetric synthesis. Cascade reactions, series of transformations that occur as a "one pot" process, often lead to remarkably short syntheses of complex molecules. In a second group of projects, we will identify novel sequences involving asymmetric metal-mediated reactions and use these to execute total syntheses of biologically active natural products, for example a cytotoxic marine diterpenoid sinulobatin B and an antiviral and antimicrobial sesquiterpene sclerocarpic acid.



Selected Publications

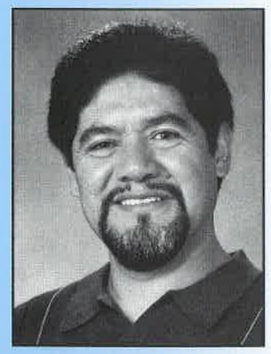
1. Malinakova, H.C.; Portscheller, J.L. Synthesis of 2H-1-Benzopyrans via Palladacycles with a Metal-Bonded Stereogenic Carbon. Org. Lett., **2002**, *4(21)*, 3679-3681.

2. Malinakova, H.C.; Liebeskind, L.S. Enantiocontrolled Synthesis of Spirooxindoles Based on the [5+2] Cycloaddition of a $Tp(CO)_2Mo$(pyridinyl) Scaffold (Tp = Hydridotrispyrazolylborate). Org. Lett., **2000**, *2(25)*, 4083-4086.

3. Malinakova, H.C.; Liebeskind, L.S. Enantiocontrolled Synthesis of Highly Functionalized Tropanes via [5+2] Cycloaddition to η3-Pyridinylmolybdenum π-Complexes. Org. Lett,., **2000**, *2(24)*, 3909-3911.

4. Stagliano, K.W.; Malinakova, H.C. Regiospecific Synthesis of 2,3-Bisnaphthopyranyl Quinones Related to Conocurvone. Effect of Substituents on Palladium-Catalyzed Cross-Coupling of Organostannanes to Naphthopyranyl Hydroxyquinone Triflates. J. Org. Chem., **1999**, *64(21)*, 8034-8040.

Mario Rivera
Bioanlytical and Bioinorganic Chemistry



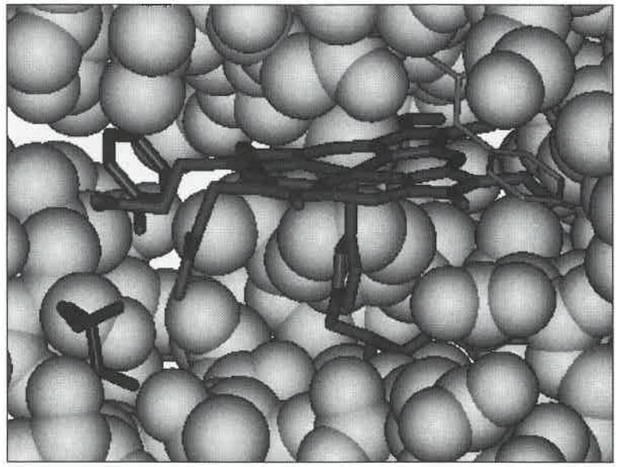
Associate Professor

B.S., 1984, Universidad Autónoma de Guadalajara; Ph.D., 1991, University of Arizona; Postdoctoral Fellow, 1991-1994, University of Arizona

Research interests:

Structure-function relationships in heme containing proteins.

The main emphasis of our program is the elucidation of structure-function relationships in heme containing proteins. Heme containing proteins are vital components of most living organisms because they participate in electron transfer reactions (cytochromes), oxygen activation and insertion reactions (monooxygenases), oxygen transport and storage (hemoglobin and myoglobin), oxygen sensing in nitrogen-fixing bacteria (FixL), heme metabolism (heme oxygenase), and regulatory functions based on nitric oxide (guanylyl cyclase, nitrophorins), to name a few. It is remarkable that despite the wide range of chemical and physiological functions displayed by heme containing enzymes and proteins, they all share the same prosthetic group, protoheme IX (heme). Consequently, elucidating how nature tunes the redox properties and reactivity of the ubiquitous heme within a protein so that the resultant activity is that of oxygen binding, oxygen activation, oxygen sensing, or electron transport at different redox potentials, is the unifying theme of our research efforts. To study structure-function relationships in redox-active hemoproteins we use recombinant DNA methodology, bioelectrochemistry, and NMR spectroscopy in our laboratory, and X-ray crystallography, EPR spectroscopy and resonance Raman spectroscopy via collaborations.



