The Carnegie Mellon Chemist

CHEMISTRY DEPARTMENT NEWSLETTER

CARNegie MELLon UNIVERSITY

March 2005

No. 14

Chemistry Undergrads

Two Classes have graduated since the last issue of these pages:

2003 Graduating Class

Twenty seven students received their bachelors degrees in chemistry at the May 2003 Commencement, 24 earning their BS degrees and three a BA. Members of the graduating class demonstrated a wide range of interests. Three students also earned Master of Science degrees, one in chemistry, one in polymer science and one in health care policy and management. Two students completed honors theses to graduate with departmental honors. One student finished the computational chemistry track. One each had additional majors in psychology, English, policy and management and French. In addition to their BS in chemistry, three students completed double degrees requiring an additional 90 units and completion of the requirements for each major, two earning additional degrees in computer science and one in physics. Six students earned minors in the following areas: one each in engineering studies, psychology, art, Spanish, biological sciences and business administration. Two students earned a Department Option for Polymer Science. Many

Continued on p. 3

A Historical Perspective of Theoretical and Computational Chemistry at Carnegie Mellon

The list of Chemistry faculty on the departmental website who have interests in theoretical and computational chemistry is long: Neil M. Donahue, Hyung J. Kim, Maria Kurnikova, Linda A. Peteau, Stuart W. Staley and David Yaron. The research interests of many of these have been topics in prior issues of this Newsletter (back copies are available via a link on that website).

As our alumni know, the research of these members of the faculty continues a tradition of theoretical and computational chemistry dating to the predecessor institutions of Carnegie Mellon: the Mellon Institute (MI) and the Carnegie Institute of Technology (CIT). Research in this area has produced some fifty Ph.D. graduates since the 50s. The focus of theoretical studies at MI in the 50s and 60s was on the statistical mechanics of polymers. This included work by Paul J. Flory, recipient of the Nobel Prize in 1974, along with that of Guy C. Berry, Edward F. Casassa, Marshall Fixman and Hershel Markovitz, with GCB, EFC and HM becoming members of the faculty of Carnegie Mellon on the merger of MI and CIT in 1967, and now all Emeriti. Quantum mechanics and quantum chemistry had a significant presence in both premerger MI and CIT, reflecting the studies of Andrew D. Liehr, Harold Conroy, Robert M. Hexter, Edwin N. Lassette, and Robert F. Stewart at MI, with the last four going to the post-merger institution, and Frank O. Ellison and Robert G. Parr at CIT prior to the merger, with only the first on the faculty at merger. John A. Pople, recipient of the Nobel Prize in 1998, held appointments in MI and CIT, and moved to the Chemistry faculty after merger.

With reference to the two Nobel Laureates, although Flory completed the studies leading to his book on the rotational-isomeric-state model for polymer chain conformations while at MI, most of his work recognized by the Nobel Prize was completed prior to his appointment at MI. By contrast, as will be elaborated in the following, Pople credits his years at Carnegie Mellon with the studies leading to his Nobel Prize. Almost all of it was carried out post merger, involving a number of Ph.D. students (a link to a list of all of the Ph.D. degrees granted in Chemistry at Carnegie Mellon is available on the Chemistry website). Moreover, Pople’s presence on the faculty was important in recruiting a number of

Continued on p. 5
The Department Head’s Column

There are always exciting events to report in the Chemistry Department. It is my pleasure to update you this year on our progress and new commitments to the future. I am very excited to report the growth of our graduate program which now has 75 students enrolled, compared to 54 in 2000. This year, we awarded 8 PhD degrees, 5 masters, and 14 undergraduate degrees. Our 2003-2004 graduate students hold positions at the University of Kansas, Eckerd College in Florida, L’Oreal USA, University of Pittsburgh, University of Texas, Weizmann Institute of Science Israel, Sandia National Laboratories, and the University of Wisconsin.

