

# I U • C H E M I S T R Y

## Model of a Living Cell

by Peter Ortoleva, Distinguished Professor of Chemistry

*On several occasions, I've asked Peter about his various research interests. Among these is the fascinating idea that a biological system as complicated as a living cell could be modeled theoretically; moreover, the model could be an evolutionary one — allowing improved accuracy as more data are acquired on individual components of the model.*

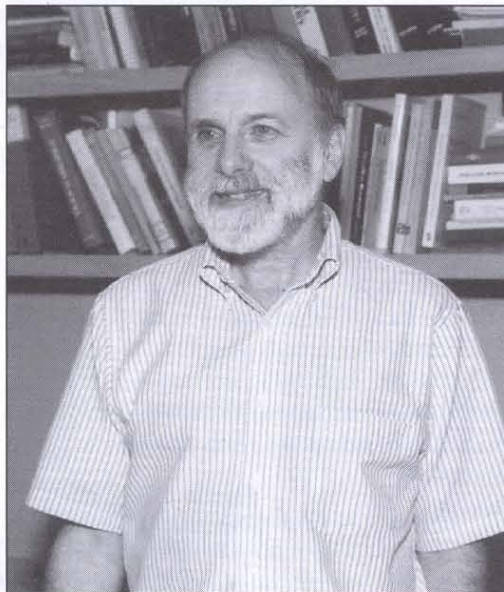
*The following is a brief commentary derived from these conversations and from a number of Peter's incipient publications by a reporter admittedly unfamiliar with some of the concepts.*

— Max Marsh

**F**or many years, Distinguished Professor **Peter Ortoleva** and his students have been developing the components of a theoretical model for a living cell. Recently, this research has received impetus through significant financial support (an \$830,000 grant) from the Department of Energy. The results to date are embodied in a comprehensive software package named "Cyber-Cell," a reaction, transport, genomic cell simulator.

The model, as it presently stands, is incomplete. There are many difficulties encountered in dealing with any such model; these are addressed in this case through an information theory approach.

Cyber-Cell accounts for zones of specialized biochemical processing (e.g. the nucleus, mitochondrion) and the transport of molecules between them. Catalyzed polymerization kinetics transcribe *RNA* from an input *DNA* sequence, while the resulting *mRNA* is used via ribosome-mediated polymerization kinetics to accomplish translation. Through post-translational processing and sequence → function rules, the resulting translated proteins are used to form the enzymes and other factors that mediate metabolism and control the transcription and translation processes. Transport between the zones of specialization



*Peter Ortoleva*

is by linear or nonlinear passive mechanisms or by active processes, all of which are mediated by electrical effects.

An information theory method is used to automate the calibration of Cyber-Cell's reaction and transport parameters via the simultaneous use of a wide range of (genomic, proteomic, bioelectric, metabolic) data of varying quality. The information theory approach is based on the construction of the probability for these parameters so that uncertainty in their estimation can be assessed. The incompleteness of the model is addressed via a probability functional approach for computing the time-dependence of the concentration of key enzymes, or other factors critical for running and calibrating Cyber-Cell. The biochemistry of these latter processes is not yet well understood.

Another challenge addressed in Cyber-Cell is the need to capture phenomena operating at the boundary of the atomic and the macroscopic scales. Small features such as ribosomes

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WE HAVE A SERIES OF ARTICLES DESCRIBING THE MANY ASPECTS OF OUR DIVERSE FIELD.

PETER ORTOLEVA SHARES HIS INSIGHTS ON THE CYBER-CELL PROJECT.

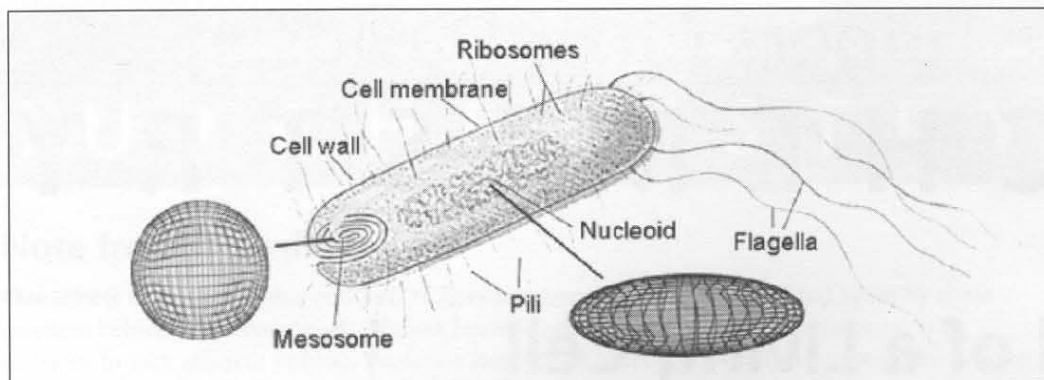
AT A RECENT SYMPOSIUM, CHEMISTS HONOR CHAIR DAVIDSON, WHO PROVES HE HAS THE "RIGHT ANSWER FOR THE RIGHT REASON."

MILOS NOVOTNY SHOWS HIS UNIQUE VIEW OF THE DEPARTMENT OVER THE YEARS.

THE INFORMATICS SECTION DEBUTS WITH ITS FIRST GRADUATES.

AND WE HONOR AND REMEMBER THE LIFE OF LYNNE MERRITT JR.

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**Figure 1.** Cyber-Cell accounts for intracellular features that evolve via mesoscopic equations solved on a hexahedral finite element grid. Key features for *E. coli* include the nucleoid and the ribosomes, while other prokaryotes have these features as well as the mesosome. Subcellular bodies carry out key biochemical functions (©Prentice-Hall Inc., 1999; grids added).

## Model cell

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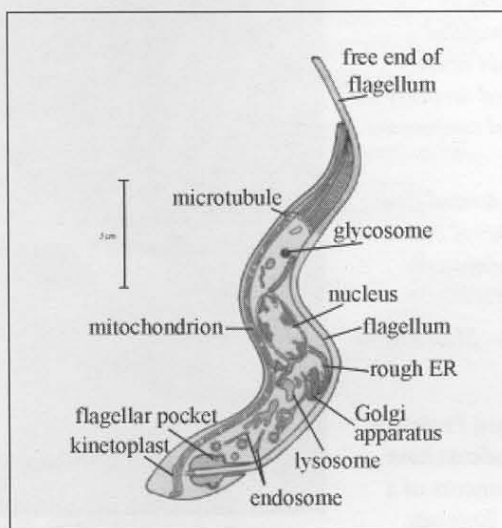
or viruses behave in ways that rely on their atomic scale structure but that take place in the overall (macroscopic) balance of metabolic reaction and transport. Thus, in Cyber-Cell, there is an option whereby these zones may be treated in more detail via the solution of mesoscopic models using finite element methods.

In this way the composition of the medium within the mesoscopic features affects the configuration of macromolecules, and the latter property, in turn, affects the reaction and transport of small molecules to yield a self-consistent mesoscopic approach. The Cyber-Cell simulator and the information theory shell program (by which it is automatically calibrated, run, and generalized) represent major advances in cell biophysics and biochemistry.

Cyber-Cell considers the many compartments into which a cell is divided and within each of which specialized biochemical processes take place (Figures 1 and 2).

One of Ortoleva's major concerns is the realization that the development of drug resistance among infectious agents is occurring at an increasing rate. Unless there is a shorter time scale for drug discovery and development, the battle will be in favor of the disease microorganisms.

Cyber-Cell will offer the opportunity to rapidly identify drug targets. In addition, it will allow examination of cell response to a drug in terms of its effect on other cell processes. Differences in rate coefficients for biochemical reactions between normal and pathogenic states in a cell can then be identified and exploited in drug design. Insight can be gained with regard to the mechanism of development of drug resistance.



**Figure 2.** Diagram of the internal compartments of *Trypanosoma brucei* (intermediate bloodstream form of the African Sleeping Sickness parasite) presently being modeled using Cyber-Cell (from Kang, X., 2001, "Antigen Variation: Investigation of GPI-Anchoring of the Variant Surface Glycoprotein in *Trypanosoma Brucei*," Dissertation, der Fakultät für Chemie und Pharmazie der Eberhard-Karls-Universität Tübingen).

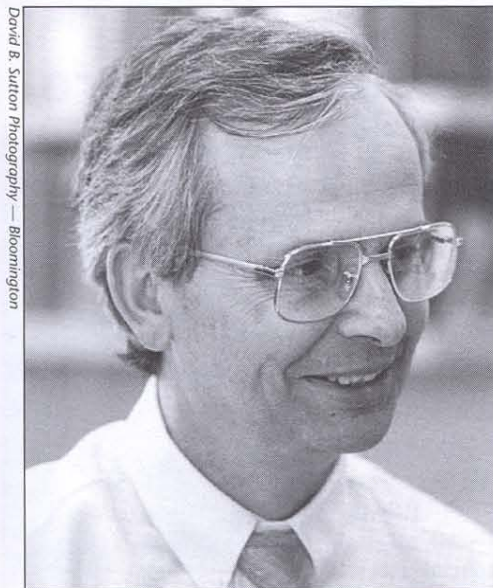
Other areas of application of the model include

- Fundamental cell research and investigation of the origins of life;
- Stem cell, organ replacement, and other medical technological function;
- Design of optimum microbes for use in various areas of biotechnology such as environmental remediation or enhanced petroleum recovery; and
- Improved synthesis of compounds of commercial interest by fermentation or other large-scale cell culture methods.

Unless there is a shorter time scale for drug discovery and development, the battle will be in favor of the disease microorganisms. Cyber-Cell will offer the opportunity to rapidly identify drug targets.



# Conference Honors Chair Davidson



David B. Sutton Photography — Bloomington

Ernest Davidson

An international group of more than 300 theoretical chemists gathered at the University of Washington in July not only to discuss the latest results in quantum chemistry, but also to honor IU chemistry chair Ernest Davidson. The theme of the conference was "The Right Answer for the Right Reason," Davidson's mantra.

A Rose-Hulman graduate who did his PhD (1961) with Harrison Shull at IU in two and a half years in an independent fashion, Davidson did a postdoctoral with Joseph Hirschfelder at Wisconsin and began his formal academic career at the University of Washington, where he stayed until he was lured back to IU in 1984. Numerous historical talks at the conference described Davidson's collaborative efforts in broad areas of analytical chemistry, experimental physical chemistry, organic chemistry, and mathematics.

One of the highlights of the conference was his introduction by Nobel Prize winner John Pople, who simply said: (paraphrasing) "Whenever I write a paper, I wonder how Ernie will feel about this, because usually I know it would not rise to his standards." Another speaker from Europe said that when he was a graduate student, he asked his preceptor who the best quantum chemist in the world was. "I then realized that this was an inappropriate question because my preceptor did not want to suggest that he was, so then I asked who was the best quantum chemist in the United States," he said. After a bit of thought, his preceptor said, "Davidson is not bad." Various collaborators described Davidson's insight and Herculean

efforts in providing a firm theoretical basis for observations. Indeed, he was often characterized as insisting on fundamental understanding, i.e. the "right reason."

Among those who provided descriptions of Davidson's efforts was our Charlie Parmenter, who listed all of the IU colleagues with whom Davidson has collaborated, along with a myriad of early photographs of Davidson. Charlie further characterized his teaching efforts with a statement about the exponential loss of attendees during the semester, ending with a slide showing Davidson in an absolutely empty Room CH122. A final dig concerned Davidson's parking spot in front of the Chemistry Building. A slide showing the parking space was displayed with a curious black square to the left (south side) of the space. Charlie explained that Davidson was "working hard to generate an executive bathroom, but as a theorist he needed to start with a model." Charlie then removed the cover over the dark portion of the slide, revealing the fixture to the south of the parking place. (For those of you who don't remember, it is a fire hydrant!)

Another one of the highlights of the conference was the presentation to Davidson of an ACS Cope Scholar Award. In this case, however, it was not the American Chemical Society but the American Cope Society. This was for his efforts in trying to characterize the Cope rearrangement transition state. The certificate was signed by Bill Doering, Harvard (Pope of the Cope), Ken Houk, UCLA (Chief BeThreeLipper), Keiji Morokuma, Emory University (First CASSER), Wes Borden, University of Washington (Dynamic Correlator), and Joe Gajewski, IU (IsotoperCoper), all scholars of "the most important reaction in organic chemistry."