Selected Publications

1. Cowley, A.B.; Altuve, A.; Kuchment, O.; Terzyan, S.; Zhang, X.; Rivera, M.; Benson, D. R. Toward Engineering the Stability and Hemin Binding Properties of Microsomal Cytochromes b_5 into Rat Outer Mitochondrial Membrane Cytochrome b_5: Examining the Influence of Residues 25 and 71. Biochemistry **2002**, *41*, 11566-11581.

2. Rivera, M.; Caignan, G.A.; Astashkin, A.V.; Raitsimring, A.M.; Shokhireva, T.K.; Walker, F.A. Models of the Low-Spin Iron(III) Hydroperoxide Intermediate of Heme Oxygenase: Magnetic Resonance Evidence for Population of the d_{xy} Electronic Ground State at Ambient Temperatures. J. Am. Chem. Soc., **2002**, *124*, 6077-6089.

3. Caignan, G.A.; Deshmukh, R.; Zeng, Y.; Eastman, M.A.; Wilks, A.; Rivera, M. The Oxidation of Heme to _- and _-biliverdin by Pseudomonas Aeruginosa Heme Oxygenase as a Consequence of an Unusual Seating of the Heme. J. Am. Chem. Soc., **2002**, *124*, 14879-14892.

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Janet Bond-Robinson
Chemical Education

Assistant Professor

B.S., Texas Lutheran College, Seguin, and the University of Texas; M.A., University of Texas; Fellow, Wright Center for Innovation in Science Education, 1994-1995, Tufts University, Boston; Ph.D., 1998, University of Iowa

Research interests:

Cognitive studies of chemical knowledge.

Our group's research studies the cognition involved to develop chemical knowledge, to understand chemical knowledge, and to teach chemical knowledge effectively. Our research techniques include (1) live and remote audio/video observation techniques for micro analysis, (2) macro-level analysis through interviews and documents, and (3) analysis through problem solving in Web-based authentic scenarios developed in Dreamweaver™ and Flash™.

Empirical chemical knowledge (ECK). We are studying the workplace of organic synthesis and how expertise develops over time with the resources and constraints of this community of practice. Differences in views of knowledge frame our work in several ways. If we cease to view science philosophically as a set of verbal axioms to be learned and view it instead as a well established community, situated learning becomes an important key to studying the practice of science scientifically. One could assume that scientists do not behave differently from other humans when using scientific reasoning, except that the standards and norms are exemplified in the tools, conversation topics, materials, protocols, expectations, and mentoring in the scientific environment.

Web-based scaffolded and complex problem solving in undergraduate chemistry. This is exciting research likely to affect chemical education contexts soon. Currently authoring problems in general chemistry using multimedia, we have just been funded to continue this work in organic chemistry and physical chemistry. We collaborate with researchers at UCLA Medical School and Clemson University in piloting authentic problems in the undergraduate curriculum. When students do problems, the path analysis is recorded at UCLA. Subsequently analysis of each student's decisions maps aspects of understanding and whether students use prolific, efficient, or sparse strategies. Thousands of student performances have been analyzed using neural nets.

Design research on innovations and research on pedagogical chemical knowledge (PCK). Members of our group, using video techniques, study teaching assistants as they conduct labs. Each GTA uses the video to analyze his or her own performance. We also use the video to study productive interactions that lead to learning, e.g., questions, explanations, talk about concepts, and talk about procedures. Research has found that the linkage is weak because most lab talk is at the shallow level of procedures and calculations rather than the deeper level of chemical concepts underlying the experiment.

Selected Publications

1. Robinson, J. Bond. New GTAs Facilitate Active Learning in Chemistry Laboratories: Promoting GTA Learning through Formative Assessment and Peer Review. J. of Graduate Teaching Assistant Development, **2001**, *7(3)*, 147-162.

