

Jayhawk Chemist

The Newsletter of The Chemistry Department at The University of Kansas

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A Chemist and a Chemical Engineer Win Historic Award for an NSF Research Center

On October 17, 2003, the final papers were signed establishing the National Science Foundation Center for Environmentally Beneficial Catalysis (CEBC), headquartered at the University of Kansas and funded at \$17 million under the NSF Engineering Research Centers (ERCs) program. The CEBC is a multidisciplinary, multi-university research center led by KU, with the University of Iowa (UI) and Washington University in St. Louis (WUSTL) serving as core partners. The five-year grant is the largest single funding award ever received by a university in Kansas. In addition to the \$17 million CEBC will receive from NSF during the first 5-year funding period, the universities (KU, UI and WUSTL) will collectively provide \$2.0 million and nearly 15 major chemical companies are expected to join CEBC as industrial partners. In addition, KU has allocated modern administration and laboratory space (nearly 12,300 square feet) at the Life Sciences Research Laboratory (LSRL) complex and will provide five new faculty positions to CEBC in support of its research and education mission. Further, the State of Kansas has pledged \$1 million to this effort through the matching grant program of the Kansas Technology Enterprise Corporation (KTEC). These additional funding streams and donated facilities are expected to bring the total package value to nearly \$30 million.



The mission of the CEBC is to develop chemistry and industrial chemical processes that are environmentally friendly, as well as economically viable. Professor Daryle H. Busch of the KU Department of Chemistry partnered with Professor Bala Subramaniam of the Department of Chemical and Petroleum Engineering at KU in an effort that extended over about six years to put together all of the parts that led to the Award. Professor Subramaniam is the CEBC director and Professor Busch is the deputy director, while Professors John Rosazza of UI and Milorad Dudukovic of WUSTL serve as CEBC associate directors at their institutions.



With an annual value of \$340 billion, the U.S. chemicals industry is vital to the nation's economy, and because environmental issues related to chemical production cost the chemicals industry \$10 billion each year, the need for this Center for Environmentally Beneficial Catalysis is particularly timely. Industry leaders understand that improvements aimed at pollution prevention, commonly called green chemistry and green engineering, are not only environmentally proactive, they could also be more cost-effective. More than 35 faculty members at three institutions contribute their expertise to CEBC research. Industrial partners will pay membership fees and will have the first opportunity to implement new technologies devised by the Center. Ultimately, CEBC

will sustain its growth and innovation with funding from industrial memberships and additional sponsors of

research projects. A successful CEBC would generate important scientific, technological, economic, academic, environmental, and social impacts that are global in scope.

The award was hailed as an important milestone for the university. KU Chancellor Robert Hemenway said this award is a testament to the commitment the University of Kansas holds to bring together technology and industry to produce tangible advances that benefit the public in numerous ways. The CEBC puts KU in the major league of research centers. There are only about two dozen Engineering Research Centers in the U.S. and they cover all areas of science and technology. This Center is unique in the way it will foster collaborative research among scientists and engineers representing various disciplines, from universities and industries worldwide, to develop environmentally friendly technologies for the chemicals processing industries. These collaborations and the resources available to CEBC make it possible to investigate both new technologies and important established process technologies in detail from the molecular scale to the plant scale using state-of-the-art research tools. Catalysis is the acceleration of a chemical reaction through the presence of a material, a catalyst, that is chemically unchanged at the end of the reaction. Catalysts are key to enabling chemical reactions essential to the production of many of the things people rely on, such as medicines, food products and even the gasoline. An important benefit of CEBC will be its academic impact as the center researchers expand the understanding of how catalysts work and invent new catalysts to do important chemistry while protecting the environment.



New High Pressure Reactors

The CEBC also will provide a unique educational experience for the next generation of engineers and scientists. Working in a multidisciplinary setting, they will have hands-on opportunities to solve real world problems. The NSF supports fundamental research and education across all fields of science and engineering, and NSF Engineering Research Centers are expected to develop powerful education programs. Engineering Research Centers are founded to advance knowledge and develop new technologies to

transform U.S. industry. The centers foster collaboration among researchers from many disciplines and provide an educational and research environment that prepares a new generation of engineering and science leaders.

The NSF backing is a landmark for KU, according to Bob Barnhill, vice provost for research and president and CEO of the University of Kansas Center for Research. "This award from the National Science Foundation represents the largest research grant ever awarded at KU or at any Kansas university. Not only will the award facilitate research important to quality of life and the environment, it also reflects and contributes to the strong momentum of research at the University of Kansas, where we are enjoying one of the largest rates of growth in research funding among the nation's public universities."

Efforts to secure the NSF award required research, organizational expertise, and institutional backing at several levels. "The CEBC had to win out in stringent peer reviewed competition in order to earn this impressive and elite NSF award," said Stuart R. Bell, dean of the KU School of Engineering. "KU is being recognized for its ability to compete on a national level as a premiere engineering institution. Building the CEBC to this level was not a short-term endeavor," he said. "The Subramaniam/Busch team gathered the essential elements and built the necessary strengths over the past several years to win this NSF Engineering Research Center. We couldn't be more thrilled for them."

The NSF award to the center will position KU and its partner institutions for greater impact in the global arena, according to Kim Wilcox, dean of the KU College of Liberal Arts and Sciences. The multi-dimensional approach taken by the CEBC faculty multiplies the effects of their cutting-edge research by adding the components of community outreach, partnerships with industry and unique educational training for tomorrow scientists, he said. This dynamic approach to research reflects KU ability to respond to the increasing demands of global competition.

