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MARTIN MARIETTA

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**Chemical and Analytical Sciences
Division Progress Report
for the Period January 1, 1993,
through December 31, 1994**

Marvin L. Poutsma
Director

MANAGED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
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**CHEMICAL AND ANALYTICAL SCIENCES DIVISION
PROGRESS REPORT FOR THE PERIOD
January 1, 1993, through December 31, 1994**

Marvin L. Poutsma
Director

Date published: June 1995

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PROGRESS REPORT FOR THE PERIOD
January 1, 1993, through December 31, 1994

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FOREWORD

Marvin L. Poutsma

This report provides brief summaries of progress in the Chemical and Analytical Sciences Division (CASD) during 1993 and 1994. The first four chapters, which cover the research mission, are organized to mirror the major organizational units of the division and indicate the scope of the research portfolio. The fifth and sixth chapters summarize the support activities within CASD that are critical for research progress. Finally, the appendices indicate the productivity and recognition of the staff in terms of various forms of external publications, professional activities, and awards.

The defining event during the reporting period occurred on January 1, 1994, when the Analytical Chemistry Division (ACD) and the Chemistry Division (CD) were merged into a single organization, CASD. This consolidation brought together all of the then CD and the major portion of the former ACD, namely the research and special analytical project functions that had not been consolidated into the Lockheed Martin Energy Systems (LMES) Analytical Services Organization that was created in mid-1993 to focus on compliance-driven analytical service work.

The stated mission of the new organization follows:

The Chemical and Analytical Sciences Division provides the leadership and focus at Oak Ridge National Laboratory (ORNL) for chemical research and its application to issues of scientific and technological importance to the Department of Energy (DOE) and the nation. It is committed to producing high quality scientific information and instrumentation, providing chemical expertise for innovative solutions to interdisciplinary problems, maintaining forefront R&D capabilities, and complying with ES&H and ethical standards. Its emphasis areas are chosen to be in congruence with ORNL and DOE missions and supportive of the needs of other federal and international agencies and the industrial and academic sectors. The important elements of CASD's mission are to perform basic and applied research in the areas of chemical syntheses, properties, structures, transformations, and analyses.

The two precursor divisions had somewhat different subject matter portfolios and research styles. The merger offered an opportunity to merge complementary strengths and experiences. The centerpiece emphasis on analytical chemistry and radioanalytical chemistry within the former ACD carried over to become a major emphasis in CASD, but the research portfolio was broadened by the addition of programs from CD in other subdisciplines of chemistry, including some less traditional areas such as materials chemistry and geochemistry. The two divisions also had somewhat different relative emphases on "basic" and "applied" research projects, and the consolidated portfolio appears closer to the desired balance. A continuing challenge to DOE's national laboratories is to better integrate basic and applied research in individual research groups in a synergistic and bidirectional fashion, without compromising the specific character of each. The new division is well poised to face that challenge.

A number of organizational changes were made to promote interactions, both in the makeup of individual research groups and in clustering these groups into sections. The Analytical Spectroscopy Section consolidates research activities in diverse aspects of inorganic and organic mass spectrometry, laser spectroscopy and miniaturization of analytical techniques, and surface science. The Nuclear and Radiochemistry Section groups together the major activities that involve radioactive materials, from basic research to special radioanalytical capabilities, and that therefore

require operation of nonreactor nuclear facilities (see below). The Organic Chemistry Section emphasizes organic analytical instrumentation and methodology as well as physical organic research. Finally, the Physical and Materials Chemistry Section contains a variety of research activities that fall into the subdisciplines of physical, inorganic, solution, and materials chemistry.

The support functions of the division were organized into an Office of Environmental, Safety, Health, and Quality Performance and Facilities Operation and an Office of Administrative Services. It was able to draw on the expertise of incumbents from both former divisions and to increase their contributions by typically increasing their span of interactions while focusing their areas of emphasis and expertise. Special attention has been given during the reporting period to improving operations and meeting compliance requirements for the division's two "nonreactor nuclear facilities," the Radioactive Materials Analysis Laboratory and the Transuranium Research Laboratory. Although requiring an expanding commitment of time and resources to maintain safe and compliant operation, these facilities continue to provide unique opportunities for significant research and special analytical projects. The division's performance in the ESH&Q arena has been noteworthy in spite of ever growing regulatory pressures.

The funding profile of CASD includes three major sponsor segments: the DOE (approximately 70%), other federal and private agencies (approximately 10%), and special analytical projects (approximately 20%) for LMES and ORNL programs in isotope production, waste management and environmental restoration, and national security. The single largest DOE sponsor is the Office of Basic Energy Sciences (OBES), with significant contributions as well from the Office of Environmental Management, the Office of Nonproliferation and National Security, and the Office of Energy Efficiency and Renewable Energy.

The division had the opportunity during the reporting period to add a number of new employees, largely by replacement of retirees, who are adding to the creativity and vitality of the research and support staffs. The work of the research staff profits from the presence of numerous long-term guest scientists. For many of them, their assignments in CASD offer valuable educational and professional development opportunities. At any particular time, some 30-35 postdoctoral fellows are in residence, along with numerous graduate and undergraduate students.

Partnerships with academia and industry have been growing as the division has placed more emphasis on making its capabilities available to other sectors of the chemical research enterprise. A number of university professors have spent significant blocks of time as guests of CASD during this reporting period. Currently active mechanisms for industrial interactions include Cooperative Research and Development Agreements (CRADAs), the Advanced Technology Program of the National Institute of Standards and Technology (ATP-NIST), and the Technology Reinvestment Program (TRP) of the Department of Defense (DOD), as well as direct industrial support for special analytical projects.

1. ANALYTICAL SPECTROSCOPY SECTION

S. A. McLuckey, Head

The Analytical Spectroscopy Section is composed of five groups: Inorganic Mass Spectrometry, Optical Spectroscopy, Organic Mass Spectrometry, Secondary Ion Mass Spectrometry, and Surface Chemistry and Heterogeneous Catalysis. Heavy emphasis throughout the section is placed on experimental research and development. Much of the work is centered on advancing the state of the art in chemical measurements with particular emphasis devoted to separations, optical spectroscopy, various forms of mass spectrometry, neutron scattering and positron spectroscopy. The Surface Chemistry Group relies heavily on various surface analysis tools, including ion scattering spectroscopy, with special current emphasis on catalytic reactions of organosulfur molecules. The section and its predecessors have also played an important historical role in the analytical support of a wide variety of research and development programs at Oak Ridge and other DOE facilities. This work is currently concentrated in the Inorganic Mass Spectrometry Group and involves, *inter alia*, high precision isotope ratio measurements in support of DOE's isotope production programs.

The section is comprised of approximately thirty full-time staff with expertise in physics, instrumentation, computers, and, of course, many subdisciplines of chemistry. Fifteen to twenty-five visitors, including visiting scientists, postdoctoral associates, graduate students, and undergraduates, work with the staff at any given time. These guests benefit from access to state-of-the-art equipment, mentoring by mature scientists, and participation in exciting research activities while at the same time bringing new ideas, new capabilities, and added enthusiasm to the section.

INORGANIC MASS SPECTROMETRY GROUP; D. H. Smith, Leader

Research Activities

Glow Discharge Mass Spectrometry -- An investigation into the cause of anomalously high ion intensities for materials deposited as solutions on the sample cathode led to the conclusion that reactive sputtering was almost certainly the explanation. The utility of using argides, metallic dimers, and +2 species for quantification was demonstrated. ZnAr^+ was observed to be present at anomalously high concentrations (up to 30% of the Zn^+); the current explanation for this phenomenon is that Zn sputters much more efficiently than the other metals investigated. An evaluation of the ability to measure isotope ratios using a glow discharge source yielded precision as good as $\pm 0.03\%$; this value was realized with several elements (Pb, Cu) and almost certainly reflects an instrumental limitation. This work is on hold pending arrival of a Fisons Plasma-54 mass spectrometer which is equipped with seven collectors; substantially improved precision is anticipated when a glow discharge cell is interfaced to this instrument. Development of an rf cell for analysis of nonconducting samples continued with design of a cell that accommodates flat specimens (as opposed to the conventional pin shape). A new electrical interface was developed as well. This combination resulted in improved mass resolution and sensitivity in comparison to previous efforts. It offers promise for depth profile analysis of nonconducting films. A glow discharge cell was interfaced to our new Teledyne ion trap. This work is in its early stages; signal-to-noise ratios have been improved; selective ion accumulation has been demonstrated; MS-MS experiments have been performed. The immediate goal of this work is to obtain an elementally pure spectrum free of molecular interferences; if achieved, this capability will have a profound influence on the field of elemental analysis.

Secondary Ion Mass Spectrometry -- A significant advance in the measurement of isotopic ratios from insulating materials was made by using extreme energy filtering to select only those ions of greatest energy. Interfering molecular species are not formed at these high energies, and being able to measure elementally pure beams allowed attainment of unprecedented precision (0.02-0.03% for S⁺; 0.06% for O⁺); these levels reflect the ineluctable limits imposed by counting statistics. This technique has been applied to various geological systems and to studies of corrosion in vessels used in commercial power generation.

Thermal Ionization -- Using the Re overcoating technique developed several years ago, isotopic ratio measurements were made on 10⁷ atoms of Pu. This level of sensitivity compares well with that reported by other laboratories and implies that detection limits are 10⁶ atoms or lower.

Inductively-Coupled Plasma Mass Spectrometry -- Individual tree rings were analyzed by laser ablation to determine the variation of the ratio of Al to Ca over time. This ratio increased as the present day was approached, implying that changes in soil pH caused by acid rain contributed to degradation of the health of trees over the period in question. Electrochemical concentration of various elements prior to introduction to the torch resulted in improvements in detection by factors of 100 (to the mid-ppq [part per quadrillion] region!) for several elements (e.g., Tl). Interference from the matrix was eliminated as well, suggesting that this technique can be exploited to provide enhanced performance in instances where it is needed.

Support Activities

IAEA field trials to evaluate the ability of long established analytical techniques to detect clandestine nuclear activity led to heavy demands on our capacity. Over 100 samples were received and analyzed. A new glow discharge mass spectrometer obtained for support work was delivered in December 1993, but has yet to meet specification. Intense efforts on our part overcame most of the host of problems resulting from the instrument's original design; we are presently awaiting delivery of a new gas inlet system (designed in the wake of our experience) that we hope will bring the instrument up to expected performance. Our NASA project concluded with evaluation of a gas mass spectrometer for application in pre-lift-off monitoring of various signature gases. Use of our Lu double spiking procedure was enhanced by development of a hot cell chemical separation procedure. Work continued in conjunction with George Swihart (Memphis) in providing high precision analysis of B. ORNL's Stable Isotopes Program recently contracted to provide ca. 125 g per month of 95% enriched ²⁰³Tl. We provide 4 to 6 weekly isotopic analyses and monthly elemental analyses in support of this project.

Move from Y-12 -- As might be expected, our move is going far more slowly than anyone wants, but progress has been made despite innumerable bureaucratic obstacles. Two of the ORNL designed instruments are now in operation in Building 5505; the third is presently being readied for shipment. We have beneficial occupancy of the clean room (two years behind schedule). The end is in sight, at least with regard to having all operations shifted to X-10; getting free from Y-12 is an entirely different question. About 80% of the space in 9734 and 9735 has been turned over to new owners; it is anticipated that leaving the old Transuranium Laboratory will require years of effort.

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OPTICAL SPECTROSCOPY GROUP; J. M. Ramsey, Leader

This group is involved in a broad range of research and development tasks including laser-based measurement techniques that provide ultrahigh sensitivity and/or specificity, microfabrication of chemical processing and measurement devices, and crystallographic molecular structure elucidation.

Work on laser-based measurement techniques continues to include studies of single molecule detection in liquids. Single molecule detection limits by laser induced fluorescence of Rhodamine 6G has been demonstrated in a stream of droplets passing a detector at a 100 Hz rate. These results show the feasibility of performing single molecule measurements at practical analysis rates. The goal is to achieve single molecule detection limits at rates exceeding 1 KHz. Work is also progressing on understanding QED enhancements of fluorescence emission rates in microdroplets and the role of solvent dynamics. Studies of hot filament CVD diamond film growth processes have focused on monitoring of methyl and hydrogen radicals in the boundary layer region. A new frequency doubler has been put in operation to enhance resonance ionization signals of these radicals that are subsequently analyzed by time-of-flight mass spectrometry. A new atmospheric interface has been assembled to allow direct injection of aerosol particles into a quadrupole ion trap mass spectrometer. The first ever tandem mass spectrometry experiments on single microparticles has been completed. In addition, the first demonstration of the ability to use a single electrodynamic trap for both particle trapping and ion trapping was demonstrated. This combination allows nondestructive spectroscopic examination of a single microparticle with subsequent laser desorption/mass spectrometry analysis. Studies also have continued on the use of an all silica fiber optic probe to perform remote spectroscopic analysis of environmental contaminants. Enhancements to this probe are being developed to allow surface enhanced Raman spectroscopy to be performed at the distal end of the probe.

A number of new concepts have been demonstrated with microfabricated devices for chemical analysis. Micellar electrokinetic capillary chromatography (MECC) was demonstrated on a microchip device. This technique allows the separation of neutral species in a capillary electrophoresis (CE) format by including micelles in the buffer which act as a pseudo stationary phase. Separation efficiency and reproducibility were equal to or better than those of conventional capillary experiments. Devices have been fabricated out of new materials, quartz, and BK7 glass that have superior optical properties to the previously used soda lime glass. A preconcentration technique, sample stacking, has been demonstrated "on a chip." Detection enhancements of more than an order of magnitude have been observed with the worst case scenario, anions. Moreover, the first integrated chemistry devices have been demonstrated that combine chemistry and chemical analysis on a single device. CE was combined with a post-column and pre-column reaction chamber. The pre-column reactor was used to demonstrate the measurement of chemical reaction rates on a microchip device. Kinetic information can be obtained in minutes with procedures under computer control consuming approximately 100 nL of reagents. The ability to integrate chemical processing on microfabricated

devices is significant as it allows manipulation of fluid volumes many orders of magnitude smaller than that possible by using conventional techniques, and the processing is inherently automated.

The project on crystallographic computing and topology specializes in the use of Morse critical point theory and orbifolds for characterization of crystal chemistry families and simplification of space group symmetry theory applications. Development of an ORNL Orbifold Atlas that can serve as a topological supplement to the International Tables for Crystallography with descriptions of the singular set, underlying topological space, and other topological invariants for each of the 230 crystallographic space groups was started. The computing part of the project completed the software upgrade and testing of the biomolecule x-ray facilities in the Biology Division and the neutron diffraction 4-circle facilities at the High Flux Isotope Reactor (HFIR), which were upgraded in hardware by a previous Laboratory Directed Research and Development (LDRD) project. Neutron diffraction data sets were then collected and processed for 13 compounds in collaboration with users from England, Germany, Canada, and the United States.

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ORGANIC MASS SPECTROMETRY GROUP; M. V. Buchanan, Leader

This group conducts fundamental and applied research in organic and biological mass spectrometry, with particular emphasis on trapped ion techniques, both quadrupole ion trap (QIT) and Fourier transform ion cyclotron resonance (FTICR) mass spectrometry. Investigations of physical processes which occur in the ion trap are being pursued to allow new modes of trap operation to be developed and enhance the analytical utility of this device. Fundamental aspects of collisional activation and dissociation processes are being investigated to provide insight into ion energies and temperatures in a trap during ion storage and resonance excitation. Results to date indicate that resonance excitation acts as a thermal excitation source that produces a relatively slow increase in ion internal energy due to many discrete collisional excitation/relaxation events. Methods and electronics for *in situ* detection of ions in a QIT have been developed which yield improvements in signal to noise due to the ability to remeasure ion currents from the same population of ions multiple times.

Electrospray (ES) is being investigated to gain insight into the fundamental processes involved in this ionization technique. A series of experiments have demonstrated that ES can be characterized as a two electrode controlled current electrolysis cell. The potential at the metal/solution interface is a function of the ES current and the relative redox potentials and concentrations of the various species in the system, including the metal capillary. Further, the entire process is limited by both the ES current and the solvent flow rate through the capillary. Information gained from these studies is allowing new ways to expand the analytical utility of ES, such as use of ES MS as a highly sensitive and mass selective detector for electrochemical experiments and rapid, on-line electrochemical preconcentration/clean-up techniques for enhanced trace detection of metals, semivolatiles and nonvolatile organics. Electron transfer and chemical reactions have been employed to extend the application of ES to a wider range of organics, such as polycyclic aromatic hydrocarbons, fullerenes,

and others. Investigations have been conducted to increase the sensitivity of ES, especially when combined with on-line capillary electrophoresis. Sheathless electrospray sources using small i.d. gold tipped capillaries have been devised, and detection of attomole quantities of proteins have been achieved. An electrostatic ion guide, consisting of a cylindrical tube with a concentric wire, has been employed to guide ions generated in an ES source through the fringe fields of the 3T magnet of the FTICR. The guide is housed in a vacuum chamber that has three differentially pumped regions. Initial results using a variety of biomolecules have shown that ions may be trapped without the use of a pulse of buffer gas and with low trapping plate voltages, suggesting that the ions arrive at the cell with low kinetic energies. Experiments are now under way to reduce the pressure in the overall system and deflect ions after excitation and detection events to improve mass resolution and other performance characteristics.

Fundamental aspects of matrix assisted laser desorption/ionization are also being investigated using a specially designed time-of-flight instrument. Optical and other methods are being used to probe chemical and physical parameters which affect the success or failure of the MALDI experiment. The results from these studies are being used to extend the mass range and sensitivity of MALDI, especially for oligonucleotides. Other approaches for enhanced MALDI generation of oligonucleotides are also being investigated. Electrophore tags are being attached to the 5'-terminus of an oligonucleotide so electron capture conditions can be used to form ions more efficiently and with less fragmentation than with conventional MALDI conditions. A number of these tags have been synthesized (by Phillip Britt of the Physical Organic Group) and are stable in the MALDI process. The time-of-flight instrument is being modified to permit MALDI under electron capture conditions.

Development of gas phase processes to yield more detailed structural characterization of organics and biomolecules remains a major area of emphasis in the group. Collision induced dissociation processes have been employed with FTICR and MALDI to characterize a series of adducts of DNA oligomers, including identification of the adduct, site of attachment to the nucleobase, and location of the adducted base within the oligomer. New off-resonance excitation techniques have been applied to collisional dissociation studies of MALDI generated ions from oligonucleotides. These new techniques provide increased fragmentation and thus enhanced structural information for these singly charged ions. MALDI FTMS is also being used to identify and structurally characterize a variety of nanoclusters ranging from endohedral fullerenes to gamma radiolysis products of C_{60} . For example, it was found that the ionization potentials of $La@C_n$ are substantially lower than the corresponding values for the empty fullerenes, implying that the lanthanum atom donates electron density to the fullerene cage. The relative gas phase acidities for nucleobases have been determined using ES QIT and will be used to understand the decomposition behavior of multiply charged oligonucleotides via collisional activation. This information will provide insight into oligonucleotide sequence. Investigations of ion/ion reactions in a QIT with ES generated multiply charged ions have revealed that these reactions are more energetic, efficient, and rapid than ion/molecule reactions. Further, ion/ion electron transfer has been observed to yield more extensive fragmentation than ion/ion proton transfer. Ion/molecule reactions involving proton transfer with an ion at a specific m/z value have been explored as a means of enhancing mass resolution of ES spectra where individual charge states are not resolved.

Both MALDI and ES are being explored for rapid, confident detection of polymerase chain reaction (PCR) fragments that are widely used in clinical, forensic, biochemical, and other laboratories to

identify people, heritable diseases, and pathogens. Working with a team of researchers from the Biology and Health Sciences Research divisions, we have demonstrated that both ionization techniques may be used to detect synthetic oligomers and PCR products. In the latter case, we have detected DNA fragments diagnostic of cystic fibrosis in humans and fragments specific to *Legionella* bacteria.

The group is actively involved in a number of projects in which the unique capabilities of ion traps are employed for rapid, confident detection of trace compounds and for chemical analysis in the field. We have continued work on the combination of the ORNL atmospheric sampling glow discharge ionization source (ASGDI) with tandem mass spectrometry. Specific attention has been focused on interfacing the source with a small commercial QIT and reducing source pumping requirements by a factor of ten over the normal source. The ORNL ASGDI was recently introduced commercially by Teledyne MEC and exhibited at the Pittsburgh Conference in February. Ion trap instrumentation is being developed as part of a CRADA with the automotive industry to design and build a small, easy to operate instrument for characterization of ultra low emission vehicles (joint with the Instrumentation group). Both ASGDI with NO^+ attachment and *in situ* chemical ionization are being investigated for real-time characterization of emissions from a vehicle being tested on a dynamometer. Methods are also being developed for the rapid detection of target compounds in foods and physiological media using ion traps, especially in combination with new ES techniques. In collaboration with the Knoxville Police Department, we have initiated investigations to help explain why latent fingerprints from children disappear from surfaces faster than those from adults. Initial investigations of the chemical components of fingerprints from children and adults have revealed distinct differences, primarily in the types and molecular weight distribution of compounds that support these observations. Based on these studies, Reza Dabestani and Mike Sigman (Physical Organic Group) will develop an improved method for visualization of fingerprints.

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SECONDARY ION MASS SPECTROMETRY GROUP; P. J. Todd, Leader

Research in the Secondary Ion Mass Spectrometry (SIMS) Group centers around development of new analytical capabilities, with special emphasis on spatially resolved analysis (i.e., imaging), along with improvements in ion optics and methods of data acquisition. We receive funding from a variety of sources which covers projects from basic research of fundamental problems to instrumental and data systems development. The interplay among these various projects is such that barriers to progress found in areas of development in one project stimulate basic research to understand and overcome these barriers. Funding sources over the past two years include the DOE Office of Basic Energy Sciences, the Office of Research and Development, the National Institutes of Health, the Laboratory Directed Research and Development Program, and support from the Mass Spectrometry Development Group at Y-12.