Chemistry faculty continued to receive University and National recognition for their accomplishments in 2003 and 2004. Catalina Achim received the Camille Dreyfus Teacher-Scholar Award, one of the 13 awarded in 2003. In 2004, Achim also received the National Science Foundation’s most prestigious award for new faculty members, the Faculty Early Career Development (CAREER) award. Krzysztof Matyjaszewski, J. C. Warner Professor of Chemistry, received the 2004 Cooperative Research Award in Polymer Science and Engineering from the American Chemical Society (ACS). He was also the recipient of the 2004 award of the Foundation for Polish Science. Guy Berry, a university professor of polymer science and chemistry, was selected as one of the American Chemical Society’s Polymeric Materials: Science and Engineering Fellows. The PMSE Fellows program honors significant contributions to the science and engineering of polymeric materials. Richard McCullough, Dean of MCS, received the 2003 ACS Akron Section Award. David Yaron received the 2003 MERLOT Classic and Editors’ Choice Awards for Exemplary Online Learning Resources and was awarded the 2004 Carnegie Science Center Education Award for Excellence as a University/Post-Secondary Teacher. Bruce Armitage received the Julius Ashkin Teaching Award. Terry Collins, Thomas Lord Professor of Chemistry, received the 2004 Pittsburgh Award from the American Chemical Society’s Pittsburgh Section. Karen Stump, teaching professor and director of undergraduate studies of chemistry, is the recipient of the 2005 Ryan Award for meritorious teaching.

It is my unhappy duty to inform you of the loss of three former faculty since the last issue of these pages: Leroy E. Alexander, John A. Popie and Anton (Tony) J. Streiff. Additional information on these individuals and their careers is detailed elsewhere in this issue. Perhaps here, it is appropriate to remember their many contributions to the Department over their years on the faculty of Carnegie Mellon.

Hyung J. Kim

Faculty Profiles

This issue profiles two of the newest members of the Chemistry faculty:

Newell R. Washburn
joined the Department of Chemistry as assistant professor in 2004, with a joint appointment with Biomedical Engineering. His research interests lie in the synthesis of polymers for tissue engineering. He is currently developing materials with specific affinities for signaling proteins involved in inflammation and tissue regeneration. The Washburn Group uses fluorescence-spectroscopy techniques such as fluorescence correlation spectroscopy and fluorescence lifetime measurements to investigate the diffusion and binding of important signaling proteins in biological materials, such as demineralized bone matrix or porcine submucosa, that have been shown to be effective in tissue regeneration. These data will be used as design principles for synthetic polymers. A parallel effort is under way in the development of peptide- or carbohydrate-based ligands having strong, specific affinities for these signaling proteins. These ligands will be incorporated in biocompatible, polymeric matrices to impart similar affinities for these signaling proteins as the biological materials. The final step in the materials-development process is to create new materials for implantation.

Maria G. Kurnikova
joined the Department of Chemistry as assistant professor in August, 2003. Before coming to Carnegie Mellon, Kurnikova was an assistant professor at Marquette University in Milwaukee, WI. She has done important work in ion channels and was the first to develop a model that connected a microscopic description of the channel to experimentally measured ion currents. Her more recent research is in the area of computational chemistry and biophysics, particularly understanding the work of membrane proteins and ion channels. She has an excellent grasp of both biology and theoretical methodologies. Her experience in molecular mechanics of biomolecules makes her an addition to the Chemistry Department that will broaden the computational chemistry research program and encourage collaborations with Biological Sciences. Kurnikova received her Ph.D. from the University of Pittsburgh and did her postdoctoral work at the University of Tel Aviv.
Undergrads (from p. 1)

members of the 2003 Graduating Class received honors in recognition of their scholarship: eleven students graduated with University Honors and five with MCS College Research Honors. Eleven students received Carnegie Mellon Senior Leadership Awards, three were inducted into Phi Beta Kappa and two into Phi Kappa Phi. The graduates left for a range of positions: in industry including Merck and Microsoft; in Ph.D. programs at institutions such as Case Western Reserve, the University of Maryland, the University of Hawaii and Columbia University; in government with the National Institutes of Health; and in medical school at the University of Southern California and the University of Pittsburgh.