—Daryle H. Busch

To learn more about the center, its mission and the people at its core, go to <http://www.ku.edu/~cebc/main.shtml>;
To learn more about the National Science Foundation's Engineering Research Centers go to the ERC website at website <http://www.eng.nsf.gov/eec/erc.htm>.

Notes from the Chair



Dear Chemistry Alumni and Friends:

Greetings from Malott Hall. It has been another active year in Lawrence. The basketball team made the Final Four again, the football team is going to the Tangerine Bowl, and Chemistry continues its growth. Although the state budget remains bleak and funding for education is still down, we are adding faculty, attracting more students, bringing in more grant funds, and renovating Malott Hall. The generous donations from you, alumni and friends, are a significant reason we have been able to continue to grow in these tough financial times. So I want to start this letter with a heartfelt thank you to all of our donors.

This year saw the retirement of two members of the faculty. Barbara Schowen retired at the end of the academic year, leaving a big hole in both Chemistry and the Honors Program. She has now joined Dick in his world travels. Al Lata retired as Director of General Chemistry Laboratories after more than 35 years at KU. He left an indelible impression on the General Chemistry laboratory. Al was last seen on the Lawrence Community Theater stage. We wish both Barbara and Al well.

We have been fortunate to be able to add faculty this year. Professor Mario Rivera joined the faculty in July. Professor Rivera is a bioanalytical chemist studying protein structure. He came to us from Oklahoma State University where he had established an internationally recognized research program. We also welcomed Dr. Roderick Black to the faculty as the Director of General Chemistry Laboratories. Dr. Black earned his Ph.D. at the University of North Carolina – Chapel Hill. We think the trade of Roderick for Roy was a pretty good deal for the Chemistry Department.

Several Chemistry faculty received honors this year. Kristin Bowman-James received the ACS Midwest Regional Research Achievement Award in Chemistry. Daryle Busch was awarded the Basolo Medal for Outstanding Research in Inorganic Chemistry and was given honorary membership in the Chemical Society of Japan. Bob Carlson was a finalist for the H.O.P.E. Award for outstanding teaching. Helena Malinakova received an NSF Career Award. Finally, Cynthia Larive was promoted to full Professor this year.

The Chemistry Department faculty had a very successful funding year. Research expenditures in the Department exceeded \$4.3M. Chemistry faculty were also central in winning several major federal grants. KU was awarded two NIH COBRE grants, one on drug discovery and the other on proteomics, that will provide \$10M in funding each had several members of the chemistry faculty as key contributors. Professor Daryle Busch is the co-PI along with Professor Bala Subramanian in engineering of an NSF Engineering Research Center (ERC) on environmentally beneficial catalysis that contributes over \$30M in funding. Four of the focus groups of the ERC will be lead by members of the Chemistry Department faculty. Finally, NIH has announced a \$10M grant to Professor Jeff Aube of Medicinal Chemistry and Courtesy Professor of Chemistry on combinatorial synthesis. Again, several members of the Chemistry Department are key contributors to this grant. These initiatives continue to expand the opportunities for both our graduate and undergraduate students to pursue research at KU.

I would like to extend a special thank you to Don Leedy who established the Ted Kuwana Fund through a major donation. The Kuwana Fund will be used to establish a graduate fellowship in honor of

Professor Ted Kuwana's distinguished career. We are also extremely grateful to Ozzie Wong for a major donation to establish the Barbara Schowen Fund. The Barbara Schowen Fund will provide scholarships in Barbara's name to outstanding undergraduate chemistry majors. We could not provide the programs we do without the outstanding generosity of alumni like Ozzie and Don. We are extremely grateful for every donation, of whatever size, that we receive.

I again extend a warm invitation for you to visit the Department whenever you have the opportunity. On behalf of the faculty, staff, and students, we all look forward to seeing you again.

Craig E. Lunte

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KU AND UNC TRADE

Three years ago when Roy Williams was first recruited by the University of North Carolina – Chapel Hill but decided to remain at KU, the Chemistry Department felt it appropriate to give our colleagues in chemistry at UNC a consolation prize. An appropriate tee-shirt autographed by the faculty was sent to UNC.



Mark Wightman, Professor of Chemistry at UNC and KU alumni (Adam's postdoc), models the shirt.



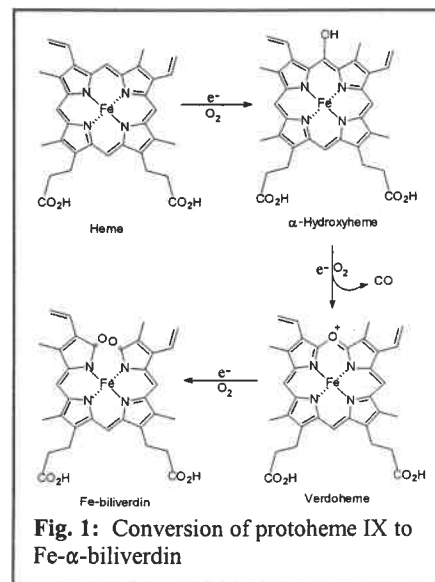
With Coach Williams recent departure to UNC, their chemistry department has kindly returned the favor with an autographed tee-shirt of their own. This shirt is now proudly displayed in the Chair's Office.

RESEARCH NEWS FROM NEW ASSOCIATE PROFESSOR, MARIO RIVERA-LAOS

The main emphasis of research in the Rivera laboratory has centered on the elucidation of structure-function relationships in heme containing proteins. Heme containing proteins and enzymes are known to be vital components of most living organisms. Heme proteins 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 my research efforts.