We have overcome the fundamental barrier to imaging organic compounds known as the static SIMS limit. This limit is the dose of primary ion (ca. 10^{13} primary ions/cm²) beyond which organic compounds cease to emit *characteristic* secondary ions. This limit has been a profound barrier to mapping the distributions of organic compounds in tissue. Overcoming the static SIMS limit means that the surface of a sample can be cleaned in vacuum, greatly simplifying sample preparation. Furthermore, analysis of dilute samples by summing and averaging data, as well as obtaining depth profiles of organic samples, becomes possible. We accomplished this feat by coordinated use of a primary beam of massive, multiply charged glycerol clusters and our Cs⁺ ion beam. The Cs⁺ beam is routinely used for imaging because it can be focused and rastered. The cluster beam can neither be focused nor rastered. However, by alternately turning the Cs⁺ beam on and off in complement with the cluster beam, images can be obtained with the Cs⁺ beam and the damaged surface molecules removed with the molecular beam.

Use of the cluster gun has also enabled us to analyze lipids and sugars directly by SIMS without any sample preparation. In fact, we have observed secondary ions characteristic of lipids directly from biologic tissue. These observations represent a major milestone in the application of SIMS to imaging and analyzing biologic tissue. Two major barriers to the ultimate goal of imaging biologic tissue for drugs and their metabolites, namely the static SIMS limit and the lack of characteristic secondary ion emission from tissue, have been overcome.

We have developed a routine and general method of charge compensation for secondary ion imaging of large heterogeneous insulating samples. Most organic samples, in particular biologic tissue samples, are insulators. If the charge which accumulates on the surface of an insulating sample when bombarded by the primary ion beam is not neutralized, analysis by SIMS becomes impossible. With our technique, the secondary ion extraction field is synchronized with a periodic primary Cs⁺ beam to allow a sheetlike beam of 5 eV electrons to pass over the sample surface. Electrons are attracted to and neutralize any points on the sample that have accumulated positive charge. We now use the technique routinely for static SIMS imaging of biologic and other insulating samples.

We have advanced the field of time-of-flight (TOF) mass spectrometry by experimentally demonstrating that an ion mirror can be constructed which compensates for initial ion kinetic energy distributions in both the ion extraction field as well as the field free drift region. Ion kinetic energy distributions are often the limiting factor in determining mass resolution for TOF mass spectrometers since a distribution of energies (or velocities) leads to a distribution of ion flight times, unless properly compensated for. Conventional ion mirrors compensate only for the drift region. By careful analysis of the entire TOF mass analyzer, we were able to devise a suitable modification to the conventional mirror design and then experimentally demonstrate this capability. The consequence of these measurements is that the ion extraction region no longer needs to be very small relative to the rest of the TOF spectrometer. The removal of this limitation opens the way for development of large field-of-view imaging TOF microprobes and compact TOF SIMS instruments. Although the prototype TOF SIMS instrument compensates for initial kinetic energy distributions in both the extraction field and drift regions, it is very sensitive to small variations in the sample surface potential. In other words, ions (of the same mass) leaving the sample with a distribution of energies have essentially the same flight time through the mass spectrometer, leading to a well defined TOF mass peak. If the sample surface potential changes, however, this peak shifts in the TOF spectrum. We were able to exploit this feature of our TOF spectrometer to measure small changes in the surface potential

of insulating samples subjected to TOF SIMS analysis. We were able to demonstrate that the equilibrium surface potential reached with charge compensation using low energy electrons could be measured and was a function of the charge compensating electron current. This technique should be useful for fundamental studies of surface charging, as well as a method for evaluating the effectiveness of various charge compensation schemes.

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SURFACE CHEMISTRY AND HETEROGENEOUS CATALYSIS GROUP; S. H. Overbury, Leader

This group contains two programs. The objective of one program is to understand fundamentals of catalytic reactions of organosulfur molecules occurring at metallic surfaces and to understand how these molecules affect and are affected by the surface structure and composition. The approach is experimental but is complemented by theoretical modeling used as an interpretive tool. Adsorbates chosen for study include thiols, substituted thiophenes, bifunctional molecules such as benzenethiol and mercapto-ethanol, related organic molecules, and partially deuterated derivatives of these molecules. Substrates are metallic and bimetallic single crystals, ultra thin films grown on metal single crystals, and these surfaces following sulfidation or oxidation. The objective of a second program is to develop and apply positron spectroscopy techniques. This involves fundamental studies of the interactions of positrons with materials, applications of the techniques to practical samples, and development of instrumentation and collaborations.

Various methods were applied to study sulfidation of surfaces. High resolution soft x-ray photoemission spectroscopy (SXPS) experiments were performed on the U-13 undulator at the National Synchrotron Light Source to characterize the sulfidation of Ni(111). Combined with other data, a new structural model of the high coverage sulfided surface has emerged and demonstrates the ability of SXPS to determine the bonding environment of S atoms. Low energy alkali ion scattering, ISS, has been used to determine the interaction and structures of co-adsorbed S and Ni on the W(001) surface. The goal of this study was to determine how a strongly bonded adsorbate, sulfur, interacts with a well characterized bimetallic system.

Growth and structural evolution of Ni and C overlayers deposited on W(001) were studied by ISS and W 4f_{7/2} SXPS. This work allowed comparison between structural details obtained from ion scattering with measurement of the electronic environment sampled by SXPS. The correlation of structural and electronic information shows that the W core levels are less sensitive to the type of nearest neighbors they have than they are to their location relative to the surface. For the carbided surfaces, peaks associated with W atoms bonded to two, three, and four C atoms are evident in the spectra.

ISS studies were undertaken of the structure and surface composition of the (110) and (100) surfaces of FeAl alloy single crystals. First and second layer compositions were determined for each crystal face. An investigation of the structure of clean and Pt covered ZnO by ISS was initiated. To understand supported catalysts it is important to develop new techniques to probe the structure of oxide surfaces and their interaction with metals deposited upon them. Analysis of bulk and thin film oxides will be a major future research emphasis.

Reaction studies of methanethiol, benzenethiol, and dimethyldisulfide (DMDS) on Ni(111) were undertaken during this period. Reaction products, desorption profiles, and preliminary spectroscopic results were obtained. Extensive studies were made of methyl thiolate formed from methanethiol and DMDS. SXPS data proves the presence of two types of molecular intermediates at high coverage. Consideration of HREELS, SXPS, and computational modeling indicates the two intermediates are adsorbed on bridge and hollows sites. Benzenethiol yields only one type of thiolate with C-S bond tilted with respect to the surface normal. Extensive studies of the kinetics of C-S bond scission using SXPS during isothermal anneals provide evidence of hydrogen assisted C-S bond scission in benzenethiol.

SXPS experiments have been conducted on the reaction of methanethiol on ultra thin Ni and C films deposited on W(001). It is found that thin pseudomorphic Ni films increase selectivity for methane production compared to total decomposition, higher than from clean W or Ni surfaces. The reactivity of methanethiol can be correlated with the structure of the Ni films on W(001), known from ion scattering measurements. On the C modified surface, selectivity for methane formation is also high, and molecular methanethiol is stabilized to higher temperatures. Isotopic labeling indicates that there is little incorporation of the sulfhydryl hydrogen in the methane desorption products. The stability of the thiolates in the bridge sites is also higher than that of thiolates in four-fold sites on the clean surface.

Reactions of thiophene and methyl substituted thiophenes were examined on clean and hydrogen treated Ni(111) surfaces to determine both reaction mechanisms and the effects of hydrogen on the reactions. Thiophenes desulfurize to form mono-unsaturated alkenes. Increasing the availability of hydrogen increases the selectivity toward alkene production but does not result in alkane formation. Steric effects were observed in the reaction as 2,5-dimethyl thiophene underwent rapid cleavage of the methyl groups resulting in only C_4 products, while 3-methyl thiophene produced significant pentene. The data are interpreted in terms of either a "metallocycle" intermediate or a π -bonded allyl fragment. Such detailed understanding may allow altered hydrocarbon product selectivity in HDS reactions.

The ability of a laser to remove surface defects from Si(100) was studied by STM. Using sequential, low power, green laser pulses, the dimerized first layer of Si(100) could be mostly removed leaving a vacancy free underlayer with altered structure. This selectivity is believed to be due to the reduced coordination of Si atoms at steps or adjacent to vacancies. This work has implications for possible new methods for the processing of semiconductor surfaces.

Positron and electron induced luminescence were compared to learn more about the mechanisms for positron excitation. Optical spectra of the light emitted from anthracene dissolved in polystyrene were obtained for bombardment by 3 keV positrons or electrons. Differences are attributed to the fact that electron bombardment produces electron hole pairs, while positron excitation can give rise to unpaired holes which ultimately decay with an impurity or defect. Positron induced luminescence may therefore be a useful probe of defects, impurities, and material structures. Measurement of the energy broadening of positron annihilation radiation was tested as a diagnostic probe of paint weathering. It was found that changes due to simulated weathering for periods of a few weeks could be detected compared to control specimens and that there were variations depending upon the presence of pigments and the type of binders. The depth of weather penetration was determined by variation of the energy of the probing positrons. Molecular ionization of gas phase molecules, induced by

positrons with energies from 0.3 to 3 eV, were studied. It was found that positrons with very low energies, below the threshold for positronium formation, can yield significant fragmentation in large alkane molecules. The cross section for fragmentation depends upon the size and structure of the molecule.

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2. NUCLEAR AND RADIOCHEMISTRY SECTION

J. R. Stokely, Head

The Nuclear and Radiochemistry Section is composed of four groups which perform research, development, and special support for a number of different DOE and LMES programs and a few private corporations. Most of the work conducted by the section involves the handling of radioactive materials in special experimental facilities designed for this purpose. There is considerable variation in the type of work done by the different groups ranging from fundamental chemical R&D to short-term studies needed to meet specific project objectives. Studies and special support are performed in the following general areas: investigation of the fundamental chemical and physical properties of the actinide elements and compounds, characterization of radioactive waste to provide information needed for remediation efforts or environmental compliance, chemical and radiochemical analyses to support the ORNL transuranium element production program, and utilization and advancement of neutron activation analysis for characterization of materials. Applied support and R&D activities within the section often yield new methodology and insight which allow contributions to be made to methods compendii, program reports, or scientific publications or presentations.

NEUTRON ACTIVATION ANALYSIS GROUP; L. Robinson, Leader

The Neutron Activation Analysis (NAA) Group continued conceptual design efforts in support of the Advanced Neutron Source (ANS) project. The ANS project supported personnel for a two week visit to the research reactor at the National Institute of Standards and Technology. During this visit, research was conducted that confirmed the applicability of both thermal and cold neutron prompt gamma ray analysis to the determination of trace elements in soils taken from the Oak Ridge Reservation.

Delayed neutron counting (DNC) was applied in a number of studies in which fissile element content was of interest. Due to a high neutron flux at the High Flux Isotope Reactor (HFIR) and an extremely low delayed neutron background, a detection limit of approximately 10 nanograms per gram was established. This allowed the group to participate in a nuclear nonproliferation study in conjunction with the DOE and the International Atomic Energy Agency (IAEA) designed to determine fissile materials in environmental matrices. Samples included pine needles, tree bark, grasses, mosses, soil, water, and smears from laboratory bench tops. If levels of uranium (or plutonium) were above typical levels for a given matrix, then these materials were subject to additional analysis by mass spectroscopy. Other studies involving the use of DNC were gross fissile content of Gunite Waste Tank samples and transuranium waste samples from ORNL, uranium content of treated soils from the DOE's Fernald and Portsmouth sites, and uranium content in ocean floor sediments. In many of these studies DNC was used in conjunction with conventional NAA to determine the isotopic ratio of ^{238}U to ^{235}U .

In 1993 the NAA Group concluded a joint effort with researchers in the Environmental Sciences Division (ESD) to determine baseline concentrations of 35 elements in soil taken from around the Oak Ridge Reservation. This study was a follow-up to the 1991-1992 East Fork Poplar Creek project in which 4000 samples from the creek's floodplain were analyzed for eight elements by NAA. In the

baseline characterization study, about 140 samples were analyzed. The quality assurance standards in both programs were deemed comparable to existing protocols established by the Environmental Protection Agency (EPA) for the Contract Laboratory Program (CLP).

A Monte Carlo integration method has been developed to solve the integral form of the solution of the Boltzmann transport equation. The approach is used to treat neutron transport in a system with a californium-252 neutron source. The flux of cold neutrons is studied as a function of the moderator and cooling materials and as a function of the geometry of the system. This appears to be the first time that a Monte Carlo method has been used to obtain such results. These results are compared with those from the diffusion form of the solution of the Boltzmann equation and from experiments. The relationship between the momenta of two particles before and after collision are written in a new way. This relationship is that imposed by the conservation of energy and momentum in an elastic collision. These calculations could serve as the basis for the development of an actual cold neutron source which would have applications in trace element analysis and moderator development.

Neutron activation analysis continues to be used to detect ppm concentrations of ^{129}I in spent reactor fuel rods. Following chemical separation of unwanted fission products, iodine is retained on an ion exchange resin loaded directly in a small irradiation insert. These inserts are loaded directly into rabbits, irradiated, and counted the following day.

A neutron activation analysis procedure was developed to determine sub-ppb levels of molybdenum and tungsten in high purity silica gel. This work was prompted by a Work-For-Others (WFO) request by the General Electric Company (GE). GE fabricates quartz optical fibers from the silica gel, and apparently the presence of Mo and W causes embrittlement of the fibers. This project will help GE to select raw materials of the highest purity and to find sources of contamination in their manufacturing process.

A project to assist the Southwest Naval Engineering Command to determine naturally occurring radionuclides in building materials continues. Materials analyzed include gravel, sand, soil, rocks, cement, and finished concrete. Among the radioisotopes measured by high resolution gamma ray spectroscopy are ^{40}K , ^{238}U , and ^{232}Th . Radon emanation rates are determined by storing samples in dessicators for several days and sampling the air inside the dessicator with a Lucas cell. The Lucas cell has a zinc sulfide coating on one face, and light pulses produced in the cell by alpha particles are measured in a phototube.

A novel method for the determination of aluminum and phosphorus in biological material has been developed. It is extremely difficult to determine microscopic amounts of aluminum in the presence of macroscopic amounts of phosphorus due to the production of ^{28}Al from fast neutron reactions in stable ^{31}P . This new method takes advantage of the uniquely different neutron flux spectra of the two pneumatic tube systems at HFIR. The apparent Al production rates are determined in both systems using standards. Samples are then irradiated and counted similarly. Final concentrations of Al or P are determined from the solution of a set of simultaneous equations. This method has been validated using standard reference materials. Over 100 biological samples have been analyzed including brain, kidney, liver, and fingernails.

The application of NAA to geology and geochemistry continued via the group collaboration with geochemists from The University of Tennessee at Knoxville. Over 150 geological and lunar samples

have been analyzed. This association has led to two publications and the dissertation of one graduate student.

Since 1991 the NAA Group has collaborated with researchers in the ESD on a program to monitor airborne mercury levels in the vicinity of the Y-12 plant. Samples are taken by pumping a metered amount of filtered air through iodated charcoal traps. The charcoal in these traps is placed in high purity graphite rabbits and irradiated for up to five minutes. Radioactive ^{203}Hg is measured three to four weeks later.

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RADIOACTIVE MATERIALS ANALYSIS LABORATORY GROUP; J. M. Keller, Leader

The Radioactive Materials Analysis Laboratory (RMAL) develops new methodology for the inorganic and radiochemical analysis of radioactive materials. Most of the current work is directed toward the characterization of radioactive waste from underground storage tanks and radioactive sludge stored in drums. In addition, the group provides technical and analytical support to numerous programs and special projects within the laboratory. Over the past year the group has expanded to include a number of special projects involving environmental levels of radioactivity which include wildlife monitoring and a Noble Gas Monitoring System for the HFIR stack. A selection of the special projects and programs are discussed below.

Method development studies for the clean-up of radioactive waste samples for characterization are sponsored by the Analytical Services Division (ASD) of DOE/HQ. The purpose of the project is to develop more efficient methods for the characterization of radioactive waste samples from DOE facilities and to distribute these methods to potential users. Traditional methods are not well adapted to the handling of high levels of radioactivity in samples. Also, the standard method cannot handle interferences from the complex sample matrices typical of DOE radioactive wastes. Improved methods must consider as low as reasonably achievable (ALARA) practices, waste minimization, and contamination control. These improvements involve methodologies that reduce or replace hazardous reagents/solvents, can be performed remotely, require less time, and can be easily adapted to automation. These studies are presented in the form of procedures which are included in the *DOE Methods for Evaluating Environmental and Waste Management Samples* (DOE Methods Compendium), a compendium of sampling and analysis procedures for DOE waste samples, published by the ASD.

During 1993, method development studies focused on three main areas: clean-up of radioactive samples for (1) metals determination by Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS), (2) alpha spectrometry, and (3) radioactive strontium determination. These studies resulted in the development of new methods using extraction chromatography which reduce waste, time, and personnel exposure as compared to traditional techniques using solvent extraction and precipitation techniques. Results of these studies were presented at the 44th Pittsburgh Conference and Exposition on Analytical Chemistry and Applied Spectroscopy in

Atlanta, Georgia, and at the 1993 Analytical Chemistry Information Meeting Poster Session in Oak Ridge, Tennessee. The studies on metal determinations were published as an ORNL Technical Report, *Separation Techniques for the Clean-up of Radioactive Mixed Waste for ICP-AES/ICP-MS Analysis*, in March 1993. As a result of the strontium determination studies, a procedure, *Determination of Total Radioactive Strontium Using Extraction Chromatography*, was submitted to the ASD and included in the DOE Methods Compendium.

During 1994, studies concentrated on the determination of ^{99}Tc in radioactive wastes and contaminated oils. The studies of ^{99}Tc in radioactive wastes were combined with 1993 studies and presented at the American Chemical Society (ACS) National Meeting in Washington, D.C. The oral presentation has been submitted for publication in the proceedings of the national meeting. A new sample preparation method for ^{99}Tc , *Determination of ^{99}Tc in Oils Using a Muffle Furnace and Extraction Chromatography*, was also submitted to the ASD for inclusion in the DOE Methods Compendium.

The GAAT Treatability Study is a large program being conducted by the LMES Environmental Restoration Division for Environmental Restoration and Waste Management (ERWM)/LMES to determine the options for removing radioactive waste from the inactive gunite storage tanks located within the ORNL Waste Area Grouping (WAG) 1. RMAL became involved with this project in the summer of 1994, and we are currently funded at about \$800 K/year for analytical and technical support on the physical, inorganic, and radiochemical characterization of the tank waste. The data generated by the project will support planning in the areas of waste management, risk assessment, safety, design, and structural integrity.

RMAL is the lead analytical laboratory for the DOE Waste Isolation Pilot Plant (WIPP) Transuranic (TRU) Waste Characterization Program (TWCP). This work is supported by the DOE Carlsbad Area Office (DOE/CAO) and is currently funded at \$1.5 M/year. Waste characterization data will be collected to support regulatory compliance programs associated with the WIPP facility.

The TWCP requirements for WIPP involved the upgrade of facilities, procurement of analytical instruments and equipment, and the development of many procedures and project plans. The procurement and installation of several GC and GC/MS systems, new glove boxes, high pressure microwave dissolution systems, a mercury cold vapor AA system, and a data management system were completed during the 1993-94 time frame. Also completed during this period were the upgrades to several laboratories and modifications to the HVAC system for new glove box installations. The required procedures were developed, written, and approved during the past year. Quality assurance (QA) documents were prepared which included the development of the *Radioactive Materials Analysis Laboratory-Oak Ridge National Laboratory (RMAL-ORNL) Quality Assurance Project Plan (QAPjP) for the Transuranic Waste Characterization Program (TWCP)*. This QAPjP was submitted for review and approval to Idaho National Engineering Laboratory (INEL) in September 1994.

RMAL personnel provide radiological support and collaboration to LMES/TWRA/DOE for monitoring wildlife throughout the Oak Ridge reservation. These efforts mostly include the annual deer hunts held each fall and monitoring/tagging studies done on geese and turkeys. The total number of deer taken during the 1994 hunts was 495, consisting of 309 bucks and 186 does. The total number of deer not released to the hunter over the past two years is fifteen, which is below the average

retention percentage of about 3% for all hunts. Of the deer retained during the 1994 hunts, two were kept because of ^{137}Cs being present above the release limit of 5 pCi/g. This was the first time in ten years that deer were retained due to ^{137}Cs contamination (all other retained deer were due to ^{90}Sr contamination).

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TRANSURANIUM ANALYSIS GROUP; C. D. Parks, Leader

The Transuranium Analysis Group (TAG) is located in the Radiochemical Engineering Development Center (REDC), Building 7920. The group is currently made up of four staff members, four technical support members, and two subcontractor employees. The primary objectives of the group are to provide around-the-clock analytical support to the transuranium isotope production efforts by the REDC of the Chemical Technology Division (CTD) and to provide monitoring of radioactive and non-radioactive process waste streams for the Waste Operations Section of the Waste Management and Remedial Action Division (WMRAD). In addition, the group provides analytical support to a variety of laboratory programs including waste tank characterization projects, remedial action programs, radioactive waste solidification projects, and support of health physics throughout the laboratory for the identification of nuclides from various contamination events.

The analytical support provided for the REDC/CTD throughout CY 1993 and for much of the first half of CY 1994 entailed Mark-42 Fuel Assembly processing and development. The Mark-42 Fuel Assemblies were irradiated at the DOE Savannah River Site and are processed for the recovery of plutonium, americium, and curium. The first two of a planned ten fuel assemblies to be processed were completed during this period. Development support on the Mark-42 processing included a series of PUREX experiments to characterize the separation of plutonium from other transuranic elements and TRUEX experiments intended to validate the computer model (developed at Argonne National Laboratory) of the process which removes transuranic elements from waste solutions. The TAG also conducted experiments in conjunction with researchers from CTD on the removal of high levels of cesium from the MK-42 waste solutions using a resorcinol formaldehyde resin in order that the waste stream resulting from the processing is not as highly radioactive when discharged to the waste tanks. The level of support for the MK-42 processing included the analysis of 1,400 samples with approximately 17,000 analytical determinations during the period.

