# IU•CHEMISTRY

Letter to the Association of Indiana University Chemists from Adam W. Herbert, Indiana University president

Dear esteemed colleagues and alumni,

Since joining this distinguished university community, I have taken great pleasure in learning about the long, prestigious history of chemistry at Indiana University. From past commercial successes and theory contributions to recent discoveries in analytical chemistry, organic chemistry, and proteomics, the bright past of IU Chemistry shines unfiltered into an equally bright future.

This legacy of scientific excellence does not appear *de novo*. Rather, it reflects the strength of our faculty and broad community support — colleagues in chemistry and related sciences, departmental administrators and staff, graduate school leaders, and members of past IU administrations. It is with this continuity in mind that I affirm my support for chemistry in its many forms and for basic and applied sciences in general, throughout IU.

With the goal of further expanding IU's research productivity and capabilities, we must seek out new, external funding opportunities for IU science faculty. We must facilitate and encourage interdisciplinary collaboration. We must expand initiatives related to the life sciences and information technology. We must support intercollegiate projects that can benefit our chemists. And we must do whatever is needed to attract ever more outstanding chemistry faculty to our university.

Already under way is a 10-year push to broaden and deepen scientific research throughout the university. The construction of three new multidisciplinary science buildings on the Bloomington campus and the meteoric growth of the Indiana University-Purdue University Indianapolis scientific community demonstrate our commitment to that end.

In the last year for which information is available, 2002–03, IU's sponsored research totaled more than \$392 million. With a slew of new, multimillion-dollar research grants this summer from the National Science Foundation and the National Institutes of Health, it is hard to imagine anything but good news in coming years.



Adam W. Herbert

IU Chemistry also graduates future chemists who go on to do impressive work as scientists, teachers, physicians, and in many other areas of scientific endeavor. Chemistry's commitment to involving students in research at an early stage in their graduate careers, in numerous sponsored seminars and in research colloquia clearly fosters an exceptional educational environment. Thus, it is no coincidence that IU Chemistry graduates are coveted by graduate schools and industry across the nation.

I am very proud of IU Chemistry and look forward to supporting efforts to advance further its distinguished international reputation of excellence.

> — Adam W. Herbert President, Indiana University

We welcome Adam
W. Herbert as our
new president, and
we are sure that
the Department of
Chemistry will
benefit from his
ongoing support.

- THE EDITORS \*

# New developments in inorganic chemistry at IU

### by Ken Caulton

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Ligands controlling reactivity and metallatherapeutic reagents designed to attack tumor tissue are only two of the several inorganic research efforts in our department. Inorganic chemistry suffered major losses in the past two years with the departures of Malcolm Chisholm and then George Christou. Both had outstanding research programs and were active and insightful departmental citizens. While the search for a senior inorganic faculty member here continues, we have been active in hiring at the junior level, and in this way we have imported research activity in a number of recently developing research areas.

Assistant Professor Dan Mindiola began in the department in July 2002. His prior educational path took him from Michigan State University (undergraduate research with Kim Dunbar) to MIT (PhD with Kit Cummins) and then to the University of Chicago (postdoc with Greg Hillhouse, PhD'80). Dan's expertise in synthetic and mechanistic molecular chemistry of the transition metals has focused on multiple bonds between metals and C, N, or P. Dan is active with all of the transition metals in the periodic table, as well as with low valent lanthanides. His initial research focus at Indiana is the use of sterically bulky bidentate nitrogen donor ligands to access unusually low coordination number metals (see fig. 1), which therefore have high reactivity and sometimes catalytic potential. Dan is a synthetic "wizard," and his students have a hard time matching Dan's energy level.

Mu-Hyun ("Mookie") Baik (pronounced "bake") joined the department in July 2003, from his bachelor's degree in Germany, his PhD with Cindy Schauer (University of North Carolina), and a postdoc with Rich Friesner (Columbia University). Mookie is one of the new generation of applied computational chemists: those who use the spectacularly practical density functional theory to produce useful quantum mechanical descriptions for molecules of complexity equal to those actually studied by contemporary experimental molecular researchers. The DFT methods enable





**Fig. 1.** Using steric bulk to protect a rare Ti=P bond.

calculation (i.e., prediction) of any observable: energy, structure, vibrational frequencies, NMR parameters, rate constants, and thus mechanisms, etc. Mookie's special interest is in transition-metal-containing molecules, ranging from bioinorganic (see cis-platin model, fig. 2) to catalytic to organometallic systems. Mookie's special talent is his ability to choose broadly important problems unsolved by experimental studies and apply computations to their solution. He is an exceptionally interactive scientist, having already collaborated and published with experimentalists in three countries outside the United States.

Dongwhan Lee began as assistant professor in July 2003, following his BS and MS degrees in Korea, then his PhD with Steve Lippard and postdoc with Tim Swager, both at MIT. Dongwhan is an expert in synthetic bioinorganic modeling by "designer ligands," the skill of using ligand donor atoms, and constraints linking these together to alter reactivity of transition metal complexes of biological relevance. Dongwhan's postdoctoral research in the area of organic materials (site-isolated polypyroles, fig. 3) has led him to begin work at Indiana with functional polymers responsive to injection and removal of electrons. By using sulfur-rich polymers having redox-active heterocyclic junctions, he hopes to develop conductive materials appropriate for sensing applications. The most important fundamental skill for his research group is organic synthesis of the sophisticated polymer architectures he intends to create.

Mookie and Dongwhan share a coincidental link in their research backgrounds, since both have advanced the understanding of how nature selectively functionalizes methane under ambient conditions: the enzyme methane monoxygenase. In his PhD work, Dongwhan designed and synthesized diiron complexes having close structural and functional similarity to those found in the enzyme active site. Mookie, in his postdoctoral research,

Fig. 2. A model of cisplatin (cis-diammin edichloroplat inum(II)) attacking DNA, leading to tumor cell death. did density functional calculations with the aim of predicting the mechanism of this same reaction.

At Indiana, Mookie also holds an appointment in IU's new School of Informatics, a field whose goals include "mining" huge amounts of data, involving many independent variables, for their underlying causal factors. For example, "bioinformatics" currently seeks structure/function relationships among observations on a variety of homologous biopolymers. The field of "chemical informatics" is still defining itself, and Mookie is involved in that evolution. For example, advances in computing power now allow semi-automated searches of a huge range of molecular structures, to the extent that the researcher has trouble evaluating such volume of output. Chemical informatics can hope to establish some few "criteria of quality" by which a huge volume of data can be automatically prioritized, then brought to the attention of the researcher.

Jeff Zaleski continues to optimize ligands with conjugated functionality. When these are complexed to a metal, both geometric and electronic factors influence the temperature needed to cyclize the conjugated acyclic system to a *p*-phenylene diradical (see fig. 4). The goal of this project is to use the reactivity of the diradical as a "metallatherapeutic" reagent, to attack tumor tissue. In addition to the design of metalloenediyne therapeutics, the Zaleski lab has additional interests in the development of metal-diazo compounds that use metal-ligand photochemistry to release dinitrogen, generating reactive radicals that can attack biological substrates. He also has productive collaborations with the Chisholm group (OSU) in the design and function of liquid crystals with magnetic alignment properties, and with Carl Bauer in the biology department of IU, focused on the details of metal and chromophoremodulated gene expression (on/off production of proteins) in the presence and absence of light.

My own interests center on a concept of "product adapted geometry," dictated by a new macrocyclic ligand class, which destabilizes a metal reagent



**Fig. 4.** Cyclizing a magnesium-complexed "ene-diyne" damages DNA by double Hatom abstraction.

complex to the extent that it will cleave the C-H bond of methane, and convert ethane to ethylene. Another type of ligand, again tridentate, has the property of making a metal highly reducing even in oxidation state +2 (see fig. 5). Finally, a French postdoc in my group has developed a ligand that is alternately bidentate or tridentate, and the former thus leaves the metal able to bind

substrates with negligible activation energy.

All together, recruiting efforts for new graduate students and postdocs in the areas of inorganic chemistry continue to benefit from the friendly and outgoing personalities of the faculty. Our current graduate students, who are very positive about the educational program, including development of all communication and related professional skills, probably are the most persuasive ambassadors for our program. The research output of the inorganic chemistry faculty also benefits from undergraduate researchers, financed in part by a National Science Foundation grant to the department to bring about 20 students to our department for 10 weeks each summer. Postdoctoral researchers constitute another important part of the departmental intellectual atmosphere; those currently or recently

here include PhDs from the United States, India, Russia, France, Germany, and China. All told, inorganic chemistry takes on numerous new faces, both human and thematic, but is marked by enthusiasm, optimism, and good rapport between faculty and younger researchers.



Ken Caulton



**Fig. 3.** Isolation of a  $\pi$ -conjugated polymer backbone with a "canopy" of hydrocarbon groups improves conductivity.



**Fig. 5.** Arriving  $C_2H_4$  molecule sterically shields the ruthenium atom by distorting the <sup>t</sup>Bu groups.

# **Building on excellence**

### by Susan D. Green

In 2003-04, Indiana University joins the University of Illinois, Ohio State, and yes, Purdue, in assessing new undergraduate students on the Bloomington campus \$1,000 in addition to the usual tuition and fees. According to the Chancellor's Office, rising costs and diminishing state support made this move imperative if Indiana University intends to keep its place in the top rung of research universities. The assessment added \$7.1 million to the base budget of the Bloomington campus this year; approximately \$28 million in base funding will accumulate over five years. These monies will be used, according to the Chancellor's Office, to support critical missions and initiatives, to recruit and retain outstanding faculty, and to provide matching funds to attract private support of graduate fellowships.

Bloomington campus schools and departments competed for these funds by submitting a total of 36 proposals to the Chancellor's Office. Seven proposals were funded, five of which enhance the status of the sciences on the Bloomington campus. "Funding for interdisciplinary environmental sciences, cognitive science, and the School of Optometry will add to the overall strength of science in Bloomington," said David Clemmer, chemistry department chair.

What really excites Clemmer, however, are two funded proposals that will impact chemistry significantly. The 21st-Century Interdisciplinary Science proposal and the Comprehensive Human Biology proposal will add a total of 37 faculty over the next five years, many of those faculty to the Department of Chemistry. First-year hiring is expected to include faculty in materials chemistry, synthetic chemistry, polymer chemistry, biochemical characterization, molecular assembly biochemistry, analytical, and organic chemistry. "The beautiful part of all this," Clemmer said, "is that we don't have to look for people at certain levels to fill certain slots; we can find the very best candidates at any level and create the slots."

"There was a concern among some science faculty that the sciences were no longer a university priority," Clemmer said. "This funding acknowledges the university's recognition of science as a 'critical mission' and should put those worries to rest. I've always believed that Indiana needs to invest in science-based technology. Because of this funding, we'll have new undergraduate and master's degree programs in applied science and human biology and biotechnology. We're also committed to a K–12 science education initiative in cooperation with the School of Education. The Commitment to Excellence program can have a huge impact, not just on the Bloomington campus, but on the whole state."

Editors' note: Susan Green is retired executive director of the College of Arts and Sciences and a devoted friend of the College.



of the summer 2003 edition of The College, the alumni magazine of the College of Arts and Sciences, and you will find another blessing for our department, a blessing beyond the one described in Susan Green's story: We will share a new \$55 million multidisciplinary science building in the heart of the old campus, between our building and Jordan Hall.

Look for your copy



# New faculty, faculty awards, and new initiatives

A s I sat down and thought about this letter and my first year as chair I was struck that this has been a year of significant transition. There are many new faces, a number of new initiatives within the department (as well as the College), and a design for a new multidisciplinary science building that will connect to the Chemistry Building. I will try to provide brief updates of each of these initiatives.

#### New faculty hires

I am happy to report that we have hired six new faculty: Mu-Hyun "Mookie" Baik, theoretical and inorganic chemistry and chemical informatics; Richard DiMarchi, biochemistry; Srinivasan "Srini" Iyengar, theoretical; Stephen Jacobson, analytical; Dongwhan Lee, inorganic; and Thomas Tolbert, biochemistry. These hires represent a significant step in replenishing our faculty ranks. Although there is still much work to be done in the coming year (and the years to follow), we have added 10 new faculty in the last two years: five at the assistant rank, two associates, and three full professors. We are further strengthened by several outstanding scientist- and clinical-rank faculty hires. This success relieves some of the pressure that we still face with the upcoming retirements of a number of our most senior and well-known colleagues.

It is worthwhile to say a few words of introduction regarding each of our new colleagues. This year four join us at the rank of assistant professor. **Mookie Baik** completed his PhD with Cynthia Schauer at the University of North Carolina and did postdoctoral work at Columbia (with Richard Friesner) and MIT (with Steve Lippard). His research cuts across many traditional boundaries, including computational, inorganic, bioinorganic, and physical chemistry/chemical informatics; he has a joint position in the new School of Informatics.

**Srini Iyengar** completed a PhD at the University of Houston, under the direction of Donald Kouri. He subsequently did postdoctoral work with Greg Voth at the University of Utah. Srini's research interests range from theoretical, computational chemistry, and physics to biological chemistry, condensed matter dynamics, and material science. We welcome him with a hearty congratulations, as he has received a Camille & Henry Dreyfus New Faculty Award. (I can't help but note that this is the second year running that a new hire of ours has been recognized with this award — Dan Mindiola won it last year.)

**Dongwhan Lee** received a PhD from MIT, working with Stephen Lippard, where he prepared and probed the reactivity of dinuclear iron compounds as models of the methane monooxygenase active site found in bacteria that convert methane to methanol. He continued his postdoctoral research there in the laboratory of Timothy Swager, where he developed novel polymeric architectures with unique structure/function relationships as precursors for novel electroactive materials. His research program at Indiana will focus on understanding materials with organic/inorganic junctions and functionally relevant bioinorganic models.

Thomas Tolbert completed a PhD at MIT, where he worked in the laboratory of James Williamson. He came to IU after a postdoctoral fellowship with Chi-Huey Wong at the Scripps Research Institute. While at Scripps, he developed techniques that use inteins and TEV protease for site-selective protein labeling and glycoprotein semisynthesis.

Stephen Jacobson joins us as an associate professor. He obtained his PhD in 1992 from the University of Tennessee, where he worked with Georges Guiochon. Upon completing his doctorate, he took a position as a Hollaender postdoctoral fellow with J. Michael Ramsey, PhD'79 (with

Hieftje), at Oak Ridge National Laboratory. Subsequently he joined the research staff at ORNL, where he worked on miniaturizing chemical assays and implementing them as simple processes that could be carried out on chips. Steve's program at IU is highly interdisciplinary and will include studies of physical and chemical phenomena on the micro- and nanoscales in artificial and living systems.