In order to understand how protein structure modulates the physical and chemical properties of the heme cofactor our group has been involved in protein chemistry, as well as methods development research. In an attempt to address the challenges posed by the study of redox active metalloproteins we combine the strengths of recombinant DNA methodology, bioelectrochemistry and NMR spectroscopy. In addition, we have established fruitful collaborations with Dr. Cai Zhang, Oklahoma Medical Research Foundation (X-ray crystallography), Dr. Pierre Moëne-Loccoz, Oregon Graduate Institute of Science and Technology (resonance Raman spectroscopy), Prof. David R. Benson, University of Kansas (protein design and structure function in heme proteins), Prof. F. Ann Walker, University of Arizona (EPR spectroscopy), Prof. Angela Wilks, University of Maryland (heme oxygenase), and Prof Krzysztof Kuczera, University of Kansas (molecular dynamics). The interdisciplinary approach to study structure-function relationships in hemoproteins has been both rewarding and productive.

Our most recent efforts are aimed at understanding the process of heme catabolism at the molecular level. Heme catabolism in mammals is carried out by the enzyme heme oxygenase. The metabolic breakdown of heme is remarkable in that heme oxygenase utilizes heme in a dual role of substrate and cofactor and in an oxygen and electron-dependent set of reactions cleaves the α -meso bridge to produce CO, biliverdin and free iron (see Figure). The process of heme breakdown has recently attracted significant attention because the products of heme degradation play important physiological functions: Heme breakdown allows the efficient recycling of iron, which is typically difficult to absorb from dietary intake. CO is believed to play a role akin to that of NO in signal transduction and communication, and biliverdin is the source of bilirubin, a powerful antioxidant. Our investigations have recently demonstrated that heme oxygenase is unique among heme proteins in that the heme active site can be readily distorted from planarity. These nonplanar heme conformers, which are in dynamic motion between the confines of the protein, exhibit highly unusual electronic structures. We believe that these novel electronic structures activate the heme to participate actively in its own degradation. Thus, our current thoughts regarding the molecular aspects of heme catabolism are rooted on the fact that relatively low frequency and high amplitude molecular motions are paramount to the reactivity of heme oxygenase. Consequently, as part of our future activities we will measure and map out these types of molecular motions with the aid of NMR spectroscopy, in an attempt to paint a quantitative picture relating molecular motion and the process of heme catabolism.



We are also interested in studying the structural, thermodynamic and dynamic aspects of the interactions between heme and protein (polypeptide). To this end we are studying cytochrome b_5 , a type of protein that functions as an electron carrier by shuttling the heme iron between the +3 and +2 oxidation states. With the aid of site directed mutagenesis, thermodynamic characterization and X-ray crystal structures we have made and characterized a set of molecules with varying degrees of stability and heme binding properties. The findings so far strongly suggest an important contribution from polypeptide motion in dictating the properties of each of the proteins in our set of engineered cytochromes b_5 . We are in the process of initiating studies aimed at mapping out these functions, which we believe will provide us with a unique understanding regarding the process of assembly of the heme polypeptide complex.

-Mario Riveras-Laos

Professor Daryle H. Busch Honored in Japan

The Japanese celebrated the 125th Anniversary of the Chemical Society of Japan in high style. In a ceremony of extreme pomp (from my perspective), in the company of the royal family, and along with 5 other chemists, including 4 Nobel laureates, I was inducted as an Honorary



Daryle Busch &
Ryoji Noyori

Member of the Chemical Society of Japan. The awards were presented by CSJ President and Nobel laureate Ryoji Noyori. Two other Americans were honored, Professor Roald Hoffman (Nobel) of Cornell University and Ronald Breslow of Columbia University. The others (all Nobel) were Jean-Marie Lehn (France), Yuan T. Lee (China), and Harold Kroto (Britain). Most interesting, in conversation with the Empress I learned she has a good knowledge of Western poetry.

2003 Fred Basolo Medal Awarded

October 24, 2003, the Fred Basolo Medal for Outstanding Research in Inorganic Chemistry was awarded to Roy A. Roberts Distinguished Professor Daryle H. Busch. The Fred Basolo Medal was established by the former students of Fred Basolo in appreciation for his contributions to inorganic chemistry at Northwestern University. Professor Busch's research in basic transition metal coordination chemistry fathered modern macrocyclic ligand chemistry and created the molecular template effect. He was among the founders of the subject of ligand reactions and an early researcher and proponent of bioinorganic chemistry. He first described the phenomenon called *preorganization* in 1970. His research is presently focused on green homogeneous catalysis, bioinorganic chemistry, and orderly molecular entanglements, a part of supramolecular and nanochemistry.



Associate Professor Naomi Hoshino of Hokkaido University, former graduate student of Dr. Busch; Dr. Busch; Professor Tasuko Ito, Distinguished Professor at Tohoku University, former Busch post-doctoral researcher.

CHEMISTRY AND SHOW BUSINESS: STRANGE BEDFELLOWS?

The ACS student affiliates (KU Chemistry Club) has been extremely busy during the fall 2003 semester taking on new challenges as they shape their new and original, chemically-charged, interactive multimedia chemistry show entitled, "Frozen Flames University: Chemistry Tonight!" Taking both its audience members and its cast on the most exciting scientific journey to date, "Frozen Flames University" is breaking new ground in the attempt to reach out to the university and community and encourage both to embrace chemistry even more. The show pits Dr. Pyro against Dr. Cool in an information-filled hour of "temperature swings" that will both excite and educate the aspiring mind. The initial version of the show debuted at the University Open House on September 20, 2003. A newly released version will be presented in Spring 2004 to several of the local schools. More information on the show schedule and times, a viewable trailer for the show, and additional links can be found at our website at [acs.chem.ku.edu/students/]. This show hopes to attain new heights with your continued support and sponsorship.