2. Bond-Robinson, J.; Preece, A. The Learning Environment for Inquiry: Growth of Graduate Students in Research. Proceedings of the International History, Philosophy, and Science Teaching Annual Meeting; Denver, CO, November 2001.

3. Ellis, J.D.; Heppert, J.A.; Bond-Robinson, J.; Mason, S. Problem Solving in the Chemistry Laboratory. J. of Col. Sc. Teaching, **2002**, *XXXI(5)*, 322-326.

4. Bond-Robinson, J. Becoming Scientists: Empirical Grounding of the Nature of Scientific Inquiry (submitted).

5. Bond-Robinson, J. Becoming Scientists: Conceptual Change in Science and in Members of a Community of Practice (submitted).

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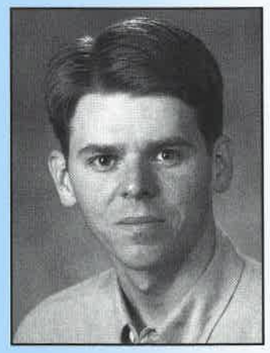
Ward H. Thompson

Theoretical Chemical Dynamics



Assistant Professor

B.S., 1991, Oklahoma State University; Ph.D., 1996, University of California, Berkeley; Postdoctoral Associate, 1997-2000, University of Colorado

Research interests:

Theoretical physical chemistry, reaction dynamics, quantum mechanical effects, energy transfer, proton transfer, spectroscopy, solvent effects.

Our research focuses on the development and application of theoretical methods for describing spectroscopy and reaction dynamics in condensed phase systems. The emphasis is on understanding at a molecular level the fundamental behavior of interesting chemical systems and phenomena. The goal of our work is to develop accurate theoretical and computational approaches that can be feasibly applied to complex chemical problems including reactions in liquids, clusters, solids, and nanostructured environments. Some of the specific problems we are addressing are outlined below.

Reactions and spectroscopy in nano-confined solvents. Nanometer-sized cavities and pores can now be routinely generated in sol-gels, supramolecular assemblies, reverse micelles, zeolites, and even proteins, giving strong impetus to improving our understanding of chemistry in confined solvents. One ultimate goal is to control the chemistry occurring in these systems by manipulating the cavity properties as well as the species present. However, this will require an understanding of the effect of cavity characteristics on reactivity. We are studying the energetics and dynamics of spectroscopy and chemical reactions in solvents confined within nanoscale frameworks using both simple models and realistic Monte Carlo and molecular dynamics simulations. The fundamental question we are addressing is how does a reaction occur differently in a confined solvent than in a bulk solvent? We are investigating proton transfer reactions, charge transfer spectra, and isomerization reactions, since these processes are typically strongly coupled to the solvent and thus should be dramatically affected by the limited number of solvent molecules, geometric constraints of a nanocavity, and solvent-cavity interactions.

Vibrational relaxation in liquids and clusters. It is difficult to overestimate the importance of vibrational relaxation since it plays a critical role in almost all aspects of chemistry (e.g., reaction dynamics and photochemistry). The timescale for vibrational relaxation ranges from ~10^{-12} seconds to ~1 second, indicating the diversity of mechanisms and the challenges in understanding and treating relaxation dynamics. We are developing simulation and theoretical methods that will provide both new insight into the molecular-level mechanisms of vibrational relaxation and practical techniques for calculating relaxation rate constants. Specifically, we are investigating the vibrational relaxation of diatomic and triatomic solutes in rare gas liquids and clusters, some of the most challenging cases for currently available methods.

Selected Publications

1. Thompson, W.H. A General Method for Implementing Vibrationally Adiabatic Mixed Quantum-Classical Simulations. J. Chem. Phys., **2003**, *118*, 1059-1067.
2. Thompson, W.H. A Monte Carlo Study of Spectroscopy in Nanoconfined Solvents. J. Chem. Phys., **2002**, *117*, 6618-6628.
3. Thompson, W.H. Mixed Quantum-Classical Simulation of Vibrational Frequency Modulations of a Diatomic Molecule in a Rare Gas Fluid. Chem. Phys. Lett., **2001**, *350*, 113-118.
4. Thompson, W.H.; Hynes, J.T. Model Study of the Acid-Base Proton-Transfer Reaction of the ClH...OH_2 Pair in Low-Polarity Solvents. J. Phys. Chem. A, **2001**, *105*, 2582-2590.
5. Thompson, W.H. Quantum Mechanical Transition State Theory and Tunneling Corrections. J. Chem. Phys., **1999**, *110*, 4221-4228.