**Richard DiMarchi** joins us as the Linda and Jack Gill Chair in Biomolecular Sciences. Richard completed his PhD in biochemistry at IU, where he worked with **Frank Gurd**. Upon leaving Bloomington, he did postdoctoral work in Bruce Merrifield's lab at Rockefeller before moving to Eli Lilly and Co. There, he rose through the ranks rapidly and took a very early retirement from his position as group vice president for Lilly Research Laboratories before joining us at IU. Richard played key roles in launching a number of Lilly products, including the molecular design *(continued on page 6)* 



David E. Clemmer

New faces and new initiatives keep our department vibrant.

\*

Chair's letter

(continued from page 5)

of Humalog. He serves on the boards of directors for IU's Advanced Research and Technology Institute and the Biotechnology Industry Organization — to mention a couple (Richard's service on state, national, and university boards is too extensive to list here). His research program is focused on understanding the chemical and physical properties of the blood-brain barrier and generally as relating to the chemical and physical properties of peptides, proteins and their modified forms.

#### New awards and recognitions

Our faculty continue to bring acclaim to our department and university by winning prestigious awards and being recognized with other honors. Congratulations go to Jeffrey N. Johnston, who recently received two national awards: the 2003 Amgen Young Investigator's Award and the 2004 Eli Lilly Grantee Award. The Amgen Young Investigator recognition was based on Jeff's commitment to academic excellence and his group's scientific contributions through research, which will have a significant impact within the industry. The Eli Lilly Grantee Award is given to untenured faculty with the potential to become leading chemical researchers. Grantees are recipients of an unrestricted grant award, focused on advancing their careers.

Milos V. Novotny was the recipient of the 2003 Tracy Sonneborn Lecture Award. This award is given to faculty members who have achieved local, national, and international distinction in both teaching and research. Milos presented the Sonneborn Lecture in the Frangipani Room on Nov. 5, which was followed by a reception in the University Club. In addition, Milos was selected to receive the 2004 Stephen Dal Nogare Award. The award is given each year to an outstanding scientist in the field of chromatography. Milos was chosen based on his contributions made to the fundamental understanding of the chromatographic process. The award will be presented at the Pittsburgh conference in March 2004.

Professor Emeritus Harry G. Day was chosen as the recipient of the highest honor given by the Indiana Academy of Science — the 2002 Distinguished Scholar Award. Harry was chosen based on his outstanding scholarship and many years of participation in the academy. It is difficult to put this award into context. With this selection, Harry joins a prestigious group of scientists, including: Herbert C. Brown (Nobel Prize 1979), Alton A. Lindsey (consultant for the Save the Dunes Council during the 1960s), Charles B. Heiser Jr. (an expert in botanical research on plants of economic importance), and our own Ernest R. Davidson (who last year won the President's National Medal of Science).

Congratulations also go to Martha Oakley, who was awarded tenure in our department this year. Upon receiving tenure, Martha took on a new appointment as the associate chair for undergraduate studies. She and a committee that she has formed are currently in the process of revising our freshman chemistry program. Along similar lines, Jeff Zaleski is now the director of our graduate studies program. This year, Andy Evans (chair of our graduate admissions committee) recruited 50 new students as our incoming class.

Last spring semester, three of our faculty members (Martha Oakley, Dennis Peters, and Jill Robinson) 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.

As noted above, **Srini Iyengar** received the 2003 Camille and Henry Dreyfus New Faculty Award. This award — given to support new faculty with research — was designed to assist outstanding scientists in realizing their promise as educators.

Congratulations go to all of our award winners for their recognized excellence!

#### New science-based initiatives

(See the full article on page 4.) During the last year, our department has been involved in the development of two new science initiatives within the College of Arts and Sciences: Human Biology and 21st-Century Interdisciplinary Science. Driving these initiatives is a new Commitment to Excellence program that will bring base funding to support 37 new science faculty (primarily chemists, biologists, and physicists and their hybrids) and will generate a number of new undergraduate majors, as well as necessary infrastructure for research.

We will begin hiring new faculty this year and expect to fill these new positions over the next five years. The Human Biology program is anticipated to include a significant molecular basis, and we anticipate expanding our biochemistry, bioanalytical, and biophysical faculty lines. The 21st-Century Interdisciplinary Science program includes a substantial initiative in molecular materials, allowing us to expand in areas of chemical synthesis, polymer, and materials chemistry, as well as new physical and analytical approaches for characterization. We owe a great deal of thanks to Professor Ted Widlanski (currently the associate dean of research at the College of Arts and Sciences), who worked with many scientists and administrators to make these initiatives possible.

#### The new Multidisciplinary Science Building

One of the primary challenges that we continue to face involves research space. Some relief is expected to come in the next three to four years with the construction of the new Multidisciplinary Science Building. This building will contain core NMR, crystallography, materials characterization, biophysical characterization, proteomics, and genomics facilities that will allow researchers to access the latest techniques in these fields. (The biophysical core was initiated this year by **Martin Stone** and **Todd Stone** and currently is located on the sixth floor of our building.) Additionally, about 10 new research laboratories are designated for chemists. It is difficult to overstate the importance of work done by many of our faculty in order to bring this project to this stage. Initial efforts to plan a building began more than three years ago, and many of us, including **David Williams, Gary Hieftje**, and **Milos Novotny**, were involved with assessing the needs of scientists at IU. During the last year **Martin Jarrold** guided the design of many of the building's core facilities as well as chemistry laboratories.

# A newly minted PhD from our department

The nicest thing that has happened during my first year as chair was that Max Marsh, BS'47, was awarded an honorary degree of doctor of science. Across the university only three honorary doctorates were awarded. The department recognized this event with a large party in the Indiana Memorial Union for Max, Jane, and their family. The night went on much longer than some of us anticipated and was filled with comments from many faculty and friends. The award ceremony included a relatively small dinner with members of the IU administration and their families and the board of trustees and their families. Following comments by Sen. Richard Lugar, Max gave one of the warmest and most inspiring acceptances that I've ever heard. The doctorate was awarded at the 2003 IU commencement ceremony in May. Long before his retirement from Eli Lilly in 1986, Max was active on our campus as a visiting scientist. He was appointed as an adjunct faculty member in the IU Department of Chemistry for the first time in 1971 and again in 1990. He has been an exceptionally loyal friend and participant in the life of our department for many years. We are very proud of you, Max.

#### New chemistry awards

Last year I reported the creation of two new chemistry awards: the **Dennis G. Peters** Undergraduate Scholarship and the **Jack K. Crandall** Award in Graduate Education. Thanks to all who contributed so generously to these endowments during the past year — both funds now generate sufficient income to award annual prizes.

#### New skills for me

I thought I'd bring this to a close on a lighter note by explaining a new skill that I've worked on with respect to one of my important jobs — the role of the host during faculty recruiting. As you might imagine, my upbringing in southern Colorado did not fully prepare me for hosting receptions for famous scientists. Wendy suggested that we take a wine-tasting course so that I could choose some nice bottles and impress candidates — until this time, my primary education came from dinners with Milos, Gary, and Dennis. To make a long story short, I found most of this to be illustrative of the power of suggestion. I would smell, taste, and try to pinpoint my impression until someone else would say "pepper" or "plum" and then I could sense it — pepper or plum. That is, until finally in about week four one wine struck me with a strong sensation that I struggled to place. Finally, I recognized it — grapes ... definitely grapes. I decided to keep this one to myself. Anyway, with guidance from others we had some nice wines and some enjoyable evenings entertaining our faculty candidates. Our six hires were from eight offers — not too bad.

Thanks, all of you who made this year enjoyable and successful: especially, **Mary Swarthout**, who simply took over and ran the show at key times and explained many of the inner workings of the department to me; Martin Jarrold, who chaired the faculty search committee; and all of the current and emeritus faculty who tirelessly met faculty candidates and their families. Our colleagues, Marvin Carmack, Ed and Dorothy Bair, Jack and Reva Shiner, Lee Todd and Marci Ankrom, and Max and Jane Marsh have an affection for IU and Bloomington that is simply contagious.

Finally, I'm not sure what we've done to deserve **Jack Crandall's** continued help as acting associate chair; his wisdom and support continue to influence and guide our department. This year, Jack's former PhD students threw him a belated retirement party. As I listened to them affectionately roast him, I got the feeling that Jack's students felt he was quite a character in his younger days. As near as I can tell, he hasn't changed much. Many thanks, Jack!

I hope all of you will drop us a line this year so that we know what you are up to. I also hope you will stop by the chair's office and visit us when you are in town.

— David E. Clemmer

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# Around IU • Chemistry

# Southern Indiana Section ACS activities

The Southern Indiana Section of the American Chemical Society has had a busy year in 2003! During 2003, SISACS has been focusing its attentions on expanding our community outreach. Starting in the fall, we expanded our chemistry tutoring service for the surrounding high school students. We will start subsidizing \$5/hour toward the usual IU tutor fee (if they use the tutor list provided by the IU Department of Chemistry) to encourage high school students and their parents to actively seek out help in chemistry. Furthermore, we have contacted the surrounding school teachers to determine how our section can better support the teaching of chemistry in primary and secondary schools. Establishing these relationships was the first step in providing our support for our community.

Starting in the fall, we announced our reinstatement of the local student affiliates chapter of the ACS. We have had moderate interest, as the word of its existence is still growing. New monthly activities include a movie night (we even bought a popcorn machine with support from the chemistry department), rock-climbing outings, bowling nights, and volunteering activities such as blood drives, Habitat for Humanity, and, closer to the holidays, food drives. We anticipate that the local student affiliates chapter will enhance our ability to perform further community outreach as well as help bolster the camaraderie of the undergraduate chemists in our section.

On Feb. 25, the SISACS hosted Thomas H. Parliament from Parliament Consulting (New York, N.Y.) who gave a captivating talk titled "The Chemistry of Coffee Roasting." We had an excellent turnout for the talk, in particular a large undergraduate population. On May 13, the SISACS hosted a seminar in IU's Department of Chemistry for Professor R. Bruce King from University of Georgia. His presentation was titled "Transition Metal Catalysis of Carbon Monoxide and Formate Reactions." Again, we had a good turnout for his talk. Both talks were followed by a wine and cheese reception for the speakers.

At the end of every academic year, SISACS gives an award to an "Outstanding Undergraduate in Chemistry" during the chemistry department's honors banquet ceremony. The recipient for 2003 was Katherine Mercer, who will graduate from IU in May 2004 with a BA in chemistry and religious studies. Her undergraduate research was in the lab of Professor Ortoleva.

The SISACS was active in the planning and execution of the 2003 National Organic Symposium that was hosted at IU June 8–12. Several

members of the section participated in staffing information booths, acted as campus guides, ran various activities such as a golf outing, a 5K run, and a wine and cheese reception for invited NOS guests on June 9. We were fortunate to have good weather, an excellent list of speakers, and a superb conference.

The SISACS sponsored several TGIF wine and cheese functions throughout 2003. The functions were held in the University Club in the Indiana Memorial Union. The TGIFs have had good attendance, with about 40–50 people. We anticipate hosting monthly TGIF gatherings in 2004. Furthermore, the SISACS hosted a very popular golf scramble in June at the local IU golf course.

On Aug. 8, the SISACS helped host the annual Undergraduate Research Symposium, where more than 30 REU students and IU undergraduates presented posters on their independent research. Every year, the entire IU chemistry department gives an excellent show of support for our undergraduates, and this year was no exception.

The SISACS sponsored National Chemistry Week to enhance the public's awareness of the wonderful contributions of chemistry. Starting in 2003, NCW was celebrated during the fourth week of October (Oct. 19-25) instead of the customary November time period. This year's theme was "Earth's Atmosphere and Beyond." The annual NCW event unites ACS local sections, industries, schools, and individuals in communicating the importance of chemistry to the quality of life. NCW is a community-based program that is run by the local ACS sections. Our section offers a series of activities including chemical demonstrations, hands-on activities for kids and families, contests and games, Boy Scout merit badges, poster competitions for students from elementary school to high school, and an open house that includes tours of the Chemistry Building at Indiana University. We habitually have a strong turn out from the area schools, and many educators incorporate the NCW into their curriculum.

The SISACS has been undertaking some fundraising strategies to ensure that our local section can maintain the money necessary to pursue our chapter goals. We have been offering two different types of T-shirts highlighting "Indiana University Chemistry" that have continued to sell well. Furthermore, we are selling the beaker mugs (with no specific decal) that students love and love to give as presents. The T-shirts sell for \$12 each, and the beaker mugs sell for \$10 (350-mL) and \$12 (600-mL). Finally, we have started selling goggles *(continued on page 10)* 



David Clemmer, left, with guest lecturer Jesse Beauchamp



Guest lecturer Roberto Car, left, with new faculty member Krishnan Raghavachari



Guest lecturer Lawrence J. Marnett, left, with Milos Novotny

# **Lectures** Because of the Distinguished Lecture Series, our faculty, research associates, and students are able each year to learn first hand about the cutting-edge research of outstanding chemists from around the world. The lectures during this academic year were not exceptions.

LECTURE SERIES, SPECIAL LECTURES, & SYMPOSIA

Edwin Vedejs, Moses Gomberg Professor of Chemistry at the University of Michigan, delivered the V.J. Shiner Jr. Lecture on Oct. 2, 2002. He spoke about "Chiral Nucleophilic Catalysts." A native of Latvia who immigrated to the United States in 1950, Vedejs has received many awards and has served on many editorial boards.

"Adventures with Mass Spectrometry: From Cosmochemistry to Proteome Analysis" was the subject of the Frank T. Gucker Lecture given by Jesse Lee "Jack" Beauchamp, Mary and Charles Ferkel Chair of Chemistry, Division of Chemistry and Chemical Engineering at the California Institute of Technology, on Oct. 16, 2002. Beauchamp received the Pure Chemistry Award in 1978 and the Peter Debye Award in Physical Chemistry in 1999, both from the American Chemical Society. He was elected to the National Academy of Sciences in 1981.

Roberto Car, Department of Chemistry at Princeton Materials Institute and Department of Physics at Princeton University, gave the Distinguished Lecture in Computational Chemistry on Nov. 13, 2002. The lecture was titled "First Principles Molecular Dynamics: Achievements and Perspectives." Car has received the Hewlett-Packard Prize of the European Physical Society and the Rahman Prize of the American Physical Society.

The Harry G. Day Lecture, presented on April 23, 2003, by Lawrence J. Marnett, director of the Vanderbilt Institute of Chemical Biology, Mary Geddes Stahlman Professor of Cancer Research, professor of biochemistry, and professor of chemistry, was titled "Mining the Active Site of Cyclooxygenase-2: Discovery of New Inhibitors, Substrates, and Functions." Included in the awards Marnett has received are the Wayne State University President's Award for Excellence in Teaching, the American Cancer Society Faculty Award, and the Stanley Cohen Prize at Vanderbilt University. He is the founder and editor in chief of the ACS journal, *Chemical Research in Toxicology*.

Owe Orwar from the Department of Physical Chemistry and Microtechnology Centre, Chalmers University of Technology, Göteborg, Sweden, presented a Gill Center Lecture titled "Soft-Matter Nanofluidic and Bioelectronic Devices."