2004 Graduating Class

Thirteen students received their bachelors degrees in chemistry at the May 2004 Commencement, 12 earning their BS degrees and two a BA. One student earned a BS in computer science with an additional major in chemistry. Members of the graduating class demonstrated a wide range of interests beyond chemistry. One each had additional majors in history and policy and economics. One student completed a double degree requiring an additional 90 units and completion of the requirements for each major earning a BS in chemistry and a BS in biological sciences. Two students earned minors both in history. One student earned a Department Option for Polymer Science. Many members of the 2004 Graduating Class received honors in recognition of their scholarship: five students graduated with University Honors and four with MCS College Research Honors. Seven students received Carnegie Mellon Senior Leadership Awards, three were inducted into Phi Beta Kappa, three into Phi Kappa Phi and two into Sigma Xi. One student won a prestigious graduate fellowship from Phi Kappa Phi.

The graduates left for a range of positions: in industry, including Merck and Microsoft; in Ph.D. programs at institutions such as Case Western Reserve, the University of Maryland, the University of Hawaii and Columbia University; in government with the National Institutes of Health; and in medical school at the University of Southern California and the University of Pittsburgh.

Graduate Program

The Department is pleased to announce that the first Joseph A. Solomon Graduate Fellowship will be awarded in 2005, made possible by a generous bequest from Joseph A. Solomon, PhD ’69. We are also delighted to announce the addition of two new endowed fellowships: the John and Nancy Harrison Legacy Dissertation Fellowship in Chemistry and Biochemistry and the Konrad M Weis Fellowship in Chemistry. We are grateful for these generous gifts provided by John (PhD ’62, MS ’61), and Nancy Harrison, and Konrad Weis, Trustee Emeritus.

In addition, the Mellon College of Science has established a new college-wide award for excellence in graduate research in the name of Guy C. Berry, University Professor Emeritus, whose own research career sets an outstanding example for Ph.D. students in rigor and impact on research at interdisciplinary boundaries. The Guy C. Berry Research Award will be given each spring.

Finally, the Bayer Fellowship in Chemistry, announced in 2003, was awarded last year to Ke Min, a second year student in the Matyjaszewski lab. This fellowship supports her for up to 5 years and will include an internship at BayerMaterialsScience. Two graduate students, Deboshri Banerjee and Andrea Jaquins-Gerstl, were awarded travel awards from the fund created in honor of Edwin N. Lassettre. Alumni gifts enable us to maintain this fund in support of graduate student travel to present their work and participate in educational workshops.

Faculty/Staff Affairs

As highlighted in the Department Head’s column, chemistry faculty have shown themselves to excel through numerous awards over the last two years.

Catalina Achim received one of 13 Camille Dreyfus Teacher-Scholar Awards made in 2003. This award helps strengthen the teaching and research careers of talented faculty in the chemical sciences. In 2004, Achim also received the Faculty Early Career Development (CAReER) award. The five-year grant recognizes and supports the early career-development activities of teacher-scholars who are most likely to become the academic leaders of the 21st century, according to the National Science Foundation.

Guy C. Berry was selected as one of the American Chemical Society’s Polymeric Materials: Science and Engineering Fellows, due in part to his breakthroughs in rheology and the light scattering of polymers.

Richard McCullough, Dean of MCS, received the 2003 ACS Akron Section Award. The recipient of this award “demonstrates exceptional promise for making significant contributions to chemical science.”

David Yaron received the 2003 MERLOT Classic and Editors’ Choice Awards for Exemplary Online Learning Resources. The Virtual Lab allows students to experiment with standard chemical reagents through computer simulation.

Bruce Armitage received the 2004 Julius Ashkin Teaching Award. This award, which is the highest for teaching in the Mellon College of Science, was presented at the MCS.
Annual Faculty Meeting on May 4th.

**Terry Collins, Thomas Lord Professor of Chemistry, received the 2004 Pittsburgh Award from the American Chemical Society's Pittsburgh Section.** The award "recognizes contributions toward increasing chemical knowledge, promoting industry, benefiting humanity or advancing the Pittsburgh Sec

![A. Popel receiving the 1975 Pittsburgh Award](image)

19th century through its solidification after World War II.

**Krzysztof Matyjaszewski** was appointed to the rank of University Professor, Carnegie Mellon's highest academic rank, limited to 10% of the faculty at the rank of Professor. Previous University Professors in Chemistry have been Aksel A. Bothner-by, John A. Popel and Guy C. Berry.