During the second half of CY 1994 and into CY1995, analytical support provided for the REDC/CTD involved TRU Campaign #69. The TAG performed a wide variety of chemical and radiochemical analyses in support of the processing and purification of curium, berkelium, californium, einsteinium, and fermium. The transcurium actinides are produced through the irradiation of curium targets in the HFIR, and radiochemical analyses are required throughout the purification to verify the processing steps and to quantify the amounts of material present. Development work during the campaign included the testing and implementation of a procedure to separate berkelium from cerium using Eichrom's TEVA•Spec extraction chromatography resin. The effort provided by the group for TRU Campaign #69 included the analysis of 941 samples with approximately 8,300 analytical

determinations. During the period CY 1993 and CY 1994, the total number of samples analyzed in support of TRU Campaign operations was 2,344 with approximately 19,000 analytical determinations performed.

The TAG performs both chemical and radiochemical analyses in support of ORNL's Waste Operations monitoring of various waste streams at the laboratory. Among the streams monitored are waters prior to release to the Clinch River, various ponds and creeks inside the laboratory for possible releases of radioactivity, and process water in areas prior to work. Routine samples are also taken from the Low Level Liquid Waste (LLLW) Facility to monitor the effectiveness of columns used on the LLLW stream to remove radioactive constituents. Samples from various nonradiological streams (Process Water Treatment Plant, Sewage Treatment Plant, etc.) are also monitored to ensure that activity is not being introduced. During the period CY 1993 and CY 1994, the TAG performed nearly 93,000 analyses on 30,000 samples received from the WMRAD.

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TRANSURANIUM ELEMENT CHEMISTRY GROUP; R. G. Haire, Leader

The Transuranium Element Chemistry Group's objective is to perform systematic investigations regarding the fundamental chemistry, physics, and materials science of actinide metals, alloys, and compounds. The goals are to advance the basic science of these materials and to provide information conducive to technologies that are relevant to various missions of the DOE.

The experimental research focuses on vapor and solid state science of the f-elements, with the emphasis being on the actinides through fermium. Several scientific disciplines are employed in the experimental studies; these include high pressure x-ray diffraction and/or spectroscopy, high temperature x-ray diffraction and mass spectrometry, laser ablation mass spectrometry, thermal analyses, solid state spectroscopy (Raman, absorption, fluorescence), and novel synthetic techniques. The chemistry of the actinides and transactinides is also considered theoretically using quantum and statistical mechanics.

Our high pressure studies explore the effects of pressure on materials. One of the principal effects of pressure is to decrease the atomic separations in materials, which can induce large changes in their chemical and physical properties and provide insight into their fundamental science. Collaborative investigations with the Institute for Transuranium Elements during this period have involved x-ray diffraction and resistivity studies of americium and einsteinium metals as well as several actinide bismuthides. For the metals, the focus was on the delocalization of the f-electrons and the occurrence of a metallic valence change due to pressure. From such studies we have established pseudo Hill limits, which are very useful for interpreting the behaviors of actinide compounds. Studies of the actinide monobismuthides searched for potential valence fluctuations brought about by pressure and allowed systematic comparisons to be made between their pressure behaviors and those of other actinide mononictides or monochalcogenides. Attempts were made to explain the structural transformations and volume collapses observed in terms of the electronic configurations of atoms comprising the compounds.

We have also pursued high temperature studies of f-elements which concern thermochemical and physicochemical properties of vapors and condensed phases. These studies have involved the actinide elements, alloys and compounds, and dealt with gas-solid reactions of uranium halides and technetium compounds; the vaporization and phase behaviors of actinide oxides; and the high temperature physicochemical properties of several actinide alloys systems.

High temperature gas solid chemical studies probed materials in special environments, revealing novel species and bonding not encountered under conventional conditions. Mass spectrometric Knudsen cell studies involving reactive gases with both technetium and uranium have identified aspects of their chemistries that may be problematic in remediation technologies. New vapor species of technetium have been identified (e.g., TcO_3Br , TcO_3I , etc.), some of which have no known Mn/Re analogs. Although extensively studied, some fundamental aspects of uranium halide chemistry remain enigmatic. We have now synthesized and identified new gaseous halides, UF_3Cl and UF_2Cl_2 , which help clarify the bonding concepts for mixed uranium halides.

Oxides are one of the primary compounds of the actinides; yet many have not been characterized thoroughly, and even less was known about their high temperature vaporization/decomposition behaviors. Knudsen cell mass spectrometry and X-ray diffraction were employed in high temperature systematic studies to determine their vaporization/decomposition behaviors, which were found to be controlled by underlying roles of the element's electronic configurations and promotion energies. A relationship was devised that allowed us to correlate actinide monoxide dissociation energies with the f-electron promotion energies, which established predictions and correlations for the vaporization behaviors of all the actinides. Supplemental studies of phase behaviors at elevated temperatures complemented these vaporization studies. Such data have important implications for the speciation encountered in immobilization technologies (e.g., glasses), the vapor diffusion of actinides during high temperature processes, new synthetic concepts, etc.

The alloying behaviors of actinide metals with other f-element and transition metals illuminates bonding and electronic structures in metallic systems (e.g., roles of 5f-electrons in intermetallic bonding); they are also important for understanding and/or predicting the behaviors of actinide materials in technological applications pertinent to remediation applications, medical uses, separations, etc. Our studies of such actinide alloys have employed primarily differential thermal analysis and x-ray diffraction. We have shown that the Np-Zr system differs significantly from the U-Zr system. The Np-Fe phase diagram was found to be similar to those for U-Fe and Pu-Fe but exhibited characteristics which could not be quantitatively predicted. Similar studies were initiated for other Np-transition metal alloy systems.

Another area of research has involved the chemistry and mechanisms of laser ablation and two dimensional (mass optical) spectrometry. The fundamental insights derived from these investigations are important for understanding and predicting the behaviors of actinides in multiple chemical situations, as well as probing a new dimension in actinide chemistry. Pulsed laser ablation of solids efficiently produces vapor species for a variety of investigations. In developing experimental techniques for actinide materials, we have discovered that ablation of lanthanide oxalates produces novel lanthanide oxide clusters (Ln_mO_n^+ , with m up to 64 and $n \approx 3/2 m$). These clusters exhibit remarkable stoichiometry/valence variations that reflect subtle distinctions between the electronic structures of the different lanthanides. Other ablation techniques are being developed to probe spectroscopic properties and metal ion molecule reactions.

We have frequently used solid state spectroscopy (Raman, luminescence, absorbance, etc.) to investigate a wide range of structural, electronic, and chemical properties of f-element materials. One area of investigation incorporating spectroscopy was the characterization (valence state identification, speciation, etc.) of f-elements in glass matrices. Another was the generation and characterization of divalent states of f-elements in a tetraborate host. Following confirmation of published work on the stabilization of divalent Eu, Sm, and Yb in SrB_4O_7 hosts, it has been possible to stabilize the divalent states of Tm, Nd, Dy, and Cf in this matrix. This procedure provides access to the divalent state of f-elements for other studies and will be pursued to determine the limit of stabilization afforded by this host.

Developments in quantum and statistical mechanics approaches, and in computers and software, have provided greater capabilities for computational and theoretical chemistry. Topics addressed recently include the eigenstates of Am, quantum mechanical calculations for element 106, statistical mechanical molecular dynamics calculations, and neutron transport calculations. Several electron excitation energies for Am have been derived, and the results show that some spectroscopic terms assigned presently to experimental levels are probably incorrect. These calculated excitation energies will be highly beneficial for assigning experimental spectra and understanding electronic transitions in Am. Calculations on diatomic molecules have determined bond energies for molecular ions formed between argon and several transition metals during glow-discharge mass spectroetry studies. These energies were employed for interpreting the experimental data. A new technique for calculating neutron transport properties has been developed for the design and development of californium-252 cold neutron sources. Our calculations were in good agreement with available experimental data and with results calculated via a diffusion approach.

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3. ORGANIC CHEMISTRY SECTION

M. R. Guerin, Head

The Organic Chemistry Section performs fundamental and applied research, technology and analytical methods development, and specialty analytical support involving organic chemicals and materials. Chemical research addresses the structure and reactivity of organic chemicals in their native environments. Coals, lignin, biomass, and surface bound chemicals are receiving primary attention. Thermal and photolytic transformation chemistries for solids and water, respectively, are of special interest. Work on the chemistry of solids and surfaces is enhanced by related research in solid state nuclear magnetic resonance and chromatography based surface characterization. Applied chemical research currently addresses the development and demonstration of low emission diesel fuels and improved technologies for processing wood of promise to the pulp and paper industry. Analytical research and development addresses advanced instrumentation, high sensitivity sampling and analysis methods, and the fundamentals of chromatographic separation. Ion trap mass spectrometry continues as the primary area of instrumentation development with particular attention given to fieldable and continuous monitoring instruments. Solid sorbent air sampling and solid phase extraction of aqueous samples are combined with ion trap and chromatographic methods of analysis to yield part-per-trillion sensitivities. Specialty analytical support in this period has included direction of a national survey of exposure to environmental tobacco smoke, characterizing the headspace of underground storage tanks containing radioactive wastes, and establishing a facility for analyzing mixed wastes.

ANALYTICAL METHODS GROUP; W. H. Griest, Leader

The objectives of the Analytical Methods Group are the development of organic chemical separations and measurements methods, and their application to scientific questions and programmatic issues. Group expertise includes sample preparation, chromatographic separations and measurements, spectrometric identifications, specialty sample matrices, unusual analytes, and ultratrace determinations. The group is funded mainly by the DOE and the DOD (U.S. Army), but also is supported by other federal agencies (National Cancer Institute and U.S. Forest Service).

The analysis of environmental materials is a major focus of the group for several sponsors. Two major problems in the accurate analysis of volatile organic compounds (VOCs) in soils are the preservation of VOCs during sample shipment and their incomplete extraction in analysis. Optimum refrigerant packing conditions which preserve samples in coolers for shipment up to five days have been identified and demonstrated in a field study, and a hot methanol extraction method which recovers VOCs from soil more efficiently than the EPA purging protocol has been developed. It is suspected that VOCs sequestered in micropores and fissures of soil particles are displaced and released more efficiently by the hot polar solvent than by the bubbling action of the conventional gas purge.

Unusual environmental contaminants determined for military sponsors include a rocket propellant and phosphorus- and sulfur-containing chemical warfare agent decomposition products and

manufacturing byproducts. The method for determining N,N-dimethylnitrosamine (a propellant constituent) in groundwater was developed, certified, and applied with excellent results to approximately 50 groundwater and water treatment process research samples. The 2 parts-per-trillion level of sensitivity is unmatched by any other method or laboratory. It is achieved by the novel combination of a large volume injection (0.2 mL of a 1 mL solvent extract concentrate from 1 L of water) using a solid phase sorbent column and a short path thermal desorber, and gas chromatography (GC) with a chemiluminescence detector operated in the nitrosamine selective mode. More recent work aims to replace the 24-hour continuous solvent extraction with a carbonaceous solid phase sorbent. Development and certification is nearly complete for the alkylphosphonic acids method (detection limit of ca. 1 ppb in water), which features solid phase extraction with a quaternary amine anion exchanger substituted column medium, elution with an alkaline derivatizing agent which forms the methyl esters upon injection into the GC inlet, and detection/quantitation using a phosphorus selective flame photometric detector.

Explosives also are an important focus of method development and applications. The standard method for determination of explosives in soils requires an overnight ultrasonic extraction using acetonitrile, followed by high performance liquid chromatography (HPLC) with diode array ultra-violet absorbance detection. Initial investigations into a faster method based upon supercritical fluid extraction (SFE) provided evidence for the first time that nitramine explosives (important as a component of plastic explosives and some propellants) could be extracted by SFE. The important factors were a relatively high SFE temperature and a polar modifier in the supercritical fluid.

An unusual law enforcement related environmental analytical activity conducted for the U.S. Forest Service was the identification of unique compounds which could be used for the rapid detection at a distance of marijuana gardens (ideally, using airborne direct sampling ion trap mass spectrometry [DSITMS]). In a study conducted in collaboration with the Instrumentation Group and the Environmental Monitoring Group, air samples were collected within an experimental marijuana garden maintained by the U.S. Department of Agriculture and were analyzed using several techniques including GC-MS and DSITMS. Two sesquiterpenes, beta-caryophyllene and (-)-isocarophyllene, were identified as very promising indicators because of their relatively high abundance. Monoterpenes were not unique and were found in background sources such as pine and cedar.

Analytical methods for and investigations of hazardous and mixed wastes also are a major focus of the group. The efficiency of composting for decontaminating and detoxifying explosives laden soils and sediments has been investigated in a multidisciplinary study led by this group for the U.S. Army. Analyses of explosives and their microbial metabolites in soils and composts and determinations of the bacterial mutagenicity and leachable aquatic toxicity showed greater than 98% reductions in explosives content and similar decreases in toxicity by the composting process. The fate of the major explosive, 2,4,6-trinitrotoluene (TNT), also was briefly investigated. The TNT was not mineralized (converted to carbon dioxide, water, and nitrogen oxides), but rather biotransformed into an insoluble product which resists release into the environment. The evidence suggested that an amino derivative of TNT was covalently bound to humic substances in the soil. These findings were instrumental in the acceptance by the State of Oregon and EPA Region X of windrow composting for remediating explosives lagoon sediments at the Umatilla Army Depot activity site.

Not only explosives but also munitions have been the subject of analytical methods development and programmatic investigations. Studies for the Army demonstrated that adhesive joint failure in combustible cartridge case munitions is caused by an interdependent, multifactorial mechanism including heat and nitroester migration into the case wall from the propellant charge. A method for micro-sampling and analyzing the case wall without destroying the structural integrity of the round was developed. Current methods of sampling and analysis damage the round and make it unsuitable for further testing or firing. The nitroester migration in the case wall of M829 antitank rounds was mapped and found to be uniform circumferentially around the round but varied along the length of the round. This prompted the development of a prototype nitroester indicator patch which could signal the accumulation of nitroesters from the propellant in the case wall and identify rounds which are unsafe and liable to structural failure.

The group has developed many analytical methods for characterization of radioactive mixed wastes (RMWs) and is part of the unique analytical capabilities of the RMAL. For several years, EPA and other analytical methods have been adapted and their performance validated for their application to RMW analysis in glove box, hot cell, and radiochemical hood operations. Methods for extracting and analyzing volatile organic compounds, Resource Conservation and Recovery Act Toxicity Characteristic ("TCLP") semivolatiles and pesticides have been adapted, validated, and published in a DOE manual of methods for waste and environmental sample analysis. A particularly difficult achievement was the development, production, and performance validation of the prototype equipment for conducting the TCLP zero head-space extraction (ZHE) of VOCs. The equipment developed for the ZHE of RMW was found to perform better than the EPA TCLP protocol ZHE in preserving and recovering VOCs from wastes. The second phase of the project is now focusing on modifying state-of-the-art methods and instrumentation such as GC-ITMS and HPLC-MS to RMW analyses. It has been demonstrated that the GC-ITMS is 10^2 - 10^3 more sensitive in the analysis of semivolatile organic compounds than is the EPA protocol GC-quadrupole MS, and allows smaller sample amounts or more diluted extracts to be analyzed.

A unique laboratory has been set up at the RMAL for the preparation and organic chemical analysis of transuranic wastes on a custom production scale. Sample extraction, purification, and solvent concentration equipment has been set up in glove boxes and radiochemical hoods. A custom volatiles purging apparatus has been obtained and installed in a glove box and interfaced to a trap/desorption module and GC-MS located outside of the box. Other GCs and a GC-MS for analysis of semivolatile organics, nonhalogenated/water soluble volatiles, and PCBs have been set up in radiochemical hoods or laboratories. Method performance demonstration and procedure documentation are under way in preparation for regulatory analyses of transuranic waste sludges to be placed in the WIPP.

The development of methodologies for health effects issues and bioanalytical chemistry included the investigation of volatile organic carcinogens in food, the search for dibenzo(a,l)pyrene (DbalP, the most carcinogenic polycyclic aromatic hydrocarbon [PAH] yet discovered) in materials relevant to human exposure, and a mutagenic antibiotic that only affects female germ cells. A unique blender purge and trap device was developed to allow the accurate analysis of benzene and other VOCs in foods at low to sub-ppb concentrations. The method was demonstrated to be highly reliable and accurate, and the benzene content of many raw and cooked foods was determined. Of particular interest was the observation of a linear correlation between the benzene content and the level of

gamma irradiation (for preservation) of chicken meat. However, the levels of benzene were in the low ppb range even at the highest dose of irradiation (1.77 ppb at 3 KGy). A very extensive 16-step method consisting of solvent and pH partitioning, sorption column chromatography, and sequential HPLC on reverse phase/size exclusion/reverse phase columns was developed to isolate a very narrow PAH subfraction extending in ring size from benzo(ghi)perylene to anthanthrene in complex mixtures. Application to tobacco, charcoal and coal smoke particulates, a coal liquefaction heavy oil, and roofing tar indicated that DbalP concentrations are very low, and definitive evidence for its presence is exceedingly difficult to obtain. The upper limits to its concentration ranged from 75 ppb in combustion particulates from Chinese smoky coal to 4 ppb in tobacco smoke condensate. The main difficulty was the complexity of the isolate and the very low relative concentration of DbalP, which prevented positive ultraviolet spectral identification.

The antibiotic bleomycin affects female (but not male) germ cells. Means of detecting it in female germ cells are needed for studies of its mode of action. Methods were developed and demonstrated to harvest large numbers of oocytes from mice, expose them *in vitro* to bleomycin, extract bleomycin taken up by the cells, and detect it using matrix assisted laser desorption ionization time-of-flight mass spectrometry.

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ENVIRONMENTAL MONITORING GROUP; R. A. Jenkins, Leader

The Environmental Monitoring Group conducts applied research on the development and application of analytical methods for the determination of toxic species in complex matrices, with special emphasis on airborne and environmental mixtures. An important additional specialty is the area of enhanced biomass processing and fuels chemistry, with particular emphasis on process optimization. The group is funded primarily by the DOE, but is also supported by the Westinghouse Hanford Co., the DOD, and the Center for Indoor Air Research (CIAR).

A long term focus of the group has been the generation, sampling, and/or chemical characterization of complex airborne matrices. For example, we have developed sampling and analytical methodology bases for the determination of airborne organic species in the underground storage tanks at DOE's Hanford Site. The technology has been based on the collection of organics of a very wide range of volatilities on traps containing sequentially packed multiple sorbents, followed by gas chromatographic/mass spectrometric analysis. Fugitive emissions from these tanks over the years have resulted in a number of flammability and worker exposure concerns. To date, we have applied the methodology to the headspace characterization of more than 35 tanks at the site.

We have been conducting studies through a large CRADA with Cincinnati Milacron (CM). CM is one of the country's largest providers of machining fluids for the metal working industry. Aerosols of the fluids resulting from the machining process can often be irritating to workers. Studies in our laboratories have been directed toward the determination of particle size distribution of fluid aerosols

generated for inhalation toxicology studies of these fluids. Cascade impaction has been employed to provide size fractionation, relying on UV or fluorescence spectrophotometry for quantification of stage loading. In addition, we have been using HPLC to determine distribution of aerosol components as a function of particle size. Results to date have indicated a wide range of size distributions, depending on specific fluid compositions.

One of our most interesting recent studies has been the determination of human exposure to environmental tobacco smoke (ETS). Approximately 100 subjects were recruited from each of 16 cities around the country to wear personal sampling systems, both at work and away from work. Samples were analyzed for eight components of ETS, and individual samples of saliva were collected and analyzed for a metabolite of nicotine (cotinine) to assess smoker status and to compare individual ETS nicotine exposure with levels of salivary cotinine. The field phase of the study was concluded in June 1994, and data evaluation is ongoing. Preliminary conclusions from the study are that individuals living with smokers receive a greater ETS exposure at home than do individuals who are exposed in the workplace. In addition, the fraction of individuals who misreport their smoking status (i.e., claim to be lifetime never smokers but are in fact current active smokers) is much higher than that reported in previous studies. The latter finding has profound implications for the assessment of risk to lung cancer from ETS exposure.

A second focus of our group is the development and evaluation of technologies for more rapid and/or complete characterization of sites contaminated with organic wastes. To this end, we have been developing two subsurface sampling systems. One of these, the multisorbent arrayed sampler, consists of an array of six multisorbent traps, identical to those validated for the tank headspace characterization studies described above, in a remotely operated assembly designed to function in conventional 4" diameter monitoring wells. The sampler has an integrated packer so that the zone being sampled in the well can be isolated. Quantitative samples of vadose (unsaturated) zone soil gas can be collected on the sorbent traps and returned to the surface for analysis by a variety of analytical techniques. The sampler was deployed during two field trials each at DOE's Savannah River and Hanford sites. As a result of the Hanford deployments, several previously unreported semivolatile contaminants of the subsurface were identified. The DOD has been supporting the development of a membrane interface sampling system for both vadose and saturated zone implantation. This system is designed to be deployed with the Army's cone penetrometer system and permits contaminants, which pass through the interface, to be swept to the surface where they can be analyzed in real time using a direct sampling ion trap mass spectrometer. Unique features of this system will permit quantitative determination of soil gas levels of contaminants, independent of the soil permeability. We are exploring the patentability of the interface system. Laboratory evaluations are nearing completion, and the system is due to be field tested in the first half of CY 1995.

Another aspect of our enhanced site characterization efforts has been the evaluation of field analytical technologies, with the end product of the studies being the development of SW-846-type analytical methods for inclusion in the DOE Methods Compendium. During the past two years, we have tested and developed methods for several immunoassay kits for the determination of PCBs, mercury, and fuel components in soil and water, and colorimetric test strips for the determination of lead, chromate, nickel, and nitrate in water. In addition, we have developed methods for the determination of selected VOCs in water and soil, using the Bruel and Kjaer Model 1302 photoacoustic infrared monitor. All of these methods have been submitted and reviewed and are now a part of the Compendium.