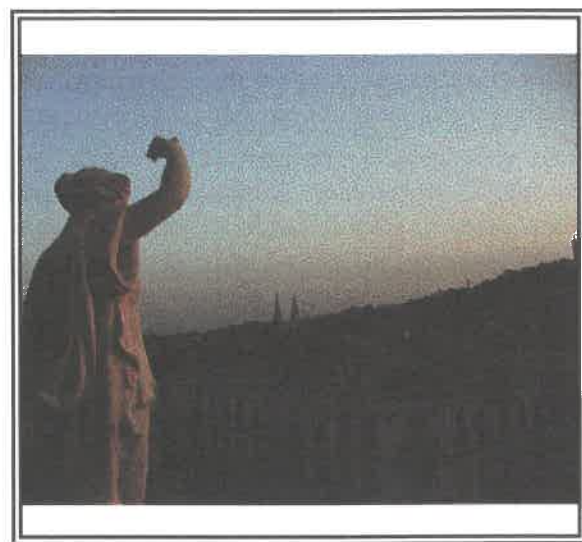
If you are able to help by visiting our website [acs.chem.ku.edu/students/] and pledging funds to this show, you can help make chemistry come alive for the generations to come!!!

-Paul Hanson

INTERFACE SCIENCE AND BAGUETTES

This past summer, I had the honor and opportunity to co-organize and attend a workshop on *Crystal-Melt Interfaces: Structure, Dynamics and Growth* that was funded and hosted by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) at the Ecole Normale Supérieure in Lyon, France. My co-organizers in this international endeavor were Dr. Ruslan Davidchack, a former graduate student/postdoc in

my group here at KU, currently a lecturer in Applied Mathematics at the University of Leicester in England, and Prof. Mark Asta, Professor of Materials Science at Northwestern.



View from Les Muses de la Opera – the venue for the workshop banquet.

Our goal in this workshop was to bring together, in a common forum, theoretical and computational scientists (and even a few experimentalists to keep us honest!) from materials science, engineering, physics and chemistry with a mutual interest in the study of crystal-melt interfaces. The motivation for such a meeting was recent advances in interfacial simulation methodology and computer power that complement similar advances in the continuum modeling of crystal growth to make possible true multi-scale modeling of such technologically important processes, such as dendritic growth in metal alloys to protein crystallization, starting from an atomic-level description. By bringing together a diverse group of interface scientists, the workshop was successful in helping to break down disciplinary barriers and has already nucleated a number of international collaborations. Oh yeah, and the food was good too!

Further information and images from the meeting can be obtained from the workshop website: <http://weizen.chem.ku.edu/CECAM/interfaces.html>

-Brian B. Laird

NEW, STATE OF THE ART RESEARCH LAB

Those of you who attended KU before the mid 1990's will remember the 6th floor of Malott being occupied by the Government Document and Science Libraries. Those libraries have since been moved to different locations, and just this past year, half of the old stack area of the Science Library was remodeled into state of the art laboratory space for Dr. Andy Borovik and his group. After the demolition of the old stacks the west side of the area was converted to include a 1540 square foot lab and 653 square foot student office space.

The lab was remodeled to have a very open design to allow the students easy access to all features. The design allows Dr. Borovik to place his instruments (glove boxes and EPR) in a safe and efficient manner. The remodel included three Labconco Fume Hoods, suspended electrical outlets; central gas cylinder storage; and a flammable storage room.



The office was designed with windows that look out into the laboratory. Students and visitors are able to watch experiments taking place without entering the lab. The office area can accommodate up to twelve students and has a built in counter top for desks and built in file cabinets. In addition there are two smaller rooms that can be used by students for tutoring or studying.

TRANSITIONS

Two new faculty members join the Department!

Laboratory Director Roderick S. Black moved to KU in January 2003 to pursue his interest in undergraduate science instruction. He is currently working with colleagues to introduce additional laboratory experiments to the undergraduate chemistry curriculum. He also coordinates the daily operation of the general chemistry laboratories, and assists with the training and supervision of teaching assistants.



Associate Professor Mario Rivera-Laos came to KU in August 2003 from Oklahoma State University. Mario earned his B. S. degree from Universidad Autonoma de Guadalajara in Mexico and his Ph. D. in Analytical Chemistry from the University of Arizona under the supervision of Professor Quintus Fernando. Mario carried out postdoctoral studies in the laboratory of Professor F. Ann Walker, where he developed his interest in heme containing proteins and bioinorganic chemistry. Mario's research is currently aimed at understanding the mechanism of heme catabolism, which is carried out by the enzyme heme oxygenase. He is also interested in applying the lessons learned from studying the structural and dynamic properties of heme proteins to the design of relatively sturdy heme proteins exhibiting useful catalytic properties, such as electron transfer and oxygen activation.

Two esteemed faculty members retire!

Professor K. Barbara Schowen Retires

On May 31, 2003 family, friends, and colleagues of Barbara Schowen attended a reception by the Department to honor her on her retirement after 26 years of teaching, research, and service to the University of Kansas. Recognized by a Kemper Fellowship for teaching and advising excellence in 1997, Barbara has had a significant impact on the lives of her students, the curriculum of the Department of Chemistry, advising in the College of Liberal Arts and Sciences, and the growth and development of an Honors program that has enriched the educational opportunities for hundreds of outstanding students throughout the College.