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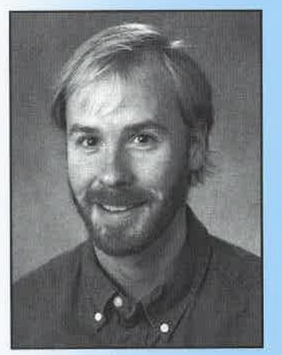
Jon A. Tunge

Asymmetric Transition Metal Catalyzed Organic Transformations



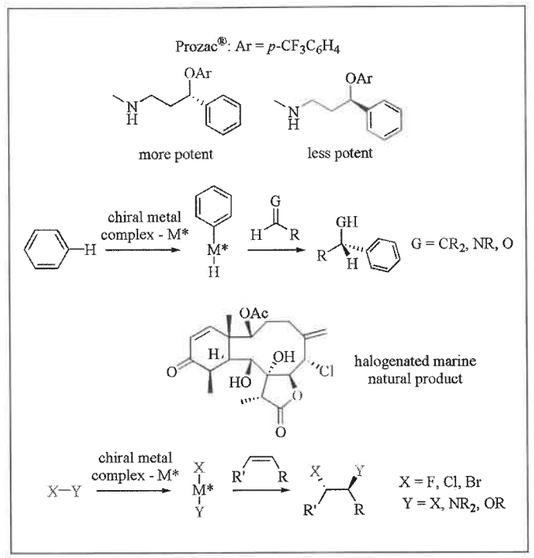
Assistant Professor

B.S., 1995, University of Idaho; Ph.D., 2000, Columbia University; Postdoctoral Associate, 2000-2002, University Wisconsin, Madison

Research interests:

Development of new catalysts that control the stereochemistry of organic reactions.

It is now widely known that biological systems distinguish a pair of enantiomers as different molecules. This is particularly important when designing new pharmaceuticals, as one enantiomer of a drug may be beneficial while the other may be toxic. This knowledge has prompted chemists to come up with more sophisticated approaches to chemical synthesis that allow construction of molecules as a single enantiomer. The expansion of the "chiral pool" (small molecules readily available as a single enantiomer) is important in providing the building blocks necessary to construct more complex molecules such as natural products. We are interested in using metal catalysts to control the enantioselectivity of organic reactions thus expanding the chiral pool and providing the methodology necessary for introduction of stereocenters into complex molecules.



The asymmetric functionalization of C-H bonds. C-H bonds are normally thought of as inert; however, recent efforts have shown that C-H bonds can be "activated" toward reaction by transition metals. It is one of our goals to functionalize C-H bonds providing new routes to molecules from simple hydrocarbons.

The asymmetric halogenation of C-C double bonds. C-X (X = halogen) bonds are among the most synthetically versatile, allowing substitution with retention or inversion of configuration. Creation of halogenated compounds as single enantiomers will provide molecules that can be further manipulated to provide a multitude of interesting compounds using conventional chemistry. We use a variety of techniques to understand how metals control the course of chemical reactions. With a fundamental understanding of the reaction mechanism, new and better catalysts can be designed.

Selected Publications

1. Tunge, J.A.; Gately, D.A.; Norton, J.R. Asymmetric Formation of α-Amino Acid Esters through Dynamic Kinetic Resolution: A Cyclic Carbonate as an Optically Active CO_2 Synthon. J. Am. Chem. Soc., **1999**, *121*, 4520-4521.
2. Chen, J.-X.; Tunge, J.A.; Norton, J.R. Asymmetric Synthesis of Silylated α-Amino Acid Esters through Dynamic Kinetic Resolution. J. Org. Chem., **2002**, *67*, 4366-4369.
3. Tunge, J.A.; Czerwinski, C.J.; Gately, D.A.; Norton, J.R. Mechanism of Insertion of Carbodiimides into the Zr-C Bonds of Zirconaaziridines. Formation of α-Amino Amidines. Organometallics, **2001**, *20*, 254-260.
4. Casey, C.P.; Lee, T.-Y.; Tunge, J.A.; Carpenetti, D.W. II. Direct Observation of a Nonchelated Metal-Alkyl-Alkene Complex and Measurement of the Rate of Alkyl Migration to a Coordinated Alkene. J. Am. Chem. Soc., **2001**, *123*, 10762-10763.