Matyjaszewski received the 2004 Award of the Foundation for Polish Science, which is commonly called the Polish Nobel Prize. The award was granted for the "discovery and commercialization of new methods of controlled radical polymerization". The award, which has been granted by the Foundation annually since 1991, is widely viewed as the most prestigious science award in Poland. It is given to outstanding scientists whose achievements and discoveries within the last four years "constitute an important contribution towards the advancement of science, spiritual life and civilization in Poland, and grant our country an important place in the international community of science". This year's other recipients are Prof. J. adwiga Staniszewicz (sociology), Prof. J. anusz Limon (medicine), and Prof. W. jciech J. Stec (chemistry). The awards, amounting to 100,000 ZLP ($25,000), were presented at the award ceremony in the Royal Castle in Warsaw.

**Robert F. Stewart** retired in January 2005 as Professor Emeritus. Bob joined the department as an Assistant Professor in 1967, coming from the Mellon Institute.

**Karen H. Stump** has received the 2005 William H. and Frances S. Ryan Award. The award is given annually to faculty at Carnegie Mellon who have demonstrated unusual devotion and effectiveness in teaching undergraduate or graduate students. The award recognizes excellence in teaching in several dimensions: outstanding classroom teaching, creation of challenging and innovative courses, creation or use of new and innovative teaching methods and course materials, effective supervision of research or creative projects and effective supervision of undergraduate honors students and graduate students.

**Roberto Gil** joined Chemistry in 2002 as a Research Scientist and Director of the NMR Facility, coming from the faculty of the Cordoba National University in Argentina. The new NMR Facility opened in July 2003 with 300 and 500 MHz state-of-the-art Bruker Avance Spectrometers for liquid NMR spectroscopy, equipped with broadband probes that allow modern multinuclear and multi-dimensional NMR experiments using Gradient Assisted Spectroscopy. For further information, see the url: [http://www.chem.cmu.edu/cma/nmr.html](http://www.chem.cmu.edu/cma/nmr.html).

**Andrew Potratz**, senior systems/software engineer in the Department of Chemistry, received the MCS Outstanding 2004 Achievement Award.

**Nicole Reading**, graphic designer and webmaster for the department and the Mellon College of Science received the MCS Rookie of the Year award in 2002.

**Citation Index.** Carnegie Mellon ranks second among high-impact U.S. universities in organic chemistry & polymer science for average citations per paper. The index is based on publication and citation statistics of ISI* of the number of times the papers were cited from 1998 through 2002: Carnegie Mellon's 177 papers had an average of 14.55 citations per paper. Others in the top five were Caltech (21.44), MIT (10.18), University of Pittsburgh (10.02), and Harvard (9.42).

**Faculty Profiles** (from p. 2) perform cell culture experiments to test cellular responses to these materials. Given the complexity of these systems, combinatorial methods will be used to provide a global understanding of the interplay be-
between materials, signaling proteins, and cellular responses. Washburn received his bachelor's degree in Chemistry at the University of Illinois (Urbana-Champaign) and his Ph.D. in Chemistry at the University of California (Berkeley). After post-doctoral training in chemical engineering at the University of Minnesota (Twin Cities), Newell spent four years at the National Institute of Standards and Technology (Gaithersburg, MD), first as a National Research Council Post-Doctoral Fellow then as Leader of the Biomaterials Group in the Polymers Division. During this time he was also Adjunct Professor at Johns Hopkins University in the Graduate Program in Biotechnology. He is currently an Assistant Professor of Chemistry and Biomedical Engineering at CMU and a member of the faculty of the McGowan Institute for Regenerative Medicine at the University of Pittsburgh.

Theoretical and Computational Chemistry (cont. from p. 1)

faculty in theoretical and computational chemistry before his retirement in 1993, including Charles L. Brooks III, since moved to the Scripps Research Institute, and several of the current faculty named above with research interests in quantum chemistry or statistical mechanics.

The antecedents of research in theoretical and computational chemistry that is still a very active component in the Department may be traced to the research of chemistry faculty members Ellison and Parr in the 50s and early 60s. Parr collaborated with R. Pariser (of duPont) to develop a quantum mechanical theory of the structure of organic molecules in the early 60’s. At the same time, Pople was independently developing such a model in the UK, and these efforts, which eventually became known jointly as the PPP-theory, have enjoyed a productive history. Pople elected to leave the UK in 1964 and accept joint positions (one-half time each) in the Mellon Institute and the Dept. of Chemistry of CIT.