Martin Stone, left, with guest lecturer Christian Schöneich



Guest lecturer Owe Orwar

Another Gill Center Lecture, " Reactive Oxygen Species and Selective Protein Oxidation in Biological Aging and Disease: Lessons from Proteomic Studies and Physical-Organic Chemistry," was given by Christian Schöneich, Department of Pharmaceutical Chemistry at the University of Kansas. (continued on page 10) (continued from page 9)

#### Organic chemists meet at IU

In June, our department hosted the National Organic Chemistry Symposium. This biennial event sponsored by the Division of Organic Chemistry of the American Chemical Society and organized locally by Joe Gajewski and Mike Martinelli (formerly of Eli Lilly) consisted of 14 plenary lectures as well as poster sessions after the evening program. The Roger Adams Award winner, Albert Eschenmoser, who gained fame for his participation in the synthesis of vitamin  $B_{12}$ and more recently for his studies of the origin of the genetic code, gave one of the plenary lectures, speaking about his career, a career in which his studies included terpenes as well as nucleic acids. The subjects of the other plenary lectures ranged from complex organic syntheses to a mathematical description of how life must have evolved using a recently discovered reaction as a model to a possible cure for cancer.

The symposium was a great success, attracting 1,060 participants and nearly 500 posters. But the week's events were not confined completely to organic chemistry. A 5K run with more than 70 runners, a golf outing, and a dinner under tents around Showalter Fountain featuring food from Terry's and music from Pat Harbison (IU faculty member from the School of Music) added to the symposium's collegiality.

#### Another honor for David Williams

Which faculty has received more Tracy Sonneborn awards than any other? The answer is the chemists from our department, and as our chair mentioned briefly in his letter published in last year's *IU*•*Chemistry*, David Williams was the recipient for 2002.

Each year, this award is given to the faculty member who has achieved local, national, and international recognition in both teaching and research. Williams received his award and presented his lecture titled "A Fusion of Art and Science: The Natural World of Organic Chemistry" on Dec. 9, 2002, in the Indiana Memorial Union's Whittenberger Auditorium. With a masterfully chosen series of vignettes, he showed that studies of the organic chemistry of natural products reveal themes of elegance and simplicity.



David Williams

#### Symposia from 2002

Every year at least two symposia occur at about the time we are going to press. As a result, we have not provided coverage. This year for the first time, we describe the symposia from the previous year so that you, the reader, can have a better idea of the complete happenings of our department.

The 12th annual Inorganic Alumni Mini-Symposium occurred on Oct. 4, 2002. After opening remarks by Jeff Zaleski, the principal speakers were William Buhro (postdoctoral associate with Malcolm Chisholm) from Washington University; Elisa Seddon, PhD'01 (with George Christou), from Lubrizol Corp.; Hillary Eppley, PhD'96 (with George Christou), from DePauw University; Alan Cooper, PhD'98 (with Ken Caulton), from Air Products; and Gregory Hillhouse, PhD'80 (with Barry Haymore), from the University of Chicago. A dinner at Le Petit Café followed the symposium. A picnic at Hardin Ridge on Lake Monroe, a longtime tradition and a great favorite of the inorganic group and returning alumni, occurred the next day.

Sponsored by Eli Lilly, the second Annual Symposium for Excellence in Undergraduate Research took place on Sept. 28, 2002. Seven faculty members at colleges and universities from the surrounding region were honored for their contributions in their important work as research mentors who encourage undergraduate students to pursue science. Richard DiMarchi, who was then group vice president of research at Eli Lilly and who is now a professor in our department, gave the keynote address. P. Andrew Evans, who organized the symposium, was pleased with the program, stating, "This year's honorees maintained the standard of excellence established by last year's awardees. Most of us, graduate students and faculty alike, had our first research experience in undergraduate laboratories like these. It's only fitting that we recognize these faculty and the important work they do." The symposium concluded with a dinner and awards ceremony.

### Southern Indiana ACS

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in the chemistry department to offer students the ability to buy goggles when they forget or lose theirs for lab.

For the calendar year 2003, Rick Mullins is the chair, Kate Reck is the chair-elect, Tim O'Dea is the secretary, and Steve Wietstock is the treasurer. The National Chemistry Week coordinator is Jill Robinson, and Steve Wietstock remains our career services coordinator. Jeff Zaleski is our local section councilor.

— Cathrine Reck



It has been a busy year for the faculty with the successful recruitment of six new colleagues being a major focus of our effort, as you have read in the chair's letter. Of course, individual faculty members still found time to pursue their many research and teaching activities, a number of which are highlighted below.

**Don Burke** spoke at the ACS meeting in New Orleans at a symposium honoring Ian Scott, winner of the Nakanishi Award. His talk was titled "Ribozyme Engineering and Evolution." Don also chaired a session, "Sequence Evolution in the RNA World and Beyond," at the Gordon Conference on the Origins of Life.

Ken Caulton served on the NSF panel for the evaluation of proposals for CAREER grants for new faculty. This past summer Ken hosted a research scholar from Moscow State University.

In addition to his new duties as the chair, David Clemmer gave keynote lectures at the 19th LC/MS Symposium in Montreux, Switzerland, and the 16th International Mass Spectrometry Conference in Edinburgh, Scotland, on the research of his group on multidimensional separation methodologies for analysis of highly complex mixtures using gas-phase ion-mobility and mass spectrometric techniques. In addition, David was an invited speaker at the Symposium on Fundamentals of Electrospray Ionization at the March ACS meeting in New Orleans, which honored John Fenn, the 2002 Nobel laureate in chemistry. He also gave talks at Gordon Conferences on Analytical Chemistry and Biological Molecules in the Gas Phase.

A number of Jack Crandall's former graduate students assembled in Bloomington on June 9 for a belated retirement celebration. The event was organized by Stan Sojka, PhD'72, and attended by Jack Arrington, PhD'69; Tim Ayers, PhD'92; Joyce Brockwell, PhD'75; John Burks, PhD'79; Al Clark, PhD'70; Larry Crawley, PhD'73; Luan-Ho Lin, PhD'67; Don Paulson, PhD'68; Bob Seidewand, MS'69; Joe Wehlacz, MS'70; Rex Widener, PhD'77; and Tony Wiederhold, MS'03, as well as many of their spouses. The day started with a reception at Jack's place, followed by a tour of the Chemistry Building (which had changed considerably since many of the attendees had last been there), and finished up with a nice banquet at the Uptown Café, including an assortment of fine wines personally selected by Jack for the occasion. A splendid time was enjoyed by all with a lot of catching up and exchanging of old war stories. Jack really appreciated the opportunity to visit with so many of his former associates.

**Richard DiMarchi**, PhD '79 (Gurd), has begun a second stint at IU after retiring from Eli Lilly, this time as the Jack and Linda Gill Distinguished Chair in Biomolecular Science. He maintains an association with his former employer as a Visiting Lilly Scholar. Richard has founded, with Peter Schultz from Scripps, a new biotech company called Ambrx, which will focus on the discovery of biosynthetic proteins containing unnatural amino acids. Richard gave the plenary lecture, "Clinical Effects and Challenges in the Registration of Forteo," at the American Peptide Symposium.

**Bogdan Dragnea** has been awarded an NSF grant from a special biophotonics program for study of near-field optical trapping and spectroscopy of single viruses. Bogdan also contributed an article, "Chemical Imaging with Near-field Scanning Optical Microscopy," to the *Encyclopedia* of Nanoscience.

Andy Evans has been elected as a member at large to the executive committee of the Organic Division of the ACS. He was also appointed to the Board of Consulting Editors for Tetrahedron and Tetrahedron Letters. Andy delivered invited talks on aspects of his group's work on metal-catalyzed chemistry at two different Gordon Conferences; one on organic reactions and processes, the other on heterocycles.

Andrew Feig presented a paper on the use of bioinformatics and molecular visualization in undergraduate biochemistry courses at the annual meeting of Cottrell Scholars.

In addition to co-organizing the National Organic Symposium, an event we described earlier, **Joe Gajewski** also found time last year to produce the second edition of his monograph, *Hydrocarbon Thermal Isomerizations*.

Gary Hieftje was the organizer for the "Turkey Run" conference in November 2002, which brought together analytical chemistry faculty and students from Indiana and Purdue for an amicable exchange of chemistry at McCormick's Creek State Park. He also chaired a symposium titled "New Capabilities and Instrumentation in Plasma-Source Mass Spectrometry" at the 2003 Pittsburgh Conference in Orlando. Plenary lectures were delivered by Gary at the European Conference on Analytical Chemistry in Dortmund, Germany, and the Beijing Conference and Exposition on Instrumental Analysis. Gary continues to serve on the review committee for the Chemistry Division at Los Alamos National Laboratory.

Martin Jarrold organized a Gordon Conference in July on biological molecules in the gas phase. He was selected to present a series of Conférences de Troisième Cycle en Chimie at several Swiss universities. In addition, Martin gave a plenary lecture at the 11th International Symposium on Small Particles and Inorganic Clusters in Strasbourg, France.

**Jeff Johnston** had a busy summer during which he presented three invited talks describing ongoing synthetic projects in his group at separate

### **Faculty news**

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Gordon Conferences on free radicals, organic reactions and processes, and natural products. Jeff was also selected to participate in the NSF Workshop on Organic Synthesis and Natural Products and the Procter and Gamble Pharmaceuticals Colloquium on Organic Chemistry.

Dan Mindiola has started his independent research career impressively with five articles accepted for publication during his first year at IU. In addition, Dan was one of only three individuals selected to give oral presentations of their posters at the Gordon Conference on organometallic chemistry. Dan, who was a Ford Foundation Minority Postdoctoral Fellow before coming to IU, gave a presentation sponsored by the Ford Foundation in Puerto Rico that aimed at encouraging minority students into careers in the physical sciences.

In September, **Mike Montgomery** was an invited speaker at the Fifth International Symposium on Crystalline Metals, Superconductors, and Ferromagnets at Port-Bourgenay, France, where he spoke on the synthesis of a novel synthetic metal/superconductor precursor.

As usual, Milos Novotny was invited to discuss the work of his research group in a number of lectures at meetings around the world, including the International Symposium on Capillary Electroseparation in Helsinki, Finland; the Biochemistry Centenary Symposium on Signaling the Future in Liverpool, England; the High Performance Capillary Electrophoresis International Symposium in San Diego; the 26th International Symposium on Capillary Chromatography and Electrophoresis in Las Vegas; and the 28th International Ethological Conference in Florianopolis, Brazil; as well as at the New York ACS meeting. His paper in Chemical Reviews, titled "Structural Investigations of Glycoconjugates at High Sensitivity," was designated as an Editor's Choice article.

**Dennis Peters** presented two invited papers on his work on transition-metal complexes as catalysts in organic electrochemistry at the May meeting of the Electrochemical Society in Paris, France. At this same meeting, Dennis was elected to serve a two-year term as the chair of the Organic and Biological Electrochemical Division of the society. Dennis gave a related invited talk at the ACS meeting in New York in September.

Krishnan Raghavachari gave a series of invited lectures on his research in quantum chemistry in Taiwan last December as well as talks at the Indian Institute of Technology, Madras, India, and the Center for Atomic Research, Kalpakkam, India, in March. He presented papers at a workshop titled "Grand Challenges in Modeling the Assembly and Properties of Nanomaterials" at Argonne National Labs and at the conference of Foundations of Molecular Modeling and Simulation in Keystone, Colo., in addition to two invited talks at the New Orleans ACS meeting.

Kate Reck participated in an interesting project

last fall when she recreated six of Issac Newton's experiments from his original notebooks for inclusion in a television production aired by BBC in Britain last June, titled *Newton: The Dark Heretic*. NOVA is scheduled to present a revised program later this year.

Jim Reilly continues to direct work in proteomics, which has generated several patents concerned with mass spectrometric techniques for biomolecules.

John Richardson officially retired at the end of the past academic year, although he and Lislott are spending this year in the lab finishing up a last project. John continues to serve on the editorial board of the *Journal of Biological Chemistry*, and he recently published an invited minireview, "Rho factor," in *Cell* that summarizes of much of the work of his lab during the past 30 years.

Romualdo de Souza was designated as a 2003 SBC Fellow for his pioneering use of teaching and learning technologies. This award supported a summer workshop on the application of his CALM computer-assisted quiz program in high school courses. Romualdo was also coordinator of a session on silicon strip detectors at the Workshop for Experimental Equipment for the Rare Isotope Accelerator held at Oak Ridge, Tenn.

Vic Viola presented a plenary lecture at the International Conference on Nucleus-Nucleus Collisions in Moscow, Russia, and served on the organizing committee for the Heavy-Ion Conference '03 in Montreal, Canada. Vic also recently completed a chapter on nuclear reactions for the *Handbook of Nuclear Chemistry*.

Ted Widlanski has been appointed for another year as the associate dean of the College for Science and Research.

**Gary Wiggins** is chairing the American Chemical Society Joint Board-Council Committee on Chemical Abstract Services in 2003. He also received the Meritorious Service Award of the ACS Division of Chemical Information at the fall 2003 ACS meeting.

David Williams continues to lead his research group in their efforts directed toward the total synthesis of natural products, with notable recent completions of the syntheses of leucascandrolide and phorboxazole. We have already described Dave's recent Sonneborn lecture. In addition to a number of talks at universities and pharmaceutical companies, Dave gave an invited lecture at the IUPAC Symposium on Stereoselective Organic Synthesis in Ottawa, Canada.

Jeff Zaleski delivered an invited lecture in a session titled "Metals in Medicine" at the 35th International Conference on Coordination Chemistry in Heidelberg, Germany, last summer. This year, Jeff is hosting a German exchange student from Freiburg in his lab.

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## FACULTY & STAFF PROFILES: Vernon 'Jack' Shiner

Jack Shiner retired only recently, but he came to IU in 1952, when the faculty size was around 20 and was struggling to develop a strong research presence. Jack had just finished a year of independent research nominally under the guidance of Paul Bartlett at Harvard, and in a short period of time he became well known for his contributions to physical organic chemistry utilizing deuterium isotope effects.

In 1962, Jack became chair and began writing a proposal that would further solidify enormous research gains at IU over that period. By 1966, the faculty size was nearly 45, including administrators like Ward Schaap and Lynn Merritt, who spent most of their time at Bryan Hall. At that time, IU's research reputation had developed so that it was rated 15-20 in the country, judging by publications and grant income. What Jack and other members of the chemistry department and the physics department did was to write a proposal for a "Centers of Excellence" grant. This grant provided for the development of the IU Cyclotron Facility and for expanded hiring of faculty and staff in chemistry for a five-year period. The NSF provided \$5 million and the university was to pick up the salaries after five years. Unlike some other universities receiving this type of grant, IU fulfilled its promise. This is one of the reasons that IU's Department of Chemistry enjoys such strong support in the machine, electrical, computer, and glass shop even today.