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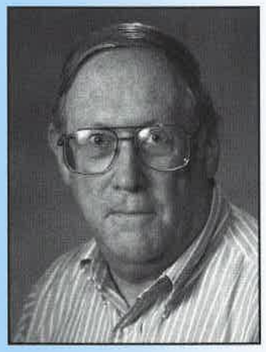

George S. Wilson
Bioanalytical Chemistry

Higuchi Professor of Chemistry and Pharmaceutical Chemistry

A.B., Princeton University, 1961; M.S., University of Illinois, 1963; Ph.D., University of Illinois, 1965; National Institutes of Health Post-Doctoral Fellow, 1965-66, University of Illinois

Research interests:

Biomolecular recognition, biosensors, flow injection immunoassays, cytogenetics.

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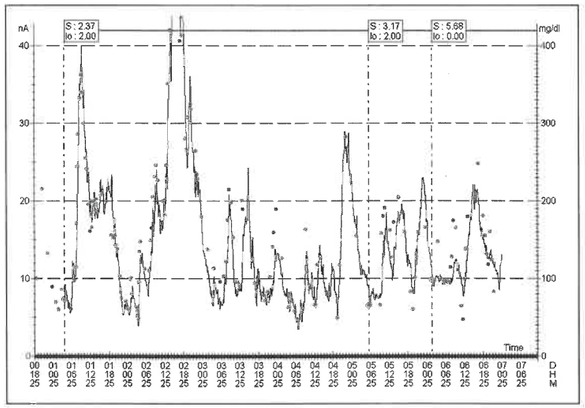
The measurement of analytes in complex biological media continues to be a challenge. High sensitivity and selectivity are essential, and time-dependent changes in analytes can make continuous *in-vivo* measurements necessary. We are developing a number of approaches to biomolecular recognition as means to simplifying analysis.

Biosensors. We have developed a subcutaneously implanted glucose biosensor now applied to continuous estimation of blood glucose in diabetic patients. Other microbiosensors can monitor lactate, glutamate, and oxygen in the brain of laboratory animals, making possible short time resolution of neurobiological events. Characterization of the tissue interaction with implanted sensors is a major focus.

Immunochemistry. Antibodies have been used to recognize conformational changes in proteins adsorbed on surfaces, as catalysts for reactions of analytical interest, and for a variety of applications in medical diagnosis and environmental assessment. These can be implemented in the form of sensors and/or as part of a microfluidic system.

Cytogenetics. It is now recognized that the regulation of gene transcription is controlled by chromatin, a chromosome substructure that includes nucleosomes containing histones, small proteins that are post-translationally modified. These modifications are believed to influence gene regulation, and we have been developing systematic approaches to quantitative evaluation of histone modifications.



Real Time Glucose Measurement in Diabetic Patient

Selected Publications

1. Qian, Q.; Wilson, G.S.; Bowman-James, K; Girault, H.H. MicroITIES Detection of Nitrate by Dual Facilitated Ion Transfer. Anal. Chem., **2001**, *73*, 497-503.

2. Matsumoto, N.; Chen, S.; Wilson, G.S. Fundamental Studies of Glucose Oxidase Deposition on a Pt Electrode. Anal. Chem., **2002**, *74*, 362-367.