A final focus of our group is on the development of environmentally friendly technologies. Research areas include low emission diesel fuels which incorporate biomaterials, wood processing technologies which lower process chemical use, and development of effective electrochemical methods for decontaminating and recycling metals from gaseous diffusion plants. Efforts to formulate and evaluate emission reducing diesel fuels have been funded by a variety of sources, including DOE/EE, in-house support (LDRD and seed money), and a USCAR partnership. Stable diesel fuels which have conventional performance, contain 20% or more renewables, and reduce NO_x by 25% have been formulated and evaluated. A thermal pretreatment technology which increases chemical penetration into whole wood has been under development with LDRD support. This technology permits direct hydrolysis of individual constituents within whole, bark-on wood by chemical catalysts and bio-catalysts. Results of kraft pulping tests indicate substantial increases in yield (up to 10%) coupled with reductions in lignin content (30-50%) and effective alkali (25%). Longer term funding for this research will be sought in 1995. Methods for removing radioactive contaminants (⁶⁰Co, ⁹⁹Tc, and U) from gaseous diffusion plant scrap are being evaluated. It appears that a combination of purification methods and electrochemical processing could purify the nickel sufficiently for reuse at DOE facilities. The availability of effective process technology could decrease the DOE's costs of maintaining contaminated nickel as a legacy waste.

An important addition to our specialty facilities during this period has been the installation of a room sized controlled experimental atmosphere chamber in Building 5507. The chamber has interior stainless steel walls and an air recirculation system capable of maintaining a wide range of temperatures and relative humidities at a variety of circulation conditions. To date, the facility has been used to generate dilute atmospheres of typical subsurface environmental contaminants and homogeneous atmospheres of environmental tobacco smoke. However, its capabilities afford the opportunity to perform large scale monitoring instrument validations, enclosure of bench scale chemical processing to assess fugitive emissions, and generation of battlefield obscurant and security related aerosols.

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INSTRUMENTATION GROUP; M.B. Wise, Leader

The Instrumentation Group conducts basic and applied research in the area of analytical instrument development and novel applications of existing analytical technologies. Projects span all aspects of instrument evolution including concept, design, construction, testing, validation, and technology transfer. Special capabilities exist particularly in the areas of mass spectrometry, quadrupole ion trap mass spectrometry, sampling hardware and techniques, computers, electronics, and field instrumentation. Areas which are currently being emphasized include instrumentation and methods for on-site field analysis of organic pollutants, automated instrumentation for process monitoring, mass spectrometry detection of chemical warfare agents and precursors, and downsized instrumentation for man portable and specialized applications.

Many of the ongoing projects in the Instrumentation Group are related to the development and application of DSITMS. DSITMS is a combination of sampling and measurement technologies for the rapid determination of organic pollutants in a wide range of samples including air, water, soil, and waste media. With this technology, low levels of pollutants can be quickly determined without the need for extensive sample preparation or compound separation methods. Demonstrated detection limits range from 10 ppb to 10 ppt, depending on the analyte, the sample matrix, and the exact analytical method used. Sample analysis time is generally less than 5 minutes, allowing the results to be available to the customers almost immediately and greatly reducing the cost relative to conventional laboratory analysis.

The application of DSITMS to the rapid analysis of organic pollutants in the environment has been a major thrust of our research during the last several years. This work has been sponsored by the DOE Office of Technology Development (EM-50), the DOE Waste Management (EM-40), the U. S. Army Environmental Center (AEC), the Program Manager for Rocky Mountain Arsenal, and the LMES ERWM programs. Much of this project has a special focus on the development of DSITMS instruments which can be operated either in a laboratory or in the field for site characterization, compliance monitoring, and remediation monitoring activities. The benefits of rapid on-site analysis capability include more thorough site investigations, quick access to analytical results by site engineers and geologists, and reduced analytical costs by minimizing the number of samples which must be shipped to an off-site laboratory for routine analysis. Field demonstrations of the DSITMS technology have been successfully conducted at a number of DOE and DOD sites across the country. In addition, DSITMS instruments are currently deployed for routine use at the Oak Ridge sites, the Savannah River site, and Rocky Mountain Arsenal. Gaining acceptance of the DSITMS technology by regulatory agencies continues to be a focus area of the environmentally related projects. A DSITMS method for screening VOCs in groundwater was approved by the EPA Office of Solid Waste Organic Methods Working Group during July 1994 for tentative inclusion in a future update of the SW-846 manual. Commercialization of the technology is currently being addressed by Teledyne Electronic Technologies as the result of the ARPA Technology Reinvestment Program (TRP). This TRP also includes as partners ORNL, Monsanto, Phillips Petroleum, Scientific Instrument Services, Inc., and Synergist, Inc.

Current work for the U.S. AEC involves the development of DSITMS methods for environmental contaminants of special interest to DOD including explosives, chlorinated solvents, and fuels. In addition, DSITMS is being tested in conjunction with the Army's cone penetrometer truck which is used for rapid site characterization. The cone penetrometer is a hydraulic system for pushing sensors and sampling probes into soil and groundwater, and is a low cost alternative to conventional soil boring and well drilling. The DSITMS is being evaluated as a real time monitor for the characterization of volatile organic compounds in soil gas which is sampled through the tip of the cone penetrometer as it is pushed into the ground. The fast response and high sensitivity of the ion trap should provide the ability to produce high resolution depth profiles of VOCs in soil.

In addition to the environmental applications described above, there are several other projects in the Instrumentation Group which utilize variations of ion trap technology for other applications. One of these projects is funded by the Edgewood Research Development and Engineering Center (ERDEC) and is focused on using ion trap mass spectrometry for the on-site detection of chemical warfare

agents and precursors for treaty verification purposes. This project primarily involves evaluating the performance characteristics of a fieldable ion trap mass spectrometer which is manufactured for ERDEC by Bruker-Franzen.

The high sensitivity and rapid response capabilities of the ion trap have also made this technology a major cornerstone in a project cofunded by the U.S. Forest Service and the DOE which is aimed at the remote detection of hidden marijuana gardens. This has been a joint project between the Instrumentation Group, the Environmental Monitoring Group, and the Analytical Methods Group. The goal of this work has been to collect and characterize samples of airborne vapors from marijuana plants with the intent of identifying unique markers or a combination of markers which might be used to help locate illegal marijuana gardens planted in the national forests.

Another collaborative project is being conducted in conjunction with the Environmental Research Consortium and personnel from McClellan Air Force Base. This project is part of a CRADA with the U.S. automotive industry and will result in a prototype hydrocarbon and oxygenated hydrocarbon speciation monitor based on an ion trap mass spectrometer with low to sub-ppb detection limits. The target compounds were selected because of their toxicity or contribution toward smog. The ORNL focus is on ion source design (i.e., atmospheric sampling glow discharge and *in situ* chemical ionization), characterizing ion chemistry (i.e., proton transfer, NO⁺ attachment), methods development, and providing input on overall system design. Experiments have been performed on static samples to demonstrate instrumental capabilities, and experiments in a dynamometer test facility using the prototype instrument are scheduled for early 1996.

Although applications of ion trap mass spectrometry constitute much of the work in the Instrumentation Group, there is also a significant effort which is devoted entirely to advancing the state of the art of ion trap technology. One project which is funded by the DOE (NN-20) is being conducted in conjunction with the Analytical Spectroscopy Section. This work is aimed at the development of new modes of ion trap operation which could improve the analytical speed, specificity, selectivity, and detection limits. Work which has been specifically conducted in the Instrumentation Group has focused on characterizing the performance of ion trap mass spectrometers using air as a buffer gas as opposed to helium. The results have clearly demonstrated that there are operating parameters outside of the normal operating conditions in which the use of air as a buffer gas does not seriously degrade the instrument performance for compounds with molecular weights of less than 200 amu. This could be a significant advantage in terms of increasing the portability of the instrument and reducing the complexity of sample inlets. In addition, operational conditions have been discovered which permit improved performance for the ion trap in its more traditional mode of operation using helium as the buffer gas.

Another related project is also funded by the DOE, NN-20, and is aimed at the development of a full featured, man portable ion trap. This project is being conducted in collaboration with Phil Hemberger at Los Alamos National Laboratory. The final product will be an instrument which has all of the capabilities of a research grade laboratory ion trap, yet is packaged in a case which can be carried on board an aircraft. Los Alamos will be contributing to the design and construction of the mass analyzer hardware and control software. Work at ORNL will involve completion of the analyzer hardware, the design and construction of the vacuum system, interfacing of the sample inlets, final packaging, and development of interactive software for instrument control and data reduction.

Both of the projects which are aimed at the development of advanced ion traps are also supporting the development of a general purpose analytical instrument control and data manipulation system which is based on the VXI bus. This system will provide generic hardware for controlling and acquiring data from ion traps and, in principle, other types of analytical devices. The VXI bus provides an industry standard which is used for a variety of applications including process control and monitoring. Modular devices are linked together by the VXI bus in order to form a functioning control and data system. Software for control of the system is being written using LabView, which provides a convenient means of interacting with the VXI modules. For the advanced ion trap projects, the VXI system will provide an upgradable and customizable data acquisition and control platform for implementing and evaluating new ion trap operating modes which would be difficult to investigate using the commercial ion trap hardware and software.

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PHYSICAL ORGANIC CHEMISTRY GROUP; A. C. Buchanan, III, Leader

The Physical Organic Chemistry Group conducts research that addresses the structure and reactivity of organic chemicals and materials, particularly in complex settings. An integrated approach is employed that involves chemical synthesis, product analysis, determination of reaction kinetics and mechanisms, structural interrogation *via* spectroscopic methods, and computational methods. Emphasis areas include structure and reactivity of fuel materials such as coal, kerogen, and biomass; development of advanced NMR spectroscopic methods for analysis of complex carbonaceous solids such as fossil fuels, polymers, and fullerenes; thermal or catalyzed decomposition reactions for organic compounds, polymers, and surface-bound organic films; photochemical reactions of hazardous organic compounds at environmentally related solid-air and solid-liquid interfaces, and in aqueous solutions; development and investigation of photocatalysts for degradation of organic chemicals; and optical spectroscopic investigation of organics in heterogeneous environments. Major projects are summarized below.

The objective of our fuel related research is to gain new knowledge on the chemical structure and reactivity of coal, lignin, and biomass. This research contributes to the scientific foundations required for the commercial development of novel processes for the conversion of fossil and renewable resources into chemicals or fuels in an environmentally acceptable manner. Reaction mechanisms that underpin thermal and catalyzed reactions of coal and lignin have been explored through the use of representative organic model compounds. Silica immobilized compounds are employed to study interfacial reactions in dispersed solids, and dramatic effects of clay minerals on thermochemical reaction pathways for coal and lignin model compounds have been observed. The impact of restricted mass transport on reaction pathways involving free radicals has also been addressed, and a novel radical relay mechanism involving serial hydrogen transfers on a surface has been demonstrated. Hydropyrolysis reactions have been investigated isothermally and by temperature programmed reduction (TPR) with online detection by mass spectrometry. High pressure TPR experiments on immobilized organosulfur model compounds have permitted an analysis of the

corresponding sulfur species in coals and kerogens. Pyrolysis pathways for model compounds containing key coal heteroatom functionality such as ethers and sulfides have been investigated in fluid phase and silica immobilized forms. Model compounds and polymers containing carboxylic acid functionality have been prepared and their pyrolysis behavior investigated to reveal reaction pathways associated with low temperature cross-linking events observed in the pyrolysis of low rank coals. Solid state NMR methods are being developed to obtain structure/reactivity information in chemically modified coals and lignins. NMR techniques under development include high resolution solid state ^{19}F -NMR, and triple resonance ^{13}C -NMR techniques that exploit the ^{13}C - ^{19}F dipolar interaction to reveal information on local structure in ^{19}F -labeled organic molecules, polymers, and coals. Fluorination chemistry under investigation included the conversion of specific oxygen functional groups in low rank coals into fluoride derivatives using diethylaminosulfur trifluoride and sulfur tetrafluoride. The combined fluorination and NMR approach provided the first evidence for primary alcohols in a lignite and also provided a novel method for differentiation of aliphatic and aromatic carboxylic acids.

The emphasis of our photochemistry program is on fundamental investigations into the influence of local chemical environment on the photochemistry of hazardous organic materials. Studies of photochemical events at interfaces (solid/liquid and solid/gas) and in aqueous media are of central importance to this research. Results from these studies enhance the basic understanding of photochemical processes occurring in industrially and environmentally important settings. In addition, the research will lead to an improved understanding of the factors that control the environmental fate and residence times of these organics. The photochemistry of polycyclic aromatic hydrocarbons (PAHs) has been the focal point for recent studies because of connection between these materials and fossil fuel production and consumption, and the status of many PAHs as EPA priority pollutants. Product analysis and *in situ* spectroscopic techniques are the primary methods used in the investigations. A systematic study of PAH structure has allowed the elucidation of contributions from electron transfer and singlet molecular oxygen mediated PAH oxidation pathways. Highly polar surfaces, such as that of SiO_2 , have been shown to have dramatic effects on the photochemistry of weakly interacting organics, as typified by unsubstituted PAHs. Investigations using spectroscopic interfacial probes have revealed PAH pairing effects on the surface and permitted a quantitative measure of the nature of PAH surface interactions. Likewise, water has been shown to be a medium that exerts significant influence on the rates and product distributions observed for PAH photochemistry. Photooxidations of several PAHs have been observed principally to involve energy transfer mechanisms with singlet oxygen as a key intermediate. Recently, semi-empirical SCF calculations have been employed which indicate that the pathway for singlet oxygen addition to phenanthrene and acenaphthalene is through a peroxirane intermediate. In related research, photocatalysts are being designed to photooxidize PAHs in waste waters that are difficult to bioremediate. Immobilized photosensitizers have been prepared that can oxidize dilute aqueous solutions of PAHs under solar irradiation. This research helps form the foundations for development of new remediation schemes.

A collaborative project with the Organic Mass Spectrometry Group aims to develop a new DNA sequencing technique based on matrix assisted laser desorption time-of-flight MS coupled with DNA labeling. Synthetic methods have been developed for derivatization of aminohexyl modified DNA with several electrophore tags. MS characterization of electrophore tagged 17-mers have shown that the derivatives are stable under the analysis conditions. Research continues to focus on improvements in the MS desorption/ionization efficiency for these derivatives.

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ORNL/UTK RESEARCH PROGRAM GROUP; G. A. Guiochon, Leader

In an attempt to derive a method for characterizing the surfaces of pulverulent materials, we have studied the distributions of the adsorption energies (AED) of different probes on the surface of adsorbents. These AEDs are derived from experimental data acquired by gas GC. The adsorption isotherms of the probes are calculated from nonlinear elution profiles obtained by GC, using the characteristic points method of finite concentration chromatography. The AED is then calculated from the classical linear Fredholm integral equation of adsorption using these adsorption isotherms. The problem is mathematically ill posed. It is solved with an iterative maximum likelihood method called expectation-maximization (EM). The algorithm was programmed and run on a massive parallel supercomputer. Parallelization and use of the matrix-vector routines supplied by the vendor provide substantially faster run times than that executed with the sequential code by other mainframe computers, allowing the economical use of the EM algorithm for these types of problems. Theoretical models for the local adsorption include the Langmuir, Jovanovic, Fowler-Guggenheim (both random and patchwise), and Brunnaer-Emmett-Teller local isotherms.

Experimentally, porous layer open tubular capillary columns (PLOT) are prepared from a slurry of the adsorbent powder in a compatible solvent. The column, filled with the slurry and closed at one end, is slowly coiled inside an oven at a temperature slightly above the solvent boiling point. A thin homogeneous layer is obtained. The performance of these columns was to be considerably better than that of packed columns in terms of their ability to supply accurate isotherm data and AEDs. The effect of the finite column efficiency and the limited loading factor on the accuracy of the estimated energy distributions was investigated. It was shown that the accuracy decreases with decreasing efficiency and that approximately 5000 theoretical plates are needed (PLOTs have consistently more than 20,000 plates) when the loading factor, L_f , equals 0.56 for sampling of a unimodal Gaussian distribution. Increasing L_f further increases the contribution of finite efficiency to the AED and causes a divergence at the low energy endpoint if too high. This occurs as the retention time approaches the holdup time. These results indicate that the accuracy of estimated AEDs with respect to the true underlying distribution of the surface is poor for most studies of this nature.

The adsorption energy distributions of the molecular probes are calculated from their adsorption isotherms using the expectation-maximization (EM) method of parameter estimation. EM does not require prior knowledge of the distribution function or the isotherm, requires no smoothing of the isotherm data, and converges with high stability toward the maximum likelihood estimate. The method is therefore robust and accurate at high iteration numbers. The EM algorithm was tested with

known energy distributions corresponding to unimodal Gaussian, bimodal Gaussian, Poisson distributions, and the distributions resulting from Misra isotherms, using a procedure which simulates the whole determination process. The results are contrasted to those obtained with conventional methods and shown to be superior in terms of both robustness, accuracy, and information theory. The effect of undersampling of the high pressure/low energy region of the adsorption is reported and discussed for the EM algorithm, as well as the effect of signal-to-noise ratio on the degree of heterogeneity that may be estimated experimentally.

The estimation of adsorption energy distributions on DAVISIL, IMPAQ, and VYDAC silica samples was considered in detail. Chemical derivatization of these samples was also considered. The adsorbates studied include diethylether, methanol, ethanol, tetrahydrofuran, pyridine, and heptane. The effects of temperature and maximum solute partial pressure on the AED estimation were studied. The validity of the technique is assessed, and it was concluded that adsorption energy distributions may only be calculated accurately and without bias for systems in which the majority of the adsorption energy is 10 kJ/mol greater than the heat of vaporization of the solute. For adsorption energies less than this, intermolecular interactions decrease the accuracy and confidence of the results. Other experimental parameters, including the detector range and resolution and the injection profile, also limit the scope of studies of this kind. The major obstacle is the difficulty in sampling the entire range of adsorption energies, especially the low energies which correspond to the required measurement of the retention times corresponding to high solute partial pressures.

The determination of the thermodynamic data required for the modeling of chromatography must be done with an accuracy which seems to exceed what the current level of column-to-column reproducibility of these data permits at present. An investigation of this important scale-up problem is on-going. Isotherm data were measured by frontal analysis and elution by characteristic points for 2,6-dimethylphenol, 3-phenyl-1-propanol, and methyl benzoate on columns packed with four commercial octadecyl silica (KROMASIL, VYDAC, YMC, and ZORBAX, all average particle size, 10 μ m), using methanol/water (45 x 55, v/v) solutions as the mobile phase. Seven 10 x 0.46 cm and two 25 x 0.46 cm columns were packed for each phase. The column efficiencies and capacity factors were also determined for a series of compounds: m-cresol, benzyl alcohol, methyl benzoate, benzyl acetate, and 2-isopropylphenol, all eluted under infinite dilution conditions. The average total column porosities were derived from the uracil retention volume, the internal and external porosities by reversed size exclusion chromatography, from the calibration curve obtained with a series of polystyrene standards with molecular weights ranging from 456 to 20,600,000 Dalton.

The retention factors and isotherm coefficients depend on the packing density which varies markedly from column to column and is also a function of the column length. This observation is consistent with the results of previous work, which has shown that the beds of packing materials in conventional packed columns consolidate to a marked extent during an initial period. Therefore, a procedure for the accurate and precise determination of the external porosity of columns is necessary. The internal and external pore volumes (hence, porosities) of the columns can easily be determined with accuracy from the plots of the logarithm of the molecular weight of the probes versus their retention volume. Corrections of isotherm data based on the difference between column retention factors and phase

ratios do not compensate correctly for the deviations observed. Corrections based on the difference of external porosities of the columns do better.

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4. PHYSICAL AND MATERIALS CHEMISTRY SECTION

R. E. Mesmer, Head

The research in this section represents a mix of basic and applied research in the areas of chemical separations, geochemistry, high temperature aqueous chemistry, inorganic materials chemistry, and polymer science. There are 23 Ph.D. and 3 B.S. and M.S. staff in this section. The principal sponsors include the Office of Basic Energy Science (Divisions of Chemical, Materials, and Geosciences), Office of Technology Development, Office of Energy Efficiency and Renewable Energy, Electric Power Research Institute, and Office of Health and Environmental Research.

The Chemical Separations Group addresses solvent extraction/ion exchange of cations, anions, and ion pairs; design, synthesis, and evaluation of macrocyclic ligands for molecular recognition; structures of extraction complexes; and separations in environmental restoration. The Geochemistry Group addresses experimental studies of hydrothermal and magmatic systems; crustal materials and fluid-rock interactions; metal ion complexing; stable isotope geochemistry; and high temperature thermodynamics of C-H-O-N systems. The High Temperature Aqueous Chemistry Group addresses thermodynamic properties and reaction thermodynamics of solutes in water at high temperature; experimentation and modeling; nonideal electrolyte behavior; and applications to energy production and waste treatment. The Inorganic Materials Chemistry Group addresses the synthesis and characterization of ceramic, optoelectronic, and superconducting materials; thin films; sol-gel synthesis of multicomponent oxides; reactive sputtering for nanocomposites; and CVD. The Polymer Science Group addresses experimental and computational characterization of polymer structure and dynamics; semicrystalline and amorphous materials; polymer blends; and use of molecular dynamics and neural networks in materials science.

CHEMICAL SEPARATIONS GROUP; B. A. Moyer, Leader

CASD's Chemical Separations Group strives to elucidate principles of chemical recognition and separations and to develop applications supporting the missions of its sponsors, including DOE programs in Basic Energy Sciences (BES), Office of Environmental Management (OEM), and the Office of Health and Environmental Research (OHER). Research themes primarily deal with the coordination chemistry of synthetic organic ligands designed to selectively complex metal ions and effect their separation from complex matrices. Within this broad area, the group has earned an international reputation as a leader in solvent extraction and ion exchange, both in fundamental and applied aspects. In large part, the special strength that the group has developed in the area of crown ethers, macrocyclic compounds, and designed ligands has been responsible for this success and has led to a number of noteworthy accomplishments in recent years. One recent applied accomplishment, for example, has been the development of a novel solvent extraction process that uses crown ethers for removing the radioactive contaminant technetium from aqueous waste. In addition to waste treatment, potential applications of the systems developed by the group include groundwater remediation, hydrometallurgy, nuclear separations, analytical chemistry, and biotechnology. Systems selective for such metals as lithium, sodium, cesium, strontium, barium, radium, manganese, copper, and zinc have been characterized. Further, the binding of lanthanides and actinides is a major topic in several projects.