An excerpt from Pople’s autobiography offers his assessment on some aspects of his work in the period 1964-93:

"I was late in recognizing the role that computers would play in the field— I should not have been, for Frank Boys was continually urging the use of early machines back in Cambridge days. However, by 1964, it was clear that the development of an efficient computer code was one of the major tasks facing a practical theoretician and I learned the trade with enthusiasm. Mellon Institute, where I had an adjunct appointment, acquired a Control Data machine in 1966 and my group was able to make rapid progress in the dingy deep basement of that classic building. In 1967, Carnegie Tech and Mellon Institute merged to become Carnegie Mellon University (CMU) and I remained on the faculty there until 1993. Almost all of the work honored by the Nobel Foundation was done at CMU. That institution deserves much of the credit for their continuing support and encouragement over many years.

"The scientific details of the Pittsburgh work are related, in part, in the accompanying (Nobel Prize) lecture. Over the years, we were able to keep abreast with the rapid developments in computer technology. Around 1971, the work was moved to a Univac 1108 machine and then, in 1978, we were fortunate enough to acquire the first VAX/11-780 minicomputer from the Digital Equipment Corporation for use entirely within the chemistry department. This became a valuable workhorse as we began to distribute programs to the general chemical community. In more recent years, of course, the techniques have become available on small workstations and personal computers. The astonishing progress made in computer technology has had profound consequences in so many branches of theoretical science. From 1981 to 1993, I continued to run my research group in Pittsburgh, commuting frequently and communicating with my students by telephone and modem. Northwestern University kindly offered me an adjunct appointment and I became a full member of their faculty in 1993. I am very grateful for them for the opportunity to continue my research program and interact with other members of the chemistry department."

The full text of the autobiography may be found at the url: http://www.nobel.se/chemistry/laur eates/1998/pople-autobio.html

The VAX/11-780 computer, operating at 13.3 MBytes/s, and standing shoulder high.

As noted in his autobiography, the acquisition by the Chemistry Department of the VAX/11-780, the first shipped by Digital, was important to Pople’s research. That acquisition was made possible by a grant from the NSF in response to a proposal put together by Pople, with Mort Kaplan, for his studies in nuclear chemistry, and Bob Stewart, for his studies in x-ray analysis.

An obituary for Pople, written by Bob Parr and published in Chemical Heritage 22(2) 27-9, 2004, provides an interesting summary of some of the interactions that led to Pople joining CIT in 1964.

Many of you will appreciate the
impact of Pople’s contributions, and their continuing legacy in research in the Chemistry Department of Carnegie Mellon and many other institutions. These have been summarized nicely in an obituary published in *Physics Today*, in press (2005) authored by Mark Gordon, Hyung Kim and Mark Ratner: “John Pople’s greatest contributions lie in the insights he provided, in the students he trained, and in the methods he developed and shaped. The most striking methods lie in *ab initio* electronic structure theory. John took as his challenge the development of both techniques and tools to allow scientists and engineers to understand molecular electronic structures. Such development required major advances, including overcoming the electron correlation problem, providing reliable basis sets for actual calculations, norming computation methodologies against reliable experimental data, and constructing and making available a set of robust and efficient software codes. John accomplished all of those. Notations, devised by Pople and his colleagues such as MP/2 theory in the 6-31G* basis set are familiar to molecular scientists worldwide. The MP/2 describes the type and level of perturbative corrections to the self-consistent field method, and the 6-31G* describes the one-electron basis set. John and his group took delivery of the third VAX minicomputer ever made, and thus began a trend away from central processors toward work stations. The group also produced Gaussian 68, the first widely applicable code for molecular electronic structure calculations. He and his students wrote, optimized and commercialized many software tools that changed the way scientists do chemistry."

Aspects of Pople’s science may be found to varying degrees in the work of the present faculty in Chemistry listed above in the area of Theoretical and Computational Chemistry. For example see profiles or research summaries in issues of this newsletter for Donahue (2001), Kim (2002), Kumikova (this issue), Peeteau (2001), Staley (1997), Stewart (2001) and Yaron (2003), or visit the website for the department.