Jack's administrative efforts extended to the Office of the Dean of the College of Arts and Sciences. He began in that position during the recession of 1973, a particularly difficult time for U.S. universities. His efforts helped preserve the very strong international reputations of not only the chemistry department, but also the English, German, psychology, and biology departments. The latter was particularly noteworthy because four different departments in Jordan Hall were combined into the current biology department during Jack's tenure. Characteristic of Jack's deep analytical sense was his statement at the time: "What you do in Hard Times is more important than what you do in Good Times."

In 1982, Jack was recruited again to be chemistry department chair when plans for a \$40 million renovation of the Chemistry Physical Plant were to be executed. Jack oversaw the building of the south and east additions, the renovation of the '64 annex, and the renovation of the original chemistry building. Among the many concerns during that effort was the air handling system, which was new for academic buildings, although more or less standard for new industrial labs. A modest, but relatively new, innovation was an ethyleneglycol heat recovery system to increase efficiency.



These unselfish efforts were not Jack's only contribution to IU chemistry. His research group, while never large by synthetic chemistry standards, was productive and important in their impact. Hyperconjugation as a stabilizing force for cations received its confirmation in Jack's lab. The characterization of solvolysis reactions, particularly the sequence of formation of intimate, then solventseparated, then free ions was also confirmed and delineated for particular systems in Jack's lab. The calculation of isotope fractionation factors and the recognition that solvent isotope effects could be characterized by changes in vibrational frequencies due to hydrogen bonding came out of Jack's lab. It is particularly significant that one of Jack's students, Brown Murr, who when he began his independent research career at Johns Hopkins, utilized deuterium kinetic isotope effects to show that solvolytic generation of the 2-norbornyl cation occurred with participation by the beta C-C bond. That is, he showed that the cation was nonclassical, thereby settling an important question in the '60s and '70s, long before the development of NMR and theoretical techniques that ultimately provided the same answer. One need only attend the Gordon Conference on isotope effects to witness the enormous esteem in which Jack's scholarly efforts are held. But Jack's scientific interests go well beyond isotope effects. Those of us privileged to know him over the years have profited from his many penetrating questions to seminar speakers in diverse areas of chemistry.

In addition to his scholarly and administrative activities, Jack lent his expertise to the American (continued on page 14) Vernon "Jack" Shiner

If Harry Day was the heart of chemistry, then surely Jack Shiner was its head.

\*

### Shiner

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Joe Gajewski has described Vernon 'Jack' Shiner to me as a scholar, administrator, teacher, sports car enthusiast, gentleman farmer, and patron of the arts. I concur heartily, but I hasten to add one more word of description: insightful — he hired me! - RUPERT WENTWORTH

\*

Chemical Society, serving on the Committee for Science (and for one year as its chair) and on the Human Rights and Scientific Freedom subcommittee for the International Affairs Committee, whose chair is Zafra Lehrman of Columbia College of Chicago. Zafra, Jack, and others have collaborated on a new approach to teaching non-science majors chemistry. Zafra pioneered the integration of chemistry and the arts because her college specializes in the latter. On a few occasions, she brought a group of her students to IU to demonstrate their projects, which included a dance of the elements and interesting TV/chemistry combinations. Of all the interactions with Jack, Zafra remembers the time their van transporting students to IU broke down and Jack's willingness to drop all and become their "savior."

Jack's coming to IU had more than the usual number of twists and turns. As a student at Texas Western College of Mining (now UTEP), he developed an interest in organic chemistry, but World War II intervened. After a one-year training period as a radar technician that took him to Chicago, then to Oklahoma, then to Washington, D.C., he finished the war in the Pacific on a destroyer that he helped commission. After finishing his bachelor's degree in another semester, he went to Cornell University, where before the fall semester started he worked at the Agricultural Experiment Station in Geneva, making long chain hydrocarbons to compare with mineral oil used as insecticidal pre-emergent sprays for fruit trees. His PhD work with John R. Johnson revealed the structure of the ketene dimer, a study that involved addition of deuterio methanol to ascertain where the proton added, which then could provide information on the structure. Students might recognize that this was before NMR spectrometers were developed, so analysis for deuterium was particularly difficult (think gradient density techniques). It was here that his interest in isotope effects developed, and they matured in a postdoctoral with Sir Christopher Ingold at the University College London and later as a senior postdoctoral fellow in the Bartlett Laboratory.

Jack returned to London on sabbatical twice and was a frequent visitor not only to the United Kingdom, but to the continent as well. He did bring back an early silver E-type (a Jaguar XKE for the non-aficionados of sports cars), a legendary six-cylinder, three-carburetor, beautifully aerodynamic machine that could cruise at 140 mph. Ernie Campaigne swore he would never again accept a ride from Jack after a very fast trip to northern Indiana. Jack recently restored the car, and it sits almost like a museum piece in his garage, although it still occasionally sees the light of day and meets the concrete of the road.

But Jack has a somewhat more sedate side. Those driving Arlington Road between Bloomington and Ellettsville can catch a glimpse of Jack working in a very large garden or tending to fruit trees. Judy Harmony tells of stopping at Jack's place on a Sunday drive and seeing the dean in overalls, which removed him from the ranks of the officious, in her mind. At Jack's side through these many years has been his wife, Reva, who as a dancer in former years has been a patron of the Bloomington Playwrights Project and has contributed an award for writers. Her hospitality, good will, and *joie de vivre* have been enjoyed by many in the Bloomington community.

Finally, as famous as Jack is for his many efforts, he will not surpass the fame of the brew named for a small town in east Texas that bears the family name. Shiner Bock Beer is a Texas staple.

— Joe Gajewski

### **Faculty news**

#### (continued from page 12)

A number of professors emeriti have also been involved in noteworthy activities over the past year. **Frank Gurd** has forwarded from Albuquerque an article in *Biophysical Chemistry* 

— co-authored with Fred Richards — that provides a special perspective on the career of their mentor, John Edsall. Marvin Carmack has relocated from Arizona back to Bloomington, where he is a lively participant in many departmental and university social functions. A reception honoring **Ed Bair** took place on the occasion of the dedication of the Edward J. Bair Mechanical Instrument Services facility last December. During a series of lectures on ice physics in Fairbanks, Alaska, last December, **George Ewing** had the misfortune to be in an automobile accident involving a moose, but he has recovered from this incident and is back at work in the lab, doing NSF-sponsored research on the properties of thin-film water and ice. **Lee Todd** recently completed the construction of a fully functional laboratory on his farm in Monroe County, where he plans to pursue some new research ideas.

**Evelyn Jabri** has left IU to become an assistant editor for *Nature Structural Biology*. **Joe Zwanziger** has relocated to Dalhousie University in Nova Scotia.

— Jack Crandall



PROFILE: Charlie Parmenter

### Another side of Charlie Parmenter

Like a fine gem, Charlie Parmenter has many facets. Teacher, researcher, father, and grandfather are a few that are obvious, but how many know of his passion for photography? Charlie has been recording the life around him for a long time, including poignant scenes in Germany nearly 50 years ago and, more recently, the gaiety of his grandchildren. All of his work is striking, but here are three photos, out of several thousand, that I find really appealing. I hope you enjoy them too.

— Rupert Wentworth





# profile: John Huffman

# Making crystallography easier and better

Ever affable with an infectious laugh and rapidfire speech, John Huffman has graced our department for 45 years, as an undergraduate student, a graduate student, and more recently as director of the department's Molecular Structure Center. I am happy to write about John as paltry payment for the many times that his crystallography gave structural answers to my graduate students and me, answers for which we had sometimes not yet formulated the correct questions.

For anyone from our department who has been associated with the syntheses of new compounds, John Huffman has often been the last arbiter when we want a molecule's structure, especially when all other spectroscopic techniques failed to point to that structure.

And it was in his role of last arbiter that I first became acquainted with John: I had given Bill Streib, a professor and crystallographer in our department, a crystal whose analysis indicated it was [Ni(cis,cis-1,3,5-triaminocyclohexane),2](NO<sub>3</sub>),2. I



John Huffman

hoped that ligational energies were great enough to force the triamine ligands out of their natural equatorial conformation into an axial conformation, allowing the amine groups to coordinate to the metal ion on the trigonal faces of an octahedron. While the compound's electronic spectrum supported my hope, the spectrum could hardly be regarded as proof of structure. Bill gave the crystal to John, who at that time was a graduate student. Working with Bill and Rick Jackson, another graduate student, John found the crystal's space group was C2/m with the metal at the origin. A Patterson map quickly revealed the image of the molecular ion, showing that its structure was exactly what I had hoped. Because solving the structure was so easy, John concluded (erroneously) that crystallography was an easy exercise requiring no thinking. Of course, he has faced many crystallographic challenges requiring serious thought since then.

Before he faced those challenges, however, John was born and raised in Kokomo, Ind., attending Kokomo High School. He received his BS in chemistry from IU, his master's degree from Jerry Schmidt in this department, and his PhD while working under the tutelage of Bill Streib. John was appointed director of the department's Molecular Structure Center in 1974.

Although he and his colleagues have solved the structures of thousands of compounds, all of them intriguing according to John, he has always been interested in doing crystallography better. In fact, he has a simple rule based on this interest: Spend half of the time doing crystallography and spend the other half figuring out how to do it easier and better. He says the rule has been invaluable. My own quick look around the IUMSC's laboratories showed me all kinds of equipment, computers, and diffractometers, all dedicated to making the IUMSC's crystallography easier and better.

When I began to give crystals to John many years ago, the most dreaded words I could hear were, "We can't solve the structure because the crystal is twinned," or "We can't do it because the crystal is split." Those seeking John's services today are not likely to hear those words of defeat because John has made his crystallography easier and better. To prove his ever-increasing prowess to himself, he once put five different crystals together in the same X-ray beam, decided which spots went with which crystal, and then solved each of the structures.

John's wife, Caroline, has also solved crystal structures for me and others, and we are everlastingly grateful, but the family involvement does not end there. His son, named John like his father, has also contributed to the success of the IUMSC. When he was a student at Purdue, he constructed the IUMSC's first Web site, and while he was doing it, he devised a method for feeding in a molecule's crystallographic coordinates, and then converting them to Cartesian coordinates so that he could rotate the molecule to any desired orientation. His method was unique enough to lead to father and son presenting an invited paper and workshop at the 1996 meeting of the International Union of Crystallography in Seattle. As if that were not enough good fortune, John the son also met his future wife at that meeting.

The IUMSC's Web site at www.iumsc.indiana.edu has continued to evolve since its inception. A lot of information can be found there. For example, *(continued on page 17)* 



#### Annual awards honor staff

This year, once again, one of our staff members, Stacy Felton, was a recipient of the University Outstanding Staff Award. She was one of two support staff honored for her meritorious service at a university-wide reception in December. This was held in the Frangipani Room at the Indiana Memorial Union and was hosted by IU Bloomington Chancellor Sharon Brehm, who spoke of Stacy's accomplishments. Gary Fleener was the recipient of the department's Outstanding Staff Award, which was presented at the Annual Staff Reception held in April at the Tudor Room. Gary's meritorious service was acknowledged by several faculty and his former supervisor, John Dorsett. Additionally, we honored 11 staff for their IU anniversaries: 10 years - Alice Dobie-Galuska (coordinator of undergraduate services), Brian Ferguson (research machinist III), Becky Hanson (coordinator of administrative computing), and Judi Roberts (administrative secretary to the chair); 15 years - John Poehlman (manager of the electronic instrument services) and Amy Van Pelt (manager of chemistry business); 20 years - Brian Crouch (manager of information technology) and Stacy Felton (research secretary to professors Williams and Johnston); 25 years — Delbert Allgood (research machinist III); 30 years - Judy Crandall (personnel and grants manager); and 35 years - Don Chatten (lab prep coordinator for the organic teaching labs).

#### Secretarial changes

Jeanette Ash left the department in January and relocated in Columbus, Ohio, to catch up with her husband, Jason. Jason transferred to Ohio State University's chemistry graduate program. Jeanette had been in the department for a little over two years, first in the business office and later in technical services as their office services assistant. Nicholas Parfitt picked up some of Jeanette's former responsibilities as an hourly assistant for ITG, EIS, and MIS. Nicholas is a third-year computer information systems student who recently moved here from South Africa.

**Bill Unrue** joined us in February as research secretary to professors Burke, Oakley, Richardson, and Stone, replacing **Tanya Kinnick**. Bill is a chemistry major who has a wide variety of experience, including work as a lab technician and medical transcription processor.

Jennifer Kelley left her position in May as research secretary for professors Caulton, Mindiola, and Zaleski for a wonderful opportunity in HPER's public health master's program. She was offered an assistantship and paid internship. Jackie Chandler joined us in June, replacing Jennifer. She had just completed her bachelor's degree in chemistry from Hanover College and had relocated to Bloomington. Jackie had worked previously as a bank teller, a teacher, and a tutor to calculus students. Among her other skills, she also holds a minor in math.

Judy Summerville retired from the university in August to pursue her practice in oriental medicine. She has been asked to take a position as head acupuncturist at a clinic in South Bend, Ind., as well as to take over a holistic practice of a colleague in Columbus, Ind. Judy will also be starting her own practice in Bloomington. She continues to teach for Indiana University Bloomington. Judy previously had a career in opera and as a weaver and designer; we wish her the best with this new career opportunity. Becky **Baugh** returned to the department in September, replacing Judy as scheduling officer. Becky has had a good deal of IU experience, having received an optometric technology degree as a student, as well as working in the registrar's office, the chemistry undergraduate office, the School of Optometry, and more recently the Department of Theatre and Drama. Becky gained very relevant experience from her former position in the chemistry undergraduate office, as well from her previous position where she served as the scheduling officer for the Department of Theatre and Drama.

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### Huffman

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you can take a visual tour of the laboratory and offices. You will also find that the projects of principal current interest to John are (a) structure analysis, as you would expect, (b) remote access to instrumentation, allowing continuous monitoring of work in progress in the IUMSC's laboratory and eventually allowing access to synchrotron and neutron sources at other sites, (c) the reciprocal net, a project still under development that is used by research crystallographers to store molecular structure information that is generally available to the public, (d) analysis and visualization of instrument-driven data, a venture that will be used for storage and preliminary analysis of crystallographic data from local instruments as well as those located elsewhere, and (e) molecular visualization, a joint project with the Advanced Visualization Laboratory and the School of Informatics with a current goal to develop a series of scalable graphics that can be used for molecular visualization. The Web site also lists the IUMSC's personnel and their interests. For example, you will find that one of John's hobbies is gardening, and some excellent views of his garden are available. Unexpectedly, you will also learn about whistle pigs and you will hear their call.