Those of us who were privileged to attend will attest to the high regard accorded our chair by this distinguished group of scientists. It was a special event, which was also hosted by Reba Davidson. IU faculty and spouses who attended were Charlie and Pat Parmenter, Harrison and Will Shull, Stan and Elaine Hagstrom, and Joe Gajewski. Also attending were Bob Cave, who is currently on the faculty of Harvey Mudd College, and Andrzej Jarzecki, a postdoctoral at Princeton (both former postdocs with Davidson); Julia White, PhD'91, currently at Battelle Northwest Laboratories; and Viktor Staroverov and

(continued on page 5)

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## Endowments and awards: Facilities for the future

It is my pleasure to announce that the Keith Ault Scholarship/Fellowship was established earlier in the year through memorial gifts from his family and friends. The fund will exist in perpetuity and was established to support graduate and undergraduate students needing financial assistance. **Frederick (Keith) Ault**, MAT'67, and his wife, Gloria, founded the VitaChlor Corp., and Mr. Ault was president of the company for 20 years. Before that he was a faculty member at Ball State University and taught at Brown County High School.

**David Williams** was given the Harry G. Day Chair earlier in the year. Emeritus Professor Harry G. Day graciously donated the proceeds from his earlier Crest research to endow the chair to be awarded to faculty in the area of biochemistry or bio-related disciplines in chemistry. Williams' research interests lie in the development of chemical methodology for the total synthesis of targeted, biologically active natural products. Present studies are directed toward new agents for treatment of cardiovascular disorders and neoplastic diseases as well as new antibiotics.

The Lilly Endowment made a major gift (called the Indiana Genomics Initiative) to the IU Medical School. A small part of this is being shared with the Bloomington campus, and a fraction of that is being used to develop a proteomics research and development facility in chemistry. This provides an opportunity to link our expertise and future developments to research activities of the IU Medical School. By design the facility will focus on developing new analytical methodologies and instrumentation for protein and glycoconjugates. This facility will be the basis for developing a center of excellence in elucidating the proteomics of mammalian and non-mammalian systems. Initially, the faculty associated with the facility will be **Milos Novotny**, **David Clemmer**, and **Jim Reilly**, with Novotny serving as director. The budget will provide more than \$1.5 million for new instrumentation in addition to start-up funds for two senior hires.

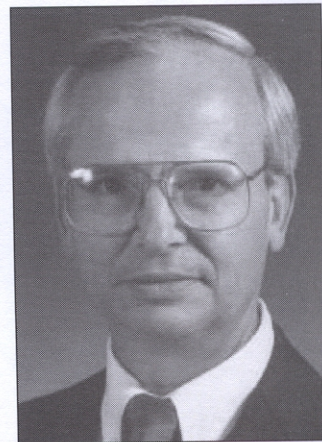
We continue to have changes in our faculty. During the past year, **George Christou** departed to the University of Florida. **David Clemmer** was promoted to full professor after only one year in rank as an associate professor.

We hired Assistant Professor **Bogdan Dragnea**, who is establishing a laboratory to use near-field probes to study single-molecule dynamics and bio-molecular machines. Several more retirements are expected this year. With the support of the administration, we are searching for several additions to our faculty at both the junior and senior levels.

**Maren Pink** joined the Molecular Structure Center. In addition to her general crystallography skills, she is a recognized expert in twinning and has been asked to present papers and act as instructor at several national workshops (see also page 15). **Cathrine Reck** joined the teaching ranks and is developing a new undergraduate laboratory course in inorganic chemistry.

Our faculty members continue to receive university and national recognition. Since our last newsletter, many of our faculty have been honored. **David Clemmer** was selected to receive the inaugural Pittsburgh Conference Achievement Award, sponsored by the Society for Analytical Chemists of Pittsburgh and the Pittsburgh Conference for 2002. The award will be presented during an award symposium that will be held as part of the Technical Program of the 2002 Pittsburgh Conference (New Orleans, March 18–21, 2002). **Jack Crandall** received the 2000 Leo F. Solt Distinguished Service Award presented by Research and the University Graduate School, Indiana University. The award recognized his contributions to the excellence of graduate education at IU. **P. Andrew Evans** received the 2001 Johnson & Johnson Focused Giving Award, given by the Johnson & Johnson Corporate Office of Science and Technology. The program was established in 1980 to stimulate exploration in medical science (broadly defined). Nominees must have served with special distinction as teachers of chemistry at any level (see also page 12).

**Gary Hieftje** received the 2001 Pittsburgh Spectroscopy Award. Exceptional contributions to spectroscopy and the Spectroscopy Society of Pittsburgh were the driving forces behind the nomination, submitted by a group of earlier recipients of the award. A symposium was held in Hieftje's honor at the Pittsburgh



Ernest Davidson

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## LECTURES & PRESENTATIONS



A group of special lectures embellished the ongoing departmental Distinguished Lecture Series this year.

The first of these was actually presented late last year by David Bartel. He is an associate member of the Whitehead Institute and, in 1999, was appointed to the Irwin and Helen Sizer Career Development Professorship at the Massachusetts Institute of Technology. On Nov. 8, he discussed "The Creation and Evolution of New Ribozymes."

Another special occasion was the presentation of the 2000 Phi Lambda Upsilon Fresenius Award to our own Professor **David Clemmer** on Jan. 17. On hand to personally confer the award was Jack D. Graybeal, one of the national officers of the chemistry honorary fraternity.

For his award address, Clemmer spoke on "Anhydrous Protein Ions: Understanding Elements of Structure and Applications in

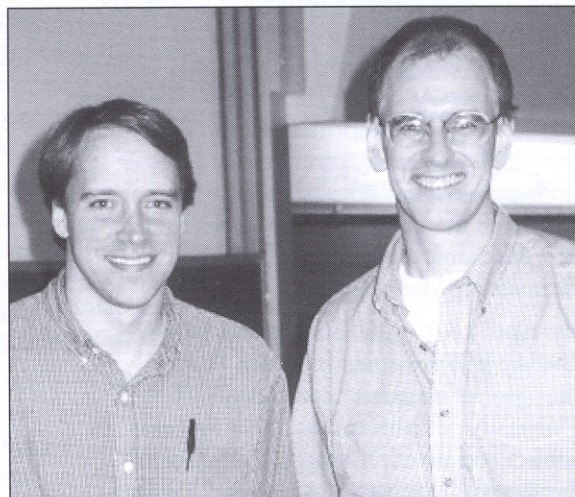
Proteomics." Following the lecture, a reception was held in the faculty lounge.

A lecture on the burgeoning field of chemical informatics represented another special occasion in the department on Feb. 28. Peter Willett, head of the Computational Informatics Research Group at the University of Sheffield, discussed

"Chemoinformatics: Where It Has Come

From, Where It Is Now, and Where It Is Going." Willett is also the chair of the Governors of the Cambridge Crystallographic Data Centre and president of the Chemical Structure Association in England.

On March 28, an Eli Lilly Distinguished Lecture was presented by Jiri Janata. Janata is the Georgia Research Eminent Scholar at the Georgia Institute of Science and Technology in Atlanta. His subject was "Conducting Polymers and Layers for Solid State Gas Sensors."



David Bartel, left, with our Don Burke

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## Chair's letter

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Conference in New Orleans on March 6, 2001. Hieftje was also selected by the Indiana Academy of Science to be Speaker of the Year. He gave a presentation titled "Instrumentation Science in the New Millennium" at Indiana University East, Richmond, Ind. (see also page 13). **Milos Novotny** was the recipient of the 2001 Eastern Analytical Symposium Award for Outstanding Achievements in the Fields of Analytical Chemistry. The governing board of the EAS selected Novotny for his numerous outstanding contributions to the fields of analytical chemistry. The award was presented at Atlantic City in October (see also "Faculty Profile," page 8). In November, **Dennis Peters** received the 2001 James Flack Norris Award for outstanding achievement in the teaching of chemistry. The Norris Award, one of the oldest awards given by a section of the American Chemical Society, is presented annually by the Northeastern Section. Nominees must have served with special distinction as teachers of chemistry at any level. In addition, Peters was selected from among more than 50 nominees to

receive the Alpha Lambda Delta (IU chapter) Favorite Faculty Award for 2000. This award recognizes excellence and distinction in teaching, particularly at the freshman level.

Last April, **Jeffrey Johnston** and **Martin Stone** received Trustees' Teaching Awards, established by the IU Board of Trustees in recognition of classroom excellence. Courses taught, course enrollments, and student evaluations provided the principal basis for selection.

At the 2001 commencement ceremony in May, **Jack M. Gill**, PhD'63, was awarded an IU honorary doctor of science degree, one of the highest academic recognitions Indiana University can bestow. In addition, he was the recipient of the 2001 College of Arts & Sciences Distinguished Alumni Award in November. **Allen R. Siedle**, PhD'73, received the 2000 Distinguished Alumni Award of the University Graduate School. This award was given to Siedle in recognition of his excellent achievements in his career as an IU alumnus.

Congratulations to all!

— Ernest Davidson

## Davidson

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Aurora Clark (current graduate students). Other attendees included Larry Schaad (postdoc'59-61), professor at Vanderbilt; IU Adjunct Professor Odile Eisenstein; and IUPUI chemistry Professor Cliff Dykstra. The saddest part of the meeting was the revelation that the Davidsons will retire to Seattle in the not-too-distant future.

— Joe Gajewski



## AROUND IU CHEMISTRY

### Lectures and Presentations

(continued from page 5)

Josef Michl of the Department of Chemistry, University of Colorado at Boulder, gave a special lecture in the Physical-Organic Chemistry Series on April 12. The title was "Saturated Linear Chains: Conformations and Electronic Structure." The discussion involved calculations on silicon analogs of hydrocarbons and addressed the question "How Does Molecular-Size Mechanical Machinery Differ from Nanoscopic Machinery?"

On April 18, the 2001 Raymond Siedle Lecture was presented by Galen Stucky, professor of chemistry and biochemistry, University of California at Santa Barbara. His subject concerned "Composite Materials Synthesis: Learning from Nature." He was awarded the 2000 Alexander von Humboldt Research Prize. Among other responsibilities, he serves on the editorial boards of *Current Opinion in Solid State and Materials Science*, *Chemical Communications*, and *Nanoletters*.

Last in the spring semester series was the Ernest E. Campaigne Lecture on April 25. It was given by Manfred T. Reetz. Reetz is

director of the Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany. Among other honors, he is a recipient of the Nagoya Gold Medal of Organic Chemistry. His topic was "Evolution in the Test Tube As a means to Create Enantioselective Enzymes."

Just before the press deadline for *IU•Chemistry*, the Marvin Carmack Lecture, the first of the fall semester series, was given on Sept. 26. Dudley H. Williams, professor of biological chemistry at the University of Cambridge (U.K.), spoke on "Vancomycin and the Fight Against Antibiotic-Resistant Bacteria." He is the author of some 500 publications, including several books. Professor Williams was elected a Fellow of the Royal Society in 1983. The occasion of the lecture was an especially enjoyable one because Marvin Carmack returned to attend from his home in Arizona; he also remained for a few days to visit with friends.

— Max Marsh



Peter Willett



David Clemmer, left, with Jack D. Graybeal



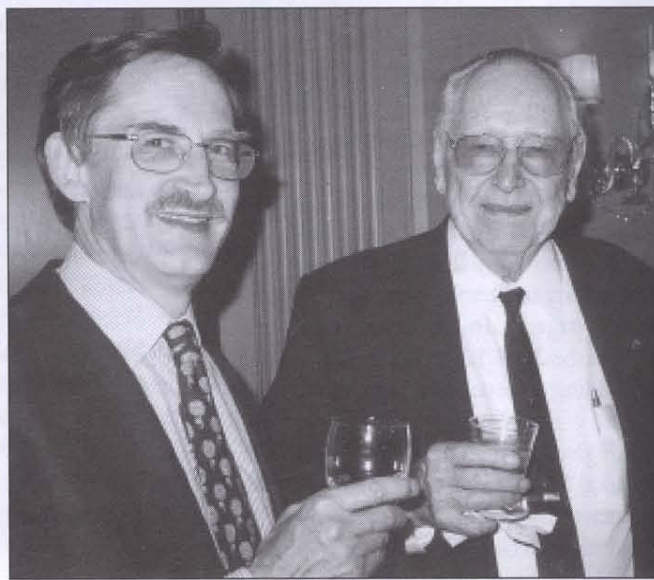
Marvin Carmack, left, with Dudley Williams



Josef Michl



Galen Stucky



Manfred Reetz, left, with Ernest Campaigne



## SCHOOL OF INFORMATICS NEWS



The first group of graduate MS students in the new School of Informatics bioinformatics and chemical informatics programs began their studies this fall at IUB and IUPUI.

A new graduate course in chemical information technology is being offered at both campuses via distance education. Polycom Viewstation equipment links the lecturers and students at the two locations. Guest lecturers in the C571 course include experts from MDL Information Systems, Barnard Chemical Information Systems, and Chemical Abstracts Service, as well as faculty from the

Bloomington and Indianapolis campuses. For the spring semester, Kevin Gilbert will team with IUPUI faculty member Samuel A.F. Milosevich to teach a graduate molecular modeling and computational chemistry course. Milosevich, a former Eli Lilly computational chemist who previously worked at the National Center for Supercomputing Applications in Urbana, Ill., is the first chemical informatics faculty member to be hired for the new program. Sun Kim, formerly of Dupont, joined the program as the first bioinformatics faculty member. MDL Information Systems gave a \$15,000 fellowship in support of the new program, and Daylight Chemical Information Systems also pledged support.