Münck Symposium

Eckard Münck, Professor of Chemistry at Carnegie Mellon University, was honored for his career accomplishments on the occasion of his 65th birthday by a Symposium entitled “Pioneering Mössbauer Spectroscopy in Chemistry and Biochemistry”. On May 24, 2003, US and foreign scientists who work in the field of bioinorganic chemistry gathered in the Mellon Institute to attend. The Symposium, organized by the biological and inorganic faculty of the Department of Chemistry, received support from the Chemistry Department and the Office of the Dean of the Mellon College of Science. The Symposium included a series of lectures in which Münck’s former graduate students, postdoctoral associates, and collaborators highlighted his pivotal role in the development of Mössbauer spectroscopy into a primary tool for studying complex iron centers in metalloenzymes and synthetic complexes, and in the elucidation of the electronic structure and function of these molecules. Many speakers added personal anecdotes to their presentations, and emphasized Münck’s role as a teacher, advisor, and friend. As a birthday present, Münck, who is a fervent opera fan, was offered tickets to the Met. A dinner cruise on Pittsburgh’s three rivers gave a cheerful conclusion to a great day of science.
performed postdoctoral research at the University of Illinois, Georgia Tech, and the University of Copenhagen before arriving at CMU in August of 1997.

Bruce leads a research group in the area of Bioorganic Chemistry. His current research is progressing in four directions. First, small molecules and oligomers are synthesized and tested for binding to specific DNA or RNA sequences and structures. Applications include sensitive detection of nucleic acids in biological samples and regulation of gene expression. In the latter case, experiments are being done in collaboration with Prof. Danith Ly. Second, fluorescent biosensors are being developed for detecting proteins of biomedical interest. This work is being done in collaboration with the Molecular Biosensor and Imaging Center (MBIC) at CMU, directed by Prof. Alan Waggone and with Prof. Bill Brown of the CMU Department of Biological Sciences. Third, the group is developing new strategies for using DNA as a template for assembling organic dye molecules into well-defined nanostructures. The resulting dye arrays exhibit interesting photo-physical properties and are being used in fluorescence imaging applications, also in collaboration with Prof. Waggone.

Bruce has taught Organic Chemistry II since 1999 and has offered a course in Bioorganic Chemistry to graduate and undergraduate students several times. He also developed a course in Supramolecular Chemistry directed toward sophomore chemistry majors. (Prof. Catalina Achim co-taught this course the past two years, broadening the content to include inorganic as well as organic chemistry.) Bruce will soon begin developing a new course titled “Chemosensors and Biosensors”, reflecting his growing interests in this field and broad interest across the University in sensing technology. He is also eager to spread the word about the field of bioorganic chemistry, giving numerous lectures at local four-year colleges as well as at the CMU West Coast campus last fall. “With two chemistry groups and the MBIC already in place and the possibility of hiring an additional assistant professor in this field in the near future, we hope to make CMU a national leader in bioorganic chemistry research and education”, says Bruce. Students and alumni are always welcome to stop by his lab!

Mike Hendrich and his group use spectroscopy to study proteins, enzymes, and biomimetic molecules containing one or more of the transition metals: manganese, iron, cobalt, nickel, copper and molybdenum. Proteins which contain metals are essential for the basic processes of life, including DNA synthesis, metabolism, detoxification, and the activation chemistry of nitrogen, oxygen, sulfur and carbon molecules required for life. The Hendrich group obtains information from a variety of spectroscopic techniques to advance an understanding of the electronic structure and chemical reaction mechanisms of these molecules. His group specializes in electron paramagnetic resonance (EPR) spectroscopy and they have developed new spectroscopic instrumentation, computer simulation software, and quantitative methodologies specifically suited to probe metalloproteins. In general, magnetic resonance techniques can provide primary determinations of concentrations of species. Such techniques have long been available for samples containing a single species with one unpaired electron per molecule. However, most of the EPR spectra that researchers consider contain multiple species and/or multiple unpaired electrons. The new software that the Hendrich group has created allows, for the first time, a detailed understanding of these more complicated spectra from a quantitative treatment of the underlying quantum spin mechanics. In other words, analogous to the weighing of a sample, the spectrum determines the amount of each species present in the sample. These advances have led to new discoveries for a variety of proteins and biomimetic complexes. A new class of enzymes containing up to 24 heme cofactors shows a novel pairing and electronic interaction between the hemes. A new allosteric interaction which affects metal loading has been detected in the enzyme ribonucleotide reductase. The activation of oxygen for insertion into substrates and oxidation chemistry is an essential role of several iron containing enzymes and synthetic complexes. His group has detected new intermediates in the catalytic mechanisms of several of these complexes. The detection and characterization of such intermediates is essential for an understanding of the chemistry and function of the complexes. His group currently has three graduate students and an undergraduate, including an enzymatic Russian, a physical beer brewer, a biochemical wrestler, and an analytical bladder.