John is not only a great crystallographer and gardener. He is also adjunct professor of informatics and director of the Informatics Research Institute. When I asked him about the relationship between crystallography and informatics, his answer was immediate and to the point. Crystallography, he said, *is* informatics. After all, informatics concerns the organization of information so that it is useful. Similarly, a crystallographer collects raw crystal data, massages it, obtains trial structures so that they can be visualized, and then organizes the information into databases so that it can be accessed.

John's eyes really lit up as he described his relationship to informatics, clearly indicating a subject of profound importance to him and leading me to believe that he is thinking of ways of making that relationship easier and better.

- Rupert Wentworth

### CHEMICAL INFORMATICS



The chemical informatics program took a giant leap forward this year with the hiring of Mu-Hyun "Mookie" Baik, who holds a two-thirds appointment in informatics and one-third in chemistry. Five students are enrolled at IUB in the School of Informatics MS in chemical informatics program. They are Jason Gretencord, Ryan Lauer, Leah Sandvoss, Kenrick Vidale, and Jianyong (Jay) Zhu. Kenrick held the \$15,000 Daylight Chemical Information Systems "Daylight Innovation in Chemical Informatics Fellowship" last year, and Jay is the 2003-04 recipient. Jason Gretencord is working with the Columbus, Ohio, firm Leadscope Inc. on an internship project this fall.

— Gary Wiggins

With the addition of six new faculty this fall, we hired two new research secretaries. Jennifer Julian joined Professor DiMarchi as his research secretary in September. She had relocated to Bloomington with her husband, Ryan, who joined Professor Clemmer's group as a postdoctoral fellow. Jennifer had worked the past two years in a similar capacity as a staff secretary/administrator at the NASA Jet Propulsion Laboratory run by Caltech. Prior to that she worked in two other academic institutions, handling a variety of responsibilities. Jennifer also completed her bachelor's in business administration recently. Angie Monts has taken a half-time position as research secretary to professors Iyengar, Caroline and Martin Jarrold, and Raghavachari. Angie previously worked in the Department of the History and Philosophy of Science as a senior faculty secretary. She also worked previously at the Monroe County Public Library and with the Bloomington Ambulance Service as the operation's coordinator. She left her position as a unit coordinator at the Bloomington Hospital to join us in September.

#### **Technical changes**

We are pleased for the new opportunity that **Doug Garvin** assumed in January as a research machinist apprentice in the Edward J. Bair Mechanical Instrument Center. This was a new position, created by the growing need in that service. Doug had provided the department with 18 years of excellent support as our shipping and receiving clerk and assisted in many other capacities within the department. We were pleased to welcome **Rick Hackler** to the department as Doug's replacement as shipping and receiving clerk. Rick also had many years of IU service from the Halls Food Service as a meat cutter and supervisor. Rick



Many personnel changes occurred in the Chemistry Library during the last year. **Gary Wiggins** transferred to the School of Informatics, and **Roger Beckman** returned to the Chemistry Library as interim head on July 1. Roger had been the assistant head of the Chemistry Library from August 1988 until he became head of the Life Sciences Library in early 1999. Jen Gerber resigned her position as campus library coordinator in July, and Justin Gardner replaced her on Sept. 1. Elizabeth Hanson, who had served as the science reference/instruction librarian for all of the IUB science libraries, was based in the Chemistry Library during the four years when Gary Wiggins had the additional duty of coordinator of the IUB Science Libraries. She will move to a new position in the library system.

Wendie Shreve completed the chemical information specialist program in the School of Library and Information Sciences and accepted a job with Eli Lilly. Hong Zhang, who worked in the Chemistry Library, is now a bioinformatics programmer at the Dana-Farber Cancer Institute, Harvard Medical School. Alison Rollins is the new SLIS graduate assistant in the Chemistry Library. Another SLIS student, Allison Tipton, also worked in the library during the 2002–03 academic year.

— Gary Wiggins

also is a bluegrass musician. He plays a banjo and dobro (resophonic guitar) and plays informally with the Stone Hill Bluegrass Band.

In March, **Scott Harrington** took the position of computer service technician, vacated by Denis Taaffe, who left to pursue his music career. Scott worked on an hourly basis in our ITG group for nearly two years, providing technical support and assisting students and staff with hardware, software, and security repairs. He has an associate's degree in applied science with a microcomputer subspecialty from Ivy Tech. He has a diverse background, including many years in the Navy and as an EMT instructor/administrator.

Jennifer Takach joined our staff in May as research technician in Proferssor Feig's laboratory. Jennifer did undergraduate research with him her senior year and completed her BS in biochemistry just prior to joining the department. She studied abroad at Adelaide University in Adelaide, Australia, from February to August 2002 and had considerable research experience at Eli Lilly in the summer of 2001 and again in the winter of 2002. In addition to these wonderful research opportunities, Jennifer has also received numerous awards and honors during her undergraduate career.

In July, **Matt Nance** joined us in a new position in the undergraduate office as demonstration technician. Matt will assist instructors with lecture demonstrations, develop new demonstrations, and test new experiments for the laboratory. Matt earned a BS in chemistry in 2001 from IU and a master's in education, also from IU, in 2002. As an undergraduate, Matt was a student in the honors chemistry courses, a member of Alpha Chi Sigma, and an associate instructor. Through his teaching experience, he is already familiar with many lecture demonstrations as well as the logistical issues associated with running a teaching laboratory.

The **undergraduate office** was reorganized, resulting in reassignment of duties and one new position, held by Matt Nance.

In closing, I regret to report the passing of a former staff member, Loyd Hudson. Loyd had a weakened immune system from a condition that he described as a precursor of leukemia, and he developed pneumonia in May. Loyd joined the chemistry department after having several other career opportunities, most in the field of music. He had a PhD in choral conducting from IU and was a faculty member and chair of the School of Music for a period at the University of North Carolina at Wilmington, and he taught English in high school for several years in Iowa. He returned to Bloomington in his later years and eventually joined the chemistry department, where he worked in the business office in different capacities over a 12-year period. Loyd officially retired from his staff position in 1992 and continued to work on an hourly basis for eight years.

# Gary Wiggins moves to School of Informatics

fter nearly 30 years and "with mixed emotions," Gary Wiggins is leaving the IU Libraries to transfer to a full-time position in the School of Informatics. He will continue as director of the program in chemical informatics, a position he has held part time for three years, and will also be interim director of the program in bioinformatics.

"There is a knot in my throat," says Gary, "as I think about the end of my formal affiliation with the IU Libraries, where I have worked in one capacity or another most of the time since 1963. This will always be a special place for me."

Gary, however, is energized by the prospect of being able to devote much more time to the development of the bioinformat-

ics and chemical informatics programs and to continue to have a role in building the School of Informatics. "It means a great deal to me to be able to help finish the job we have started in informatics," he says.

"Gary has been an invaluable member of the IUB Libraries," says Suzanne Thorin, Ruth Lilly University Dean of University Libraries and associate vice president for digital library development. "Gary's innate intelligence, his seasoned insight and commitment to integrity, his research and teaching skills, his perseverance and pursuit of high standards, his love of wisdom and fun, and his thoughtful, fair treatment of others ... [are] characteristics of the person we recognize as a leader."

"It has been my personal pleasure to have worked closely with Gary, particularly in the past few years," Thorin says, "and I wish him every success in this wonderful opportunity."

Wiggins' contributions as a librarian have been strongly shaped by his scholarly pursuits in the fields of library and information science, chemistry, and more recently informatics. He has been an active member of

AAUP and a leader in library governance and faculty issues. In addition to being head of the Chemistry Library and coordinator of the Sciences Libraries, Gary teaches chemical information courses in the IU Department of Chemistry and directs a joint program to train chemical information specialists in the School of Library and Information Sciences.

He is the author of the book *Chemical Information Sources* (McGraw-Hill, 1991) and has written a number of articles in scholarly journals. Gary is the list owner of the Chemical Information Sources Discussion List, which has more than 1,400 subscribers worldwide. He also directs the Joint Special Libraries Association/American Chemical Society Clearinghouse for Chemical Information Instructional Materials and maintains a Web guide to Internet and other chemistry resources. Gary is

a former chair of the Special Libraries Association Chemistry Division and of the American Chemical Society Division of Chemical Information.

In 1998, he was recognized with CINF's highest award, the Herman Skilnik Award for outstanding contributions in the field of chemical information, and in 2003 he will receive their meritorious service award. At IU, he has received the William Evans Jenkins Award, the W. George Pinnell Service Award, and the SLIS Distinguished Alumni Award.

Gary holds a BA in chemistry and Russian, an MA in Slavic languages and literature, and MLS and PhD degrees in library and information sciences. He began his library career at the IUB



#### Gary Wiggins

Libraries as a student in the Documents (Government Publications) Department, 1963–69, later as an intern in the Chemistry Library, 1969–70, and then as a science cataloger, 1970–71. He strayed briefly from the IU fold from 1972 to 1975, when he was employed by the University of Illinois at Urbana-Champaign Libraries as the Slavic acquisitions librarian and director of the Doris Duke Slavic Reading Room. He returned to IUB Chemistry Library in 1976.

Roger Beckman, head of the Life Science Library, has agreed to serve as the interim, part-time head of the Chemistry Library until Wiggins's replacement can be hired.

— From the office of Suzanne Thorin



During the 2002–03 school year, Professor Jeffrey M. Zaleski was director of graduate studies. Serving with him on the Standards Committee were professors Kenneth G. Caulton, Gary M. Hieftje, Lawrence K. Montgomery, Martha G. Oakley, and Charles S. Parmenter.

The Graduate Admissions Committee was chaired by **P. Andrew Evans**. Evaluating the hundreds of dossiers submitted to the department were professors **Bogdan G. Dragnea**, **Martin F. Jarrold**, **Andrew L. Feig, Gary M. Hieftje, Evelyn Jabri, Jeffrey N. Johnston, Dennis G. Peters, Daniel J. Mindiola**, and **Jeffrey M. Zaleski**.

#### Award winners

Gerardo Gamez was awarded the 2003 Kirkbright Bursary Award. The Association of British Spectroscopists gives this very prestigious award. He obtained a BS in 1999 from the University of Texas at El Paso with a major in chemistry and a minor in biology. He started his graduate research at Indiana University in 2000 with Gary Hieftje, Distinguished Professor and Robert and Marjorie Mann Chair. His present research involves the fundamental study of plasmas that are routinely used in analytical spectrochemistry, such as the inductively coupled plasma and glow discharge, through laser scattering, laser induced fluorescence, and emission based techniques.

Aurora E. Clark was awarded the Kraft Fellowship. She completed her undergraduate education at Central Washington University in 1999, where she received a BS degree in chemistry. While at Central Washington University, she was involved in undergraduate research under the guidance of JoAnn DeLuca and aided in the development of a strategy for carbene generation using phenyliodonium ylides. She started her graduate research at Indiana University in 1999 with Distinguished Professor Ernest R. Davidson and Professor Jeffrey M. Zaleski. Her initial research efforts were directed toward the use of electronic structure codes to elucidate the mechanisms of thermally and photochemically induced Bergman cyclization of enediynes and metalloenediynes. These studies led to the definition of new quantum chemical operators that may be applied to such systems and result in the calculation of new molecular properties such as  $S_A$  and  $S_A S_B$  found in the Heisenberg Hamiltonian. She completed her PhD degree in April.

The Eli Lilly Fellowship in Analytical Chemistry was awarded to Danielle M. Goken. She earned a bachelor's of science degree in chemistry at Northern Illinois University in 1999. Under the auspices of Presidential Teaching Professor Chhiu-Tsu Lin at Northern Illinois University, she prepared and tested various sol gel samples to ascertain the optimum conditions for encapsulation of divalent europium cations into optically transparent xerogels. She has worked in Herman T. Briscoe Professor Dennis G. Peters's laboratory since becoming a graduate student at Indiana University in 1999. Her initial research focused on synthesizing [2,2'-([2,2'-bipyridine]-6,6'divl)bis[phenolato]-N,N',O,O']nickel(II). She determined that reduction of this compound in the presence of alkyl halides results in a short-lived catalytic cycle in which carbon-halogen bonds are broken and the nickel-containing catalyst is subsequently destroyed in follow-up reactions with alkyl radicals. She continues to study the fate of various transition metal-containing catalysts during indirect reduction of halogenated organic compounds in an ongoing effort to design better electrochemical catalysts.

Rajesh Viswanathan was the recipient of the Lubrizol Fellowship. He received a MS degree in



Rajesh Viswanathan

chemistry from the Indian Institute of Technology, Kanpur, India. He began his graduate studies at Indiana University in the fall of 1999, under the direction of Assistant Professor Jeffrey N. Johnston. His research in the Johnston group has focused on the

development of free radical-mediated aryl amination reactions. After establishing the scope of this reaction, he developed it as part of an asymmetric synthesis of indoline  $\alpha$ -amino acids. This synthetic study also led to the discovery of the cyclopentenyl carbinyl radical isomerization. His current efforts are devoted to the total synthesis of ambiquine G, an indole natural product, using free radical-mediated aryl amination as a strategic method.

The Procter & Gamble Fellowship was awarded to Lori A. Watson. She graduated from the University of Kentucky in 1999 with a BS degree

in chemistry. She is currently a doctoral candidate at Indiana University in the labs of Distinguished Professor Kenneth Caulton. Her research interests include the experimental and computational exploration of unsaturated transition metal species. Currently, she is examining the



Lori Watson

structure and reactivity of ruthenium complexes containing a particularly reducing pincer ligand. She is also working on collaboration with the group of Professor P. Andrew Evans to elucidate the active catalytic species and its mechanism of reaction in the recently discovered regioselective rhodium-catalyzed allylic substitution reactions.

**David K. Leahy** was the recipient of the E.M. Kratz Fellowship (endowed by Mr. and Mrs. W.W. Gasser Jr.). He received a BS degree in chemistry from Lebanon Valley College in 1998. Following



his graduate studies at the University of Delaware under the direction of Professor P. Andrew Evans. He moved with Evans to Indiana University in the spring of 2001 to complete his PhD in organic chemistry. His research in the Evans group has

graduation he began

David Leahy

focused on expanding the scope of the regio- and enantiospecific rhodium-catalyzed allylic alkylation reaction to new nucleophiles including phenols, copper(I) alkoxides, and copper enolates. He is also working on the total synthesis of the PAF antagonist kadsurenone, as well as the potent antitumor antibiotic fredericamycin A.

The Richard Slagle Fellowship was awarded to **David C. Johnson**. He received a BS in chemistry from Baldwin-Wallace College in 1999. In the fall of that year he started graduate school



at Indiana University in the Department of Chemistry. Under the direction of Professor Theodore Widlanski, he is currently working on the synthesis of dinucleosides containing non-hydrolyzable phosphate-diester mimics. Such molecules may have potential application as antiangiogenesis agents

David C. Johnson

(cancer therapeutics). The *N*-acyl sulfonamide, sulfonimide, and imide functional groups have been selected as the target phosphate-diester mimics. Methodology for the incorporation of these functional groups onto nucleoside scaffolds has been and continues to be a goal of this research. Concurrent with this project, he is also investigating new synthetic methods for the construction of di- and triphosphate-monoesters. The goal of this project is to access nucleoside di- and triphosphates as well as sugar di- and tri-phosphates non-enzymatically in high-yield.