In 1987, after teaching 13 years at Baker University and another 10 years as a half-time Lecturer in the Department of Chemistry at KU, Barbara became a full-time faculty member in the Department where she was Coordinator for Undergraduate Studies with responsibilities for overseeing the undergraduate educational mission, running the undergraduate research program, and teaching courses in both general and organic chemistry. For years she also served as a primary advisor to the pre-health science students in the College. Nearly every weekday afternoon students could be seen in her office where she would give them special encouragement, accurate information, and sound advice.

In August of 1996, she was appointed as Director of the University of Kansas Honors Program while remaining half time in Chemistry. It was during the period 1996-2003 that she helped to achieve more than a 50% increase in both the number of honors course offerings and more than a 40% increase in the number of

participating students. Equally significant were her successful efforts to enhance the role of undergraduate research in the curriculum of the numerous departments throughout the campus. She played a key role in bringing various educational opportunities outside the classroom to the attention of students. These experiences together with careful mentoring led to students receiving 20 Goldwater Scholarships, three Marshall Scholarships, one Rhodes Scholarship, nine Udall Scholarships, and four Truman Scholarships during her tenure as Director.

Barbara has been a leader at the local and national levels in promoting the importance of an undergraduate research experience for science majors, and was recognized for these efforts by her presentation of invited papers for the National Research Council, the National Science Foundation, and the American Chemical Society followed by her receipt in 1996 of the ACS Midwest Award for Mentoring Undergraduate Research. At KU, she has been coordinator or co-coordinator of 18 years of a successfully funded Summer Undergraduate Research program.

Professor Schowen's research interests in organic, bio-organic, and biochemical reaction mechanisms has focused on proton-transfer and tautomeric catalysis and how these processes differ in aprotic, protic, and



ixed solvent systems. Her expertise in the applications of solvent isotope effects to these studies led to her authoring or co-authoring (with R. L. Schowen) several chapters and articles on how solvent isotope effects and the proton inventory method can be used to help elucidate enzyme and other reaction mechanisms. These publications remain as frequently cited works to the present time. Above are a few pictures taken at her retirement reception.

Barbara plans to spend time traveling with her husband Dick and spending more time with her two daughters and two grandchildren. We all wish her the very best in the years to come, but her extensive and high quality contributions to the Department and the University will be greatly missed.

Alfred J. Lata Retires

Alfred J. Lata officially retired this past summer after 38 years of service to the Department of Chemistry. Alfred was part of the department's "Princeton connection" that included KU Professors Ralph Adams and Clark Bricker. When Alfred was a freshman at Princeton, his laboratory instructor was Ralph Adams, and Ralph served as Alfred's research advisor during his senior year. Alfred took two years of analytical chemistry at Princeton with Clark Bricker, who also served as his junior year advisor and mentor. Alfred completed his BA degree in chemistry at Princeton in 1954.



Alfred's years at Princeton were followed by two years in the US Army where he was an officer in a 280-mm gun battery and serving also as an atomic projectile officer. He then entered graduate school at Western Reserve University, where he completed an MA degree in education a year later. He taught for the next eight years at Shaker Heights High School in Shaker Heights, Ohio. During this period Alfred sang under the direction of the famous Robert Shaw, and he also carried out laboratory research toward a graduate degree in chemistry at WRU. Before he could complete this degree, however, he received a call from Clark Bricker in the Department of Chemistry at KU. Clark had come to KU in 1963 to run the general chemistry program, and he wanted Alfred to oversee the laboratory portion of his courses. Alfred accepted the offer and became a member of KU's Department of Chemistry in 1965. Clark and Alfred established a rigorous general chemistry program at KU that was ranked among the

best in the country. Also, for many years during the summer, Alfred and Clark ran an NSF-sponsored institute designed to enhance the chemistry backgrounds of high-school teachers.

In their early years at KU, Alfred and Clark Bricker wrote a series of laboratory experiments that was used, with yearly modifications, in the general chemistry labs at KU for approximately 30 years. Alfred also wrote experiments designed for KU's liberal arts chemistry course. Years later, with suggestions and encouragement from Barbara Schowen, Alfred and Grover Everett modified these experiments for eventual publication in 1988 by Harcourt Brace Jovanovich in a manual entitled "Experiments in General, Organic, and Biological Chemistry", co-authored by Arne Langsjoen and Paul Lieder. In 1995, Alfred and Grover selected twelve of these experiments for a smaller manual, "Experiments in Chemistry 125", published by HBJ and intended for use in the laboratory portion of the liberal arts chemistry course at KU.

Alfred was one of the first to experiment with the use of computers for chemical education. He worked with the GE-Honeywell time-sharing system, which was among the earliest systems to be operated in an interactive mode. He wrote Fortran and BASIC programs for computer assisted instruction, for simulation of qualitative analysis, and to keep records for the general chemistry program. Alfred was invited to speak on the topic of computer assisted instruction at a number of schools and at regional, national, and international meetings. For a number of years, he was a member, and served as Chairman, of the ACS Division of Chemical Education's Committee on Computers in Chemical Education.