![A subunit of the 24-heme enzyme hydroxylamine oxidoreductase](image)

**IN MEMORIUM**

**John A. Pople (1925-2004)**

John C. Warner University Professor Emeritus, passed away on March 15, 2004. Since published obituaries are referenced above (p. 5), and additional copy is available via a link on the department webpage, we will refrain from presenting additional details here.

**Anton (Tony) J. Streiff (1915-2004)**

Administrative Officer and Principal Chemist Emeritus, passed away on 1 April 2004. Chemistry De-
partment graduates, receiving their degree between about 1960 and 1986 will remember Mr. Streiff as their advisor and their friend, and a strong advocate for the Chemistry Department. He began his career as a research chemist for the National Bureau of Standards improving petroleum refining methods for the war effort. In 1950, Tony moved to the Carnegie Institute of Technology in Pittsburgh, where he continued his work on pure chemicals and authored 20 journal articles and a book. This research was sponsored by the American Petroleum Institute and involved the separation, purification, and characterization of the components of standard crude petroleum. Few undergraduate chemistry students ever knew that buried next to the stairwell in Doherty Hall was a distillation column running from the basement level to above the third floor, used for the separation of petroleum components. In 1966, Tony was named executive officer of the Chemistry Department and in 1972 he was promoted to Principal Research Chemist. In 1986, he retired as the Administrative Officer and Principal Chemist Emeritus of Carnegie Mellon University. After retiring, he returned to Jackson, Michigan. In 1999, he received the Ethelene Jones Crockett Distinguished Alumni Award from Jackson Community College.

Leroy E. Alexander (1910-2004)
Professor Emeritus, came to the Department of Chemistry of CMU via Mellon Institute at the merger in 1967, having joined the x-ray diffraction laboratories in MI in 1946. He and Harold R. Klug coauthored the classic book "X-Ray Diffraction Procedures" in 1954, and he authored a second book in 1969 titled "X-ray Diffraction Methods in Polymer Science". Both books had a significant impact on the field, and are in use even today. By the time of his retirement from Carnegie Mellon in 1976, Alexander had also published 50 research papers in the refereed literature on x-ray analysis and methods, including work on both small molecules and polymers. In all of these published works, Alexander demonstrated his depth of knowledge of x-ray diffraction, and his talent for style and clarity in his writing.

ALUMNI NEWS
Your generous responses to the questionnaire in the Newsletter are much appreciated—we now have heard from nearly 300 of you—please keep them coming! As usual, capsules from your questionnaire responses are included below.

Tony Parker BS, 1958, PhD (Penn State) 1963, who was with the Dow Corning MI Fellowship from 1963 to 1967 wrote to identify the person to the right of Earl Warrick in the photo in the last issue of these pages as John Speir, who remained with Dow Corning at Midland, MI, for the remainder of his career. Tony is with Seton Hall College in Greensburg, PA.

Doris Zimmerman BS, 1964, is to be congratulated for earning a PhD in December 2004, from Kent State University. A studious lady she, having now earned two MS degrees, (Chemistry and Materials Engineering), from Youngstown State University. She has been teaching in various visiting and adjunct roles in several universities in the area, and is active as an officer in the local sections of American Chemical Soc. and the Soc. for the Advancement of Material and Process Engineering.

Robert H. Neilson, BS, 1969, earned a Ph.D. in chemistry from Duke University in 1973. He joined the staff of Texas Christian Univ. in 1978, became a full professor in 1987 and served as chair from 1997 to 2003. In 1995, Neilson received the TCU Chancellor’s Award for Distinguished Research & Creative Activity. He received the 2003 W.I. Doherty Research Award for his research in inorganic polymer chemistry, especially the preparation of new monomers and polymers based on phosphorus, boron, and silicon. The award, given by the ACS Dallas-Fort Worth Local Section, consists of $1,500 and an engraved plaque. Established in 1972, the award is named in honor of one of the founding trustees of the Robert A. Welch Foundation, which supports chemistry research in Texas.