The Merck Analytical/Physical Fellowship was awarded to Robert T. Hart. He received a BS degree in chemistry from the University of Wisconsin-Madison in 1999. He started graduate school at Indiana University in 1999 under the direction of Professor Josef W. Zwanziger. His research in the Zwanziger group has focused on a class of glass ceramics that show optical second harmonic generation, which may become important in waveguides and telecommunication. The design of such devices relies on predictive models of their optical coefficients. This research involves experimentally measuring structural parameters by solid-state NMR and Raman spectroscopy, as well as neutron and X-ray scattering. These data are used to generate structural models that can offer the ability to make predictions towards material optimization.

Two students held National Science Foundation Fellowships. Jennifer M. Kindy, who received a BS in chemistry from Wake Forest University, is a student of Robert and Marjorie Mann Professor David E. Clemmer. Lori A. Watson, a graduate of the University of Kentucky with a BS in chemistry, is a fourth-year student of Distinguished Professor Kenneth G. Caulton. The Department of Chemistry had been selected by the U.S. Department of Education to participate in the Graduate Assistance in Areas of National Need Fellowship Program. Last year, a GANN fellowship was awarded to **Richard Beardsley**, who is working with Professor James Reilly.

Other fellowship recipients were Parichatr Vanalabhpatana, Anandhamahidol Foundation Scholarship; George Chee-Yuen Chan, Croucher Foundation Scholarship; Gerardo Gamez, Dean's Fellowships; Thaddeus Jones, Mays Fellowship; William J. Andrews, James C. Klein, Amy N. Walstrom, and Christopher S. Weitzel, Paget Fellowships; Vanvimon Saksmerprome, Royal Thai Government Fellowship; and Amy L. Rosen and Lori A. Watson, Women in Science Fellowships.

Research and University Graduate School Fellowships were awarded to: William R. Alley, William J. Andrews, Brad C. Bailey, William C. Broshears, Jesse D. Carrick, Chao Chen, Jianmiao Fan, James C. Klein, Ruwan T. Kurulugama, Michael J. Lawler, Yali Li, Michael J. McCoy, Nathan A. Miller, Partha P. Nag, Julie A. Pigza, Gregory D. Schilling, Levi S. Simpson, Bianna H. Smith, Amy N. Walstrom, Matthew B. Worthington, and Ryan A. Yoder.

#### Annual honors and awards

At the Chemistry Honors Banquet in April 2003, the following students were honored:

E. Campaigne C500 Award: Peter J. Mikulecky

*Eli Lilly Fellowship*: Michael J. Lawler and Julie A. Pigza

McCormick Science Fellowship: Khuloud Jaqaman

Wendell P. Metzner Memorial Award: Benjamin M. Nugent



Benjamin M. Nugent



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Graduate students Michael J. Lawler, left, and Julie A. Pigza won Eli Lilly fellowships.

### Graduate notes

(continued from page 21)



Parichatr Vanalabhpatana

# Charles N. Reilley (Pharmacia Corp.) Award: Richard L. Beardsley

Felix Haurowitz Award: Gerardo Gamez

Instructor Awards: Daniel G. Gurnon, Jack L. Hayes, Benjamin M. Nugent, Timothy P. O'Dea, and Amy L. Rosen

William P. Klinkenberg Award: Parichatr Vanalabhpatana

John H. & Dorothy McKenzie Award: David K. Leahy

#### PhD degrees awarded

Aliaga, Nuria (inorganic, Christou, April 2003)

**Bhaduri, Sumit** (inorganic, Christou, August 2002)

**Burlingham, Benjamin** (organic, Widlanski, July 2002), assistant professor, Mount Union College, Alliance, Ohio

**Canada Vilalta, Christina** (inorganic, Christou, January 2003), product support scientist, Indianapolis

**Clark, Aurora** (physical, Davidson/Zaleski, April 2003), postdoc, Los Alamos National Lab, Los Alomos, N.M.

Click, Damon (inorganic, Chisholm, August 2002)

**Dailey, Robert** (physical, Davidson, June 2002), assistant scientist information analyst, Chemical Abstracts Service, Columbus, Ohio

Engel, David (organic, Montgomery, December 2002), GE corporate research, Schenectady, N.Y.

Harris, William (analytical, Reilly, September 2002)

Huang, Yunping (analytical, Novotny, July 2002)

Ihle, David (organic, Williams, January 2003), postdoc, Oregon State University, Corvallis, Ore.

Joo, Chan (physical, Zwanziger, October 2002)

Kammler, David (organic, Williams, October 2002)

Kraft, Brian (inorganic, Zaleski, April 2003), postdoc, Los Alamos National Lab, Los Alamos, N.M.

Marchenko, Alexei (inorganic, Caulton, August 2002), postdoc, University of Oregon, Eugene, Ore.

Maxwell, Dustin (analytical, Nie, April 2003)

McClain, Diana (biological, Oakley, July 2002), Federal Drug Agency, Washington, D.C.

Que, Amy (analytical, Novotny, December 2002), scientist, Pharmacia, St. Louis, Mo.

Quinlan, Kristine (inorganic, Chisholm, August 2002)

Sharrow, Scott (biological, Novotny, December 2002), scientist, Eli Lilly, Indianapolis

Soler, Monica (inorganic, Christou, April 2003)

Taylor, Jason (analytical, Nie, July 2002), lecturer, University of Maryland, Baltimore County

Zhang, Zhenfeng (physical, Ewing, December 2002)

#### MS degree awarded

Ash, Jason (physical, Zwanziger, May 2003)

Lorenz, Tara (physical, Jabri, August 2002)

Prendergast, Tara (analytical, Clemmer, December 2002)

Rosen, Amy (analytical, Hieftje, May 2003)

**Strelow, John** (biological, Widlanski, January 2003)



Meeting with 2003 Nobel laureate John Fenn (third from left) are students, from left, Sunnie Myung, Stormy Koeniger, and Amy Hilderbrand.

# UNDERGRADUATE

This has been an exciting and busy summer for everyone involved with the IU undergraduate chemistry program! Because the undergraduate office has undergone reorganization, I will introduce each member of our team separately. It is my privilege to work with this terrific group of faculty and staff whose primary responsibilities are to work with our undergraduates, to design and implement curriculum improvements, and to maintain the high level of undergraduate training for which our department is known all over the country.

Alice Dobie-Galuska, formerly our general chemistry coordinator, has been promoted to the position of coordinator of undergraduate services. Alice's main responsibilities are to manage the undergraduate office, to serve as the departmental adviser, and to run the job placement office, which serves both graduate and undergraduate students. This change leaves Steve Wietstock, our coordinator of curriculum development and outreach, free to use his considerable expertise in curriculum development to make our chemistry curriculum a model for others to follow. He has already played a major role in the revision of our general chemistry curriculum (see below). He has also initiated several exciting outreach activities to Indiana high school teachers and students that will improve student preparation for college chemistry courses, to attract top students to IU, and to improve recruiting and retention of underrepresented groups.

There are several new faces in the UGO this fall. Heather Brummett, now a familiar fixture behind the reception desk in C021, will take a maternity leave and will be replaced by Danusha Goska during her absence. We wish Heather the best during these exciting months! We are also pleased to welcome Becky Baugh back to our department. Becky, who worked for a year as the UGO receptionist, is now our department scheduling officer. Last but certainly not least, we welcome recent IU graduate Matthew Nance, our new demonstration technician. In addition to assisting faculty with lecture demonstrations, Matt is involved with curriculum development in our lab classes and with various outreach activities that target current IU chemistry and biochemistry students.

We are also fortunate to have two outstanding teaching faculty associated with the UGO. Jill **Robinson** joined our faculty last year after a stint at the University of Wyoming. She obtained her PhD in analytical chemistry from the University of Colorado. In her first year at IU, she was very successful teaching general chemistry for majors and nonmajors, and she has also been actively involved in our efforts to revise our general chemistry curriculum for chemistry and biochemistry majors. Kate Reck obtained her PhD in inorganic chemistry from Wayne State University and carried out postdoctoral work at the University of Chicago. Since joining our faculty in the summer of 2001, Reck has taught more than a dozen different courses in general chemistry, inorganic chemistry, and organic chemistry. She has developed an inorganic lab course and has also been a key player in our general chemistry curriculum reform efforts. She also advises undergraduate research students in collaboration with Professor Jeff Zaleski. Somehow, amidst all that, she has found time to assist a faculty member in the Department of History and Philosophy of Science with a film project about Isaac Newton on the BBC this fall.

Our major task during the last year has been to revise our general chemistry curriculum for majors. Beginning this fall, we have replaced C105 and C125 with a five-credit integrated lecture and lab course, C117 Introduction to Chemistry and Biochemistry. The second semester course in this sequence, C118, will be offered for the first time in the spring of 2004. Our goal in these courses is to teach students fundamental chemistry concepts using modern examples to illustrate these concepts. This work was begun last fall by Dennis Peters and Adam Allerhand. Faculty participating in the sequence this year include Caroline Jarrold, Martin Jarrold, Dan Mindiola, Dennis Peters, Kate Reck, Jill Robinson, Jeff Zaleski, and myself. A key goal in these classes is to expose students to modern careers in chemistry or biochemistry by inviting visiting speakers. If you would like to assist us with this effort by giving a short talk about your career, please contact the undergraduate office at (812) 855-2700.

Finally, in the spring of 2004, we plan to hold our first internal Department of Chemistry graduation ceremony, at which we will individually recognize each chemistry or biochemistry major who will graduate in 2004. This ceremony will be combined with a brunch to allow the families and friends of our graduates to meet faculty, staff, and other students. We are proud of our graduates, and we think each one deserves time alone on a stage to celebrate his or her accomplishments!

— Martha G. Oakley

#### Scholarships and awards

ACS Award: Katherine Joan Mercer

Analytical Chemistry Award: Katherine Elaine Hersberger

William H. Bell Awards: Amy M. Fang, Shawn Travis Greathouse, Paul Hae-Yong Park, Misha Lee Taber, and Jennifer Christine Takach

John H. Billman Summer Scholarship for 2003: Brandon Lee Steele

CRC Press Freshman Award for 2003: Denver J. McDaniel

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## ALUMNI PROFILE: Albert C. Yates

# Yates retires as Colorado State president

In June 2003 Albert C. Yates retired, after 13 years in office, as president of Colorado State University and chancellor of the Colorado State University System. Al is a native of Memphis, Tenn., where he attended Memphis State University after a stint in the Navy as an assistant navigator aboard the carrier *Kitty Hawk*. At Memphis State, Al earned a double major in both mathematics and chemistry. Following his graduation from



Courtesy photo, Colorado State University

Albert C. Yates

college, Al spent three years as a graduate student in my research group and graduated with a PhD in chemical physics in 1968. His thesis in theoretical study explained the experimental results for the scattering of spin polarized electrons by molecules. After graduating from IU, Al spent a postdoctoral year at USC working with Howard Taylor in theoretical chemistry before joining the IU chemistry faculty as an assistant professor. He was promoted to the rank of associate professor of chemistry in 1974 before leaving for the University of Cincinnati to become the associate dean of the graduate school. In 1977 he was promoted to the position of vice president and

dean of graduate studies, a position he held until 1981, when he was chosen to be the executive vice president and provost of Washington State University in Pullman. After serving for nine years in that post, Al was selected as the 12th president of Colorado State University in Fort Collins, where he served until his retirement.

I have a number of fond memories of Al, which I would like to share. Although a brilliant student in the field of theoretical chemical physics, Al gained a certain degree of notoriety during his student days after he fleeced a group of fellow graduate students who had challenged him to a game of pool at the Memorial Union. It seems he showed up for the challenge match carrying a very professional looking pool cue case, which earned him the moniker of "Memphis Fats."

Al told me once that one of the big thrills of his life had been bringing the aircraft carrier *Kitty Hawk* into San Francisco Bay as the ship's navigator. Although he was only the assistant navigator at the time he had to take over the job because the chief navigator was sleeping off "a night on the town."

I was privileged to be in attendance at his inauguration as president of Colorado State University in Fort Collins in 1990 and enjoyed listening to the stories told by Al's family members concerning his wayward youth. Especially humorous was the take about the principal of Al's high school, who at an honor assembly announced that Albert C. Yates had been awarded the National Merit Scholarship. When Al stepped forward to receive the award, the principal, who knew Al intimately by his many non-voluntary office visits, but only by a nickname, refused to believe that this was indeed the award winner.

Al has received numerous awards, including three honorary doctorates, election to the Hall of Fame of the Memphis City Schools in 2000 (www.memphis-schools.k12.tn.us/admin/ communications/Hall of Fame/Albert Yates.htm.), a Distinguished Service Award from the College of Arts and Sciences of Washington State University in 1990, a Distinguished Alumnus Award from Memphis State University in 1992, and honorary degrees from the Colorado School of Mines and University of Denver. Of particular note was the establishment of several scholarship funds for minority students in Al's name, including the Albert C. Yates Fellows and Scholars Program at the University of Cincinnati, established in 1995, and the Albert C. Yates Leadership Development Institute, founded at Colorado State in 2001. In that same year, Feb. 28 was declared Albert C. Yates Day in the state of Colorado, and in 2002 Al was given the Citizen of the West award by the National Western Stock Show Association. Some of the previous winners of this award include Supreme Court Justice Byron White, Vice President Dick Cheney, and Senator Alan Simpson.

# ALUMNI PROFILE: Max Marsh Marsh honored for 'high standards of excellence'

"I know of no other scientist of this period [who] has maintained such a persistent and active role in the service of science. ... The only thing Max has lacked is a formal diploma testifying to his doctoral knowledge." These powerful words referring to Max Marsh, BS'47, were from a colleague at Eli Lilly. They are now out of date, however, because Max no longer lacks a doctoral degree. He received an honorary doctor of science degree from Indiana University at commencement on May 10. In his supporting letter, the dean of the College of Arts and Sciences, Kumble R. Subbaswamy, said, "Max Marsh easily meets the first criterion for an honorary degree, namely the achievement of high standards of excellence."

High standards of excellence did indeed mark the career of this native of Indianapolis. After graduating from Shortridge High School and starting extension night classes at IU, he began working for Lilly in 1942 as a laboratory assistant in the analytical department. He was drafted in 1943 and served in India. When he returned at the end of World War II, a leave of absence from Lilly allowed him to complete the requirements for his bachelor's degree in chemistry at IU. With that degree in hand, he worked as a chemist in the analytical department for another 10 years until he and other colleagues formed the analytical research department. Eventually, he served as its head. High standards of excellence were again obvious when Max became a research associate in 1961 and a research adviser in 1966. In 1967, he became director of the Physical Chemistry Research Division, a division that included analytical research as well as a group devoted to molecular structure determination and a small group of electrochemists. After two years and at his request, he returned to his role as a research adviser, a position he kept until his retirement in 1986.