More than 25,000 students satisfied their laboratory requirement for general chemistry during Alfred's career at KU, and approximately 600 teaching assistants had their first experience in teaching under Alfred's supervision. Alfred was renowned for his highly-organized, weekly TA meetings and well-run laboratory courses. His personal laboratory was the venue for modification of laboratory experiments, and it also served as a repository for the "unknowns" used in qualitative analysis. Alfred's office was frequented by both TA's and undergraduate students, and often there was a queue outside his door. Alfred was reluctant to discard anything, and over the years the visiting space in his office shrank. Eventually all that remained was sufficient room for the door to open and an aisle leading to his desk that could be traversed by a thin person walking sideways.

Alfred's service to the university and the community includes six years in University Governance with the University Council, a year on the University Senate Executive Committee, and ten years as Chairman of the Douglas County Science Fair.

Within the Lawrence community, Alfred is best known for his wonderful voice and his acting talents. He has been involved with the University Theater and the Lawrence Community Theater for many years, both on the stage and in off-stage production. To date, he has participated in more than 50 productions in Lawrence. Alfred was one of the founding members of *Voci de Camera*, a singing group started by Ralph Christoffersen of KU's Department of Chemistry. Alfred still sings with the Lawrence Motet Singers, and he is frequently asked to sing at weddings and funerals.

Alfred and his wife, Winston, plan to remain in Lawrence.

Cynthia Larive Promoted to Full Professor

Cindy Larive's research on the development and application of new NMR methods is impacting the fields of both bioanalytical and environmental analytical chemistry. A major focus of her research has been in analytical applications of NMR spectroscopy. One area of study is understanding the nature of interactions between small molecule ligands and proteins. NMR diffusion measurements are a useful way to study ligand-protein binding, because changes can be detected when a small molecule (like a pharmaceutical agent) interacts with a macromolecular target without the need for special labels. Her group has developed 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 cases where several ligands are studied simultaneously. In addition to providing information about the strength of the interaction, the build-up of transferred-NOE during the diffusion experiment can provide insight into the nature of ligand-protein binding and can be used to prepare an epitope map of the ligand, which is useful for the elucidation of structure activity relationships.

One of the major limitations of NMR as an analytical tool is the relatively poor sensitivity of this technique. Although a number of innovations continue to enhance the sensitivity of this method, including high field magnets and cryogenically cooled probes and preamplifiers, challenges remain in this area. NMR microcoil probes can greatly improve the mass sensitivity of NMR measurements and facilitate coupling with on-line capillary separation techniques. Microcoil NMR probes constructed in Dr. Larive's laboratory, capable of measuring volumes of 1 μ L or less, permit NMR detection with capillary isotachopheresis (cITP) or capillary HPLC separations. The Larive group is using these separation methods coupled with NMR detection to study a number of problems related to structure elucidation including the characterization of humic substances and oligosaccharides.

Research in the Larive group also has an environmental focus. In order to understand the breakdown pathways and processes involved in the transformation of a contaminant it is necessary to identify and quantify the products of these processes as well as the rates at which they occur. However the structure elucidation and quantification of breakdown products of pollutants in aquatic ecosystems presents a significant analytical challenge. Because of its high specificity and low detection limits, LC/MS/MS provides important information for structure elucidation of unknown compounds. The complementary information provided by NMR generally makes it a valuable addition to MS, however the relatively low sensitivity of NMR has thus far limited its application to environmental problems. In conjunction with LC/MS/MS we are using conventional LC/NMR instrumentation along with capillary separations interfaced with specially constructed microcoil NMR probes to study the fate and effects of antibiotics in aquatic ecosystems. An important and unique aspect of our research involves field experiments conducted in collaboration with colleagues in the Departments of Civil and Environmental Engineering and Ecology and Evolutionary Biology at the University's Nelson Experimental Studies Area, one of largest ecological research stations in the world.

-Cynthia Larive

IN MEMORY

John L. Margrave, Ph.D. 1950, one of our most illustrious students, died in Houston December 18, 2003 at age 79 of complications following heart surgery. At the time of his death, he was the E. D. Butcher Professor of chemistry at Rice University. During a career spanning five decades, Dr. Margrave made a multitude of professional and personal contributions across diverse settings, exemplifying his commitment to scientific excellence and the larger community. He loved teaching and interacting with students of all ages, and his inspiration brought many students to the study of chemistry. He was recently honored by the American Institute of Chemists with the Chemical Pioneer Award for his ground-breaking research in the field of fluorine chemistry and for his work with high temperature liquid metals. In July 2003, he received the R & D 100 Award for his innovative work on fluorinating carbon nanotubes. His research, including more than 800 scientific publications, consistently expanded the frontiers of chemistry. He was elected to membership in the National Academy of Sciences in 1974. He was also elected as Fellow of the American Institute of Chemists, the American Physical Society, and the American Association for the Advancement of Science.

Dr. Margrave and his research group often presented chemical magic shows for youth in libraries, schools, and the Houston Museum of Natural Science. He mentored more than 100 graduate students and 100 post-doctoral researchers during his career. Interacting with his students and sharing in their success and

interests provided deep satisfaction in his professional life. For many years, Dr. and Mrs. Margrave have been Faculty Associates at Rice's Graduate House. He founded the journal, "*High Temperature Science*" and served as its editor, innovator, and reader of all submissions.