— Gary Wiggins



### ACS Southern Indiana Section wins ChemLuminary Award

Graduate student Kris Quinlan, organizer of the 2000 National Chemistry Week Open House at IUB, saw her hard work rewarded at the 2001 American Chemical Society National Meeting. The ACS Southern Indiana Section was selected as the recipient of the first-place award for the best open house in 2000.

### Department hosts symposium

On Friday, Sept. 8, 2001, the department hosted the Symposium for Excellence in Undergraduate Chemical Research. The daylong symposium was the first of what we hope will be an annual event to recognize and to honor those faculty members from small colleges who excel at research and provide their undergraduate students with high-quality research experiences.

The attendees were welcomed by the chemistry department's Professor **P. Andrew Evans** and by **Kumble R. Subbaswamy**, dean of the College of Arts and Sciences.

Each of the honored professors presented a seminar on their work that spanned all areas of chemistry and biochemistry. At a beautiful banquet in the Federal Room of the Indiana Memorial Union, each of the visitors received a plaque in recognition of their achievements.

Also attending the symposium were a number of undergraduate research associates from the laboratories being honored, providing them an opportunity to see IU. In addition to the seminars by the invited guests, there was a poster session highlighting some of the work going on in the chemistry department here at IU, a facilities tour, and a seminar by Mike Martinelli, Lilly Research Fellow from the process group at Eli Lilly & Co. Martinelli shared with us his perspectives on chemistry in

the pharmaceutical sector and the challenges of bringing novel synthetic compounds to the clinic and the marketplace.

— Andrew Feig

### This year's honorees

**Judith Ambergey-Peters**  
College of Wooster  
**David Bailey**  
Illinois Wesleyan University  
**Scott Feller**  
Wabash College  
**Edward Fenlon**  
Xavier University  
**Barbara Lawrence**  
Eastern Illinois University  
**Bryan Lynch**  
University of Evansville  
**Albert Matlin**  
Oberlin University  
**Serge Schreiner**  
Randolph-Macon College



Professor Andrew Evans (right center) with honorees at the IU Undergraduate Research Symposium



## Faculty Profile: Milos Novotny

*When I think of separations using chromatography, I think of Milos Novotny. A Distinguished Professor who holds the Lilly Chemistry Alumni Chair, he has been active in this field since his postdoctoral experiences at the Czechoslovak Academy of Sciences and the Karolinska Institute in Sweden and throughout his eminent career at Indiana University. He has carried his unique experience with difficult separations into an intense investigation of mammalian pheromones, research that led him to establish the Institute for Pheromone Research as a principal vehicle for enhancing interdisciplinary research in the field of chemical communication. We offer our readers the following interview with this unique chemist.*

— Rupert Wentworth

### All things seem to change with time. How has IU changed since you arrived?

I fell in love with Bloomington and the IU campus at once. It was during the spring of 1971 during my interview trip, which was quite late in the faculty recruiting season. The flowering trees, combined with the grace of limestone architecture greatly impressed me during my visit — frankly, I rather expected a conglomeration of “functional” buildings in the middle of cornfields. Additionally, to a European freshly transplanted into a new-world environment, there was a spirit of traditional university, with its emphasis on arts, music, and exotic languages, all in coexistence with an excellent science department. I accepted at the end of my visit — coming from abroad, I was rather naïve about such things as salary negotiations and set-up arrangements. I just accepted. Before coming here, I had always lived in a much larger city, and there was some uncertainty as to whether I could be happy at this location. However, 30 years later, my love affair with Bloomington and the IU campus continues unabated.

While I was hired initially as an analytical chemist, I appreciated greatly the fact that IU had a biochemistry component right in the Department of Chemistry. (Biochemistry had been the subject of my graduate studies before coming to the United States.) And, what a group of distinguished scientists: Gene Cordes, Frank Gurd, Henry Mahler, and, yes, Felix Haurovitz! Both Felix and I came from the same part of the world, and, in very different times and circumstances, we were forced to

leave our homes. Initially, I hesitated to call him “Felix” because of our age difference, but he firmly insisted on breaking away from the old European ways. Knowing this warm, scholarly, and collegial individual has been one of the highlights of my time in Indiana.

The excitement of my beginning academic career seemed endless: new laboratory and the boxes arriving with new equipment, C500 interviews, and discussions with my new colleagues could easily fill my days. By the October NIH deadline, in the first semester of my residence, I submitted my fourth grant proposal. In those days, released teaching time was never discussed; I taught full time the first year and anytime after. Regrettably, there was little time left to appreciate the beauty of southern Indiana’s fall and spring during my first year. In 1971, the analytical chemistry group at IU was the youngest division in the department, with John Hayes and Gary Hieftje having arrived just one or two years ahead of me. Dennis Peters was the only senior research-active analytical chemist. There was a strong desire to build and succeed. We complemented each other in expertise and approach to graduate education. There was competitive spirit, and perhaps no one on the faculty believed that all young analytical chemists would receive tenure. The rest is history.

To every junior faculty member, a dose of professional and social approval by their senior colleagues appears essential. I fondly remember the kindness of Ernie Campaigne, Marvin Carmack, Walter Moore, Jack Shiner, Ward Schaap, and Dennis Peters during my beginning years at IU. Research mentorship was not common then, but I certainly found friends, tennis partners, and lunch companions among my senior colleagues. I developed a very special relationship with Marvin Carmack. Marvin was the man who made me aware of the important biological literature on mammalian pheromones. To this day, I still talk about pheromones with Marvin. Over the years, we shared ideas, traveled to scientific meetings, and published several papers together. In short, IU would not be the same place to me without Marvin Carmack.

As our reputation in analytical chemistry began to grow during the late 1970s, our program underwent significant changes. We grew



Milos Novotny



substantially in the number of graduate students, group size, and research programs. In 30 years, we experienced excitement, national prestige, and pride, but also some turmoil. It has been proven over and over again that sustaining excellence in analytical chemistry without the overall departmental strength is difficult, if not impossible. During the most recent period, we lost some valuable colleagues. I have felt the loss of Mark Wightman, a very dear friend and colleague, most. Mark shared with me a research philosophy and views on graduate education, and we became engaged in several common research projects.

I feel lucky to have experienced a substantial increase of our department's national reputation. I am sure that I am not alone in feeling gratitude to Adam Allerhand for showing us the need for sustaining excellence and high standards during the late 1970s. As a result, we now enjoy outstanding laboratories and departmental facilities that few other departments have. We must not slip on our path to scientific excellence! When my age group eventually leaves the scene, it will be up to the likes of Dave Clemmer, Martin Stone, Jeff Zaleski, and others to sustain and improve on what has been generated. Even more important, we need to identify new talent and see new directions through vigorous faculty recruitment.

### **Have the students and their attitudes changed since you arrived?**

I think they have changed, but so have we and the world around us. Naturally, we tend to think of the days of our scientific youth in superlatives. Regardless, I feel fortunate to have had some absolutely stellar graduate students during the 1970s and early 1980s. Students such as Milton Lee, Mike McConnell, Jim Jorgenson, Jerry Rhodes, Vicki McGuffin, and Jenny Gluckman come readily to my mind in judging their dedication to science, superb knowledge and skills, and just about any other quality we seek in our graduate student body. They were no bookworms, either — most played hard and worked hard. Their on-going success in academia and industry thus appears natural. Of course, there were other outstanding students during more recent years as well. I have graduated both analytical chemists and biochemists from my group. Pharmaceutical industry, biotechnology, and scientific-instrument companies employ many of the recent graduates.

The attitudes of our society toward science, in my view, substantially affect the dynamics of what we see in our student body, both gradu-

ates and undergraduates, over the time.

During the periods of relative prosperity when jobs are plentiful, the attitudes of some students change considerably. I have seen the same phenomenon with the European and Japanese societies as well. Rather than “adjusting” our standards, we have to work harder to win the best students over. The revolutionary developments currently taking place in biological sciences and the biomedical field, in particular, are bound to secure a leading role for chemistry in the years to come. But chemistry is not a “soft science,” and our students must be made aware of both the opportunities and challenges. We are a major research institution, and recruiting the best talent, worldwide, remains one of our top priorities.

### **How has your research evolved since you arrived at IU?**

Separation science has often been central to my research activities. But when I entered academia, I was somewhat surprised at how little the analytical chemists in the United States identified with the separation science as a part of their field. There were only a handful of academicians working in chromatography. Thirty years later, the situation is completely changed, and I like to think that my contributions and those of my students have helped change the situation. Analytical separations have become one of the most exciting fields, impacting many aspects of modern science and technology. They are also central to bioanalytical chemistry, biotechnology, proteomics, and glycobiology. Besides the enormous advances in chromatography during the last three decades, electromigration techniques emerged as a major area of separation science. The major stimulus for these developments was provided by the pioneering work of a former student, Jim Jorgenson, on capillary zone electrophoresis. Capillary electrophoresis has been repeatedly the subject of numerous symposia, attended by thousands of participants on an annual basis. The set of related techniques revolutionized biosciences, including the recent completion of the Human Genome Project.

I have always been a problem-oriented analytical chemist. I never believed in developing a “toolbox” just for the sheer beauty of it. While my entire scientific career has been based on developing new types of separation and measurements, the biochemist in me is concerned about advancing knowledge of some biological process. This combination has

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## Faculty profile

*(continued from page 9)*

worked for me on more than one occasion. I also seem to be attracted to difficult problems and complex situations. Receiving tenure at IU brought to me a certain liberation, permitting me to get deeply involved in two areas that might or might not have been fruitful: (a) miniaturized separations and detection; and (b) research on mammalian pheromones. In retrospect, both directions worked, but not without the years of intensive research and a fair amount of frustration. Miniaturization has become an important trend in separations, and to my satisfaction, all currently practiced capillary separation methodologies have connections to Indiana University. Turning to pheromones, during the mid-1980s, we were finally able to demonstrate the action of the first pheromones ever to be definitely identified in a mammal (house mouse). Both Marvin Carmack and I were gratified by this initial success, showing that relatively simple molecules (not unlike those found in the insect world) can serve as important messengers in mammals. The pheromone research remains a frontier area of scientific endeavor to this date. Without combining different types of expertise in one laboratory, we would not have been able to achieve success. Highly efficient separation techniques, combined with sensitive structural tools, have been the key to identification of pheromones, while organic synthesis and biological testing were essential to complete the task. Structural elucidation of the first mouse pheromones (and many other constituents of complex biological mixtures throughout the years) and syntheses were accomplished through the unique skills and expertise of a long-time associate, Donald Wiesler. Even after his retirement, Don maintains great interest in our research and continues advising my current students on structural aspects. The pheromone biology was brought to our group as the necessary component in the early 1980s by Professor Anna Marchlewska-Koj from the Jagiellonian University (Poland) and was continued for a number of years by her former student, Bozena Jemiolo, and more recently, Weidong Ma. While we still

continue identification of pheromones in other mammalian species, the most current research has centered around the mechanisms of pheromone perception at the level of olfactory tissues and, more specifically, pheromone-protein interactions.

I have always enjoyed working with scientists from other fields and adding my chemical expertise to a complex scientific problem. Pheromone research has been to me an outstanding example of interdisciplinary research that gives us an opportunity to interact with other scientists, both at IU and elsewhere. Within the newly established Institute for Pheromone Research, we have just started to develop several international collaborations. Our work in capillary liquid chromatography and capillary electrophoresis has enabled us to study peptides and glycoconjugates at unprecedented resolution and sensitivity. This, in turn, now allows us to play a leading role in the emerging fields of proteomics and glycobiology. Together with my faculty colleagues, Dave Clemmer and Jim Reilly, we are currently developing a number of exciting collaborative projects with the IU School of Medicine.

### **What were some of your memorable moments at IU?**

Not too long after I joined the faculty at IU, I happened to have the opportunity to participate in one of the notable projects of the space program, the 1975 Viking Mission to Mars. It all started as a modest project to evaluate

*(continued on page 11)*

## The Lilly Chemistry Alumni Chair

Last year's award to Professor Novotny of the Lilly Chemistry Alumni Chair was the culmination of more than 13 years of dedicated support by several Department of Chemistry alumni and friends. Charles J. Paget and Max Marsh initiated the endowment fund in 1986, while both were research advisers in the laboratories of Eli Lilly and Co. in Indianapolis. They enlisted the help of the IU Foundation, the College of Arts and Sciences, and the Department of Chemistry in reaching out to other Lilly employees and retirees who were alumni or friends of the department. Not only was the initial response enthusiastic, it was maintained over the span of many years. In all, more than 35 donors have contributed to the endowment fund. Matching funds from Lilly also added significant amounts, as did income from the foundation's investment program. The original goal was to provide an endowment to be used at the discretion of the department chair; however, there was a gradual consensus that the fund be allowed to accumulate until it reached a size sufficient to support a chair. This was realized last year when the value reached \$1 million. The fund remains open for additional contributions; money not required to support the chair will again be allowed to accumulate and be used to meet other departmental needs. Other chairs and professorships that have been awarded to chemistry department faculty included the Robert and Marjorie Mann chairs (Ernest Davidson and Gary Hieftje), the Harry G. Day Chair (David Williams), and the Herman T. Briscoe Professorship (Dennis Peters).