While working at Lilly, the subjects of his 41 publications ranged from wet chemical methods to new instrumentation for chemical measurement, and extended into quantum chemical calculations. "He was the first in the entire pharmaceutical industry," a colleague at Lilly wrote, "to initiate a sustainable program for the use of rational drug design and of theoretical chemistry." Along with Wayne W. Hilty, he also published a now classic review titled *Pharmaceutical and Natural Drugs*, a review that they revised and republished three additional times because of the rapid growth in this field.

Throughout his career at Lilly, he maintained his interest in our department and visited it frequently. He became our second industrial professor in 1971, a position that required him to spend a few

weeks on campus each year. It was a position he held until 1976. A colleague, describing Max in this role, said, "He became a facilitator for collaboration, the solution of problems, and the advancement of science." After his retirement from Lilly, he came back to Bloomington and IU permanently, doing molecular design work. But that was not all: He was instrumental in getting

work. But that was not all: He was instrumental in getting the chemical informatics program at IU started; he took the lead in raising endowment funds from other alumni at Lilly; and he is an esteemed member of the advisory board for the Dean of the College of Arts and Sciences. He became associated with this magazine — then a simple newsletter — in 1992 and provided a sustaining interest in quality and invaluable leadership until he retired

Colleagues, both at Lilly and in our department, are passionate in their praise of Max. One said, "He stands out for demonstrating the timeless values of intelligence, integrity, honor, character, modesty, service, loyalty, kindness, and generosity."

Perhaps the best way to close this tribute to Max Marsh is to quote a colleague from the department: "His contributions have been both enduring and unwavering. He represents, quite simply, the best that IU can or should produce." Congratulations, Dr. Marsh!

- Rupert Wentworth

### Yates

#### (continued from page 24)

as one of the editors last year.

When Al stepped down from the Colorado State University presidency, university officials renamed the chemistry building Yates Hall, created the Yates endowed chair in mathematics, and set up a generous scholarship fund in his name. Al has been extremely active in community service, having served on boards or committees for 17 different organizations. Talk about taking on impossible tasks!

Since Al is retiring at a young age, at least by my standards, I am wondering what he will be up to next? Perhaps a run for a U.S. Senate seat?

— Russell A. Bonham



Max Marsh

### ALUMNI NEWS



# 50 YEARS AGO

Several alumni attended the Symposium on Coordination Compounds held in August. They included **G.W. Leonard**, BS'47; **J.W. Faucett**, BA'32, MA'32, PhD'48; **E. Lauterman**, PhD'51; **H.S. Rothrock**, AB'26; **R.L. Patrick**, PhD'51; **T.H. Chao**, BS'35, MA'36; and **W.O. Bea**vers, BA'39, MA'41.

# 25 YEARS AGO

Herbert S. Gutowsky, AB'40, received the National Medal of Science for pioneering studies in nuclear magnetic resonance spectroscopy. He is without doubt the chemist most responsible for developing and applying NMR techniques to chemical problems.

**R.L. Patrick**, PhD'51, manager of the Harris Research Laboratories at the Gillette Research Institute, received the ASTM Adhesives Award for 1978 at a meeting in San Antonio. The award was presented by another alumnus, **Robert H. Gillespie**, BS'38.

The coal strike produced an energy shortage that reduced the Chemistry Building's temperature to that of an alchemical laboratory in the Middle Ages. We operated at 55 degrees until the university closed for three weeks in March. It was quite a year for **Alli Abraham**, BS'98. Writing to David Clemmer, she says that she works for Pfizer in a little town in Connecticut called Groton. Her letter shows her excitement: Starting slowly as she got oriented while learning day-to-day procedures in the Analytical Division, she began to meet deadline after deadline, guided by an excellent supervisor and working with a great group of people. She enjoys living in Groton because it is within easy driving distance of New York City and Boston.

**George M. Bodner**, PhD'72, was honored by the American Chemical Society with the 2003 George C. Pimentel Award in Chemical Education. The award recognized his achievements, both in the classroom and laboratory, in shaping how educators can more effectively teach chemistry and other sciences. He lives in West Lafayette, Ind.

**Stephen M. Bonsib**, BA'72, MS'76, MD'78, was appointed director of surgical pathology at the IU School of Medicine in February 2002. He lives in Indianapolis.

Anne Caraley, postdoc'00–'02, accepted a faculty position at SUNY Oswego.

**Gregg A. Dickerson**, BA'80, MD'84, a radiation oncologist in Jackson, Miss., has been inducted as a fellow in the American College of Radiology. He lives in Madison, Miss.

**G. L. Dike-Birbeck**, BA'90, was recently awarded a \$378,000 grant from the National Institutes of Health to study the social and economic impact of epilepsy in Zambia. The assistant professor at Michigan State University lives with her husband, Matthew, in Mason, Mich., and can be reached at gretchen.birbeck@ht.msu.edu.

**Philip A. Downing**, BA'69, is the manger of analytical services for BASi Evansville in Evansville, Ind.

**Thomas Driver**, BS'99, a graduate student at the University of California, Irvine, received a graduate fellowship from the ACS Division of Organic Chemistry.

**David Ginger**, BS'97, has accepted a faculty position at the University of Washington in Seattle. He was a Marshall Scholar who received his PhD from Cambridge in 2001 and then completed his postdoctoral work at Northwestern, where he was supported by NIH and Dupont fellowships.

Anthony J. Iannarelli, BA'01, is in the MAT program at IU and hopes to be teaching soon. He lives in Bloomington.

Hugh W. Johnston, PhD'48, writes, "I'm a volunteer in the archives at both Whitworth College and Eastern Washington Historical Society, processing manuscripts in the areas of college history, protestant church history, and history of the Inland Empire." He lives in Spokane, Wash.

Demetrios N. Kaiafas, BA'89, MD'93, writes, "I have left my medical practice in Indiana and now

practice in Florida." The Belleair Beach, Fla., resident can be reached at dkaiafas@tampabay.rr.com.

Jane C. Krauhs, MA'71, PhD'75, was reelected treasurer of the American Medical Writers Association. She is a senior scientist at Wyle Laboratories Inc., Life Sciences, Systems, and Services and lives in LaPorte, Texas.

Mark A. Krockover, BA'93, is in his 10th year as a teacher at Maine East High School in Park Ridge, Ill. He is the head coach of varsity coed cheerleading, which won the 2002 Illinois Cheerleading State Championships. He recently received a second master's degree in educational leadership from Northeastern Illinois University.

Lisa A. Lear, BA'83, was inducted into the International College of Dentists at this year's annual ADA meeting in San Francisco. The Tucson, Ariz., resident can be reached at lisalear@aol.com.

**Paul R. Loconto**, MS'73, published his first book, *Trace Environmental Quantitative Analysis* (Marcel Dekker, 2001). He is now a laboratory scientist and specialist for the Michigan Department of Community Health, Bureau of Laboratories. He and his wife, Priscilla, live in Okemos, Mich.

**Steven D. Long**, BA'63, is retiring and leaving California to return to Indiana.

**Peter Mahaffy**, PhD'79, a professor of chemistry at King's University College in Edmonton, Canada, is the recipient of the 2003 Union Carbide Award. His contributions include extensive work in chemical education.

William G. Mays, BA'70, MBA'73, joined First Indiana Corporation's board of directors on April 26, 2003. The president of Mays Chemical Company Inc., lives in Indianapolis and can be reached at wgmays@mayschem.com.

Nan C. Milausnic, BS'93, is a senior science recruiter with Kelly Scientific Resources in Denver. She recruits for biotech, pharmaceutical, and chemical companies in Colorado. Her husband, Michael Milausnic, BA'90, has a private dental practice in Lakewood, Colo., a suburb of Denver.

Arlan D. Norman, PhD'66, was selected from more than 100 candidates to serve as founding dean of the College of Science and Technology at Western Washington University. The professor of chemistry and associate dean for natural sciences at the University of Colorado, Boulder can be reached at normana@colorado.edu.

John M. Ramsey, PhD'79, senior corporate fellow at Oak Ridge National Laboratory in Oak Ridge, Tenn., earned the 2003 American Chemical Society Division of Analytical Chemistry Award in chemical instrumentation. He lives in Knoxville, Tenn., with his wife, Roswitha, and son, Christopher Blake.

Michael A. Raymondi, BA'88, performed with the company of "Miss Siagon" for four years be-

fore he started commercial editing for The Union Editorial. He lives in Los Angeles.

**David A. Rio**, BS'02, an Army Spc., just returned from a seven-month deployment in Afghanistan. The Oolitic, Ind., resident is stationed at Ft. Monmouth, N.J., and can be reached at superio@hotmail.com.

David A. Sasso, BM'98, BS'98, composed Indianapolis' first professional children's opera "The Trio of Minuet," presented by the Indianapolis Children's Choir in May. He is now working toward a combined MD/MPH at Northwestern University Medical School where his wife, Dana Small, BM'98, BS'98, is an assistant professor of neurology. They live in Chicago.

James F. Schooley Sr., BA'53, was honored as a member of IU's 1953 men's national championship basketball team on March 3, 2003. He and his wife Mary A. Schooley, BS'53, live in Gaithersburg, Md.

Elisa J. Seddon, PhD'01, and Eric Seddon, PhD'01, celebrated the birth of their daughter, Gwyneth Theresa, on June 23. They live in Cleveland.

### Undergraduate

(continued from page 23)

Harry G. Day Summer Scholarships for 2003: James Travis Patterson, Paras Batuk Ramolia, Christian Ross, Deepthi Yavarthi, and John Michael Zaborske

Grim Scholarships for 2002–03: Katherine Elaine Hersberger, Monica Joy Mann, Andrea Lindsay Nold, Brooke Marie Norman, James Travis Patterson, and Ester Marie Tristani

Russel L. and Trula Sidwell Hardy Scholarship: Joseph Matthew Lee

Howard Hughes Medical Institute Research Scholarships for 2002–03: Eric Joseph Espinosa, Shawn Travis Greathouse, Katarzyna A. Mastalerz, Paul Hae-Yong Park, James Travis Patterson, Andrew L. Paulsel, Paras Batuk Ramolia, Jennifer Christine Takach, and John Michael Zaborske

Honors Division Summer Scholarships for 2003: Michael Aaron Goodman, Theordore J. Gries, Stephen Jess Helms, Katherine Elaine Hersberger, Alan Breymann McIntosh, and Paul Hae-Yong Park

Hypercube Scholar Award: Maxim Kostylev

James C. White Award: Peter B. Conrad

Ira E. Lee Summer Scholarships for 2003: Nicole M. Vincent and Nicholas Leroy Wolf

The Lilly Organic Undergraduate Summer Research Scholarships for 2003: **Troy Sagan Alexander** and **Christopher Paul Moore**  Lilynorfeshah Mohd Shah, BS'96, is an analytical chemist in a water treatment plant in Sabah, Malaysia. She can be reached at iu1096@yahoo.com.

Lawrence T. Stanley, BA'00, received a JD summa cum laude from New England School of Law in May and was the recipient of the Dean Arthur W. McLean Award for Academic Excellence. The Quincy, Mass., resident can be reached at ltstanle@yahoo.com.

**Cara A. Tracewell**, BS'97, is working toward a doctorate in chemistry at Yale University in New Haven, Conn.

**Gretchen Schmidt Voyles**, BA'98, graduated from Butler University with a Doctor of Pharmacy. The Brentwood, Tenn., resident is a pharmacist at Vanderbilt University Medical Center.

Sherry Yennello, PhD'90, was promoted to the rank of full professor at Texas A&M University.

Charity McCoy Zink, BA'94, MS'95, conducts neuroscience research at Eli Lilly ぐ Co. She celebrated the birth of her son, Carter Daniel, in March 2002. They live in Fishers, Ind. (continued on page 29)

Andrew Loh Scholarship for Analytical Chemistry for 2003–04: Katherine Elaine Hersberger

Lubrizol Scholarships for 2002-03: Shawn Travis Greathouse, Maxim Kostylev, Katarzyna A. Mastalerz, and Paul Hae-Yong Park

Mathers Summer Scholarships: Michael Andrew Ischay, Maxim Kostylev, and Charles Chauncey L. McCrory

Merck Index Awards: Natalie Marie Best and Andre Gerardo Melendez

Mary Frechtling White Award: Jennifer Christine Takach

National Starch & Chemical Co. Scholarships for 2002–03: Troy Sagan Alexander, Natalie Marie Best, and Stephen Jess Helms

Pfizer Organic Summer Scholarship for 2002–03: Andrea Lindsay Nold

Joseph B. Schwartzkopf Award: Heather Elizabeth Burks

Sturdevant Scholarship: Shawn Travis Greathouse

Enola Rentschler Van Valer Trafford Scholarship Awards: Kathryn Mc Govern Calhoun and Brooke Marie Norman

The Votaw Undergraduate Summer Research Scholarships for 2003: Susan Kim Conroy and Frank Hrisomalos

The Francis and Mildred (Eckerty) Whitacre Scholarships for 2003–04: Stephen Jess Helms and Matthew Michael Sipze

# 15 YEARS AGO

The new south and east wings of the Chemistry Building were dedicated on Oct. 21.

#### Felix Haurowitz,

Distinguished Professor Emeritus of Chemistry and member of the National Academy of Sciences, died on Dec. 2.

# In memoriam: Harrison Shull (1923–2003)

Arrison Shull, IU Department of Chemistry faculty member from 1955 to 1979, died on Aug. 18 at his home in Monterey, Calif., after a losing battle with pancreatic cancer, marking the end of a brilliant career as a theoretical chemist and university administrator.

His early family life was enriched through contact with many scientists and others who came to visit his father, the eminent botanist and geneticist George Harrison Shull, a professor at Princeton University. He graduated from Princeton High School in 1940 and from Princeton University in 1943. He earned his PhD degree from the University of California, Berkeley, in 1948, having begun his thesis under the direction of G.N. Lewis and, after Lewis's death, completing it under the direction of Professor William Gwinn.

After serving as a National Research Council Fellow at the University of Chicago with Professor Robert Mulliken, he joined

the chemistry department at Iowa State College (now University) as assistant professor in 1949. He moved to Indiana University as associate professor in 1955, was promoted to full professor in 1958 and to research professor in 1961. He served as dean of the graduate school from 1966 to 1972 and as vice chancellor for research and development from 1972 to 1976. In 1979, he left Indiana University to become provost at Rensselaer Polytechnic Institute. He served as chancellor of the University of Colorado, Boulder, from 1982 to 1985, when he became provost at the U.S. Naval Graduate School in Monterey, Calif., serving there until his retirement in 1995.