A graduate of Rosedale High School in Kansas City, KS, he achieved the honor of Eagle Scout as well as induction into the Mic-O-Say order of scouting. Dr. Margrave received his B.S. and Ph.D. degrees from The University of Kansas, where he was a Summerfield Scholar and a Slosson Graduate Fellow. He was named a Distinguished Alumnus of KU in 1981. He pursued postdoctoral work at the University of California, Berkeley, where he received an Atomic Energy Commission Fellowship. In 1952, he joined the faculty at the University of Wisconsin, where he was an Alfred P. Sloan Fellow, a Guggenheim Research Fellow, and a recipient of the Kiekhofer Memorial Teaching Award. In 1963, he joined the faculty at Rice University. He received the American Chemical Society Award in Inorganic Chemistry in 1967, the IR-100 Award for "CFX" in 1970, the American Chemical Society Southwest Regional Award in 1973, the AIC Honor Scroll Award in 1978, the American Chemical Society Award in Fluorine Chemistry in 1980, the IR-100 Award for Cryolink Matrix-Isolation in 1993, the Sigma Xi Distinguished Achievement Award in 1994, and the Scholars Award for Excellence in Science and Technology in 1994. He served in the U.S. Army in World War II and as a Chemical Corps reservist. In recent years he served as the Navy ROTC representative for Rice.

Dr. Margrave served as Chair of the Rice University Department of Chemistry from 1967-1972 as Rice's Dean of Advanced Studies and Research from 1971-1980, and as Vice President for Advanced Studies and Research from 1980-1986. He served in various capacities at the Houston Advanced Research Center (HARC), culminating in his appointment as Chief Scientific Office in 1989. As a member of the National Academy of Sciences, Dr. Margrave served on key committees of the National Research Council related to nuclear safety, armaments, and demilitarization of chemical weapons. He was President and then Director of Sigma Xi from 1986-1992.

He was born April 13, 1924 in Kansas City, Kansas and is survived by his wife of 53 years, Mary Lou Davis Margrave, of the home. Other survivors include two children, David Margrave and Karen Margrave Bornhofen, five grandchildren, a sister, Wilma Hayward, and eight nieces and nephews.

48TH CHEMISTRY HONORS RECEPTION

The Frank B. Dains Award

outstanding first-year teaching assistant

Eric W. Crick

The H. P. Cady Award

excellent performance by first-year graduate student

Erin C. Burger

The Ray Q. Brewster Award

advanced graduate teaching award

Joseph M. Vilain

The Reynold T. Iwamoto Scholarship

award based on academic performance

Kimberly D. Bratton Elizabeth S. Erickson

The Snyder Award

graduate student of considerable promise

Leilani L. Welbes

McCollum Research Fellowship

Thomas C. Holovics Janelle L. Portscheller

Peter L. Larsen Jay R. Unruh

Sarah F. McDonald Alan Whitehead

The J. K. Lee Scholarship in Analytical Chemistry

superior academic performance and research accomplishments

by an advanced doctoral student

Stacy D. Amett

The Ernest and Marvel Griswold Scholarship in Inorganic Chemistry

superior academic performance and research accomplishments

by an advanced doctoral student

Aaron B. Cowley

The Frank B. Dains Scholarship in Organic Chemistry

superior academic performance and research accomplishments

by an advanced doctoral student

Matthew D. McReynolds

The Paul and Helen Gilles Award in Physical Chemistry

superior academic performance and research accomplishments

by an advanced doctoral student

Kenneth D. Osborn

The Higuchi Doctoral Progress Scholarship

superior post-comprehensive student(s) in his or her final year

Andrew M. Hamed

Laura H. Lucas

SPECIAL RECOGNITION

Bridget Becker--received an ACS WCC travel award to attend ACS Meeting in New York--September 2003

Andrew M. Harned--received 2002-2003 Nelson J. Leonard Fellowship sponsored by Organic Synthesis, Inc.

Laura H. Lucas--received an ACS Division of Analytical Chemistry Nine-Month Graduate Fellowship sponsored by Eli Lilly & Company

Katie R. Mitchell-Koch received an NSF Graduate Fellowship and The Fannie and John Hertz Foundation Scholarship

Cristina Vizcarra (B.S., August 2002) awarded an NSF Graduate Fellowship

DEGREES GRANTED

Bachelor of Arts

Steven G. Anderson	Eunice S. Ndærem
Quanita J. Crable	Hieu T. Nguyen
Heather D. Cunningham	Catheine C. Nodgaard
Tara R. Foxx	Jodi M A. Oldfather
Adam T. Gregg	Keely E. Olmsted
Penny M. Higginbotham, <i>Honors</i>	Bradley E. Parker
Joseph D. Johnston	Christina C. Welles
Jill K. Meyer	

Bachelor of Science

Kyle R. Brown	Katie Mitchell-Koch, <i>Honors</i>
Chad R. Hladik	Bonnie A. Sheiff, <i>Honors</i>
Huey Lih Lee	Jeanine R. Stefy
Galen S. Loving, <i>Honors</i>	Christina L. Vizcarra
Ryosuke Yamasaki, <i>Honors</i>	

Master of Science

Robert A. Doyle	NVida E. Houndonoughbo
-----------------	------------------------

Doctorate of Philosophy

Yao Houndonoughbo	Rachel Sibug-Aga
Jeffrey R. Krogmeier	Joel S. Thompson
Jennifer L. Razak	Sarah A. Vickery

2002-2003 ChemScholars

Hillary C. Compton	Christopher D. Janish
Rebecca Evanhoe	Christopher G. Lee
Jonathan W. Lamb	

ALUMNI NEWS

David Armentrout, B.S., 1961, retired at the end of 2002 after 36 years of chemical research at Dow Chemical Co., in Midland, Michigan. He was very saddened to read of the death of his mentor, Professor Ralph Adams, and send his regards to the family.