**Adam Allerhand** and **Peter Langhoff** retired after serving the department and the university for 34 and 31 years, respectively.

A former student of **Ernest Campaigne** is in the news: **Wendell Roelofs**, PhD'64, received the 2000 Kenneth A. Spenser Award from the American Chemical Society.

**Ken Caulton** participated in the national ACS meetings in San Diego and Chicago, together

with members of his research group who are from Spain, Russia, Korea, China, and around the United States. He also presented work at an NSF workshop in inorganic chemistry, where he had the distinction of being one of the oldest scientists there; however, it was an excellent opportunity to get acquainted with a broad range of academic inorganic chemists. In May, Caulton was an invited lecturer on the occasion of the retirement of his undergraduate inorganic chemistry professor from Carleton College. This summer, Caulton, together with a graduate student, mentored an NSF-sponsored summer undergraduate research

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## Faculty profile

*(continued from page 10)*

several gas-chromatographic columns (supplied by a NASA contractor) for their analytical performance. A former colleague, John Hayes, who was then funded by NASA, passed the project on to me as a "chromatography expert." Was there a form of life, as we know it, present on Mars? The so-called molecular analysis experiment, based on a miniaturized GC/MS instrument, was one of the several experiments designed to answer this question. A chunk of Martian soil, passed into a pyrolytic oven through a robot's arm, was to be analyzed for organic material — the previously analyzed samples of terrestrial soils were known to produce a fairly characteristic pattern of volatile organics (various pyrolytical products of common biopolymers). The expected mixture presented a fairly difficult analytical problem due to its substance diversity and a possible presence of large amounts of water. A poor performance of the separation column could have been a bottleneck of the entire GC/MS experiment aiming at structural analysis. Since the columns previously tested by NASA did not meet the experimental objectives, I thought of a very different column chemistry that could do the job. The rest was optimization and suitable column geometry. Our column design won acceptance by the Viking Science Team and, eventually, made it to the surface of Mars on July 4, 1976. No organics were found, but the column performed well. Occasionally, I still look at the planet during an evening walk, with a fond memory of the project.

After a number of years I spent searching for male mouse pheromones, we were finally successful in the mid-1980s to implicate 4,5-dehydro-*exo*-brevicomin and 2-*sec*-butyl-4,5-dihydrothiazole in three biological phenomena: intermale aggression, sexual attraction, and

estrus synchronizaton. A year later, we identified the female-to-female mouse puberty-delay pheromone. While probably unnoticed by most chemists, ours were the first reports of genuine mammalian pheromones in the literature. These findings have become landmark contributions in the field of chemical ecology and the cornerstone of our additional studies to this date.

I have been lucky to receive numerous awards and distinctions over the years, many more than I had ever anticipated. These include ACS awards, some medals overseas, and the 1994 Scientist of the Year Award by the *Research & Development Magazine*. Without the hard work and dedication of the many talented students and associates, I never would have been able to receive such recognition! It is particularly rewarding when the outside recognition is followed by the distinctions received locally. I have had a generous share of these as well. Indiana University has also recognized two of my best graduate students (Jim Jorgenson and Milton Lee) as distinguished alumni. I have been extremely proud of the achievements of my former students and postdoctorals. And, some students of my students are doing quite well, too. For an academic scientist, this must be the ultimate reward.

I was particularly touched by two ceremonies at which I received honorary doctorates. One elaborate, medieval-like ceremony took place at Uppsala University in Sweden; another, quite different in appearance, was in my native country of Czechoslovakia (Masaryk University). In the European tradition, receiving an honorary degree is the ultimate distinction. I have always valued my scientific contacts and friendships overseas.

I am told that many people of my age tend to wind down their research. I do not anticipate doing so yet because I am still excited about many things in science that need to be done.

❖

*I am told that many people of my age tend to wind down their research. I do not anticipate doing so yet because I am still excited about many things in science that need to be done.*

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# AROUND IU CHEMISTRY

## Faculty News

(continued from page 11)

student, whose project was so successful that it has been submitted for publication.

Before **George Christou** left the department, he received the Royal Society of Chemistry Award in Chemistry and Electrochemistry of Transition Metals for 2000.

The 2000 Phi Lambda Upsilon Fresenius Award was given to **David Clemmer** for outstanding contributions to analytical chemistry. He also received the inaugural Pittsburgh Conference Achievement Award for 2001, an award sponsored by the Society of Analytical Chemists of Pittsburgh and the Pittsburgh Conference.

A conference at the University of Washington celebrated **Ernest Davidson** and his work (see also page 3). He is also the recipient of the 2001 Schrödinger Medal by the Scientific Board of the World Association of Theoretically Oriented Chemists.

**Harry G. Day** is the author of "The Story of the First Fluoride Toothpaste," an article appearing in the fall issue of *Chemical Heritage*. A good review with some additional information may be found in the "Newsprints" section of *Chemical and Engineering News* for Sept. 17, 2001. Procter & Gamble's Crest toothpaste, introduced in the 1950s, still enjoys a flourishing market.

**P. Andrew Evans**, an organic chemist, left the University of Delaware and joined our department with the rank of full professor in January 2001. He will also receive the 2001 Johnson & Johnson Focused Giving Award. One of his students, **John Robinson**, will receive an ACS Division of Organic Chemistry Graduate Fellowship.

**Bogdan Dragnea**, a physical chemist, joined our department as a new faculty member. He received his PhD from the University of Colorado, where he worked for Professor Stefan Leone.

**Joe Gajewski** gave talks at Pacifichem (Hawaii) in December; at Ronald Breslow's 70th Birthday Symposium (Columbia University) in March; at "2001 — An Isotope Odyssey" (Zakopane, Poland) in June; and at the Quantum Chemistry Conference at the University of Washington, celebrating Ernest Davidson (see also page 3). He helped organize the effort to bring the National Organic Chemistry Symposium to IU in June 2003. He also serves on the American Chemi-

cal Society Committee on Education along with IU alumni Joe Heppert and Mary Carroll and IUPUI Professor David Malik. Gajewski serves as chair of the Southern Indiana ACS Section, and he also has been nominated (for a second time) for election as chair of the Chemistry Section of the American Association for the Advancement of Science.

Two significant events in the career of **Gary Hieftje** happened during the past year. The first was appointment (on Oct. 2, 2000) to a Robert and Marjorie Mann Chair in Chemistry. The second, as noted earlier, was receiving the 2001 Pittsburgh Spectroscopy Award. In addition to numerous invited lectures in Europe and in the United States, he presented plenary lectures at the International Conference on Analytical Sciences in Tokyo, the International Mass Spectrometry Conference in Barcelona, and the sixth Rio Conference on Atomic Spectroscopy.

**Ryan James**, a graduate student of **Ronald Hites**, was awarded the 2001 Graduate Student Award in Environmental Chemistry from the American Chemical Society.

*Chemical and Engineering News* (July 16, 2001) recently described some of the work of **Shuming Nie** and his associates on using quantum dots as "bar codes" to identify molecules in bioassays.

**Charlie Parmenter** joined 26 scientists at a conference at the German embassy in Washington, D.C., honoring the Alexander von Humboldt Senior Scientist Awards Program. Numerous U.S. scientists, including many from our department, have spent six months to a year in a German laboratory supported by these awards, which are funded by the German government. The conference was the brainchild of **George Atkinson**, PhD'70, a professor from the University of Arizona. The honored guest was Professor Edward Schlag from the Technical University of Munich, in whose lab the 26 recipients of the awards, including two Nobel Laureates, spent their productive visits. Parmenter also reached the milestone of his 50th high school reunion at the William Penn Charter School in Philadelphia. A deceased faculty member from our department, **Frank Gucker**, also graduated from this school, but a few years earlier than Parmenter. In addition to guessing whom his classmates were, Parmenter had the pleasure of joining some distinguished company by receiving the Alumni Award of Merit.

**Dennis Peters** and two of his graduate students presented two lectures at a meeting of

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Groundbreaking for the new Auxiliary Library Facility took place in Bloomington on Sept. 10. The facility, when completed by next fall, will be able to house 2.7 million volumes. As more and more backfiles of scientific journals become available in electronic format, the lesser-used paper archives of science are expected to join printed works from other disciplines in the new facility.

With the introduction at the beginning of 2001 of the new library automation system, SIRSI Unicorn, the complete holdings of the Indiana University Libraries on all eight

campuses are now visible on the Web.

Electronic acquisitions that greatly enhanced the science libraries this year included a campuswide license for the Cambridge Structural Database and a license for all journals of Academic Press. In addition, the 2000–01 fiscal year marked the first full year that Chemical Abstracts Service's SciFinder Scholar, with full substructure searching capability and 24-hour access, plus all electronic journals of the American Chemical Society, could be accessed at all eight campuses of Indiana University. The Beilstein CrossFire system, with both Gmelin and Beilstein databases, has been available to all campuses for a number of years.

### Wiggins to receive Distinguished Alumni Award

Gary Wiggins has been selected to receive the Distinguished Alumni Award of the Indiana University School of Library and Information Science. Jan. 2, 2001, marked his 25th anniversary as head of the IUB Chemistry Library. Wiggins continues to serve as a councilor of the ACS Division of Chemical Information, and he was president of the ACS Southern Indiana Section during 2000.

### Faculty News

(continued from page 12)

the Electrochemical Society in Washington, D.C. His contributions continued when he, Maria Medeiros, who is a visiting scholar from Minho University in Braga, Portugal, and two other chemists from Minho University presented a paper at the Sandbjerg Meeting on Organic Electrochemistry in Aarhus, Denmark. Peters (along with **Leo Klein**, who was a graduate student and is now a visiting assistant professor, and two chemists from the University of Rennes in Rennes, France) also presented a paper at the Electrochemical Society/International Society of Electrochemistry Joint Meeting in San Francisco. Peters will also serve a two-year term (from 2001 to 2003) as vice-chair of the Organic and Biological Electrochemistry Division of the Electrochemical Society.

**Romualdo de Souza** has become the department's associate director of instructional programs, with the intention of becoming the director next year.

Recent experiments led by a group from Indiana University together with theoretical analyses of the data by others at Michigan

State University and the Lawrence Berkeley Laboratory have provided strong evidence for the nuclear liquid-gas transition in hot atomic nuclei. The measurements were performed with the Indiana Silicon Sphere detector array at the Brookhaven National Laboratory nuclear particle accelerator. The IU collaboration was headed by **Victor Viola** and **Kris Kwiatowski** (now at Los Alamos National Laboratory).

Such a transition, analogous to the boiling of water and condensation of steam, must have occurred in the formation of neutron stars and black holes during supernova explosions. These forms of matter are the densest in the universe. For example, a typical neutron star may weigh as much as our sun but have a diameter of only about six miles.

The appointment of **Ted Widlanski** to a two-year term as associate dean in the College of Arts and Sciences is a continuation of a long line of chemists who have served as administrators for Indiana University.

**Joe Zwanziger** has become the department's associate director of graduate studies, with the intention of becoming the director next year.

— *Rupert Wentworth*





The department celebrated the annual Chemistry Staff Awards Banquet on April 26, 2001. **Heather Drake** was the recipient of the 2001 Outstanding Staff Award and was recognized for her extreme conscientiousness and dedication. In addition to her routine duties, Drake was acknowledged for the computerization of all graduate-student and alumni records.

We continue to be blessed with loyal and dedicated staff, and we recognized and honored the following for their IU service: for 30 years, **Richard Landgrebe** (assistant computer systems engineer in our research computing services) and **Deon Osman** (computer specialist, also in our research computing services); for 20 years, **Jackie Drake** (purchasing representative in our scientific storeroom) and **Don Garvin** (supervisor of glass instrumentation); and for 15 years, **Sondra Gearner** (research secretary to professors Caulton, Christou, and Todd) and **Judy Summerville** (departmental scheduling supervisor). It was great to see the smiling faces of some of our recent retirees who were in attendance: John Dorsett, Bob Ensman, Don Fowler, Carol Lettelleir, Kathryn Shirley-Koehl, and Bill and Kirsten Streib.