He was a brilliant scientist and administrator who brought a keen analytical mind and a fresh, independent perspective to problems both scientific and administrative;

consequently he was highly valued as a consultant and adviser. Especially after his election to the National Academy of Sciences in 1969, he served on numerous national committees, including the Committee on Science and Public Policy of the National Academy of Sciences, 1969–72; the Westheimer Committee to Survey Chemistry, 1964–65; the advisory committee for Chemistry of the National Science Foundation, 1966–67; the board of trustees of the Argonne Universities Association; the advisory committee for Chemical Abstracts Services, 1972–75; the visiting committee for Brookhaven National Laboratory; and many others. He was a consulting editor for Allyn and Bacon. He was highly valued as an adviser and scientific consultant to his faculty colleagues in chemistry and was influential in the direction, management, and development of our department.

Shull began his independent research work at Iowa State in both experimental and theoretical molecular spectroscopy, specifically the theoretical study of substituent effects on the electronic spectra of benzene using naïve molecular orbital theory and the

high-resolution spectroscopic studies of singlet-triplet phosphorescence in benzene and halogenated benzenes. After spending a year in Sweden with the Quantum Theory Group of Professor Per-Olov Löwdin at the University of Uppsala, Shull switched his research entirely to the then-young field of ab initio quantum chemistry, that is, the calculation of electronic properties of atoms and molecules, using mainly the method of configuration interaction. Calculations were carried out on H2+, H2, LiH, H3+ - to mention a few examples. Natural orbital analyses of the wave functions were then carried out in an effort to understand the electron correlation in these systems. To do these calculations, a great deal of basic methodology was developed and computational programs written. For example, various members of the Shull group worked on the symmetric eigenvalue problem, molecular integrals using Slater type orbitals, arbitrary precision arithmetic, etc. Some of the earliest work on Gaussian integrals was done at IU in the early '60s.

An outgrowth of Shull's several visits to the Quantum Theory Group in Sweden was an interest in the geminal method for describing the electronic structure of molecules. Computations on water and  $H_3O^+$  are examples of work in this area. The Generalized Valence Bond method subsequently developed and popularized by Goddard has much in common with the geminal method developed at IU.

His influence on the department and on Indiana University was deep, widespread, and lasting. Together with Lynne Merritt, professor of chemistry, and Marshall Wrubel, professor of astronomy, he arranged for the first purchase by the university of a digital computer, the IBM 650. Then, in 1959, the university's Research Computing Center was established, with Shull as its first

director. Many graduate students and postdocs who gained their training with Shull's research group went on to prominent careers in academic and government laboratories, including Stan Hagstrom and Ernest Davidson, who served as faculty members in our department.

Shull's interest in computational chemistry led him to establish the Quantum Chemistry Program Exchange for the sharing of computational programs among chemists, a service that brought the chemistry department at Indiana University to the attention of chemists worldwide.

Shull's wife, Will, seven children, and 10 grand children, survive him. The department, in cooperation with some of Shull's former students and the Shull family, have established a biannual endowed lectureship in his memory. Those wishing to contribute should send contributions to the IU Foundation, marked for the Harrison Shull Memorial Lectureship Fund.

— Stanley Hagstrom and Jack Shiner



# **Department mourns loss** John Henry Billman

The Department of Chemistry recently learned of the death of Professor Emeritus John Henry Billman in January 2003.

John was born Feb. 8, 1912, in Brooklyn, N.Y. He received a BS in chemistry at the University of Virginia in 1934 and MS and PhD degrees in 1935 and 1937, respectively, at Princeton University. He joined the chemistry faculty at Indiana University Bloomington as instructor and advanced to become professor of chemistry (organic) in July 1958. John held this position until his retirement in July 1977. He and his wife retired to a home on Long Island, N.Y.

He taught various courses in organic chemistry. His interests were directed toward medicinal chemistry, with a special interest in the applications of chelation therapy.

— Marvin Carmack

# Ruth Gurd

Ruth Gurd died on Nov. 11, 2002, at her home in Albuquerque, N.M., where she had lived with her husband, Frank Gurd, since their respective retirements from IU in 1988. Based in Bloomington in the medical sciences department, she was a professor of biochemistry in the IU School of Medicine. To our great pleasure, she spent considerable time in the chemistry department and seemed as a chemistry faculty member to many of her colleagues.

Ruth grew up in Paducah, Ky. After receiving a BS from the University of Michigan in 1949, she began positions as a research associate at the Presbyterian Hospital in Chicago and later at Washington University in St. Louis. Ruth completed her MD in 1957 from Washington University and moved with Frank to New York City as a postdoc at the Cornell College of Medicine.

Her life in Bloomington began in 1967 as a research assistant in the neurochemistry program of Henry Mahler and Walter Moore. In 1973, she was appointed to the medical sciences faculty, where she was active in research and was a skilled teacher and adviser to many students. Ruth was a central contributor to the development of the combined MD/PhD program.

In Bloomington, Ruth developed a productive research program focused on the structure-to-function relationship of glucagons. At a time when glucagons were a sizable synthetic challenge due to chemical and physical liabilities, her group used a number of selective chemical modifications to alter receptor function. The research provided a molecular model for glucagon action through the biophysical analysis of a set of structurally altered hormone analogs. The results continue to inspire the continued pursuit of improved glucagons agonists and antagonists for the treatment of insulin-dependent diabetes.

Beyond raising her daughter, Martha, and her son, Charles, Ruth's other life was music. She was an accomplished pianist whose musical activities were effectively on hold during her professional career. At the age of 6, Santa Claus answered her pleas for a "big piano" to begin her road to a lifetime of musical enjoyment. She attended the National Music Camp in Interlochen, Mich., where she was the principal flutist with the orchestra. Upon her retirement 40 years later, she resumed her musical immersion, again taking piano lessons and joining others in an active musical life in Albuquerque. Her January 2003 memorial was a musical tribute, attended by numerous professional musicians and many of her friends in music, as well as by former professional colleagues and classmates.

## Alumni news

(continued from page 27)

### Necrology

John Sacket McAnally, BS'38, MA'40, PhD'50 (under the direction of Harry G. Day), died Dec. 14, 2002. After completing his PhD, he spent some time on the faculty at the University of Miami School of Medicine, and in 1958, he accepted an appointment at Occidental College in Los Angeles. He continued there until his retirement in 1981. During the last three years before retirement, he divided his time between Occidental and the USC School of Medicine, where he helped to run a program for minority students who wanted to go to medical school, giving support classes in the summer. His work at Occidental involved counseling premedical students as well as teaching classes. After retirement, the McAnallys made their home in Port Townsend, Wash., looking for the peace and quiet of a smaller town after the noise and rush of Los Angeles.

John Heyward McKenzie, BA32, MA34, died Feb. 6, 2003. Graduating from the Harvard Advanced Management Program in 1949, he was general manager of American Can Co., vice president of United Carbon, founder and CEO of Agritec Inc., and a broker with A.G. Edwards. He endowed the John H. and Dorothy McKenzie undergraduate scholarship.

We received notices of the deaths of several others of our alumni since the 2002 issue of *IU*•*Chemistry*, but with no further details:

Robert Frederick Babcock, PhD'58, June 7, 2002 Malcolm Davonne Bray, BA'38, March 26, 2003 Edward T.S. Brown, BA'32, Feb. 16, 2003 John D. Christena, BS'43, April 20, 2003 Charles William Compton, BA'47, Sept. 30, 2002 Richard D. Connelly, BA'50, MD'54, March 14, 2001 Richard Eli Cowger, BA'49, Jan. 23, 2002 Clayton Clyde Curtis, PhD'59, Jan. 26, 2002 Gerald Wennen Doeden, MA'50, PhD '65, Jan. 14, 2003 Victor Dorf, BA'35, June 30, 2000 Richard M. Downey, BS'40, June 28, 2000 Donnell Dencil Etzwiler, BA'50, April 6, 2003 Charles Louis Firpo, BA'60, Dec. 23, 2002 Jay Francis Fish, BA'34, MA'35, Sept. 9, 2000 Robert H. Gillespie, BS'38, Jan. 22, 2003 George Preston Gregory, BA'42, Jan. 14, 2000 Helen P. Vernon Hartley, MA'30, Oct. 30, 2002 Phil Harter Hidy, BS'38, MA'42, PhD'44, September 2000 John Matthew Holubes, BA'50, MS'56, March 3, 2000 Thad B. Hodus, BA'47, DDS'49, Nov. 14, 2001 Howard L. Hunter, BA'44, May 23, 2003 Thomas Joseph Kennedy, BS'65, Nov. 2, 2000 Franklin S.King, BS'37, July 24, 2001 Richard Gayle Landwerlen, BS'46, June 6, 2003 Elma J. Lanterman, MA'48, PhD'51, March 9, 2003 Norman S. Lasoff, BA'49, Dec. 1, 2002 Warren H. Machleder, PhD'68, Aug. 23, 2002 Frank H. Miller, BA'39, MD'44, Res'54, April 29, 2003 Beltran G. Navarro, MS'77, MS'79, May 24, 2003 Norman Emory Parnell, BA'35, Aug. 7, 2002 Frederick Bertram Petrie, BA'50, July 22, 2002 Edwin E. Pontius, BA'44, MD'47, Res'48, May 7, 2003 Joseph L. Sheridan, BA'39, MD'43, June 30, 2003 James Douglas Stipanovic, BS'94, Oct. 11, 2002 Marjorie Ellen Svoboda, PhD'75, Sept. 28, 2002 Paul S. Visher, BA'42, Jan. 16, 2003 Robert H. Weir, BS'40, Oct. 16, 2002 Joseph Elliott Weber, BA'32, MA'33, PhD'37, March 6, 2003 Dorothy V. Nordman Wilson, BA'36, MA'38, Sept. 18, 2002 Martha E. Winstead, MS'69, July 29, 2002 Kelly Kristine Kahl Woodard, BS'01, April 27, 2003 David Paul Wooldridge, BS'56, PhD'62, Nov. 12, 2002

# CHEMISTRY HONOR ROLL 2002

Aleyamma Abraham, BS'98 Robert L. Ake, BA'60 Kent S. Alleman, MS'96, PhD'98 James W. & Ann Allen Robert C. Ammlung, BS'76 Mark R., BS'83, & Ann Anderson Cynthia J. Anderson, PhD'96 Deon S. Anex, PhD'87 Burton L. Appleton, PhD'58 George R. Aronoff, BA'72, MD'75 Michael M. Aronson, BS'67 Jack P. Arrington, PhD'69 Peter G. Arvan, MA'44 Timothy Ayers, PhD'92 Robert F. Babcock, PhD'58 William E. Jr., MA'50, & Mary E. Bacon Ann K. Bailey Donald G. Ball, MS'74 Craig A., BS'70, & Margaret Balliet Helen B. Barnes, BA'38, MD'42 John C. Bart, BS'89 Bradley B. Basinger, PhD'81 John C. Beauchamp, BA'86 Jean C. Beckman, PhD'77 James H. Beeson, BS'62 Nicholas C. Bensko, MS'74 John W. Berry, BA'37 Frank R. Berson, BA'41 Ella M. Bettinger, BS'49 Deepta Bhattacharya, BS'96 Charles H. Bibart, PhD'73 Lawrence A. Black, BS'77 John A. Bornmann Jr., PhD'58 Robert B. Bourne, BA'51, MBA'65 Charles H. Boxman, BA'53 Louis F. Bradley, BA'51, MD'55 Ludwig Brand, PhD'60 Malcolm, BA'38, & Mary E. Bray Wilfred J. Brockman, BA'42 William W. Bromer, PhD'54 Bernard Buchner, PhD'56 Robert R., BS'42, & Trudy Buck Barbara Buckley, PhD'90 Warren, PhD'64, & Judith Buddenbaum, BA'62, MA'79 Kenneth T. Burck, BS'58 Stanley L. Burden, PhD'66 John E. Burks Jr., PhD'79 Gary W. Caldwell, PhD'82 Ernest & Jean Campaigne Emily J. Canada, BA'70 Robert L. Carpenter, BA'41 William F. Carroll Jr., PhD'78 Roy D. Chisholm III, BA'80 Grace Py Chiu, postdoc'62 John W. Chung, BS'48, MA'49 Johnnie Marie Cliff, MA'64 Richard E., MA'48, PhD'51, & Janet L. Cline George W. Cochran, BS'69 Jill D. Coleman, PhD'96 Jan Arvin Combs Donald J., PhD'44, & Marion M. Cook William T. Cooper III, PhD'81 James F. Corning, PhD'84

Scott A. Cory, BA'92, MD'96 William F. Coulehan, BA'72 Joan Marie Coveleskie, MA'79 Standiford H. Cox, BA'57 Jack K. & Judy Crandall Arnold M. Crelier, PhD'71 Bradley J. Crofts Carolyn A. Cunningham, BA'63, MD'67 Leonard J. Czuba, BA'61 David Dalman, MS'67 Dwight P. Davis, BS'64 Vincent J. Davisson, MS'83 Vincent R. De Las Alas, BA'84, MD'88 Gregory DeMattia, BS'78 Richard D. Di Marchi, PhD'79 Donald E. Dieball, PhD'57 Alan Dinner, PhD'70 Gerald E. Doeden, MA'50, PhD'65 Michael P. Doherty, MS'83 David A. Dolson, PhD'81 Linneaus C., PhD'61, Or Phae H. Dorman Bryce Douglas, postdoc'53-'55 Judith A. Douglas, MS'67 Melvin L. Druelinger, BS'62 Terence J. Duffy, BA'78, MD'82 Milford E. Dulberger, BA'34 Lee G. Dunker, BA'73, DDS'77 Donald G. Earl, BA'60 Merrill Jr., BA'41, MD'44, & Louise Eaton, BA'42, MD'45 Richard F. Ebeling, MA'62 Isidore S. Edelman, BA'41 William J. Edelstein, BA'74 Keith A. Edmonson, BS'62 Douglas C. Elcock, BA'87 Leon Ellenbogen, PhD'54 Michael, BA'69, MD'72, ♂ Christine C. Elmore Donnell D. Etzwiler, BA'50 Henry L. Feffer, BA'39, MD'42 James P. Ferris, PhD'58 Lynn A. Fesenmyer, BA'89, MD'93 James J. Fields, BA72 Michael A. Fowler, BS'88, MBA'95 Emily Kaufman Frank, BA'92, MD'97 John D., BA'50, MD'53, & Martha J. Franz, MD'53, Res'58 Charles E., BS'47, MA'48, ℭ~ Evelyn Frohman, BS'43 H.R. Froning, MA'44, PhD'49 J. Garrin Fullington, MS'64 Paul J. Galley, PhD'93 David W. Garrett, PhD'74 Wilbert W. Jr., & Mary Kratz Gasser Ytbarek Gebre-Egziabher, BA'55, MD'60 Perla Gilinski, BA'56 Robert H. Gillespie, BS'38 Charles T. Gnewuch, PhD'66 Patrick E. Godici, PhD'74 Stephen Godomsky, MAT'66, EdD'70

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