W. H. Breckenridge, B.S., 1963, was awarded the University of Utah Distinguished Scholarly and Creative Research Award for 2003. This is the premier award for recognizing career national and international research contributions of faculty at the University of Utah, and is only given to three professors every year, selected from many applicants in all departments in every field (not just in the sciences). Congratulations, Professor Breckenridge!

Sterley Cole, is in his 15th year with Supelco (a division of Sigma-Aldrich) and continues to find his work both challenging and rewarding. His efforts these days revolve around strategic projects with a number of pharmaceutical companies and other business development activities. He particularly enjoys visiting with their customers and learning about the many processes they employ.

William H. Deschner, M.D., B.A., 1969, is enjoying part time practice of obstetrics and gynecology plus lots of tennis and relaxation in Palm Springs. He states he has many "great" memories of lectures in Hoch Auditorium and "lengthy" labs in Malott!!

Kale C. Gentry, B.S. 1955, M.D. 1960, retired in December of 2002.

Judson Goodrich, A.B. 1947, M.A. 1948, Ph.D. 1951, spent 35 years as a research chemist at Chevron Research Co., producing 28 patents. He retired in 1985. He now plays Freedom Horn in the Las Gallinas Valley Sanitary District Non-Marching Band, the Nova Albion brass quintet, and the Golden Gate Brass Band. Twenty arrangements for brass quintet have been published. He spent 2 weeks in Cuba during 2002 visiting national parks. Dr. Goodrich protests that there is no category in this newsletter for the 40's years. "Surely there are still a batch of us kicking around". (Ed. note, anyone who would like to contact alums from the 40's and have a section of the newsletter devoted to those alums is welcome to spearhead this project.)

Martha Ruth "Ruthie" Hagan, BS. 2000, MEd 2003, JD 2004, is about to start her 3rd year of law school at the University of Arkansas. She is clerking this summer for 2 firms in Little Rock, Arkansas.

Betty Austin Hensley, B.A. 1944, is a flute teacher, performer, and researcher. Thurlow Lieurance Indian Flute, 2nd Edition, by Betty Austin Hensley has been published by the Oregon Flute Store. The book contains a number of photos, with many in color, descriptions of the 12 historic Native American flutes, and a CD of Betty playing each flute.

Verner Nellsch, B.A. 1975, Director of the Livingston Women's Clinic, is now living on a big Texas lake, delivering babies, performing surgery, and raising 5 kids.

Dr. Katherine Prater, has been tenured and promoted to Associate Professor at Texas Wesleyan University.

Jason B. Wittner, B.A. 1993, M.D. 1997, is entering private practice in Lincoln, Nebraska with the Lincoln Pulmonary and Critical Care group. He has just completed his subspecialty fellowship in Pulmonary and Critical Care medicine. He and his wife Katie have had their first child, Nicholas.

Wayne Wolsey, Ph.D. 1962, has entered a retirement "phase-out" at Macalester College for four years. He'll be doing "professorial work" half time. A new (8th) edition of "Chemical Principles in the Laboratory", Slowinski, Wolsey, Masteron, will come out in 2004. That plus lots of volunteer work with his professional organizations occupies his time.

CHEMISTRY STAFF MEMBER EARNS MARCH 2003 "EMPLOYEE OF THE MONTH" HONORS

Richard Fritts joined the Department of Chemistry as a machinist in 1991. Since 1993, Richard has been an instrument maker. That means in addition to repairing scientific equipment and maintaining the reverse osmosis water system for the old side of Malott Hall, his routine duties include helping unload and move scientific equipment, preparing rooms for renovation, making shelves and other furniture, keeping the hallways clear and monitoring rooms for safety violations. When scientific equipment in Malott needs to be moved, Richard is the "go-to" guy. Without his expertise, the loading dock would be full of equipment that hasn't quite reached its destination. Over the past 12 months, Richard has moved a large X-ray machine, glove boxes, a nuclear magnetic resonator and other assorted items.



Recent feat(s): Last summer, the chemistry department had several simultaneous remodeling projects. One major project was the merger of the department's main office with the business office. The department was able to obtain five-foot cubicles for the new setting, but they were too small. Richard found a way to put two units together, and arrange the cubicles to optimize the workspace for each employee. In late November, Fritts was on vacation, but he called in daily to check if anyone needed anything, as he knew the department was short handed because of the holiday.

NEW ENDOWMENT FUNDS ESTABLISHED

K. BARBARA SCHOWEN UNDERGRADUATE CHEMISTRY FUND

This new fund was made possible by a generous gift from Osborne S. Wong. It will be used to provide support annually, with the possibility of renewal, for one or more deserving students in the Chemistry Department within the College of Liberal Arts & Sciences at KU. The support shall be made to Chemistry major honors students, selected by the Department Chair and designated faculty, based on need and merit.

THEODORE KUWANA GRADUATE OPPORTUNITY FUND

Donald W. Leedy, Ph.D.'s generosity made this fund a reality. It shall be used to provide awards annually with the possibility of renewal, for one or more deserving graduate students in the Chemistry Department within the College of Liberal Arts & Sciences at KU. Recipients will be graduate students pursuing studies in analytical chemistry, and will be selected by the Department Chair and designated faculty representatives. The selection of awardees will be based on, merit and need with a preference for graduate students of cultural diversity.

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Department of Chemistry
1251 Wescoe Hall Dr., Room 2010
University of Kansas
Lawrence KS 66045

We look forward to hearing from you!

Name: _____

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News, updates, comments or suggestions (feel free to enclose photos, news clippings, etc.):

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For more information:

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