Several changes in staff positions have occurred this year. In October 2000, two students within the School of Music joined the department as part-time research secretaries — **Rosemary Tarcza** as research secretary to professors Crandall, Gajewski, and Montgomery; and **Chris Howard** as research secretary to professors Clemmer, Nie, and Peters. **Lara Zabawa** left the department, also in October, to accept the position of grants manager in the School of Education. **Michelle Sicuro** took her position of editorial specialist with Professor Ortoleva. Sicuro worked at the university previously as imaging coordinator at the Registrar's Office for instructional technology. She also has a BA in English from the University of Southern Maine. **David Felker** joined us in November as our manager of instructional computing, replacing **Mike Squires**, who left in August to pursue studies within SPEA. Felker came to us from GE Appliances, where he supported an NT/Novell network. He formerly was a consultant at University Information Technology Services. **Xinfeng (Frank) Gao** joined the department in November from the University of Missouri–Columbia, where he had recently completed his PhD in physical

chemistry. He works extensively in molecular modeling and NMR in his position as chemical informatics specialist. **Ann Morris** accepted a position in contracts and grant administration as a contracts and grants administrator in February, leaving our position of research secretary to professors Burke, Oakley, Richardson, and Stone. **Toni Lady** replaced her in March, transferring from University Division, where she had worked for four years as an assistant recorder. Previously, Lady had worked at the College of Arts and Sciences for 11 years, maintaining student records and certifying undergraduate degrees.

**Richard (Rick) Moore** joined the mechanical instrument shop in April as a research machinist II. Moore graduated from Vincennes University with an associate's degree in machine trades tool and die and worked at Cook Inc. for three years, where he gained extensive experience as a machinist. **Josh Meyers** left the university in April, leaving our position of technical services secretary.

**Jeanette Ash** was promoted to this position from the business office. She vacated the position of office services assistant and was replaced by **Melissa Jayne** in July. Jayne had worked for IU in the past in financial and administrative services and in payroll. She also has an AS in interior design from Vincennes University. **Chris Howard**, who was research secretary to professors Clemmer, Nie, and Peters and was simultaneously pursuing a career in music, left his position to participate in two renowned music festivals during the summer. He was replaced by **Shawn Conner** in July, who is also working part time. Conner recently moved to Bloomington to start a graduate program in comparative literature. He has a BA in English and history from the University of Missouri–Columbia and has excellent office experience as a legal secretary.

**Michelle Sicuro** left her position in July as editorial specialist with Professor Ortoleva to start a master's program in immersive mediated environments. **Kelly Bozanic** replaced Sicuro in August. Bozanic recently moved to Bloomington so that her husband can begin a doctoral program in economics. Bozanic has a BA in philosophy from UC–Berkeley, and she and her husband returned recently from Prague, where she studied at the Goethe Institute and Charles University. Last, we saw the passing of a recent retiree, **Ken Bastin**. Bastin lost his battle with cancer and died at his home on July 4. He retired in July 1999, after having provided 30 years of skill and expertise in our mechanical instrument services — a great loss.

— *Judy Crandall, September 2001*

## Update your address book

Holly Willett and her husband, Ron, have returned to their roots and moved back to Ohio. Their new address is 29 Canterbury Drive, New Bremen, OH, 45869. Holly's new e-mail address is [hwillett@nktelco.net](mailto:hwillett@nktelco.net).



## Mechanical Instrument Services

New to the mechanical instrument services facility is an Okuma Captain L370 four-axis lathe machine. This lathe machine features the OSP-E100L computer-numerically controlled (CNC) display and is top of the line in its field. It is capable of milling, tapping, drilling, and threading functions, thus replacing the need for having to change to various machines in order to complete a job. The control is very powerful and has 2-D and 3-D tool animation and simulation for safe verification of programs. This machine also features a forceful 20 horsepower integral VAC motor/spindle drive system that gives a torque of around 241 foot-pounds from 45 to 400 rpm, while the servo drive turret index speed is an amazing 0.01 seconds. Even the slant of the bed provides higher heat stability and increased rigidity. It gives the department new capabilities to produce parts that were impossible (or impractical) to date. For example, multiple compound radiuses, which are used for ion lenses, can be easily machined. ... It seems that everything that could be envisioned was implemented in creating this incredible machine! The Okuma Captain was purchased by the Indiana Instrumentation Institute, with money made available through a grant from the 21st Century Fund.

— Gary Fleener

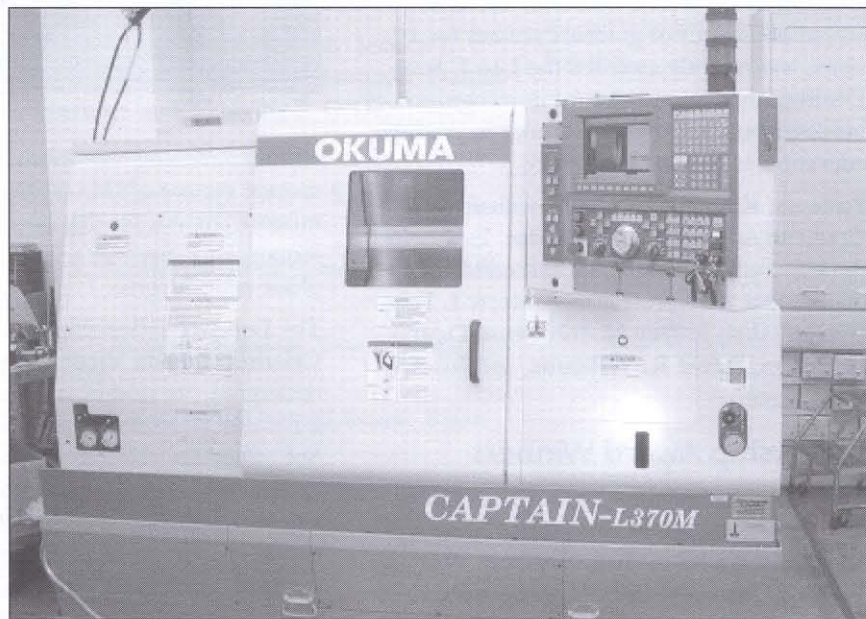
## Molecular Structure Center

There have been remarkable changes in the Molecular Structure Center during the past year. As mentioned elsewhere, **Maren Pink** joined the staff after the retirement of **Bill** and **Kirsten Streib** last year. Pink received her crystallography training in Germany and spent two years working in Victor Young's laboratory at the University of Minnesota. In addition to her general crystallographic skills, she is a recognized expert in dealing with twinned crystals.

In addition to solving structures using crystallographic techniques, the staff has been active pursuing projects in crystallographic informatics. **John Bollinger** received a grant from Compaq to build a Beowulf supercomputing cluster for the laboratory. The Beowulf is used to generate photorealistic images suitable for publication and presentations, and can be accessed using the laboratory's Web server at [www.iumsc.indiana.edu](http://www.iumsc.indiana.edu).

The unique visualization software being developed for the server contributed to **John Huffman**, Bollinger, and collaborators in the

Chemistry Library, the Department of Computer Science, the School of Education, and UTTS being granted a major award by the NSF that will make the IUMSC the central site for a molecular structure database in the National Science Engineering and Mathematics Education Digital Library. Another active research thrust of the laboratory this past year involves the access to synchrotron data. The DOE has been funding research for a "crystallography portal" (XPort) project that will allow researchers in the IUMSC and elsewhere to collaborate with colleagues working at the high brilliance synchrotron beamlines at the Advanced



*The new Okuma computer-controlled lathe in IU Chemistry.*

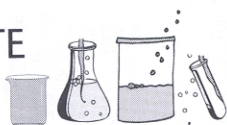
Photon Source at Argonne and the Advanced Light Source at Berkeley. The project takes advantage of IU's involvement as one of the major hubs for Internet2, the next generation research network. Central goals of the project include providing video collaboration and high-speed data transfer and access capabilities that will be important for both small-molecule and macromolecular studies by researchers in the department and university. In addition to the permanent staff of the laboratory, **Kianosh Huffman** (daughter-in-law of our director!) has been working on the XPort project. Furthermore, John Huffman was one of the principal investigators on a multi-million-dollar upgrade to the university's computing infrastructure that will help support this initiative. The informatics-related projects in the IUMSC were featured in the state of Indiana booth at the SuperComputing 2001 conference in Denver this fall.

Involvement with the national laboratories has contributed to the establishment of the Service

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## GRADUATE NOTES



During the 2000–01 school year, Professor **Jack K. Crandall** was director of graduate studies and chair of the Standards Committee. Serving with him on the Standards Committee were professors **Kenneth G. Caulton**, **Lawrence K. Montgomery**, **Milos V. Novotny**, **Martha G. Oakley**, and **Charles S. Parmenter**.

Crandall, who has chaired the Admissions Committee on several occasions and has served as director of graduate studies for 10 years, was recently awarded the Leo E. Solt Distinguished Service Award in recognition of his contributions to the excellence in graduate education at Indiana University.

Professor **Kenneth G. Caulton** chaired the Graduate Admissions Committee. Evaluating the hundreds of dossiers submitted to the department were professors **Andrew L. Feig**, **Evelyn Jabri**, **Jeffrey N. Johnston**, **Dennis G. Peters**, **David R. Williams**, and **Josef W. Zwanziger**.

### Fellowship Award Winners

**Catherine A. Srebalus Barnes** received the Eli Lilly Fellowship in Analytical Chemistry. She received a BS in chemistry from West Virginia University in 1994. Following graduation, she worked as an analytical research chemist in the pharmaceutical analysis division of Shire Laboratories Inc. in Rockville, Md. Srebalus Barnes began her graduate studies at Indiana University in 1997 under the direction of Professor David Clemmer. Her research in the Clemmer group has focused on ion mobility/time-of-flight mass spectrometry of combinatorial libraries. This ongoing research involves the use of IMS/TOF techniques for the gas-phase separation and characterization of synthetic combinatorial mixtures before and after



affinity screening. Additional research efforts include the use of IMS/TOF combinatorial mixture analysis for the investigation of sequence-to-structure relationships in gas-phase peptide ions.

The Lubrizol Fellowship was awarded to **Cristina Cañada Vilalta**, who completed her undergraduate studies in chemistry at the Universitat de Barcelona (Catalonia, Spain). She joined the research group of Earl Blough Professor George Christou at Indiana University, where she is pursuing a PhD in inorganic chemistry. The main goal of her research is the synthesis of inorganic models for the oxygen-evolving complex in the photosystem II, the center responsible for the oxidation of water to oxygen in green plants and cyanobacteria. She is also working in the preparation of new molecules with unusual magnetic properties, specifically those that exhibit single molecule magnet behavior.

The Procter & Gamble Fellowship was awarded to **Benjamin T. Burlingham**, who graduated *summa cum laude* from Grove City College in 1996 with a bachelor's degree in biochemistry. He is currently a doctoral candidate at Indiana University in the labs of

*Shell Associate Instructor Award winners, from left, are Juan Jimenez, Matthew S. Thompson, Timothy P. O'Dea, Jessica J. Hollenbeck, and Daniel G. Gurnon.*

## AROUND IU CHEMISTRY

### Staff News

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Crystallography at Advanced Photon Sources, or "SCrAPS" project. Headed by John Bollinger, the SCrAPS program gives researchers from IU and other university laboratories better access to the APS for characterizing small molecules. Both Bollinger and Maren Pink have made trips to Argonne to collect

data in association with the SCrAPS program this past year. These trips are yielding data on crystals that would not otherwise be characterized and are proving invaluable in setting up and testing the high-speed collaboration tools of the XPort project.

These and other activities of the laboratory are more fully described on the IUMSC server at [www.iumsc.indiana.edu](http://www.iumsc.indiana.edu).

— John Huffman



Associate Professor Theodore Widlanski. His research interests include the synthesis and characterization of molecules containing non-natural functional groups for use as mimics of biologically active molecules.

Two students held National Science Foundation Fellowships. **Jennifer M. Kindy**, who received a BS in chemistry from Wake Forest University, is a first-year student of Professor David Clemmer. **Lori A. Watson**, a graduate of the University of Kentucky with a BS in chemistry, is a second-year student of Distinguished Professor Kenneth G. Caulton.

Because of their outstanding undergraduate academic achievements, **Gerardo Gamez** (BS'99, MS'00, University of Texas–El Paso) and **Benjamin J. Wozniak** (BS'00, St. Norbert College) were awarded five-year Dean's Fellowships. Both students entered Indiana University in fall 2000. Gamez is doing research with Distinguished Professor Gary M. Hieftje, and Wozniak is doing research with Herman T. Briscoe Professor Dennis G. Peters. Also, because of outstanding undergraduate achievement, **Katherine J. Gill** (BA'99, Stetson University) and **Jennifer M. Kindy** (BS'00, Wake Forest University) were awarded five-year Women in Science Graduate Fellowships. Gill, who entered in fall 1999, is doing research with Distinguished Professor Ronald Hites, and Kindy, who entered in fall 2000, is doing research with Professor David Clemmer.