To accomplish its mission, the Chemical Separations Group has assembled a uniquely equipped, multidisciplinary team of scientists. In a typical R&D cycle, individual problems are analyzed, and the appropriate ligands are designed, synthesized, tested for efficacy, and probed in detail. Molecular mechanics calculations are employed in the design of extractants. The performance of extraction systems is assessed by distribution studies aided by computer modeling. Analytical tools employed in characterizing separations include ICP spectrometry, scintillation counting, ion chromatography, HPLC, capillary electrophoresis, electrochemistry, and luminescence spectroscopy. For a complete understanding of systems at a molecular level, details of structure and bonding are obtained by x-ray crystallography, NMR spectrometry, FTIR spectrophotometry, calorimetry, and other physical techniques. The group's own modeling program, SXLSQI, developed by C. F. Baes, Jr., is the most powerful and informative program available for modeling solvent extraction data.

Under the group's largest program, "Chemical and Structural Principles in Solvent Extraction," sponsored by the Division of Chemical Sciences/OBES/DOE, the molecular level behavior of crown ethers as selective extractants for several classes of metal ions has received major emphasis. The primary thrust has entailed the factors governing the ability of crown ethers to recognize the alkali metals according to size, especially at the extrema represented by environmentally important lithium and cesium. Illustrative of the many systems studied, a family of 14-crown-4 ethers having various hydrocarbon substituents has been shown to extract lithium with selectivity factors exceeding 50:1 vs. sodium ion. This ability, however, depends markedly on the particular substituents on the ring. X-ray crystallography reveals the binding of lithium cations in basket-like complexes, though the free crowns adopt twisted shapes. Significantly, calculations by molecular mechanics performed at Pacific Northwest Laboratories (B. P. Hay) show that the energy cost to "untwist" one of the substituted 14-crown-4 ethers correlates with its lithium extraction ability. To test this exciting structure-function relationship, the extraction behavior of a representative case, nonamethyl-14-crown-4, has been examined. The stoichiometry of extraction has been determined in 1-octanol by distribution measurements and ^7Li NMR, and strong solvation effects have been observed. Two dimensional NMR has aided the understanding of crown ether conformation, especially as applied to the role of functionalized sidearms attached to rigid dibenzo-14-crown-4 lariat ethers. In contrast to such small macrocycles, crown ethers having 21 or more ring atoms exhibit selectivity for the large alkali metals, cesium and rubidium. Selectivities exceeding 100:1 over sodium have been obtained, and the underlying extraction equilibria have been determined by modeling studies. Crystal structures of a number of the crown ethers with cesium salts have elucidated the roles of ring size and benzo substituents. New crown ethers bearing triptyceno and anthraceno substituents have been synthesized.

A new project entitled "Selective In-Situ Sorption of Tc from Groundwater" has been initiated under the U.S. DOE Efficient Separations and Processing (ESP) Cross-Cutting Program of the Office of Technology Development/OEM. The objective entails the development of improved resins for the removal of technetium from groundwater as targeted to the contamination problems found at the gaseous diffusion plants, especially Portsmouth and Paducah. Through collaboration with Professor S. D. Alexandratos of The University of Tennessee, Knoxville, a series of promising resins have been synthesized, and more efficient uptake of technetium than possible with commercial resins has indeed been achieved.

A new process for the removal of technetium from defense tank wastes such as found at Hanford has been developed. Under the ESP funded project "Alkaline-Side Extraction of Technetium and Acti-

nides by Crown Ethers and Other Extractants" initiated in FY 1993, it was shown that crown ethers extract technetium as pertechnetate ion from alkaline media containing high concentrations of sodium nitrate and other salts. The crown ethers offer the key advantage that the extraction cycle can be completed with an economical stripping step employing only water. Efficient conditions for the extraction cycle have been identified. In related work involving collaboration with Professor R. B. Robinson of The University of Tennessee, the extraction of technetium has also been demonstrated in supported liquid membranes. The problem of decontaminating alkaline waste solutions containing complexed actinides has also been examined, and an extraction system capable of removing trivalent actinides and lanthanides has been identified.

The group's expertise in ligand synthesis and coordination chemistry has been productively applied to the attachment of metal ion reporter groups to oligonucleotides for DNA sequencing. In projects supported by the DOE OHER Human Genome Program, the photon antenna function of aromatic groups attached to chelated lanthanide ions was demonstrated to enhance the luminescence detection of the lanthanide ions. The principle has been applied to the laser luminescence detection of a Eu(III)-labelled oligonucleotide by capillary electrophoresis. Alternatively, ferrocene groups can be attached to DNA fragments for electrochemical detection by capillary electrophoresis. A series of ferrocene and stannane reporter groups employing isotopically pure iron and tin, respectively, have been demonstrated in mass based detection schemes.

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GEOCHEMISTRY GROUP; D. J. Wesolowski, Leader

The Geochemistry Group conducts basic and applied research on the geochemical controls of matter and energy transfer in the Earth's crust, as these relate to such issues as fossil and geothermal energy resource formation, discovery, and exploitation; nuclear and toxic waste disposal and remediation; and the effects of energy utilization on the lithosphere/atmosphere/hydrosphere system such as global climate change, acid rain and acid mine drainage, and groundwater quality. Our principal approach is to conduct experimental studies of earth materials (minerals, rocks, and fluids), including their physicochemical properties and the chemical reactions among them, using a variety of state-of-the-art and/or unique facilities which enable the simulation of subsurface conditions from room temperature and pressure to 1200°C and 10,000 atmospheres. Our efforts are focused in four main categories:

(1) the speciation of elements in high temperature brines and the chemical reactions of natural brines with minerals and rocks; (2) the partitioning of the stable isotopes of hydrogen (D/H), oxygen ($^{18}\text{O}/^{16}\text{O}$), carbon ($^{13}\text{C}/^{12}\text{C}$), and sulfur ($^{34}\text{S}/^{32}\text{S}$) among minerals and fluids as a function of temperature and salinity; (3) the thermodynamic properties of natural gas and deep Earth fluids (CO_2 - CH_4 - H_2O - N_2 gas mixtures); and (4) the thermodynamic properties of silicate minerals and melts. Highlights of our recent research projects are described in the next few paragraphs.

In collaboration with the High Temperature Aqueous Chemistry Group, we make extensive use of unique pressure vessel systems fitted with platinum-hydrogen electrodes that enable extremely precise measurement of pH in aqueous solutions from 0 to 300°C. Much of our recent work with these systems has focused on the acid dissociation constants and thermal stabilities of organic acids found in natural waters and their ability to complex metal ions. These acids, which are produced by biological activity and decomposition of buried organic material in soils, aquifers, and hydrocarbon reservoirs, may play important roles in the migration of wastes as well as economically valuable metals, and may influence the hydrodynamics of groundwater and geothermal systems by enhancing permeability through selective dissolution of certain minerals. In the past two years we have determined the formation constants of Nd^{3+} -acetate complexes to 250°C in 0.1 molal NaCl solutions, Cd^{2+} -malonate and oxalate complexes in 0.1-5.0 molal sodium trifluoromethanesulfonate solutions to 75 and 125°C, respectively, and Al^{3+} -malonate complexes to 75°C in 0.1-5.0 molal NaCl solutions.

We have also initiated a detailed study of the thermal stabilities of malonic, succinic, and oxalic acids using the platinum hydrogen cells to continuously monitor the pH during the decomposition process. Finally, these facilities have been used to study several inorganic reactions, including (1) the determination of Al^{3+} complexes with SO_4^{2-} in 0.1 to 1.0 molal NaCl solutions from 0 to 125°C, relevant to acid rain and acid mine drainage environmental problems; and (2) the surface charge and H^+ sorption properties of the mineral rutile (TiO_2) in 0.01 to 3.0 molal NaCl solutions from 25 to 250°C, the first such direct measurements ever conducted at temperatures above 100°C.

In a collaborative effort involving our group and the Inorganic Mass Spectrometry and Secondary Ionization Mass Spectrometry groups, we have been utilizing ion microprobes to investigate the trace element and stable sulfur and oxygen isotope distributions in minerals formed during fluid migration sedimentary rocks of the Western Canada oil and natural gas province. Ion probes permit examination of the chemical and isotopic signatures of fluid (aqueous and hydrocarbon) sources and flow paths on the scale of individual mineral grains, which aids in the development of improved hydrocarbon exploration and development models. Innovative stable isotope measurement techniques have been developed which enable us to demonstrate that H_2S -rich "sour" gas and oil accumulations within the province are a result of thermogenic reduction of pore water sulfate in portions of the sedimentary basin subjected to very deep burial. This collaborative team has obtained a substantial LDRD grant to design, construct, and test a unique ion microprobe specifically optimized for the measurement of the stable isotope ratios of O, C, H, and S in geological materials, ceramics, and metal corrosion products, with micron scale spatial resolution.

The Geochemistry Group also conducts extensive experimental studies of stable isotope partitioning among geological minerals and fluids. Current efforts involve a detailed investigation of the rates of oxygen and carbon isotope exchange between H_2O - CO_2 fluids and the minerals calcite, quartz, and feldspar, the three most abundant minerals in the Earth's crust. We have also determined the

equilibrium fractionation of oxygen isotopes between water and the minerals magnetite (Fe_3O_4) and hematite (Fe_2O_3) in the 300-400°C range by employing a variety of novel *in situ* reactions. These iron oxides, which form in a variety of geological environments, contain a wealth of information about the sources, redox states, and temperatures of aqueous and hydrocarbon fluids associated with geothermal and hydrocarbon energy resources. A promising line of recent investigation involves determination of the stable oxygen isotope compositions of magnetite corrosion products formed on both the steam side and the fire side of steel tubing in fossil fuel burning power plants. These measurements, funded by the ORNL seed money program and performed on samples provided by the Electric Power Research Institute, indicate that the mechanisms of corrosion and the nature and diffusion rates of the corrosive oxidants (O_2 versus H_2O) can be determined by appropriately constrained laboratory and field experiments.

We are heavily involved in detailed studies of several key geochemical processes which play a pivotal role in modeling geothermal systems. Applied studies of these systems are funded by DOE's Division of Geothermal Technology Development, and these are closely coordinated with more generic, long-term studies funded by the OBES/Geoscience Research Program. Current efforts are focused on (1) the geochemistry of aluminum in geothermal systems, with recent results including the measurement of boehmite (AlOOH) solubility in NaCl brines to 250°C with *in situ* pH monitoring in our platinum hydrogen cells (the first measurements of this type ever reported); (2) the effect of dissolved salts in the system Na-K-Mg-Ca-Cl- SO_4 on the partitioning of hydrogen and oxygen isotopes between aqueous brines and coexisting water vapor and minerals to 350°C, as well as the pure water liquid vapor partitioning of both isotopes from the freezing to the critical point; and (3) the solubility of water in silicate melts (the heat engine for most active geothermal systems) and the chemical composition of separate aqueous fluids in equilibrium with granitic silicate melts as a function of temperature, pressure, and melt composition.

Finally, we have developed a unique, high temperature and pressure, vibrating tube densimeter for the determination of the pressure-volume-temperature relationships of C-O-H-N gas mixtures. This facility has produced some of the world's most accurate data on the densities of CO_2 - CH_4 - N_2 mixtures (the main components of natural gas) in the range of 50-300°C and 100-1,000 atmospheres.

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HIGH TEMPERATURE AQUEOUS CHEMISTRY GROUP; R. E. Mesmer, Leader

The High Temperature Aqueous Chemistry Group conducts basic and applied research on aqueous systems at high temperatures and pressures of importance to DOE energy related activities. Basic research is aimed at establishing fundamental principles governing chemical and thermodynamic behavior of aqueous solutions of broad classes of solutes to high temperatures and pressures through state-of-the-art laboratory studies using an exceptional arsenal of unique equipment developed over many years at ORNL. Results in this program are also advancing the disciplines of solution

chemistry and hydrothermal chemistry, as well as having important applications in several applied programs supported by DOE and other agencies.

The combination of results from measurements with potentiometry, electrical conductance, flow calorimetry and densimetry, as well as isopiestic and phase studies, provide definitive information on chemical processes occurring in aqueous solutions at high temperature. These include the equilibrium reactions ion association, hydrolysis, adsorption, precipitation, metal ion complexation with inorganic and organic species, and finally the distribution of solutes between the liquid and vapor phases. Information is being produced on the thermodynamics of reaction equilibria, especially those involving charged species, that yields models for prediction and data fitting of the complex temperature-pressure-composition relationships, particularly the divergences seen in near-critical and highly dilute solutions. The intractable nonidealities of electrolyte solutions are being systematically studied to provide input for ion interaction models for computations on real mixtures occurring in natural and technological settings such as geothermal reservoirs, power plants and steam generators, waste disposal and processing facilities, and mineral deposition processes in nature.

In this and the next few paragraphs, some highlights of both the basic and applied research efforts will be discussed. First, we have undertaken a broad research program to investigate and quantify metal complexation using the unique hydrogen electrode concentration cell developed in this program which provides an accurate measure of pH from 0 to 300°C, even in highly saline solutions. For example, the formation of zinc sulfate complexes that play a role in PWR primary side corrosion was investigated to 250°C. Similarly, the highly stable cadmium(II) complexes with naturally occurring organic acids are being measured to determine the environmental impact of releasing cadmium from waste sites. The thermodynamics of dissolved aluminum in the presence of sulfate and organic acids and kinetics of dissolution of aluminum solid phases are being investigated by potentiometry, spectroscopy, and solubility measurements to understand how aluminum is released to the environment. The first study of the complexation of a rare earth metal ion, neodymium, with an organic acid to high temperatures has now been completed. Finally, as part of an effort to quantify the adsorption of toxic metals onto mineral surfaces over the ranges of temperature, pH, and salinity found in nature, the first study of the adsorption/desorption of hydrogen ions on an oxide surface (TiO_2) has been completed to 275°C.

The isopiestic method has proven to be one of the most productive approaches to measurement of the excess thermodynamics of aqueous electrolytes; the ORNL facility is the only one capable of measurement above 100°C. During this period, new results were obtained on alkali bromides to add to the extensive list of chlorides, sulfates, hydroxides, and phosphates that have been previously studied. Preliminary examination shows similar trends with cation size as for the chlorides. Completion of a comprehensive analysis of the alkali bisulfates demonstrates that lower activity coefficients are observed for this class than for the two halides. This unique apparatus is now being readied for study of water adsorption by geothermal reservoir materials in an attempt to provide necessary data for the evaluation of reservoir behavior and lifetimes.

Electrical conductivity, as a tool to explore association behavior of electrolytes, has been pioneered in this program, especially at high temperatures, and is currently being applied to the study of the important class of alkali hydroxides in addition to NaCl(aq) and sodium triflate. Results for NaOH(aq) and KOH(aq) show association similar in type to NaCl(aq) but intermediate in magnitude between

NaCl(aq) and HCl(aq). Attempts to make measurements near the critical point demonstrated the need for greater precision, which is being sought with an improved cell design in a collaboration with the University of Delaware group of R. H. Wood.

Flow calorimetry is our best tool for measurement of excess thermodynamic properties through measurements of heats of dilution, and it has the widest temperature range of operation. The ORNL calorimeter has recently been used in studies on $\text{MgCl}_2(\text{aq})$ over a wide concentration range and on $\text{NaCl}(\text{aq})$ in the dilute range. An important and unexpected observation was the transport and re-deposition of metallic platinum in one of the capillary lines caused by incomplete removal of oxygen. Also, to improve the quality of the measurements, new heat exchanger designs have now been tested, and there is evidence for the need to preheat solutions for greatest accuracy above 300°C . In a related activity, the high temperature vibrating tube densimeter previously constructed in the program is being modified to add a capability for heat capacity measurements to supplement the heats of dilution results and give standard state heat capacities.

Currently, emphasis is being given to the study of the volatility of electrolytes for two major applications. Geothermal steam systems include varying levels of electrolytes in water and steam at high temperatures, and certain solutes in steam (e.g., HCl) are highly corrosive to piping and turbine systems (a problem of interest to the Office of Energy Efficiency and Renewable Energy of DOE). Corrosion and deposition of salts lead to problems even in the much cleaner fossil fired steam cycle (Electric Power Research Institute). We have recently determined equilibrium constants for the partitioning of electrolytes such as HCl, NaCl, Na_2SO_4 , NaHSO_4 , H_2SO_4 , NaOH, NH_4Cl , and NH_4HSO_4 , as well as some mixtures, between water and steam at high temperatures. Combined with data obtained in this program on excess thermodynamic properties (e.g., activity coefficients) in high temperature brines, these results yield models for calculating the composition of coexisting brine and steam phases over wide ranges of temperature and solute concentration. The models take into account both the production of solute contaminated steam and the formation of varying amounts of condensate liquids from the steam, and can be used to track the changing composition of condensate with varying initial boiler water concentrations, steam formation and condensation temperatures, and extent of condensation. The models are currently being used to estimate steam formation conditions in geothermal reservoirs to address the feasibility of various methods for mitigation of corrosive steam production in geothermal power cycles, and as input for revision of guidelines for the operation of fossil fired steam generator cycles in large power plants.

For the purpose of gaining an understanding of some of our macroscopic observations on a microscopic scale, an effort has been initiated on computer simulations of electrolyte solutions with P. T. Cummings and A. Chialvo. Both experimental results and quantitative empirical models based on those results are important sources of data for comparison with thermodynamic quantities calculated from molecular dynamics simulations of high temperature aqueous solutions. Recently, simulations have been carried out which give values of the equilibrium constant at infinite dilution for the formation of ion pairs in model aqueous sodium chloride at a supercritical temperature and near the critical density of the solvent. Some disagreement was found that appears largely to be due to the difference between the simulation result for the dielectric constant of the pure solvent as compared with the corresponding value for water under these conditions. When a comparison is made between quantities which are less dependent on the solvent dielectric constant, the agreement is within the combined uncertainties of the simulation and of the experimental determination. This promising

result is being pursued through simulation studies at additional state points, and testing of improved potential models.

Finally, this group is involved in a technology transfer project through a CRADA with Modell Environmental Corporation to assist in the development of the supercritical water oxidation (SCWO) process for treatment of mixed wastes, hazardous and radioactive, for DOE. The work is CRADA protected but involves laboratory phase studies on *in situ* neutralizers and an effort with CTD to upgrade the ASPEN Plus Code for aqueous electrolytes at SCWO conditions.

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CHEMISTRY OF ADVANCED INORGANIC MATERIALS; D. B. Beach, Leader

The Chemistry of Advanced Inorganic Materials Group is primarily engaged in the synthesis of inorganic solid state materials by nonclassical synthetic techniques. Classical synthesis of inorganic materials by solid-solid reaction requires long reaction times at high temperatures and often extensive grinding and mixing, the so-called "heat it and beat it" approach to synthesis. These extreme conditions are required because of slow diffusion of reactants in the solid state and often preclude the use of these materials in many technological applications. To overcome the limitations of classical synthetic techniques, we are currently using a number of techniques including aerosol pyrolysis of mixed metal nitrates as precursors to cuprate superconductors, plasma assisted chemical vapor deposition and plasma sputtering of oxide and nonoxide ceramic materials, pseudomorphic conversion of oxide ceramics to nonoxide ceramics using gas-solid reactions, ion implantation to produce electrocatalytic electrodes, and sol-gel and metal organic chemical vapor deposition of titanates for electronic applications.

High T_c Superconductors -- Studies of complex cuprate superconductors with high critical temperatures were carried out in collaboration with the Solid State and Metals and Ceramics divisions of ORNL as part of the Superconductivity Technology Center. Our primary goal was the synthesis of materials with the potential for high current applications in significant magnetic fields. To these ends, we explored the synthesis of powders of $[(\text{Bi}_{2-x}\text{Pb}_x)\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_y]$, Bi,Pb-2223, using aerosol pyrolysis of nitrate solutions to produce fine grain, intimately mixed materials. These powders were then used for the synthesis of Powder in Tube (PIT) conductors with performance superior to those made by other methods. Aerosol pyrolysis was also used to prepare powders of $\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{Ag}_{0.4}\text{O}_y$ for subsequent thallination using a multizone thallination furnace which allowed the independent control of thallium oxide vapor pressure and substrate temperature. The resulting $\text{TlBa}_2\text{Ca}_2\text{Cu}_3\text{O}_y$, Tl-1223, materials, both powders and thin films, showed excellent superconducting properties. Spray pyrolysis using nitrate solutions and subsequent thallination were used to prepare Tl-1223 films with relatively high critical currents. Finally, a sol-gel synthesis of Tl-1223 films using an all alkoxide chemistry was developed.

In addition to these more applied studies, new superconductors were synthesized for basic structure and property studies. Several recently discovered mercury containing superconductors were synthesized of the general formula $\text{HgBa}_x\text{Ca}_y\text{Cu}_2\text{O}_d$, (henceforth referred to as Hg-1XYZ). Thermopower and resistivity measurements of Hg-1223 prepared with various degrees of oxygen doping indicated that the measured T_c of 134 K could be raised further by high pressure oxygen annealing. Samples of the quaternary intermetallic superconductor $\text{YNi}_2\text{B}_2\text{C}$ were prepared, and its structure was determined by neutron diffraction.

Plasma Synthesis -- Plasma synthesis of thin films provides energy for chemical reactions without having to heat the deposition surface. Plasma assisted chemical vapor deposition (CVD) was used to generate nonoxide ceramic coatings such as SiC. In addition to CVD, plasma synthesis was also used to prepare a variety of novel nanocomposite materials by physically sputtering targets of alloys in a reactive gas ambient. For example, by sputtering a target containing gold and silicon with an oxygen plasma, a gold oxide/silicon oxide nanocomposite was formed. By heating the sample, gold oxide decomposed to form gold nanoclusters less than 100 Å in diameter. These gold nanoclusters were dispersed in an amorphous insulating matrix of silicon dioxide. Other systems studied included gold/gallium in a nitrogen plasma and gold/aluminum in a nitrogen plasma. The gold/silicon oxide system showed interesting optical and dielectric behavior, and the gold/aluminum nitride system was studied for nonlinear optical effects.

Pseudomorphic Synthesis -- This technique starts with an inexpensive, easily synthesized oxide ceramic with a desirable morphology such as a whisker or a needle and converts this oxide to a carbide or nitride by a gas solid reaction to produce a difficult to prepare ceramic material with hopefully the same morphology as the starting oxide. An example would be tungsten carbide whiskers from whiskers of sodium tungsten bronze.