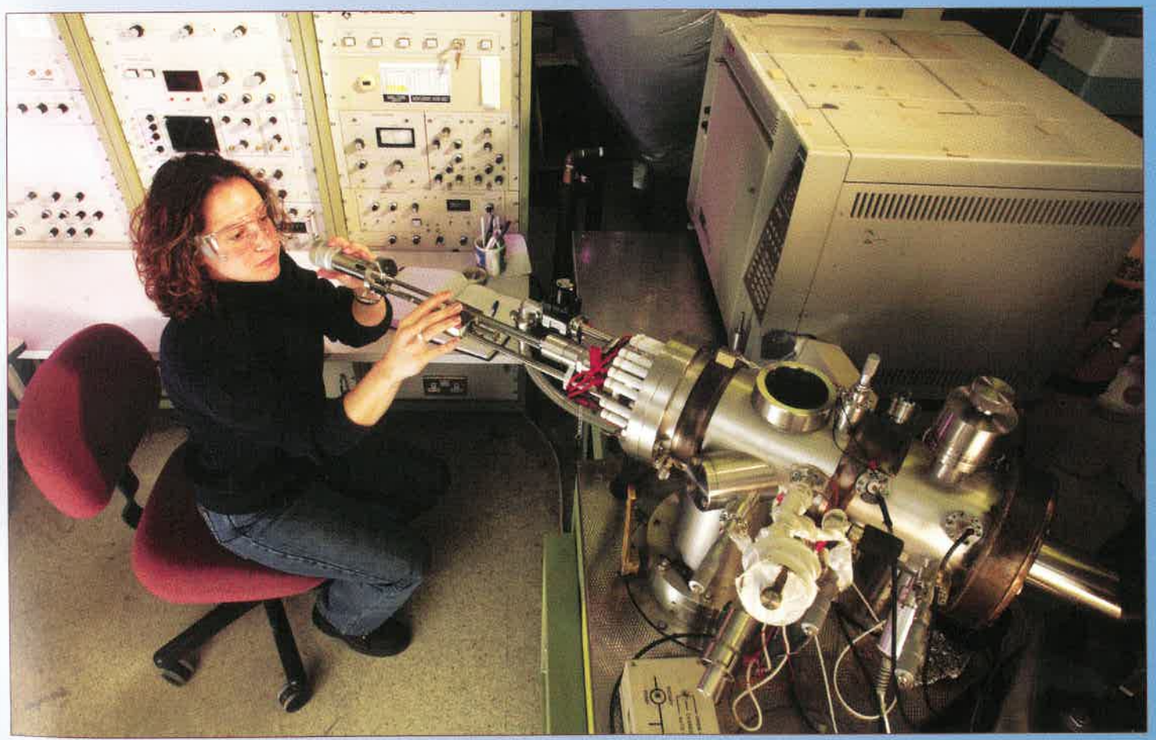
3. Chen, X.; Matsumoto, N.; Hu, Y.; Wilson, G.S. Electrochemically-Mediated Electrodeposition/Electropolymerization Yields Enzyme Microbiosensor with Improved Characteristics. Anal. Chem., **2002**, *74*, 368-372.

4. Choleau, C.; Dokladal, P.; Klein, J.-C.; Ward, W.K.; Wilson, G.S.; Reach, G. Prevention of Hypoglycemia Using Risk Assessment with a Continuous Glucose Monitoring System. Diabetes, **2002**, *51*, 3263-3273.

5. Choleau, C.; Klein, J.C.; Reach, G.; Aussedat, B.; Demaria-Pesce, V.; Wilson, G.S.; Gifford, R.; Ward, W.K. Calibration of a Subcutaneous Amperometric Glucose sensor Implanted for 7 Days in Diabetic Patients Part 2. Superiority of the One-Point Calibration Method. Biosens. Bioelectron., **2002**, *17*, 647-654.

Come Join Us

From the university's earliest beginnings in 1866, KU chemistry department faculty and student research scientists have played an important role in the expansion and application of knowledge in the chemical sciences. Although chemistry is a far more complex field today than it was more than 100 years ago, the tradition of excellence in the department continues, with many chemistry faculty members achieving international reputations for their research, teaching, and service. We are a growing department — growing in research opportunities and rightfully proud of the contributions that our graduates are making in teaching and research at institutions throughout the nation and the world. Our commitment is to a graduate program built on a foundation of excellence in research and teaching in an atmosphere of collegiality and collaboration. We invite you to join us and to share our excitement for the future.



A graduate student cycles a sample through the introduction vacuum lock for FAB analysis on a sector mass spectrometer.