Donna Mott (McDonald) BS, 1977, was employed as a chemist for seven years with Borg-Warner in Chicago and earned six patents in the area of flame retardants chemistry. Donna has been married since 1978 to Phil Mott and has three sons - Andrew 19, who is pursuing aerospace engineering at RPI; Ryan 16, and Daud 13. In 1992, she received her MA in teaching from SUNY and taught high school science. Donna is now President of the Dryden, NY school board.

Leanne J. Henry, BS, 1982, has been at the Pentagon for nearly two years, and considers her experience there to have been very rewarding. She has been working in the Directorate of Plans and Programs within the air staff, where she has been involved in the development of a real-time planning and programming tool. Besides her work, which has been very interesting, she also "witnessed history on September 11, 2001 and the subsequent rebuilding of the Pentagon."

Chris Reddick BS, 1992, earned his Ph.D. in analytical chemistry from the University of Florida at Gainesville and married fellow CMU alum, Elena Maccarone (class’91/CFA Graphic Design). For the past six years, he has been working for Bristol-Myers Squibb Pharmaceutical Company where he has been involved in drug discover/development at the Princeton, NJ facilities. In 2003, Chris became Medical Director for Cardiovascular Drug Programs with a new focus on coordinating clinical trials. A couple of years ago, Chris and Elena met fellow MCS alums John Domingos (’92), Jim
Spearman ('92) and Dino Morrelo ('92) at Spring Carnival. All were doing well, and Chris hopes to hear from other alum soon.

Jennifer Elisseeff BS, 1994, received the 2003 Young Alumni Award from the Carnegie Mellon Alumni Association—for details, see http://www.cmu.edu/mcs/about-mcs/news/031017-elisseeff.html.

Kerry McIntyre BS, 1997, completed and defended her Ph.D. thesis at Dartmouth Medical School. She is currently a faculty member at the Middlesex School, where she teaches chemistry and molecular biology and is a dorm parent. Kerry coaches girls’ ice hockey and lacrosse.

Erich C. Blossey PhD, 1963, currently Professor of Chemistry at Rollins College in Winter Park, FL. Erich was awarded the Donald J. and June M. Cram Chair in Chemistry.


Neil Ostlund PhD, 1969, is the founder and president of Hypercube, Inc. He hasn’t taught for a while, so last fall he taught a full semester of undergraduate molecular modeling at the University of Waterloo. He used his hyperchem software in every lecture! Neil and some of his CMU buddies were planning an informal reunion in Florida. Let us know how it turned out, Neil!

The Departmental Web Site
Regular improvements and additions to the department web site continue. Please feel free to contact Rea Freeland at rf51@andrew.cmu.edu, and visit us at the url: http://www.chem.cmu.edu

THANKS FOR YOUR SUPPORT!
Thanks to the many Alumni who have made gifts to the University and/or Department. These are extremely important to our efforts to provide a quality educational experience for our students. Tax-deductible gifts may be made directly to the Chemistry Department by explicit request to that effect, or by instructions that your gift to the University be directed to Chemistry. Some of you may be able to take advantage of gift-matching programs at your place of employment. Activities in both undergraduate and graduate education that benefit from your generosity include:

- Fellowships for undergraduate and graduate students
- Support for Departmental Colloquia
- Support for undergraduate research projects
- The Annual Chemistry Department Retreat
- Travel grants for students to attend scientific meetings
- Equipment for the undergrad teaching labs

2005 ALUMNI QUESTIONNAIRE

Please Complete and Return to
Department of Chemistry
Carnegie Mellon University
Mellon Institute, Box 166
4400 Fifth Avenue
Pittsburgh, PA 15213-2683

NAME: (Name at CMU if different):
ADDRESS:

PERSONAL HIGHLIGHTS & COMMENTS

BUSINESS TEL: HOME TEL: FAX:
e-mail:

Make address available to Chem Alumni?

Yes [] No []

CLASS/Degree: (Please include your degree)