Preparation and Characterization of Electrocatalytic Surfaces -- Ion implantation was used to prepare ruthenium oxide/titanium oxide electrodes by implanting ruthenium into titanium and then anodizing/oxidizing the electrode to form an electrode to model those used for electrocatalysis of brine in the chlor-alkali process. A number of analytical techniques including Rutherford back-scattering spectroscopy (RBS), x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) were used to characterize these electrodes.

High Dielectric Constant Titanates -- Work was started on the synthesis of very thin films of lead lanthanum titanate (PLT) for use as capacitors in microelectronics. The films were prepared by sol-gel techniques using a complex mixture of alkoxide precursors. Films were annealed by rapid thermal processing so as to minimize damage to the electrode and unwanted interfacial diffusion. Films with dielectric constants as high as 600 at 1000 Å of thickness were prepared.

Basic Research and Development of Radioactive Waste Management -- This research was funded by the Army to explore the basic chemistry of titanates as storage forms for the transuranic elements. The compound $\text{Pu}_2\text{Ti}_2\text{O}_7$ was synthesized, and its solid solubility in lanthanide dititanates was studied. The compounds $\text{Pu}_{2-x}\text{Ln}_x\text{Ti}_2\text{O}_7$ (Ln - Gd, Er, and Lu), $\text{Pu}_2\text{Ti}_3\text{O}_{8.7}$ and $\text{Sr}_{4-x}\text{Pu}_{2x/3}\text{Ti}_4\text{O}_{12}$ were also synthesized. Work on analogous compounds but containing americium was started.

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POLYMER SCIENCE GROUP; A. Habenschuss, Leader

In this program, we pursue fundamental structural and dynamic studies with the intent of providing a better understanding of advanced polymeric materials. To characterize the structure of bulk polymers and fibers at the molecular level, we use small angle and wide angle x-ray and neutron scattering; the motion and disorder in polymers is probed by NMR and neutron spectroscopy; scanning tunneling, atomic force, and optical microscopies can map out surface morphologies; and the bulk mechanical, transport, and thermodynamic properties are characterized with thermal and mechanical analysis. The theoretical aspects are addressed with state-of-the-art molecular dynamics and neural networks to simulate chain conformations, dynamics, and energy flow in polymers, with the simulations closely linked to experiment.

Wide angle x-ray (WAXS) and neutron (WANS) scattering are used to study the structure of liquids, polymer melts, and polymer blends to obtain fundamental information on the intra- and intermolecular interactions between molecules in these systems. For the first time, the partial H-H radial distribution functions (RDF) were obtained for three alkanes using the neutron isotopic substitution method without recourse to models of the intramolecular structure. Good agreement with molecular dynamics calculations was obtained. WAXS RDF measurements on a number of vinyl polymers were undertaken in an attempt to understand the general prediction of a "pre-peak" in the intermolecular C-C structure function by PRISM theory for vinyl polymers. The lack of a pre-peak in isotactic-polypropylene (i-PP) seems to suggest that the accepted Rotational Isomeric State (RIS) model for i-PP may be incorrect, and that it may have a structure different from other vinyl polymers. The intramolecular structure of vinyl polymers is of interest in modeling the structure of polymer blends.

A series of tetra-*n*-alkylammonium salts (TAAH) have been examined with thermal analysis, solid state NMR, atomic force microscopy, wide angle x-ray powder diffraction (Rietveld analysis), and single crystal analysis. The interest in these materials stems from the fact that these relatively small molecules display some of the same mesophases encountered in polymers. The twenty TAAHs studied undergo numerous transitions as a function of temperature, and the phases could be classified as ordered crystals, plastic crystals, or conformationally disordered (condis) crystals. Both stable and nonequilibrium behavior was analyzed. The method for distinguishing between plastic and condis crystals has already been applied to other disordered semicrystalline materials.

The ability of atomic force microscopy (AFM) to image structure at the atomic level is well established for many materials with good surface order. We have been using AFM to examine atomic scale defects, friction effects in ion implanted graphite and polystyrene, nonwoven polymer textiles, polymeric filtration materials, and the relationship of surface morphology to phase separation in alkane mixtures and polymer blends.

The mechanism of large scale irreversible deformation of semicrystalline polymers is a matter of controversy. One of the proposed explanations is that the crystalline regions must melt and

recrystallize during the deformation. In cases where hydrogenated and deuterated blends of a polymer are known to have some segregation of the components, small angle neutron scattering (SANS) has shown that deformation reduces the segregation. A similar effect occurs when the samples are melted and subjected to a fast quench. The similarity between the two processes suggests that deformation involves melting and recrystallization. SANS data collection has been completed, and analysis of the results is in progress.

A new modulated scanning calorimeter was acquired with the help of TA Instruments, Inc., and the rather interesting ability to separate reversible and irreversible phenomena was investigated. The method to measure heat capacities was extended to nonisothermal measurements, and the theory of differential thermal analysis was extended to cover the case of the glass transition. It is expected that a major advance in analyzing irreversible polymer properties will be made in the next few years. Solid state NMR was used to analyze the mobility of several polymers to establish the changes in physical properties as they are linked to molecular structure. This NMR technique has developed into the most definitive tool for the distinction between various polymer mesophases.

Polymer fibers are typically partially crystalline, however, attempts to correlate mechanical properties on the basis of a simple model of crystalline and amorphous fractions have proven to be inadequate. We have developed a systematic approach for analyzing x-ray diffraction data from polymer fibers by accounting for all intensity over two dimensional reciprocal space (full pattern two dimensional Rietveld analysis). This much more extensive analysis has resulted in the identification of three distinct structural domains in typical polymer fibers: crystalline, "oriented intermediate," and isotropic amorphous. In the "oriented intermediate" domain, the polymer chains are still parallel to the fiber axis but do not have long range crystalline order. It has been found that a number of thermal and mechanical properties of the fibers such as modulus and shrinkage are mainly determined by the amount and state of the oriented intermediate domain. The technique has been applied to PET, PPTA (Kevlar-49), and various types of PE. Complementary information is provided by small angle x-ray scattering (SAXS), calorimetry, atomic force microscopy, and solid state NMR. SAXS is also being used as a diagnostic tool for assessing the effects of variation in spinning rate and annealing procedures on morphology in the production of PET fibers.

Computational synthesis, a method for predicting the properties or for designing materials that have desired properties, was developed and tested. This method entails a novel computational paradigm for making rapid and accurate estimations of physical properties for molecular based systems. Results have been obtained for up to 16 properties of 357 different polymers, for making accurate predictions on the detonation velocity and sensitivity of energetic materials, for estimating protein degradabilities, and for predicting properties of a series of isomeric forms of saturated hydrocarbons and fluororganic compounds. In addition, the method can also be operated in the reverse direction: designing chemical structures that meet specified performance criteria. This is accomplished by using genetic algorithms to determine possible candidates based on the optimization of the trained neural network predictions. The overall abilities of the computational synthesis method provide new and far-reaching capabilities in materials design and analysis, an area which up to now has been to a large extent an empirical science.

We have also investigated the use of computational neural networks to learn the overall dynamics of a particular system in a MD simulation, and then predicting the effects of changing the size of the

system or the simulation time. This approach has been very successful and represents a major advancement in computer simulation of macromolecular systems.

We have developed computer codes that permit us to routinely run MD simulations on polymethylene crystals of size over 227 nm^3 with both united atom and full atom models. All modes of motion are allowed in these simulations; such a system is sufficiently large to serve as a model of a macroscopic polyethylene crystal. Reasonable agreements with experimental data on density, defect concentration and motion, diffusion, lamellar thickening, heat capacity, melting temperature, and the speed of sound in a polymer crystal have been reached. The large volume of detailed information of the structure and motion permits a new level of understanding of these systems.

A molecular dynamics based method was developed to compute the vibrational spectra and dispersion curves for linear macromolecules. The results are compared and contrasted with those of normal mode calculations, demonstrating the validity of the approach and providing fundamental insight into a number of dynamical processes. The strength of the method is its computational efficiency, and that it represents an exact classical dynamics approach to calculating vibrational spectra, thereby eliminating many of the weaknesses of normal mode calculations (i.e., the harmonic approximation).

Finally, we have investigated an innovative numerical integration algorithm for MD simulations which can greatly reduce the time for advancing a trajectory by a given time step. These methods, called symplectic integrators (SI), were compared with several nonsymplectic integrators which were found to lead to more significant energy drifts than the SIs.

A program on polymer blends, in collaboration with Sandia National Laboratory and the University of Illinois, aims to provide a scientific basis for the molecular design and characterization of multi-component polymer blends. The primary objective is to provide a foundation for multiphase materials development similar to the knowledge base in small molecule chemistry that underlies single phase polymers. Our approach involves polymer theory (PRISM, molecular dynamics, Monte Carlo), synthesis, and characterization (wide and small angle x-ray and neutron scattering). Some recent activity is given below.

SANS experiments are in progress on a blend with structural and energetic differences between the components. The system chosen was polystyrene/poly(p-methylstyrene) (PS/PPMS), because of the interesting observation that the FH interaction parameter (χ) appeared to exhibit a significant molecular weight dependence. The first SANS measurements have confirmed that $\chi = \chi(\text{MW}, \phi)$ is a function of both molecular weight and concentration, and further experiments to quantify the phase diagram are in progress.

The phase separation mechanisms in binary alkane mixtures have been investigated via SANS and SAXS. A 50/50 blend of $n\text{-C}_{30}\text{H}_{62}/n\text{-C}_{36}\text{D}_{74}$ showed a layered structure of single periodicity within 15 minutes of quenching from the melt, and subtle changes indicative of a superlattice occur within 30 hours. The SAXS/SANS results were in qualitative agreement with model calculations for an alternating layer structure, composed of ~80/20 mixtures.

Blends of linear and branched polymers are widely used commercially, though there is no consensus on the state of mixing of such materials. For mixtures of linear high density (HD) and long chain branched low density (LD) polyethylenes, widely different views continue to be expressed in the literature ranging from complete compatibility to phase separation in the melt. SANS and SAXS have been used to investigate the solid state morphology in linear/branched mixtures (HDPE/LDPE) and blends of HDPE with short branched linear low density polyethylene (LLDPE). The aim is to understand the influence of branching type and frequency, molecular weight, and polydispersity on melt compatibility.

The first systematic study of the influence of chain branching and backbone stiffness on the equilibrium properties of dense polymer melts has been carried out. Calculations at the atomistic, semiflexible chain, and Gaussian levels reveal the connection between polymer structure, packing, and thermodynamic properties. Theoretical predictions based on computationally convenient "intelligently" coarse grained models (in which the monomer unit is represented as a single site) were found to be in good agreement with the atomistic level results. Calculated melt solubility parameters of complicated polyolefin chains were found to be in good accord with recent PVT and neutron scattering observations.

Molecular dynamics and Monte Carlo simulations and PRISM calculations were performed for athermal polymer blends (i.e., with no heat of mixing) composed of short, freely jointed chains with different monomer size. Excellent agreement between the simulations and the PRISM predictions were found for interchain packing correlations, the excess free energy of mixing, and the effective χ -parameters. These comparisons between PRISM theory and simulations of systems of modest chain lengths ($N < 100$ segments) provide benchmark tests of the ability of PRISM to correctly predict the intermolecular packing in conformationally asymmetric athermal polymer blends.

Based on the success in describing packing correlations in athermal mixtures, thermodynamic perturbation theory was employed to compute the enthalpy of mixing effective χ -parameters and phase diagrams of various polyolefin and related blends, using a chemically realistic (atomistic) single chain model of polyethylene (PE) and isotactic polypropylene (i-PP). In accord with experiment, the theory finds that this blend is much more incompatible than predicted by FH theory. Moreover, similar large enthalpic χ -parameters were found using "intelligently" coarse grained semiflexible chain models, which mimic the conformational asymmetry associated with chain branching in polyolefin mixtures. These findings provide a theoretical basis for the use of solubility parameter approaches to polyolefin phase stability and have stimulated the development of a simple analytic solubility parameter theory of polymer alloy miscibility. Moreover, the theoretical ideas suggest new alloying and synthetic strategies based on controlled manipulation of molecular features such as chain branching and chemical microstructure to either promote or hinder phase separation.

A numerical study of structurally symmetric ("isotope-like") blends has been carried out, based on PRISM theory which uses the recently developed "molecular closures" and self consistently determines the chain conformation. Distinctive intrinsic and finite size fluctuation effects, including nonideal conformational changes for the minority component near the phase boundary are found. These non-FH effects depend on variables such as the density (ρ), concentration (ϕ), chain length and the spatial range of the van der Waals forces. Detailed comparisons with benchmark Monte Carlo simulations of Binder and coworkers show very good agreement, thereby verifying the accuracy of

self-consistent PRISM for describing density and concentration fluctuation phenomena in polymer alloys. These findings reproduce the functional dependence of χ on ϕ found via SANS in isotopic polymer mixtures at ORNL for PE, polyethylethylene, polyvinylethylene, etc. Simulation of $\chi(\phi)$ for polystyrene, which shows a qualitatively different shape of $\chi(\phi)$, is in progress.

Research Staff: B. K. Annis, A. Habenschuss, B. G. Sumpter, D. W. Noid, G. D. Wignall (Solid State Division), B. Wunderlich; *Postdoctoral Fellows:* J. Cheng, Y. Fu, A. A. Gakh, C. Getino, Y. Jin, G. Liang, J. D. Londono, J. Mueller, M. Pyda, M. Ralle, R. E. Tuzun, M. Varma-Nair, C. E. Wozny, A. Xenopoulos; *Guests:* E. G. Gakh (Moscow, Russia), R. A. Guenther (University of Nebraska), S. N. Kreitmeier (University of Regensburg, Germany), S. A. Meyer (The Colorado College), M. A. Morgenstern (The Colorado College), I. Okazaki (Toray Industries, Inc., Japan), R. Triolo (University of Palermo, Italy), Q. Wang (Lanzhou University, China); *Student Guests:* A. Boller (UT Knoxville), W. Chen (UT Knoxville), S. V. Gerdes (UT Knoxville), M. T. Spining (UT Knoxville), G. Zhang (UT Knoxville); *Collaborators:* F. S. Bates (University of Minnesota), J. G. Curro (Sandia National Laboratory), K. S. Schweizer (University of Illinois), S. Z. D. Cheng (University of Akron), L. Mandelkern (Florida State University), R. Snyder (University of California)

5. OFFICE OF ESH&Q PERFORMANCE AND FACILITY MANAGEMENT

F. J. Smith, Manager

It is the policy of the Chemical and Analytical Sciences Division (CASD) to conduct all work in a manner commensurate with maximum personal safety and health and to ensure minimal environmental impact. During 1994, CASD consolidated all Environmental, Safety, Health and Quality (ESH&Q) activities into a single office, the *Office of Environmental, Safety, Health, and Quality Performance and Facility Management*. This office, managed by F. J. Smith, provides leadership for division ESH&Q matters with special emphasis on maintaining safe and healthy working conditions and complying with federal and state laws, DOE orders, and LMES and ORNL policies and procedures pertaining to safety, conduct of operations, and environmental protection. S. D. Wright, Division Safety Officer, K. B. Thomas, Environmental Protection and Non-Nuclear Training Officer, J. L. Wagner, Quality Assurance Specialist, and R. F. Peacher, Nuclear Training Officer, provide guidance and one-on-one assistance to the research staff. The current ESH&Q and facility management "level of effort" in CASD is approximately five person years.

This year the division was the recipient of approximately 15 reviews, appraisals, and audits by external evaluators. All corrective actions are tracked on the MMES ESAMS with none overdue. Only three occurrence reports were filed with DOE for calendar year 1994 with most of those being related to contamination incidents.

1994 HIGHLIGHTS

1. The integration of individual ESH&Q activities of the predecessor divisions into a single Environmental, Safety, Health & Quality (ESH&Q) program. A single set of ESH&Q documentation was implemented.
2. Chemical and Analytical Sciences Division ESH&Q Self Assessment Program

Independent Appraisal of CASD Self Assessment Program

An ORNL ESH&Q Management Appraisal of the ORNL Chemical and Analytical Sciences Division was conducted in August 1994. Assessment of the structure, implementation, and effectiveness of the division's self assessment program identified no findings. A number of positive observations and proficiencies were noted. Among those were the use of Project ES&H Evaluation and Summary forms, the use of Management by Walking Around, and a divisional deficiency tracking database.

CASD Self Assessment Program Plan

In 1994, the CASD completed the first pass through a three year self assessment cycle. The rolling three year cycle of twelve elements covered principal ESH&Q functional areas in CASD and promoted comprehensive coverage. The elements receiving focus in 1994 were radiation protection, division-specific training, quality assurance, and division management and oversight.

Special Assessment Activities Arising from External (to ORNL) Drivers included Plutonium Vulnerability Assessment; 10CFR830.120 Price Anderson Amendments Act Compliance Assessment; Compliance Assessment for DOE Order 5480.20 Personnel Selection, Qualification, Training and Staffing Requirements for DOE Reactor and Nonreactor Nuclear Facilities; and Compliance Assessments for Compliance with Nuclear Facility Safety Documentation.

3. CASD had no lost time occupational injuries last year (only one first aid case).
4. Facility restart was achieved for the RMAL, Building 2026.
5. Radiation doses were maintained substantially below ALARA goals for the electrical upgrade of hot cells in building 2026 and for analytical support activities during the transuranium production campaign, Building 7920.
6. CASD operated over 75 RCRA waste accumulation sites last year with no significant "environmental noncompliances."
7. CASD personnel received over 3500 hours of required training during calendar year 1994. This office provided new employee orientation/training, including site-specific training, to all new employees and long-term guests of CASD.

6. OFFICE OF ADMINISTRATIVE SERVICES

S. D. Wright, Manager

The Office of Administrative Services (OAS) was formed during the merger of the Analytical Chemistry Division and the Chemistry Division. It was created in order to consolidate, where possible, the administrative functions of the two divisions. This office performs all administrative duties necessary to support a research organization of approximately 140 full-time staff members.

Those duties and the personnel responsible for them are listed below:

- ▶ Resources Coordinator, J. P. Hall
- ▶ Clerical Support, M. H. Limburg
- ▶ Finance Officer, M. Pasupathi¹
- ▶ Support Services Coordinator, L. K. Plemons
- ▶ Procurement, L. K. Woods
- ▶ Personal Computing and Network Consultation, S. D. Wright
- ▶ Manager, S. D. Wright

The Current OAS "level of effort" is 5.5 person years.

1994 Highlights

1. The integration of separate administrative organizations from the two divisions has gone smoothly. Personnel were assigned responsibilities in accordance with their personal strengths and attributes.
2. Our procurement function has constantly changed and adapted in order to meet the ever increasing requirements of MMES's ESH&Q procedures. The level of orders in this office has increased from approximately 1200 to 2400. Though it has not been without its growing pains, it continues to perform at an extremely high level of efficiency.
3. CASD began implementing a strategy to convert from the existing DCA computing network to the 10Mb/s ethernet network currently being installed at ORNL. Approximately 65% of CASD now has access to the internet through this effort. Efforts included installation of approximately 70 ethernet drops in Buildings 4500N and 4500S, as well as initiation of a project which will bring fiber optic ethernet service to four facilities (5505, 5507, 5510, and 5510A) which previously had no link to the ethernet.
4. This office coordinated the 35th Annual DOE/ORNL Conference on Analytical Chemistry in Energy Technology. There were over 400 attendees and 32 exhibitors, which made this our most successful conference ever in terms of participation.

¹Finance and Business Management Division

APPENDIX A. SOURCES OF FUNDING

FUNDING SOURCES (FY 1994)

	<u>\$M</u>	<u>%</u>
Department of Energy	17.60	64.5
Basic Energy Sciences*	10.00	36.7
Health and Environmental Research	0.53	1.9
Environmental Management	3.82	14.0
Nonproliferation	2.02	7.4
Defense-related	0.48	1.8
Energy Efficiency and Renewable Energy	0.64	2.3
Other	0.11	0.4
Work for Others	2.55	9.3
Department of Defense	1.43	5.2
National Institutes of Health	0.39	1.4
National Cancer Institute	0.28	1.0
Center for Indoor Air Research	0.26	1.0
Electric Power Research Institute	0.15	0.5
Other	0.03	0.1
Special Analytical Projects**	5.77	21.1
Laboratory-Directed R&D**	1.38	5.1
TOTAL	27.30	100.0

*Chemical Sciences, 6.64; Materials Sciences, 2.33; Geosciences, 1.03.

**Adjusted for overhead exemption.

CHEMICAL AND ANALYTICAL SCIENCES DIVISION
May 1, 1995

M. L. POUTSMA, DIRECTOR
C. J. Steele
L. R. Pyles

ESH&Q PERFORMANCE AND FACILITY MANAGEMENT

F.J. SMITH*, MANAGER
M.J. Hanner⁸, Safety and Health Representative
R.F. Peacher*, Nuclear Facilities Training
F.J. Smith*, Radiation Control Officer
K.B. Thomas*, Environmental Protection Officer
K.B. Thomas*, Non-Nuclear Facilities Training
J.L. Wagner⁸, Quality Assurance Specialist
S.D. Wright*, Division Safety Officer
D.S. Blazier*,¹¹

FACILITY MANAGERS

R.A. Jenkins*
W.H. Griest*
J.M. Keller*
S.A. McLuckey*
L. Robinson*
F.J. Smith*
S.D. Wright*

ADMINISTRATIVE SERVICES

S.D. WRIGHT*, MANAGER
J.P. Hall*, Resources Management
M. Pasupathi⁸, Finance Officer
L.K. Plemons, Services Coordinator
L.K. Woods, Procurement
M.H. Limburg¹¹

SPECIAL ASSIGNMENTS

S.A. Barshick*, Student Coordinator
D.S. Blazier*, Procedures Coordinator
P.V. Bonnesen*, Seminar Committee Chair
A.B. Dindal*, Values Committee
J.P. Hall*, Precious Metals Coordinator, United Way Coordinator
D.R. Huntley*, Improvement Council Chair
S.L. Lantz*, Employment Representative
P.M. Trentham*, Work Force Diversity Representative
L.A. Warneke*, Publications Coordinator
S.D. Wright*, Computer Security Officer, Technology Transfer Officer
J.P. Young*, Postdoctoral Coordinator

ANALYTICAL SPECTROSCOPY

S. A. McLOCKEY*, HEAD
J. D. Allgood
S. L. Lantz*

NUCLEAR AND RADIOCHEMISTRY

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L. A. Warneke*
A. R. Atwater

ORGANIC CHEMISTRY

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K. L. Hagerman
E. T. Maestas

PHYSICAL AND MATERIALS CHEMISTRY

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R. G. Violet
D. L. Greene
J. D. Patterson⁵

*MULTIPLE ASSIGNMENTS

¹GUEST SCIENTIST

²ORNL POSTDOCTORAL FELLOW

³UTK POSTDOCTORAL FELLOW

⁴GRADUATE STUDENT GUEST

⁵SUBCONTRACTOR EMPLOYEE

⁶ORNL/UTK DISTINGUISHED SCIENTIST

⁷UTK ADJUNCT R&D PARTICIPANT

⁸ON ASSIGNMENT FROM OTHER ORNL DIVISIONS/OFFICES

⁹DOE DISTINGUISHED POSTDOCTORAL FELLOW

¹⁰ORNL BES/GEOSCIENCES PROGRAM COORDINATOR

¹¹PART-TIME EMPLOYEE

¹²UNDERGRADUATE STUDENT

NUMEROUS SHORT-TERM GUESTS, SUBCONTRACTORS, AND CONSULTANTS CONTRIBUTE TO THE WORK OF THE DIVISION BUT ARE NOT SPECIFICALLY LISTED ON THIS CHART.