The Department of Chemistry has been selected by the U.S. Department of Education to participate in the Graduate Assistance in Areas of National Need Fellowship Program. Fellowships were awarded to **Aurora E. Clark**, **Nicole S. Coalter**, **Sarah B. Cortright**, **Danielle M. Goken**, **Robert T. Hart**, **Richard D. Hoang**, **David C. Johnson II**, **Brian J. Kraft**, and **Amie L. Williams**.

Other fellowship recipients were **Cherokee S. Hoaglund-Hyzer** and **Andrew M. Leach**, American Chemical Society, Analytical Division Fellowships; **Michael R. Mayer**, American Heart Fellowship; **Parichatr Vanalabhpattana**, Anandhamahidol Foundation Scholarship; **Viktor N. Staroverov**, College of Arts and Sciences Dissertation-Year Research Fellowship; **Sarah B. Cortright**, Bernard Berk Fellowship; **Julia Hoffmann**, Fulbright Fellowship; **Robert T. Hart**, John H. and Dorothy McKenzie Fellowship; **Sarah A. Webb**, National Defense Science and Engineering Graduate Fellowship; **Mark R. Herbert**, **Richard D. Hoang**, **Daniel Mutnick**, and **Benjamin M. Nugent**, Paget Fellowships; and **Vanvimon Saksmerprom**,

Royal Thai Government Fellowship.

Research and University Graduate School Fellowships were awarded to **Jason T. Ash**, **Richard L. Beardsley**, **Lewis J. Belcher**, **Nicole E. Chakov**, **Sarah B. Cortright**, **Gerardo Gamez**, **Katherine J. Gill**, **Danielle M. Goken**, **Jack L. Hayes**, **Amy E. Hilderbrand**, **Michael J. Johnson**, **David C. Johnson II**, **Jennifer M. Kindy**, **Jaime D. Vaeth**, **Lori A. Watson**, **Amie L. Williams**, and **Benjamin J. Wozniak**.

## Annual honors and awards

At the Chemistry Honors Banquet in April 2001, the following students were honored.

*Shell Associate Instructors Awards:* **Jessica J. Hollenbeck**, **Matthew S. Thompson**, **Daniel G. Gurnon**, and **Timothy P. O'Dea**

*E. Campaigne C500 Award:* **Lori A. Watson**

*William P. Klinkenberg Award:* **Samarjit Patnaik**

*Henry R. Mahler Memorial Award:* **Michael R. Mayer**

*Wendell P. Metzner Memorial Award:* **Scott V. Plummer**

*William H. Nebergall Memorial Award:* **Brian J. Kraft**

*Charles N. Reilley (Pharmacia Corp.) Award:* **William E. Doering**

*Felix Haurowitz Award:* **Khuloud Jaqaman**

## PhD degree recipients

Recent degree recipients are listed, followed by area, research professor, graduation date, and dissertation title.

**Burgess, Brandt R.** (biochemistry, Richardson, March 2001), "Investigation of  
(continued on page 18)



*William P. Klinkenberg Award winner: Samarjit Patnaik.*

*Research Award winners, from left, are Lori A. Watson, William E. Doering, Khuloud Jaqaman, Brian J. Kraft, and Scott V. Plummer.*





# AROUND IU CHEMISTRY

## Graduate Notes

(continued from page 17)

the Topological Interactions between *Escherichia coli* Transcription Factor Rho and RNA"

**Chan, Warren C. W.** (analytical, Nie, April 2001), "Semiconductor Quantum Dots for Ultrasensitive Biological Detection and Imaging"

**Chemler, Sherry R.** (organic, Roush, July 2000), "Recent Progress in Allylation Reaction Methodology: Stereoselective Reactions of Allyl- and Crotyltrifluorosilanes with  $\beta$ -Hydroxy Aldehydes"

**Clark, Michael P.** (organic, Williams, January 2001), "Studies Toward the Synthesis of Phorboxazole A"

**Coalter, Joseph N.** (inorganic, Caulton, January 2001), "Superior Routes to Ruthenium Carbenes and Carbynes"

**Cortez, Guillermo S.** (organic, Williams, August 2000), "Part I: Studies Toward the Total Synthesis of Zoanthamine Alkaloids; Part II: Total Synthesis of Lankacyclinol"

**Frank, Scott A.** (organic, Roush, December 2000), "Studies Directed Toward the Total Synthesis of (-)-Spinosyn A"

**Guzowski, John P.** (analytical, Hieftje, July 2000), "Advances in Time-of-Flight Mass Spectrometry for Atomic and Molecular Analysis"

**Hunt, Kevin W.** (organic, Grieco, December 2000), "I. Nucleophilic Bridgehead Opening of Oxabicyclic Molecules in Polar Media; II. Methods for the Construction of Advanced Intermediates for Macrolide Synthesis from Oxabicyclic Molecules: Synthesis of the C(19)-C(27) Fragment of Rifamycin S and the C(27)-C(32) Fragment of Scytophycin C"

**Iyer, Suri S.** (inorganic, Chisholm, August 2000), "Coordination Chemistry of Dirhodium and Dimolybdenum Complexes"

**Klein, Lee J.** (analytical, Peters, June 2001), "Explorations in Organic Electrochemistry"

**Leach, Andrew M.** (analytical, Hieftje, June 2001), "Recent Advances in Analytical Spectrometric Instrumentation: I. Applications of Radioluminescence in Spectrochemical

(continued on page 19)

You can find out the latest news and information about the graduate program in the Department of Chemistry and IU by visiting our Web site at [www.chem.indiana.edu/](http://www.chem.indiana.edu/)



Fellowship winners, first row, from left, are Cristina Cañada Vilalta, Benjamin T. Burlingham, Catherine A. Srebalus Barnes, Benjamin J. Wozniak, Gerardo Gamez; second row: Nicole E. Chakov, Katherine H. Gill, Sarah B. Cortright, Viktor N. Staroverov, and Robert T. Hart.



Fellowship winners, from left, are Andrew M. Leach, Cherokee S. Hoaglund-Hyzer, Julia Hoffmann, Jennifer M. Kindy, Sarah A. Webb, and Lori A. Watson.



Paget Fellowships winners, from left, are Benjamin M. Nugent, Daniel Mutnick, Richard D. Hoang, and Mark R. Herbert.



## UNDERGRADUATE NOTES



During the 2000–01 academic year, **Dennis G. Peters**, Briscoe Professor of Chemistry, continued as director of undergraduate studies. In July 2001, we welcomed Professor Romualdo deSouza, the new director of undergraduate studies. **Steven M. Wietstock** continued as the coordinator of instructional programs. In September 2000, we welcomed **David Felker** as the new manager of instructional computing. The other members of the Instructional Support Office are **Heather Kidd**, student records assistant; **Alice Dobie-Galuska**, general chemistry assistant coordina-

tor; and **Judy Summerville**, scheduling and registration manager. The ISO supports academic advising, maintains undergraduate student records, recruits, schedules classes, provides undergraduate academic computer support, supports the freshman laboratories, and coordinates information on curricular and pedagogical reform in undergraduate chemical education.

The fall 2000 recruiting program was once again a success. We had 18 companies that gave 195 interviews during the recruiting season. The companies that were on campus last fall included ArQule Inc., Array Biopharma, Baxter Healthcare, Bristol-Myers Squibb, Cargill Inc., Catalytica Pharmaceuticals

*(continued on page 20)*

## Graduate Notes

*(continued from page 18)*

Sensing. II. Investigations of an Inductively Coupled Plasma On-Axis Time-of-Flight Mass Spectrometer for Elemental Analysis”

**Seddon, Elisa J.** (inorganic, Christou, February 2001), “Synthesis of Supramolecular Iron (III) Complexes by Cluster Aggregation”

**Solyom, David A.** (analytical, Hieftje, May 2001), “The Development and Study of a Plasma-Source Mattauch-Herzog Mass Spectrograph for Elemental Analysis”

**Taylor, William P.** (biochemistry, Widlanski, November 2000), “The Mechanism and Inhibition of Protein Tyrosine Phosphatases”

**Ulrich, Elin M.** (analytical, Hites, September 2000), “Enantiomeric and Toxicological Studies of Persistent Pollutants in the Environment”

**Valentine, Stephen J.** (analytical, Clemmer, August 2000), “Probing Gas-Phase Biomolecular Ion Conformation with Ion Mobility/Mass Spectrometry Techniques”

**Yandulov, Dimitry V.** (inorganic, Caulton, August 2000), “Structural Preferences and Reactivity of Unsaturated Osmium Hydrides”

## MS degree recipients

**Coalter, Nicole L.** (inorganic, Zaleski, April 2001), “Metalloenediynes: Design, Synthesis, and Reactivity”

**Gan, Eugene C.-J.** (biochemistry, Richardson, February 2001), “Binding Studies of Escherichia Coli Rho with Fragments of  $\lambda$ Cro RNA”

**Ledezma-Gairaud, Marisol** (inorganic, Christou, May 2001), “Synthesis, Characterization and Magnetic Properties of Transition

Metal Clusters; [M = Mn, Co, Ni]”

**Lee, Young-Sam** (biochemistry, Oakley, May 2001), “Reverse and Antiparallel Basic-Region Leucine-Zipper Proteins: Expression, Purification, and Biophysical Characterization”

**Reno, Michael J.** (organic, Williams, September 2000), “Preparation of Functionalized Oxazolines and Oxazoles”

**Schmitt, Elbert W.** (inorganic, Zaleski, May 2001), “Synthesis and Structures of d<sup>10</sup>-Metalloenediynes”

**Smith, Kevin A.** (physical, Zwanziger, October 2000), “Experimental Determination of the Second and Fourth Moments of the Phosphorus Magnetic Dipole Distribution in Silver Phosphate”

**Warner, Kelly A.** (analytical, Hieftje, August 2000), “Thomson Scattering from Analytical Plasmas”

## MAT Degree Recipient

**Ford, James** (July 2000)

— Pat Stapleton

GAANN Fellowship winners, front row, from left, are Robert T. Hart, Danielle M. Goken, Aurora E. Clark, Brian J. Kraft; second row: David C. Johnson II, Sarah B. Cortright, Amie L. Williams, and Richard D. Hoang.





# AROUND IU CHEMISTRY

## Undergraduate Notes

(continued from page 19)

(Wyckoff division), Cook Imaging Inc., Dow AgroSciences, Eli Lilly & Co., General Electric Co., the Lubrizol Corp., Merck & Co. Inc., National Starch & Chemical Co., Pharmacia Corp., PPG Industries Inc., Procter & Gamble Co., Roche Diagnostics, and Sigma Chemical Co.

Our fall recruiting program for 2001 is under way and it looks as if we will once again have a full schedule of interviews.

### Scholarships and awards

The Annual Honors Banquet was held on April 17, 2001, in Alumni Hall of the Indiana Memorial Union. The following awards and honors were presented this year:

*R.J. Grim Scholarships:*

Class of 2003: Peter B. Conrad, Amy M. Fang, and Charles Chauncey L. Mc Crory

Class of 2002: Sudhir Rama Belagaje, Donald Buck, David Ming-Dar Fang, Jennifer Roberts, and Melissa Thal

Class of 2001: Bao Thien Huynh, Andrew James Moad, Kristen Elizabeth Nailor, Raju R. Rayal, and Annabeth Ryder



Chris Hughes and Elizabeth Oslos are winners of the James C. White and Mary Frechtling White Awards, respectively.



The 2001 Summer Undergraduate Research Experiences in Chemistry participants

*Lubrizol Scholarships for 2000-01:* Falk Eike Flach, Chris G. Hughes, Kelly Kristine Kahl, and Robert Tayon

*National Starch & Chemical Co. Scholarship for 2000-01:* Mackenzie Anna Ford, Samay Jain, and Melinda J. Kidwell

*Dow Chemical Corp. Scholarship:* Danielle Summer O'Donnol

*Andrew Lob Scholarship for Analytical Chemistry for 2001-02:* David Ming-Dar Fang

*Francis and Mildred (Eckerty) Whitacre Scholarship for 2001-02:* Eric Joseph Espinosa

*John H. Billman Summer Scholarship:* Eric Joseph Espinosa

*Ira E. Lee Summer Scholarships:* Samantha Ann Herbst, Jang Nee Lee

*Earl Sturdevant Summer Scholarships:* John Michael Zaborske

*Votaw Undergraduate Summer Research Scholarship:* Andrea Renee Auth, Paras Batuk Ramolia

*Frank Mathers Undergraduate Summer Research Scholarship:* Gia Charest Fazio, Annabeth Ryder, Joseph Bradley Strasburg

*Lilly Organic Undergraduate Summer Research Scholarship:* Ryan Adam Yoder

*Pharmacia & Upjohn Inc. Summer Scholarships:* Matthew Allen Anspach, Justin David Brown, Mariya K. Chhatriwala, Matthew Hardin Nett

*Honors Division Summer Scholarships:* Amy M. Fang, Joseph William Frank, Samay Jain, Jennifer Roberts, David Patrick Sullivan, Melissa Thal

*Russel & Trula Sidwell Hardy Scholarship:* Peter B. Conrad

*Merck Index Awards:* Jennifer Anne Challgren, Jason Kennard, Anna Izabela Krauze

*Analytical Chemistry Award:* Melinda J. Kidwell  
*Enola Rentschler Van Valer Trafford Scholarship Award:* Mackenzie Anna Ford, Kelly Kristine Kahl

*Courson-Greeves Prize:* Joseph William Frank

*William H. Bell Awards:* Sudhir Rama Belagaje, Joseph Peter Binfet, Falk Eike Flach

*Hypercube Scholar Award:* Allison Lisa Dill

*Joseph B. Schwartzkopf Award:* Robert Lewis Powell

*ACS Award:* Amrith Singh Malhi

*Mary Frechtling White Award:* Elizabeth Ann Oslos

*James C. White Award:* Chris G. Hughes



### Thanks to the supporters

We appreciate all the sponsors who have made these awards and scholarships for our undergraduate students possible. We congratulate these students on their achievements and express our best wishes to all of our graduating seniors for a long and successful career.

In addition to the students who received scholarships to stay on campus to work on their research projects, the department was awarded a Research Experiences for Undergraduates grant from the National Science Foundation that brought 13 additional students from other schools for a summer research experience. The summer research students participated in seminars on research ethics, career planning and placement, writing research papers, and graduate studies. The summer program culminated in an Undergraduate Research Symposium, where each student presented a poster of the work that they accomplished over the summer. The REU program was a great experience for all of the participants and we look forward to hosting additional students in the future.

This has been an exciting year for the Undergraduate Program, and we appreciate our many alumni who keep in touch with the department and who continue to provide new opportunities for our students.

— Steven M. Wietstock  
Coordinator of Instructional Programs



## Alumni Profile: Stewart Schneller

*We are always pleased to receive news about the activities of our chemistry department alumni. Occasionally, when we hear about someone whose career may be of particular interest, we request that they send us a brief bio-sketch. Dean Stewart "Stew" Schneller very kindly complied with the following.*

— The Editors

A native of Louisville, Ky., **Stewart Schneller** received his undergraduate training (BS in chemistry) at the University of Louisville and his MS at the same institution, working with Kevin Potts. He then came to Indiana University, where he pursued his PhD under E.E. Campaigne, receiving the degree in 1968. Schneller then spent two years as an NIH postdoctoral fellow at Stanford University. This was followed by a second postdoctoral period at the University of Massachusetts.

In 1971, Schneller began his academic career as an assistant professor in the chemistry department at the University of South Florida in Tampa at the time when the department was beginning its PhD program. He rose to associate professor in 1975 and full professor in 1978. He chaired the chemistry department from 1986 to 1994, at which time he moved to Auburn

University to become dean of the College of Sciences and Mathematics and professor of chemistry. He remains in those positions today.

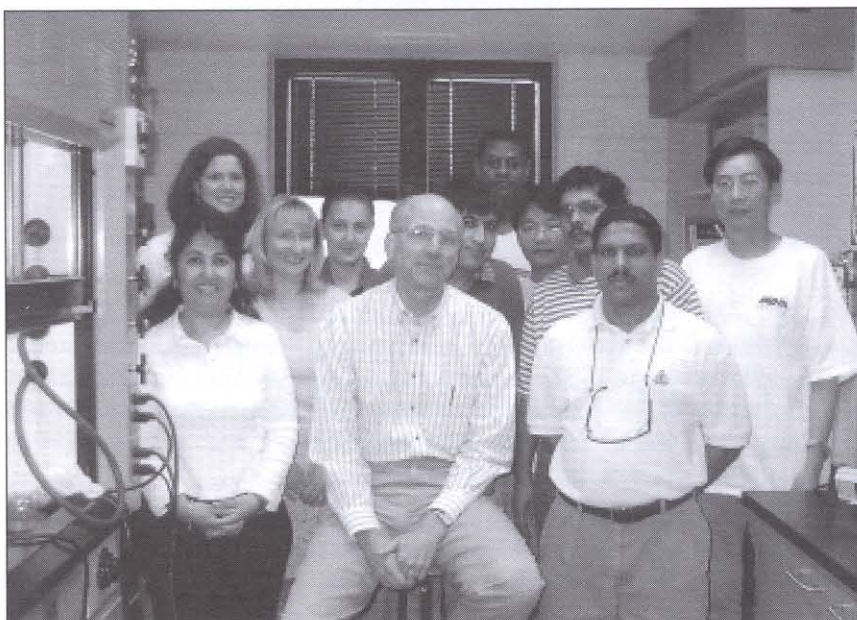
Dean Schneller has served the International Society of Heterocyclic Chemistry as president and has been a councilor of the

Division of Medicinal Chemistry of the American Chemical Society. He was also a four-year member of the Bioorganic and Natural Products NIH Study Section and a reviewer for a number of journals and granting agencies. He has presented numerous lectures worldwide. He received the outstanding professor award twice during his time at South Florida and recently was named the recipient of the 2001 Stone Will Award.

Schneller's research has focused on heterocyclic chemistry and on nucleosides, nucleotides, and nucleic acids. In fact, he has been continually funded by federal agencies since beginning his career at South Florida. As dean, he is on his second NIH grant, with the more recent one beginning in August 2000 and funded at \$2.4 million. Currently, his research group numbers four post docs and six PhD students. This has been typical throughout his career.

In addition to his academic responsibilities, Dean Schneller served as USF's NCAA faculty athletics representative for 13 years (1981–94). During his time in this role, the university added football to its program of 15 intercollegiate sports.

Schneller is married to Aina, and they have two children: Matt, now a first-year law student at Duke; and Katie, a freshman at Auburn. Schneller enjoys ham radio, reading, walking, and spending time with his family.



### Dear Alumni:

If you or your company is interested in recruiting at IU, please contact Steven M. Wieststock at (812) 855-2700 for additional information on the Chemistry Placement Program. We are also interested in setting up internship (summer and academic year) opportunities for students. If you are aware of positions, please contact the ISO at the above number. It is the strength of the department's alumni that continues to strengthen our placement and internship programs.

**Thank you!**

*Stewart "Stew" Schneller with his current research group.*





**Ron Conaway**, BA'78, and his wife, Joan, moved this summer from the Oklahoma Medical Research Foundation to the Stowers Institute for Medical Research in Kansas City, Mo. Jim Stowers, founder of American Century Mutual funds, and his wife, Virginia, created the institute with a \$50-million gift in 1994 and followed that with other gifts of stocks and cash that raised the institute's endowment to more than \$1.6 billion. Research at the institute is focused on understanding the genes and proteins that control how cells in our bodies divide, differentiate, migrate, and die. By studying these fundamental processes in cells, scientists hope to discover how genes cause many diseases, particularly cancer. The Stowers are cancer survivors. By fall 2002, the institute expects to have 16 functioning laboratories, each with a team of five to 10 researchers and technicians. The Conaways were among the first researchers recruited to the institute. When completely operational, the institute will house at least 50 independent research programs.

The Conaways shared the ASBMB-Amgen Award in 1999 for their outstanding research in the biochemistry of transcription in eukaryotic cells. Ron had been the H. Allen and Mary K. Chapman Chair in medical research at the Oklahoma Medical Research Foundation, and Joan was an associate investigator with the Howard Hughes Medical Institute at the foundation.

Ron was in the honors program at IU and did the research for his thesis in the laboratory of Professor John Richardson, who kindly supplied us with this information. Ron received his PhD in biochemistry from Stanford University.

**Gregory C. Gifford**, BA'71, MD'74, continues his practice in Kailua, Hawaii, and recently has been board-certified in hospice and palliative medicine. He is continuing as a consultant in end-of-life health care and also on legal issues.

**Mark M. Hamilton**, BA'88, MD'92, of Perkins Hamilton Facial Plastic Surgery, is the author of an article published in the spring issue of the medical publication *Aesthetic Plastic Surgery*. He is actively involved in teaching facial plastic and reconstructive surgery at IU and has authored several scientific articles and presentations.

**Marc K. Halushka**, BS'93, received an M.D. at Western Reserve in 2001 and is now a

resident in pathology at Johns Hopkins University.

**Stanley Krauhs**, MS'74, MBA'75, is a senior purchasing agent with Solvay Polymers, Houston, and is a city councilman in Shoreacres, Texas, where he and his wife live.

**James Richard Locker**, PhD'82, has been named the Clarence White Professor of Chemistry at Washington College in Chestertown, Md., where he has been professor of chemistry since 1985. His research interests include applications of analytical and physical chemistry to problems in environmental and forensic chemistry. He did his graduate research under the direction of Professor **Ed Bair**.

**Wendell L. Roelofs**, PhD'64, continues to garner recognition for his research work. He was awarded the Kenneth A. Spencer Award for Outstanding Achievement in Food & Agricultural Chemistry on Feb. 28, 2001, at the Kansas City Convention Center. The award is presented annually by the ACS Kansas City Section to encourage those engaged in research, education, and industry to continue the quest for excellence in their fields.

In his acceptance speech, Roelofs remarked, "It was a particularly special honor for me because the chemistry department at Indiana University ... nominated me for the award. ... I am mostly involved with entomology. ... Recognition as a chemist is a surprising honor."

**Steven Foster Sampson**, BS'74, OD'78, practiced in the Chicago area and was clinical instructor at Illinois College of Optometry until 1983, when he moved to Evansville, Ind. His practice has evolved from primary care and contact lenses to now include learning and visually related reading problems, crossed eyes, lazy eyes, and traumatic brain injury and stroke patients.

**James E. Schooley**, BA'53, in reply to a request from Professor Day, writes this report on his doings in recent years. He formally retired after 30 years at the National Bureau of Standards (now the National Institute for Standards and Technology) in 1990. He served as program chair of the 1992 symposium on "Temperature, Its Measurement and Control in Science and Industry" in Toronto and edited the two-volume proceedings of the symposium. In September 2000, he completed a 1,000-page history of NBS/NIST from 1969–1993, "Responding to National Needs," as part of the agency's centennial celebration.

In addition to his scientific endeavors, Schooley was inducted into the Indiana Basketball Hall of Fame in 1998.

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## 15 YEARS AGO

A groundbreaking ceremony was held on May 29, signifying the beginning of construction on the new addition to the Chemistry Building. This two-wing structure was completed and occupied four years later. It also provided an elegant new entrance at the southeast corner, facing Jordan Hall.

At this time, the department ranked second in the country in the number of bachelor's degrees awarded and sixth in the number of PhDs. Professor E. Campaigne was elected president of the Indiana Academy of Science for the coming year.



(*Alumni News*, continued from page 22)

**Robert L. Waters**, BA'62 (who also received an M.D. from the University of Chicago), sent us the following in response to a suggestion from Professor Day when Professor Waters was visiting his parents at Meadowood Retirement Community:

"My involvement with the Department of Chemistry began as a high school student, when I was fortunate to have Professor Lynne Merritt sponsor a high school science project to measure strontium 90 in rainwater resulting from atmospheric nuclear tests that were being conducted in the 1950s. I later attended IU on a research training grant under the tutelage of the late Joseph Muhler, renowned biochemist and dentist on the faculty.

"I still remember my first class in chemistry with Professor Harry G. Day and found out why it was one of the most popular classes in the university.

"The University of Chicago Medical School provided research opportunities for me while I was attending medical school, and afterwards I migrated to the University of California in San Francisco, where I finished training as an orthopedic surgeon. I took time out to serve as a fellow in the biomechanics department at UCSE, the engineering department at the University of California Berkeley and Rancho Los Amigos National Rehabilitation Center in Downey, Calif.

"I wound up in Los Angeles in 1971 at Rancho Los Amigos National Rehabilitation, where I have remained ever since — dividing my time between orthopedic surgery, research, and medical administration. I am on the faculty of the University of Southern California. RLANRC is the largest rehabilitation center on the West Coast and is affiliated with

UCLA and USC. We are a leader in applied clinical research related to rehabilitation. My own research has been in the fields of exercise physiology, kinesiology, functional electric stimulation, functional surgery, and the effects of aging on the musculoskeletal system. Most of my current research grants are in the field of spinal cord injury.

"I have held many different positions over the years. I have directed RLANRC's Spinal Cord Injury Program and was also chair of the department of surgery. Currently I am chief medical officer of RLANRC, in addition to serving as director of the Regional Spinal Cord Injury Care System of Southern California and co-director of our Research and Training Center on Aging with a Spinal Cord Injury. I have served as president of the American Spinal Cord Injury Association and as commissioner of the State of California Department of Health Services."