(see following pages for further detail)

ANALYTICAL SPECTROSCOPY SECTION

S. A. McLUCKEY*, HEAD
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INORGANIC MASS SPECTROMETRY

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M.L. Turner
R.E. Valiga
R.M. Coleman
R.L. McPherson

OPTICAL SPECTROSCOPY

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ORGANIC MASS SPECTROMETRY

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SECONDARY ION MASS SPECTROMETRY

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SURFACE CHEMISTRY AND HETEROGENEOUS CATALYSIS

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RADIOACTIVE MATERIALS ANALYSIS

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HIGH TEMPERATURE AQUEOUS CHEMISTRY

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APPENDIX C. PUBLICATIONS, PRESENTATIONS, AND REPORTS

ANALYTICAL SPECTROSCOPY SECTION

INORGANIC MASS SPECTROMETRY GROUP

Books/Book Chapters

Winchester, M. R., Duckworth, D. C. and Marcus, R. K., "Analysis of Nonconducting Sample Types," in *Glow Discharge Spectroscopies*, R. K. Marcus, ed., Plenum Publishing (1993).

Journal Articles

Barshick, C. M. and Eyler, J. R. "An Improved Ion Guide for External Ion Injection in Glow Discharge-Fourier Transform Ion Cyclotron Resonance (GD-FTICR) Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* (1993) 4, 387-392.

Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Analysis of Solution Residues by Glow Discharge Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* (1993) 4, 47-53.

Barshick, C. M., Shaw, R. W., Young, J. P. and Ramsey, J. M. "Isotopic Analysis of Uranium Using Glow Discharge Optogalvanic Spectroscopy and Diode Lasers," *Anal. Chem.* (1994) 66, 4154-4158.

Barshick, C. M., Smith, D. H., Hackney, J. H., Cole, B. A. and Wade, J. W. "Glow Discharge Mass Spectrometric Analysis of Trace Metals in Petroleum," *Anal. Chem.* (1994) 66(5), 730-734.

Barshick, C. M., Smith, D. H., Wade, J. W. and Bayne, C. K. "The Analysis of Waste Oil Samples by Isotope Dilution Glow Discharge Mass Spectrometry," *J. Anal. Atom. Spectrom.* (1994) 9, 83.

Colodner, D., Salters, V. and Duckworth, D. C. "Ion Sources for Analysis of Inorganic Solids and Liquids by Mass Spectrometry," *Anal. Chem.* (1994).

Duckworth, D. C., Donohue, D. L., Smith, D. H., Marcus, R. K. and Lewis, T. A. "Design and Characterization of a Radio-Frequency Powered Glow Discharge Source for Double-Focusing Mass Spectrometers," *Anal. Chem.* (1993) 65, 2478-2484.

Duckworth, D. C., Barshick, C. M. and Smith, D. H. "The Analysis of Soils by Glow Discharge Mass Spectrometry," *J. Anal. Atom. Spectrosc.* (1993) 8, 875-879.

Duckworth, D. C., Barshick, C. M., Bostick, D. A. and Smith, D. H. "Direct Measurement of Uranium Isotopic Ratios in Soils by Glow Discharge Mass Spectrometry," *Appl. Spectrosc.* (1993) 47, 243-245.

Duckworth, D. C., Barshick, C. M., Smith, D. H. and McLuckey, S. A. "Dynamic Range Extension in Glow Discharge Quadrupole Ion Trap Mass Spectrometry," *Anal. Chem.* (1994) 66(1), 92-98.

- Dunbar, N. B., Riciputi, L. R., Jacobs, G. and Christie, W. "Generation of Rhyolitic Melt in a Man-Made Magma: Implications for Fractional Crystallization Processes in Natural Magmas," *J. Volcan. Geotherm. Res.* (1993) **57**, 157-166.
- Hess, K. R., Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Influence of Solution-Deposited Anions on Glow Discharge Relative Ion Yields," *Appl. Spectrosc.* (1994) **48**(11), 1307-1315.
- Jin, C., Haufler, R. E., Hettich, R. L., Barshick, C. M., Compton, R. N., Puretzky, A. A., Dem'yanenko, A. V. and Tuinman, A. "Novel Molybdenum Carbide Clusters Mo_nC_{4n} , ($n=1-4$)," *Science* (1994) **263**, 68.
- Mei, Y., Duckworth, D. C., Cable, P. R. and Marcus, R. K. "Effect of Target Gas in Collision-Induced Dissociation Using a Double Quadrupole Mass Spectrometer and Radiofrequency Glow Discharge," *J. Am. Soc. Mass Spectrom.* (1994) **5**(9), 845-851.
- Riciputi, L. R., Johnson, C. M., Sawyer, D. A. and Lipman, P. W. "Crustal and Magmatic Evolution in a Large Multicyclic Caldera Complex: Isotopic Evidence from the Central San Juan Volcanic Field," *J. Volcanol. Geotherm. Res. - Special Caldera Volume* (1994).
- Riciputi, L. R., Machel, H. G. and Cole, D. R. "Ion Microprobe Studies of Diageneses: I. Carbonates in the Devonian Nisku Formation of Alberta, Canada," *J. Sediment. Petrol.* (1994).
- Riciputi, L. R., Christie, W. H., Cole, D. R. and Rosseel, T. M. "Analysis of Rare Earth Elements in Silicates by Ion Microprobe Using Doubly-Charged Ions," *Anal. Chem.* (1993) **65**(9), 1186-1191.
- Riciputi, L. R., McSween, H. Y., Johnson, C. A. and Prinz, M. "Minor and Trace Element Concentrations in Carbonates of Carbonaceous Chondrites, and Implications for the Compositions of Coexisting Fluids," *Geochim. Cosmochim. Acta* (1994) **58**, 1343-1351.
- Riciputi, L. R. and Paterson, B. A. "High Spatial Resolution Measurement of Oxygen Isotope Ratios in Silicates and Carbonates by Ion Microprobe," *Amer. Mineral.* (1994) **79**, 2027-2030.
- Riciputi, L. R., Cole, D. R. and Machel, H. G. "An Ion Microprobe Study of Diagenetic Carbonates in the Devonian Nisku Formation of Alberta, Canada," *J. Sediment. Res.* (1994) **A64**, 115-127.
- Riciputi, L. R., Cole, D. R. and Machel, H. G. "Sulfide Formation in Reservoir Carbonates of the Devonian Nisku Formation, Alberta, Canada: An Ion Microprobe Study," *Geochim. Cosmochim. Acta* (1994).
- Riciputi, L. R., Duckworth, D. C., Barshick, J. M. and Smith, D. H. "Isotope Ratio Measurements Using Glow Discharge Mass Spectrometry," *Int. J. Mass Spectrom. Ion Proc.* (1994).
- Shick, C. R., Marcus, R. K., Hunter, H. L., Wheeler, D., Smith, D. H. and Duckworth, D. C. "Radio-Frequency-Powered Ion Source for the Analysis of Flat Samples by Sector-Based GDMS," *Anal. Chem.* (1994).

Teng, J., Barshick, C. M., Duckworth, D. C., Morton, S. J., Smith, D. H. and King, F. L. "Factors Influencing the Quantitative Determination of Trace Elements in Soils by Glow Discharge Mass Spectrometry," *Appl. Spectrosc.* (1994).

Watson, C. H., Wronka, J., Laukien, F. H., Barshick, C. M. and Eyler, J. R. "The Application of Ultrahigh Mass Resolution to Glow Discharge Mass Spectrometry," *Spectrochim. Acta B* (1993) **48B(11)**, 1445-1448.

Watson, C. H., Wronka, J., Laukien, F. H., Barshick, C. M. and Eyler, J. R. "High Mass Resolving Power Glow Discharge Mass Spectrometry Using an External Ion Source FT-ICR Mass Spectrometer," *Anal. Chem.* (1993) **65**, 2801.

Zhou, F., Van Berkel, G. J., Morton, S. J., Duckworth, D. C., Adeniyi, W. K. and Keller, J. M. "Development of On-line Electrochemical Sample Pretreatment Methods for ICP-MS," *American Society for Testing and Materials, Special Technical Publication* (1994).

Presentations/Conference Proceedings

Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Isotope Ratio Measurements of Solution Residues by Glow Discharge Mass Spectrometry," 1993 European Winter Conference on Plasma Spectrochemistry, Granada, Spain, Jan. 10-15, 1993.

Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Relative Ion Yield Studies of Glow Discharge Solution Residues," Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

Barshick, C. M., Smith, D. H., Duckworth, D. C., Wade, J. W. and Bayne, C. K. "The Analysis of Waste Oil Samples by Isotope Dilution Glow Discharge Mass Spectrometry," 1993 European Winter Conference on Plasma Spectrochemistry, Granada, Spain, Jan. 10-15, 1993.

Barshick, C. M. and Smith, D. H. "Glow Discharge-Isotope Dilution Mass Spectrometry," 41st American Society of Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Barshick, C. M. and Smith, D. H. "Direct Analysis of Oils by Solution Residue Glow Discharge Mass Spectrometry," DOE/ORNL Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Barshick, C. M., Watson, C. H., Wronka, J., Laukien, F. H. and Eyler, J. R. "The Application of Glow Discharge-Fourier Transform Ion Cyclotron Resonance (GD-FTICR) Mass Spectrometry to Isotope Ratio Measurements," 41st American Society for Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Barshick, C. M., Duckworth, D. C., McLuckey, S. A., McKown, H. S. and Smith, D. H. "Ion Kinetic Energy Spectrometry of Inorganic Ions," American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Barshick, C. M., Shaw, R. W., Young, J. P. and Ramsey, J. M. "Uranium Isotope Ratio Measurements Using Diode Laser Optogalvanic Spectroscopy," American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Barshick, C. M., Shaw, R. W., Young, J. P. and Ramsey, J. M. "Glow Discharge Atomization Coupled with Optogalvanic Detection for Isotopic Analysis," 1994 Winter Conference on Plasma Spectrochemistry, San Diego, CA, Jan. 10-15, 1994.

Barshick, C. M., Duckworth, D. C., McKown, H. S., McLuckey, S. A. and Smith, D. H. "Collisional Dissociation of Diatomic Ions Produced in a Glow Discharge," 13th International Mass Spectrometry Conference, Budapest, Hungary, Aug. 29-Sept. 2, 1994.

Barshick, C. M., McLuckey, S. A., McKown, H. S. and Smith, D. H. "Mass Analyzed Ion Kinetic Energy Spectrometry of Inorganic Ions," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Glow Discharge Mass Spectrometry: It's Not Just for Metals Any More," 35th DOE/ORNL Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 11-13, 1994.

Cole, D. R., Riciputi, L. R. and Machel, H. G. "An Ion Microprobe Study of Sulfur Isotope Variability in Pyrites from Devonian Carbonates, Western Canada Sedimentary Basin, Alberta, Canada," Strasbourg, France, April 1-5, 1993, abstracts of the European Union of Geosciences VII (in press).

Duckworth, D. C., Barshick, C. M., Smith, D. H., McLuckey, S. A., Yelton, R. and Hess, K. R. "Mass Spectrometric Investigations of Glow Discharge-Generated Ions with a Quadrupole Ion Trap," 35th DOE/ORNL Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 11-13, 1994.

Duckworth, D. C., Barshick, C. M., Smith, D. H., McLuckey, S. A., Yelton, R. and Hess, K. R. "Design and Characterization of a New RF-Glow Discharge Mass Spectrometer," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Duckworth, D. C., Barshick, C. M., Smith, D. H., McLuckey, S. A., Hess, K. R. and Yelton, R. "Glow Discharge Mass Spectrometry Using a Quadrupole Ion Trap Mass Analyzer," 13th International Mass Spectrometry Conference, Budapest, Hungary, Aug. 29-Sept. 2, 1994.

Duckworth, D. C. "Design and Characterization of a Radio Frequency Powered Glow Discharge Source for the VG9000," 3rd International Conference on Plasma Source Mass Spectrometry, Durham, UK, Sept. 13-18, 1992.

Duckworth, D. C., Riciputi, L. R. and Smith, D. H. "Direct Analysis of Soils by Radio-Frequency Powered Glow Discharge Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Duckworth, D. C. and Smith, D. H. "Fundamental Considerations for Quantitative Analyses of Non-conducting Materials by RF-GDMS," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

Duckworth, D. C., Barshick, C. M. and Smith, D. H. "Analysis of Soils by Glow Discharge Mass Spectrometry," European Winter Conference on Plasma Spectrochemistry, Grenada, Spain, Jan. 10-15, 1993.

Fraracci, K. N., Taylor, L. A., Jerde, E. A., Snyder, G. A., Clayton, R. N., Mayeda, T. K., Riciputi, L. R. and Sobolev, N. V. "Two Unusual Diamondiferous Eclogite Xenoliths from the MIR Kimberlite in Yakutia, Siberia," Geological Society of American Meeting, Boston, MA, Oct. 25-29, 1993.

Jin, C., Haufler, R. E., Hettich, R. L., Barshick, C. M., Compton, R. N., Puretzky, A. A., Dem'yanenko, A. V. and Tuinman, A. A. "Novel Metal Carbide Clusters MnC_4n , ($n=1-8$)," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Limbach, P. A., Marshall, A. G., Duckworth, D. C. and Buchanan, M. V. "RF Glow Discharge Ionization with FT/ICR/MS Detection," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Machel, H. G., Krouse, H. R., Burton, E. A., Foght, J. M., Riciputi, L. R. and Cole, D. R. "The Nisku Sour Gas Play: A Unique Natural Laboratory for the Study of Thermochemical Sulfate Reduction," American Association of Petroleum Geologists Meeting, 1993.

Machel, H. G., Krouse, H. R., Riciputi, L. R. and Cole, D. R. "The Devonian Nisku Sour Gas Play, Canada - A Unique Natural Laboratory for Study of Thermochemical Sulfate Reduction," Geochemical Transformations of Sedimentary Sulfur American Chemical Society Symposium Series, 1993.

Machel, H. G., Krouse, H. R., Foght, J. M., Riciputi, L. R. and Cole, D. R. "Sour Gas in the Nisku Formation of Central Alberta: Geochemical Evidence for Biologic and Thermochemical Sulfate Reduction," CSEG/CSPG Exploration Update Meeting, 1994.

Marcus, R. K., Shick, C. R., Sharpe, J., Hunter, H. L. and Duckworth, D. C. "Radio Frequency Glow Discharge (GDMS) Analysis of Nonconductive Materials," Pittsburgh Conference and Exposition '94, Chicago, IL, Feb. 28-Mar. 4, 1994.

McSween, H. Y., Riciputi, L. R., Johnson, C. A. and Prinz, M. "Trace Element Concentrations in Calcite and Dolomite from Carbonaceous Chondrites Determined by Ion Microprobe, and Coexisting Fluid Compositions," Annual Meteoritical Society Meeting, Vail, CO, July 19-23, 1993.

Morton, S. J., Van Berkel, G. J., Duckworth, D. C., Keller, J. M. and Smith, D. H. "Development of Electrochemical Sample Pretreatment for Inductively Coupled Plasma Mass Spectrometry," ASTM Symposium on Applications of ICP/MS to Radionuclide Determinations, Gatlinburg, TN, Oct. 13-14, 1994.

- Paterson, B. A., McSween, H. T. and Riciputi, L. R. "High Spatial Resolution Sulphur Isotopic Analysis of Troilite in Ordinary Chondrites by Ion Microprobe," 25th Lunar and Planetary Science Conference, Houston, TX, Mar. 14-17, 1994.
- Riciputi, L. R., Duckworth, D. C., Barshick, C. M. and Smith, D. H. "Isotopic Analyses by Glow Discharge Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 31-June 5, 1993.
- Riciputi, L. R., Cole, D. R. and Machel, H. G. "Sulfur Isotope Variations in Devonian Carbonates of the Western Canada Sedimentary Basin, Alberta, Canada: An Ion Microprobe Study," Geological Society of America Meeting, Boston, MA, Oct. 25-29, 1993.
- Riciputi, L. R., Barshick, C. M., Duckworth, D. C. and Smith, D. H. "An Evaluation of Glow Discharge Mass Spectrometry for the Measurement of Isotope Ratios," 2nd Alfred O. Nier Symposium on Inorganic Mass Spectrometry, Durango, CO, May 10-12, 1994.
- Riciputi, L. R., Paterson, B. A., Cole, D. R. and Machel, H. G. "Ion Microprobe Investigations of $\delta^{34}\text{S}$ Variability in Sulfides from the Obed Sour Gas Reservoir, Alberta, Canada," Society for Sedimentary Geology Research Conference, Lake Ozark, MO, May 21-25, 1994.
- Riciputi, L. R. and Paterson, B. A. "In-situ Analysis of Oxygen Isotope Ratios in Silicates and Carbonates by Ion Microprobe," *Proc., Goldschmidt Conference*, Edinburgh, Scotland, Aug. 28-Sept. 2, 1994, in *Mineral Mag.* (1994) **58A**, 770-771.
- Riciputi, L. R. and Paterson, B. A. "Analysis of Oxygen Isotope Ratios of Silicates, Carbonates, and Phosphates In-Situ by Small-Radius Ion Microprobe," Annual Geological Society of America Meeting, Seattle, WA, Oct. 20-25, 1994.
- Shaw, R. W., Barshick, C. M., Young, J. P. and Ramsey, J. M. "Laser Spectroscopy for Practical Isotope Ratio Measurements," IV Laser Applications to Chemical Analysis Meeting, Jackson Hole, WY, Mar. 8-11, 1994.
- Shaw, R. W., Young, J. P., Barshick, C. M. and Ramsey, J. M. "Diode Laser Spectroscopy for Practical Isotope Ratio Measurements," ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.
- Shick, C. R., Marcus, R. K., Hunter, H. L. and Duckworth, D. C. "Development and Characterization of a Flat Sample Holder for RF Glow Discharge Mass Spectrometry," 1994 Winter Conference on Plasma Spectrochemistry, San Diego, CA, Jan. 10-15, 1994.
- Srinivasan, K., Riciputi, L. R. and Walker, K. R. "REE Geochemistry of Cambro-Ordovician Platform Carbonates: Implications for Sources of Diagenetic Fluids," Annual Geological Society of America Meeting, Seattle, WA, Oct. 20-25, 1994.
- Smith, D. H., Carter, J. A. and Bostick, D. A. "Lutetium Double Spiking: An Independent Method of Inventory Verification," 2nd International Tank Measurement Conference, Ispra, Italy, Oct. 5-8, 1993.

Smith, D. H., Duckworth, D. C., Bostick, D. T., Coleman, R. M. and McPherson, R. L. "Analysis of Femtogram-Sized Plutonium Samples by Thermal Ionization Mass Spectrometry," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Snyder, G. A., Taylor, L. A., Jerde, E. A. and Riciputi, L. R. "Evolved QMD-Melt Parentage for Lunar Highlands Alkali Suite Cumulates: Evidence from Ion Probe Rare-Earth Element Analyses of Individual Minerals," 25th Lunar and Planetary Science Conference, Houston, TX, Mar. 14-17, 1994.

Swihart, G. H., McBay, E. H., Smith, D. H. and Carpenter, S. B. "Boron Isotopic Study of the Tertiary Bedded Borate Deposits of Furnace Creek, California," Annual Geological Society of America Meeting, Boston, MA, Oct. 25-28, 1993.

Swihart, G. H., Barshick, C. M., McBay, E. H. and Smith, D. H. "Instrumental Techniques for Boron Isotope Analysis," Annual Geological Society of America Meeting, Seattle, WA, Oct. 24-27, 1994.

Teng, J., King, F. L., Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Determination of Relative Sensitivity Factors for the Quantitative Analysis of Clays by Glow Discharge Mass Spectrometry," DOE/ORNL Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Teng, J., King, F. L., Barshick, C. M., Duckworth, D. C. and Smith, D. H. "Parameters Influencing Relative Sensitivity Factors for Trace Element Determination in Clays by Glow Discharge Mass Spectrometry," 1994 Winter Conference on Plasma Spectrochemistry, San Diego, CA, Jan. 10-15, 1994.

Teng, J., Barshick, C. M., Duckworth, D. C., Smith, D. H. and King, F. L. "GDMS Characterization of Trace Elements in Soil Samples," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Valiga, R. E., Duckworth, D. C. and Smith, D. H. "Quadrupole Glow Discharge Mass Spectrometry as a Routine Multiple Element Analysis Technique," Colloquium Spectroscopicum Internationale, Leipzig, German, Aug. 27-Sept. 6, 1994.

Van Berkel, G. J., Zhou, F., Morton, S. J. and Duckworth, D. C. "Electrochemical Preconcentration/Cleanup Techniques Coupled On-line with Inductively Coupled Plasma-Mass Spectrometry and Electrospray-Mass Spectrometry for Enhanced Trace Element Determination," 35th ORNL-DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 11-13, 1994.