**Shirley Jean Yennello**, PhD'90, was the recipient of the 2000 Sigma Xi Young Investigator Award for scientific accomplishment, relevance of research, and communication of research. Yennello is currently an associate professor in the Department of Chemistry at Texas A&M University and a scientist at their University Cyclotron Institute. Robert A. Kennedy, Texas A&M vice president for research and associate provost for graduate studies, said, "She is in a unique role — an outstanding scientist who also sees the importance of playing a leading role in the formulation of science policy."

Yennello previously has been awarded many recognitions, among which are National Science Foundation Young Investigator Award, Oak Ridge Associate Universities Junior Faculty Enhancement Award, the GE

(continued on page 24)

## 25 YEARS AGO

The departmental molecular structure center was created when several scattered facilities were gathered together in a large Quonset hut located just east of Owen Hall. John Huffman became the director. Most large-scale computing involving crystallographic data was done on IU's central CDC 6600 system via interactive terminals in the center. Harry G. Day became professor emeritus in July; he was also editor of the AIUC newsletter. Gary Wiggins became head of the Chemistry Library.

## 50 YEARS AGO

Professor Harry G. Day was acting head of the chemistry department; he was appointed associate editor of the *Journal of Nutrition*, official publication of the American Institute of Nutrition.

John R. Kuebler, AB'12, MA'15, began his 25th year as secretary-treasurer of AXΣ, the national professional chemistry fraternity. Kuebler was a longtime teacher of chemistry at famed Shortridge High School in Indianapolis. J.C. Warner, PhD'23, president of the Carnegie Institute of Technology, and his wife visited the campus and met members of the chemistry faculty at a tea at the home of Dean and Mrs. Frank T. Gucker Jr.

The new radiochemistry laboratory was occupied in the fall semester. Located behind the east wing of the Chemistry Building, it was an all-concrete structure (even the roof was composed of concrete slabs). It was eventually removed in the course of later expansion of the Chemistry Building.



(*Alumni News*, continued from page 23)

Foundation Faculty for the Future Award, an Amoco Fellowship, the Chemistry Merit Award, and the Felix Haurowitz Award for Excellence in Research.

## Necrology

**Ronald W. Collins**, PhD'62, died from a heart attack in his home city, Ypsilanti, Mich., on Feb. 1, 2001. He was 64. His late wife, Geraldine, preceded him in death. The closest survivors are daughters Debbie and Sharon.

As reported in the Ypsilanti newspaper (Feb. 3 2001), Collins became an assistant professor at Eastern Michigan University in 1965 and a full professor six years later. He headed the chemistry department before becoming provost and associate vice president for academic affairs in 1980. EMU president Samuel Kirkpatrick was quoted, "Ron has been an integral part of this institution for more than 35 years and has led academic efforts for the past 18 years." In addition, the president stated, "He cared deeply about EMU and provided exemplary academic leadership."

Collins was born and raised in Dayton, Ohio, where he earned a BS at the University of Dayton. This was followed by four years at the Wyandotte Chemicals Corp. in Michigan. In 1957 he began his graduate studies at IU under the direction of W.H. Nebergall and completed work for the PhD with a thesis titled "Reactions of Tin (II) Compounds with Calcium Tin (II) Hydroxyapatite."

In Collins' progression to the status and high responsibility as provost of EMU, there were several events and actions that greatly exemplified his high academic capability and achievements. Notably, while he was professor and head of the department of chemistry at EMU, on April 15, 1980, the university accurately and properly issued a special report titled "Collins Selected for National Honor." It referred to him as "an expert on the use of computers in chemical education," and noted that he was "one of four individuals selected by the Chemical Manufacturers' Association to receive this year's prestigious Catalyst Award for teaching excellence and excellence in chemical education."

*We received notices of the deaths of several other alumni, but with no further information:*

- **George H. Ahlering**, BS'42, Oct. 27, 2000
- **Leon James Aiken**, BS'60, Feb. 2, 2001

- **Frederick Keith Ault**, MAT'67, Nov. 14, 2000
- **Richard Eugene Bayer**, PhD'59, June 30, 2000
- **Carolyn A. Fischer Bovenkerk**, PhD'71, July 26, 2000
- **Rexford Hale Bradt**, BA'30, Feb. 5, 2001
- **Hadley Louis Conn**, BA'42, MD'44, Dec. 3, 2000
- **Julius Mosher Coon**, BA'32, June 19, 2000
- **Edward Weir Cullipher**, BS'28, MD'32, March 25, 2001
- **Samuel J. Davis**, BA'37, MD'40, Feb. 22, 2001
- **George Thomas Gifford**, BA'32, April 10, 2001
- **Karl Kurt Haber**, BS'38, Oct. 2, 2000
- **Raphael A. Hardrick**, BA'56, Sept. 24, 2000
- **Joseph V. Hartman**, BS'38, Nov. 5, 2000
- **Randall Clark Jordan**, BA'72, MD'77, Jan. 16, 2001
- **Charles Marion Kerr**, BS'44, MD'46, Nov. 6, 2000
- **Michael Kim Lomax**, BA'67, MD'70, March 31, 2001
- **William G. McDonald**, BA'43, MD'46, Nov. 4, 2000
- **Edith Maxine McGuire**, BA'50, Nov. 9, 2000
- **Geraldine Georgia Germek Moss**, BS'59, Aug. 20, 2000
- **Axel Harding Peterson**, PhD'52, Sept. 19, 2000
- **John T. Pinkston**, PhD'40, Feb. 1, 2000
- **Helen Ann Viney Porter**, BA'57, May 12, 2000
- **Charles Austin Raney**, BA'32, June 20, 2001
- **William Bradley Reid**, PhD'46, April 27, 2001
- **Charles Caspar Rhetts**, BS'41, JD'77, June 3, 2001
- **James B. Robinson**, BS'36, June 30, 2001
- **Alma Burkin Rosen**, MA'50, Sept. 23, 2000
- **Andrew Salm**, BA'38, MD'42, Nov. 17, 2000
- **Philip Everett Smith**, BS'70, May 22, 2001
- **Milton Stern**, PhD'62, May 24, 2000
- **Ernest Franklin Stevenson**, BA'36, MA'37, July 8, 2001
- **Kenneth E. Thompson**, BS'48, March 27, 2000
- **Willard W. Tryon**, BA'31, Oct. 17, 2000
- **Harvey Eugene Wagoner**, BS'30, April 8, 2001
- **Harry Lewis Zeitels**, BA'40, Oct. 23, 2000



## In Memoriam: Professor Emeritus Lynne L. Merritt Jr. (1915–2001)

Lynne L. Merritt Jr. was born on Sept. 10, 1915, in Alba, Pa. From Wayne State University in Detroit, Mich., he earned a BS in both chemistry and physics in 1936 and an MS in 1937. For the three years from 1939 to 1942, Merritt was an instructor of chemistry at Wayne State University. In 1940 he received a PhD in analytical chemistry from the University

of Michigan. In 1942, Merritt, with his wife, Lucille, and two young children, moved to Bloomington as an assistant professor of chemistry. He rose through the academic ranks to become professor of chemistry in 1953. Only six years later, Merritt began to accept major administrative responsibilities in addition to those of teacher and researcher, a move that would be a hallmark of his other significant contributions to Indiana University, even after his general retirement in 1982.

As a faculty member here, Merritt immediately developed a course dealing with instrumental methods of analysis. Later, after introducing a course on radiochemical methods of analysis, he assisted a number of colleagues in their use of isotopes as tracers for investigations of a variety of chemical and biochemical reactions, and he played a seminal role in the creation of the Radiochemistry Building next to the Chemistry Building. Over the years, Merritt focused his own research program on the preparation and characterization of reagents for chemical analysis, embracing the technique of X-ray crystallography as a tool for determining the structures of molecules, and providing the impetus for the eventual creation of the internationally recognized Molecular Structure Center in the Department of Chemistry. Not to be overlooked is Merritt's passion for computational methods, first experienced during a sabbatical semester at the California Institute of Technology (1949–1950).

Upon returning from leave, Merritt quickly took the initiative in the development of a universitywide research computing system that ultimately became the Wrubel Computing Center. Across the nation and around the world, Merritt became most well known as coauthor of the highly acclaimed textbook *Instrumental Methods of Analysis*, six editions of which appeared over the years from 1948 to 1981.



*Professor Lynne L. Merritt Jr. and his wife, Lucille (May 1993 photo).*

Merritt started his administrative service as associate dean of the College of Arts and Sciences in 1959 and became associate dean of the faculties in 1962. During the period 1963–64, Merritt was acting dean of the faculties. In 1965, he began a 10-year term as vice president and dean of research and advanced studies. From 1975 to 1980, he took on the duties of special assistant to the

university president and dean for research coordination and development, and he retained the former position after reaching administrative retirement age in 1980. He became acting university grand marshal in 1978 and assumed full responsibility for that position in 1980. After his general retirement in 1982, Merritt commuted regularly from Bloomington to teach chemistry at IU Northwest, and he served twice as acting dean of academic affairs for that campus.

Merritt was recognized by awards and memberships in numerous societies. He was honored with a Guggenheim Fellowship in 1955–56 and a Fulbright Fellowship in 1963–64. In 1959, Merritt received a Distinguished Alumni Award from Wayne State University, and in 1988 he was awarded an Honorary Doctor of Science degree from Indiana University. He was on the Advisory Committee on Analytical Chemistry for the Oak Ridge National Laboratory (1957–61), the Committee on Analytical Chemistry of the National Research Council (1960–63), and the Advisory Committee for the Chemistry Section of the Air Force Office of Scientific Research (1953–73). He held memberships in the American Chemical Society and the American Crystallographic Association, and he was a Fellow of the American Institute of Chemists, of the Indiana Academy of Science, and of the American Association for the Advancement of Science. Locally, he was president of Sigma Xi (1959–60), as well as secretary (1959–61) and president (1964–65) of Phi Beta Kappa.

Merritt's service to Indiana University and the nation touched many other bases. He was the first director of the Bureau of Institutional Research. He played important roles in the formation of the Developmental Training Center, the School of Public and Environmental Affairs,

*(continued on page 27)*



# Chemistry Honor Roll 2000

- Mel E. Abascal  
Robert L. Ake, BA'60  
Timothy J. Anders, BA'89  
Mark R., BS'83, & Ann  
Anderson  
Cynthia J. Anderson  
Burton L. Appleton, PhD'58  
George R. Aronoff, M.D.,  
BA'72  
Peter G. Arvan, MA'44  
William E. Jr., MA'50, &  
Mary E. Bacon  
Ann K. Bailey  
Steven M. Bakeis, BS'90  
Jay R. Baker, BA'92  
Craig A., BS'70 & Margaret  
A. Balliet  
Helen B. Barnes, M.D., BA'38  
John C. Bart, BS'89  
Bradley B. Basinger, PhD'81  
John C. Beauchamp, BA'86  
Jean C. Beckman, PhD'77  
Mohammad Behforouz,  
PhD'65  
Nicholas C. Bensko, MS'74  
Marcia A. Berggren, BA'65  
Ella M. Bettinger, BS'49  
Lawrence A. Black, BS'77  
Alvin M. Borders, PhD'37  
Max I. Bowman, PhD'37  
Charles H. Boxman, BA'53  
Joanna Dickey Bradt, MA'33  
Wendy S. Braun, BA'93  
Malcolm, BA'38, & Mary E.  
Bray  
Thomas M. Brink  
William W. Bromer, PhD'54  
William W. Brubaker, PhD'98  
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## In Memoriam

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and the International Activities Center (which he later directed). In connection with the last of these, he traveled to nearly 40 countries throughout the world, working particularly with universities in Afghanistan, Indonesia, Iran, Italy, Japan, Pakistan, and Thailand. Merritt represented Indiana University through his membership and leadership roles in numerous educational organizations: Board of Trustees of the Universities Research Association, Board of Directors of Midwest Universities Consortium for International Activities, Advisory Council of the Organization for Tropical Studies, Board of Directors of the Association of Universities for Research in Astronomy, Council on Federal Relations of the Association of American Universities, and National Council of University Research Administrators. He also served as campus coordinator for the USAID/IU Higher Education Administration Project at Kabul University and for the Ford Foundation/IU Project at the University of Islamabad. For eight years, he was a member of the Indiana State Scholarship Commission, and he was on the Board of Overseers of St. Meinrad College and Seminary for nine years.

Merritt passed away in Bloomington on Jan. 11, 2001, at the age of 85. He is survived by three daughters — Peggy Reed, BS'61, of Boulder, Colo.; Lucy Williams, BS'67, MS'73, of Bloomington; and Linda Marler, BS'73, MS'78, of Indianapolis — by eight grandchildren, and by three great-grandchildren. His wife, Lucille, and his son, Lynn Robert, preceded him in death.

— H.G. Day, D.G. Peters, and V.J. Shiner Jr.

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