Watson, C. H., Barshick, C. M. and Eyler, J. R. "Using Ion-Molecule Reactions to Enhance High Resolution Glow Discharge FTICR Mass Spectrometry," 41st American Society for Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Watson, C. H., Wronka, J., Laukien, F. H., Barshick, C. M. and Eyler, J. R. "Development of a Pulsed-Gas Glow Discharge Ion Source for High Mass Resolution on a Fourier Transform Ion Cyclotron

Resonance Mass Spectrometer," 41st American Society of Mass Spectrometry Meeting, San Francisco, CA, May 31-June 4, 1993.

Young, J. P., Barshick, C. M., Shaw, R. W. and Ramsey, J. M. "Application of Diode Lasers to the Isopiestic Selective Determination of Uranium in Oxides by Laser Enhanced Ionization," 7th International Symposium on Resonance Ionization Spectroscopy and Its Applications (RIS-94), Bernkastel-Kues, Germany, July 3-8, 1994.

Zhou, F., Van Berkel, G. J., Duckworth, D. C. and Morton, S. J. "Electrochemical Stripping Analysis Combined On-Line with Inductively Coupled Plasma-Mass Spectrometry for Enhanced Trace Metal Determination," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Zhou, F., Van Berkel, G. J., Duckworth, D. C. and Morton, S. J. "Stripping Analysis Combined On-line with Inductively Coupled Plasma-Mass Spectrometry for Enhanced Trace Metal Determination," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Conference, St. Louis, MO, Oct. 2-7, 1994.

Reports

Smith, D. H., McKown, H. S. Bostick, D. T., Coleman, R. M., Duckworth, D. C. and McPherson, R. L. *Analysis of Femtogram-Sized Plutonium Samples*, ORNL/TM-12632 (1994).

OPTICAL SPECTROSCOPY GROUP

Books/Book Chapters

Young, J. P. "Foreword for Radiation and Society," in *American Chemical Society Advances in Chemistry Series Book*, J. P. Young and Rosalyn Yalow, eds. (1994).

Journal Articles

Barnes, M. D., Brooks, P. R., Curl, R. F. and Johnson, B. H. "Probing Chemical Reactions: Evidence for Exploration of an Excited Potential Energy Surface at Thermal Energies," *Science* (1993) **261**, 1434.

Barnes, M. D., Ng, K. C., Whitten, W. B. and Ramsey, J. M. "Detection of Single Rhodamine 6G Molecules in Levitated Microdroplets," *Anal. Chem.* (1993) **65**, 2360-2365.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Probing Femtosecond Dynamics in Solution on a Picosecond Timescale: Cavity Enhancement of Spontaneous Emission Rates in Levitated Microdroplets," *Chem. Phys. Lett.* (1994) **227**, 628-632.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Single Molecule Detection in Liquids," *Anal. Chem.* (1994) (in press).

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Enhanced Fluorescence Yields Through Cavity-QED Effects in Microdroplets," *J. Opt. Soc. Am. B*, (1994) **11**(7), 1297.

Dai, S., Mamantov, G., Coffield, J. E., Begun, G. M. and Young, J. P. "Accurate Procedure for Determining the Calibration Curve of High-Temperature Molten Salt Systems via Raman Spectroscopy," *Appl. Spectrosc.* (1993) **47**, 1286-1288.

Dai, S., Coffield, J. E., Mamantov, G. and Young, J. P. "Reduction of Quartz Fiber Raman Backgrounds in High Temperature Fiberoptic Raman Spectroscopy via the Measurement of Anti-Stokes Raman Spectra," *Appl. Spectrosc.* (1994) **48**(6), 766-768.

Dale, J. M., Yang, M., Whitten, W. B. and Ramsey, J. M. "Chemical Characterization of Single Microparticles by Laser Ablation/Desorption in a Quadrupole Ion Trap Mass Spectrometer," *Anal. Chem.* (1994) **66**, 3431-3435.

Jacobson, S. C., Koutny, L. B., Hergenroder, R., Moore, A. W. and Ramsey, J. M. "Microchip Capillary Electrophoresis with an Integrated Postcolumn Reactor," *Anal. Chem.* (1994) **66**, 3472-3476.

Jacobson, S. C., Hergenroder, R., Koutny, L. B. and Ramsey, J. M. "High Speed Separations on a Microchip," *Anal. Chem.* (1994) **66**(7), 1114-1118.

Jacobson, S. C., Hergenroder, R., Koutny, L. B. and Ramsey, J. M. "Open Channel Electrochromatography on a Microchip," *Anal. Chem.* (1994) **66**(14), 2369-2373.

Jacobson, S. C., Hergenroder, R., Koutny, L. B., Warmack, R. J. and Ramsey, J. M. "Effects of Injection Schemes and Column Geometry on the Performance of Microchip Electrophoresis Devices," *Anal. Chem.* (1994) **66**(7), 1107-1113.

Jacobson, S. C., Hergenroder, R., Moore, A. W. and Ramsey, J. M. "Pre-Column Reactions with Electrophoretic Analysis Integrated on a Microchip," *Anal. Chem.* (1994) **66**, 4127-4132.

Stump, N. A., Burns, J. B., Dai, S., Mamantov, G., Young, J. P. and Peterson, J. R. "Europium Oxide Absorption Spectroscopy as an Optical Probe of Temperature," *Spectrosc. Lett.* (1993) **26**(6), 1073.

Presentations/Conference Proceedings

Barnes, M. D., Ng, K. C., Whitten, W. B., Arnold, S. and Ramsey, J. M. "Detection of Single Molecules in Microspheres," in *Proc., Society for Optical Engineering '93 Conference*, Los Angeles, CA, Jan. 16-22, 1993.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Digital Molecular Detection of Fluorescent Molecules in Liquid Microspheres," 20th Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "QED-Enhanced Fluorescence Yields in Levitated Microdroplets," in *Proc., U.S. Army Edgewood Research and Development Engineering Center Conference on Obscuration*, Aberdeen Proving Grounds, MD, June 22-24, 1993.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Solution Dynamics and Cavity-QED in Liquid Microdroplets," Annual Optical Society of America Meeting, Toronto, Canada, Oct. 3-8, 1993.

Barnes, M. D. "Solution Dynamics and Cavity-QED Effects in Microdroplets: Probing Ultrafast Dynamics via Fluorescence," Seminar at Rice University, Houston, TX, Oct. 28, 1994.

Barnes, M. D. "Solution Dynamics and Cavity-QED in Microdroplets: Probing Ultrafast Dynamics via Fluorescence," Yale University Mini-Symposium on Physics of Droplets, New Haven, CT, May 25-27, 1994.

Barnes, M. D. "Solution Dynamics and Cavity-QED in Microdroplets: Probing Ultrafast Dynamics via Fluorescence," Department of Physics, New Mexico State University, White Sands Missile Range, NM, Dec. 1, 1994.

Barnes, M. D., Whitten, W. B. and Ramsey, J. M. "Single-Molecule Detection in Microdroplets," Laser Applications to Chemical Analysis IV Meeting, Jackson Hole, WY, Mar. 8-11, 1994.

Barshick, C. M., Shaw, R. W., Young, J. P. and Ramsey, J. M. "Glow Discharge Atomization Coupled with Optogalvanic Detection for Isotopic Analysis," 1994 Winter Plasma Conference, San Diego, CA, Jan. 10-15, 1994.

Barshick, C. M., Shaw, R. W., Young, J. P. and Ramsey, J. M. "Uranium Isotope Ratio Measurements Using Diode Laser Optogalvanic Spectroscopy," American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Burnett, M. N. and Johnson, C. K. "Euclidean and Spherical 2-Orbifolds," Annual American Crystallographic Association Meeting, Atlanta, GA, June 25-July 1, 1994.

Coffield, J. E., Dai, S., Young, J. P. and Mamantov, G. "Analysis of Fluoride in Molten Salt Mixtures Using Microwave Digestion," DOE/ORNL Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Dai, S., Coffield, J. E., Mamantov, G., Young, J. P. and Begun, G. M. "Reduction of Quartz Raman Backgrounds in High Temperature Fiberoptic Raman Spectroscopy," Pittsburgh Conference on Analytical Chemistry, Atlanta, GA, Mar. 1993.

Hergenroder, R., Jacobson, S. C., Koutny, L. B., Warmack, R. J. and Ramsey, J. M. "Microchip Capillary Electrophoresis," 5th International Conference on High Performance Capillary Electrophoresis, Orlando, FL, Jan. 25-28, 1993.

Hergenroder, R., Jacobson, S. C., Koutny, L. B. and Ramsey, J. M. "Microscale Liquid Phase Sensors: Chromatography on a Chip," ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Hergenroder, R., Jacobson, S. C., Koutny, L. B. and Ramsey, J. M. "Microminiaturized Chemical Instruments: The Ultimate Chemical Sensors?," Pittsburgh Conference and Exposition, Chicago, IL, Feb. 27-Mar. 4, 1994.

Jacobson, S. C., Hergenroder, R., Koutny, L. B. and Ramsey, J. M. "Microchip Capillary Electrophoresis Devices," 4th Annual Frederick Conference on Capillary Electrophoresis, Frederick, MD, Oct. 19-20, 1993.

Jacobson, S. C., Koutny, L. B., Hergenroder, R., Warmack, R. J. and Ramsey, J. M. "Liquid Phase Separation on a Microchip," 17th International Symposium on Column Liquid Chromatography, High Performance Liquid Chromatography Meeting, Hamburg, Germany, May 9-14, 1993.

Jacobson, S. C., Hergenroder, H., Koutny, L. B. and Ramsey, J. M. "High Speed Electrophoretic Separations on a Microchip," High Performance Capillary Electrophoresis Meeting, San Diego, CA, Jan. 31-Feb. 3, 1994.

Jacobson, S. C., Hergenroder, R., Koutny, L. B. and Ramsey, J. M. "Electrochromatography on a Microchip," 18th International Symposium on Liquid Chromatography, Minneapolis, MN, May 8-13, 1994.

Jacobson, S. C., Hergenroder, R., Koutny, L. B. and Ramsey, J. M. "Micro-Scale Liquid Phase Sensors: Chromatography on a Chip," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Jacobson, S. C., Hergenroder, R., Moore, A. W. and Ramsey, J. M. "Electrically Driven Separations on a Microchip," Solid-State Sensor and Actuator Workshop, Hilton Head, SC, June 13-19, 1994.

Jacobson, S. C., Moore, A. W. and Ramsey, J. M. "Microfabricated Instruments for Liquid Phase Analysis," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Johnson, C. K. and Burnett, M. N. "Crystallographic Orbifold Atlas," 2nd Canadian Computational Chemistry Conference, Queen's University, Kingston, Ontario, Canada, May 21-25, 1994.

Johnson, C. K. and Burnett, M. N. "Euclidean Orbifolds and Their Singular Sets," Annual American Crystallographic Association Meeting, Atlanta, GA, June 25-July 1, 1994.

Koutny, L. B., Hergenroder, R., Jacobson, S. C. and Ramsey, J. M. "Microchip Capillary Electrophoresis of Proteins with an Integrated Post-Column Reactor," Pittsburgh Conference and Exposition, Chicago, IL, Feb. 27-Mar. 4, 1994.

Moore, A. W., Jacobson, S. C. and Ramsey, J. M. "Microchip Separations Using Micellar Electrokinetic Capillary Chromatography," Frederick Conference on Capillary Electrophoresis, Frederick, MD, Oct. 25-26, 1994.

Ramsey, J. M., Hergenroder, R., Jacobson, S. C. and Koutny, L. B. "Microchip Liquid Phase Separation Devices," 15th International Symposium on Capillary Chromatography, Riva del Garda, Italy, May 24-18, 1993.

Ramsey, J. M., Barnes, M. D. and Whitten, W. B. "Microdroplet-Based Ultrasensitive Analysis," Annual Optical Society of America Meeting, Toronto, Canada, Oct. 3-8, 1993.

Ramsey, J. M., Barnes, M. D. and Whitten, W. B. "Fluorescence Spectroscopy in Microspheres: Fundamentals and Applications," International Conference on Luminescence and Optical Spectroscopy of Condensed Material, Storrs, CT, Aug. 9-13, 1993.

Ramsey, J. M. "The Adventures of Fluorescence Spectroscopy in Microspheres," University of Utah, Salt Lake City, UT, April 8, 1993.

Ramsey, J. M. "Microdroplet Fluorescence Spectroscopy: Detection and Photophysics," 28th Colloquium Spectroscopicum Internationale, York, United Kingdom, June 29-July 4, 1993.

Ramsey, J. M. "Fluorescence Detection of Single Molecules in Solution," Bowling Green State University, Bowling Green, OH, April 20-21, 1993.

Ramsey, J. M. "Detection of Single Fluorescent Molecules in Solution," University of British Columbia, Edmonton, Alberta, Feb. 22-23, 1993.

Ramsey, J. M. "Chemical Measurement of the Future: Think Small," University of Wisconsin, Madison, WI, May 6, 1993.

Ramsey, J. M. "Chemical Measurement at the Micron Scale," University of Toledo, Toledo, OH, April 19, 1993.

Ramsey, J. M. "Chemical Characterization of Microparticles Using Electrodynamical Traps," East Tennessee Mass Spectrometry Discussion Group, Knoxville, TN, April 13, 1993.

Ramsey, J. M. "Microminiaturized Instrumentation for Chemical Separations," Workshop on Field/Portable Mass Spectrometry, 41st ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Ramsey, J. M. "Chemical Measurements on the Micron Scale," Brigham Young University, Salt Lake City, UT, April 6-7, 1993.

Ramsey, J. M., Hergenroder, R., Jacobson, S. C., Koutny, L. B. and Moore, A. W. "Process Sensing with Microminiaturized Chemical Instrumentation," WATTEC Conference and Exhibition, Knoxville, TN, Feb. 22-25, 1994.

Ramsey, J. M., Dale, J. M., Yang, M. and Whitten, W. B. "Mass Spectrometry of Individual Micro-particles in an Ion Trap," IV Laser Applications to Chemical Analysis Meeting, Jackson Hole, WY, Mar. 8-11, 1994.

Ramsey, J. M. "Miniature Chemical Instrumentation: The Next Generation?" Abbott Laboratories, Chicago, IL, Aug. 11, 1994.

Ramsey, J. M., Jacobson, S. C., Hergenroder, R. and Koutny, L. B. "Microchip Liquid Phase Analysis Devices," 6th International Symposium on High Performance Capillary Electrophoresis, San Diego, CA, Jan. 31-Feb. 3, 1994.

Ramsey, J. M. "Single Molecules and Microchips," University of South Carolina, Columbia, SC, Dec. 9, 1994.

Ramsey, J. M. "Ongoing Activities in Micromachining at ORNL," Micromanufacturing Technology Center Workshop, Oak Ridge, TN, Feb. 21, 1994.

Ramsey, J. M. "Miniaturization of the CE Process," Advanced Lab Exposition and Conference (ALEX '94), San Jose, CA, Oct. 25-27, 1994.

Ramsey, J. M. "Miniature Instruments for Liquid Phase Analysis," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Ramsey, J. M. "Miniature Chemical Instrumentation: The Next Generation?" Stanford University, Stanford, CA, Sept. 1, 1994.

Ramsey, J. M. "Micromachined Devices for Performing Chemical Reactions and Separations," National Institute of Standards and Technology, Gaithersburg, MD, Nov. 15, 1994.

Ramsey, J. M. "Microfabricated Chemical Instrumentation for Chemical Sensing," Section Meeting of American Institute of Chemical Engineers, Knoxville, TN, Oct. 13, 1994.

Ramsey, J. M. "Microfabricated Chemical Instruments," Gordon Conference on Bioanalytical Sensors, New London, NH, July 17-22, 1994.

Ramsey, J. M. "Microfabrication of Chemical Instruments," Fourth International Workshop on Bioanalysis, Lawrence, KS, July 10-13, 1994.

Ramsey, J. M. "Counting Molecules: The Ultimate Approach to Chemical Analysis," Society of Applied Spectroscopy Speakers Tour, Detroit Section, Dearborn, MI, April 11, 1994.

Ramsey, J. M. "Analysis of Ultradilute Solutions Based on Single Molecule Detection in Micro-droplets," Gordon Conference on Bioanalytical Sensors, New London, NH, July 17-22, 1994.

Ramsey, J. M. "Analytical Chemistry on a Small Scale: Microdroplets, Microchips, and Micro-particles," Society of Applied Spectroscopy Speakers Tour, Minnesota Section, Mendota Heights, MN, April 12, 1994.

Ramsey, J. M. "Analytical Chemistry on a Small Scale: Microdroplets, Microchips, and Micro-particles," Society of Applied Spectroscopy Speakers Tour, Penn-York Section, Corning, NY, April 13, 1994.

Ramsey, J. M. "Chemical Measurements of the Future: Think Small," University of North Carolina, Chapel Hill, NC, April 18, 1994.

Ramsey, J. M. "Chemical Measurements of the Future: Think Small," Glaxo Corporation, Research Triangle Park, NC, April 19, 1994.

Shaw, R. W. "Fieldable Instrument for Isotope Ratio Measurements," DOE EXPO '93, Oak Ridge, TN, May 3-7, 1993.

Shaw, R. W. "In Situ Laser Diagnostics for the CVD Growth of Diamond Film," Optical Diagnostics Workshop, Oak Ridge, TN, Dec. 1-2, 1993.

Shaw, R. W., Young, J. P., Barshick, C. M. and Ramsey, J. M. "Diode Laser Spectroscopy for Practical Isotope Ratio Measurements," ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Shaw, R. W., Barshick, C. M., Young, J. P. and Ramsey, J. M. "Laser Spectroscopy for Practical Isotope Ratio Measurements," IV Laser Applications to Chemical Analysis Meeting, Jackson Hole, WY, Mar. 8-11, 1994.

Whitten, W. B. "Atmospheric Sampling of Aerosol Particles," DOE EXPO '93, Oak Ridge, TN, May 3-7, 1993.

Whitten, W. B. "Ultrasensitive Fluorescence Detection/Biological Threat Detector," DOE EXPO '93, Oak Ridge, TN, May 3-7, 1993.

Whitten, W. B., Shapiro, M. J., Ramsey, J. M. and Bronk, B. V. "Identification of Individual Micro-organisms by a Microsphere Fluorescence Immunoassay," in *Proc., U.S. Army Edgewood Research and Development Engineering Center Conference on Obscuration*, Aberdeen, MD, June 22-25, 1993.

Whitten, W. B., Shaw, R. W. and Ramsey, J. M. "Raman Spectroscopy of Levitated Diamond Micro-crystals," Annual Optical Society of America Meeting, Toronto, Canada, Oct. 3-8, 1993.

Whitten, W. B., Shapiro, M. J., Ramsey, J. M. and Bronk, B. V. "Morphological Resonances for Multicomponent Immunoassays," IV Laser Applications to Chemical Analysis Meeting, Jackson Hole, WY, Mar. 8-11, 1994.

Whitten, W. B., Ramsey, J. M. and Bronk, B. V. "Microsphere Fluoroimmunoassay for Microorganisms - An Update," in *Proc., U.S. Army Edgewood Research and Development Engineering Center Conference on Obscuration and Aerosol Research*, Aberdeen Proving Ground, MD, June 22-24, 1994.

Yang, M., Dale, J. M., Whitten, W. B. and Ramsey, J. M. "Optical and Mass Spectrometry of Individual Microparticles in Electrodynamical Traps," American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Yang, M. and Ramsey, J. M. "Nitrocellulose Destruction by Laser," U.S. Army Construction Engineering Laboratory Workshop on Nitrocellulose Research, W. Lafayette, IN, Nov. 4-5, 1993.

Yang, M., Dale, J. M., Whitten, W. B. and Ramsey, J. M. "Laser Desorption Mass Spectrometry of Individual Microparticles in an Ion Trap," in *Proc., Laser Spectroscopy Symposium*, KAERI, Taejon, Korea, Nov. 3-4, 1994.

Yang, M., Dale, J. M., Whitten, W. B. and Ramsey, J. M. "Laser Desorption Mass Spectrometry of a Single Levitated Microparticle in a Quadrupole Ion Trap," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Young, J. P., Dai, S., Coffield, J. E., Mamantov, G. and Claus, K. G. "Raman Sensor Development in Molten Salt Systems: A Recently Completed CRADA," Optical and Diagnostics Symposium, Pollard Auditorium, Oak Ridge, TN, Dec. 1-2, 1993.

Young, J. P., Shaw, R. W. and Ramsey, J. M. "Application of Diode Lasers to the Determination of Lanthanides and Actinides," 12th Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

Young, J. P. "Resonance Ionization Mass Spectrometry Developments at Oak Ridge National Laboratory," 2nd Symposium on Laser Spectrometry, Yusong, Taejon, Korea, Nov. 2-4, 1994.

Young, J. P. "Review of RIS and RIMS at ORNL," Seminar, Korea Institute of Geology, Mining, and Minerals, Daejeon, Korea, Apr. 18, 1994.

Young, J. P., Barshick, C. M., Shaw, R. W. and Ramsey, J. M. "Application of Diode Lasers to the Isopiestic Selective Determination of Uranium in Oxides by Optogalvanic Spectroscopy," in *Proc., 7th International Symposium on Resonance Ionization Spectroscopy and Its Applications (RIS-94)*, Bernkastel-Kues, Germany, July 3-8, 1994, H. Jurgen Kluge, James E. Parks and Klaus Wendt, eds., pp. 111-114 (1994).

Young, J. P., Barshick, C. M., Shaw, R. W. and Ramsey, J. M. "Application of Diode Lasers to the Isotopically Selective Determination of Uranium in Oxides by Optogalvanic Spectroscopy," Resonance Ionization Spectroscopy '94 Meeting, Bernkastel-Kues, Germany, July 3-8, 1994.

Young, J. P., Dai, S. and Mamantov, G. "All-Silica Fiberoptic Probe; Recent Studies and New Directions," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Reports

Young, J. P. and Mamantov, G. *In-Line Sensors for Electrolytic Magnesium Cells -- 10th Quarterly Report*, ORNL/M-2666 (1993).

Young, J. P. and Mamantov, G. *In-Line Sensors for Electrolytic Magnesium Cells, 11th Quarterly Report*, ORNL/M-2808 (1993).

Young, J. P., Coffield, J., Dai, S. and Mamantov, G. *In-Line Sensors for Electrolytic Magnesium Cells -- Final Report*, ORNL/M-3003 (1993).

ORGANIC MASS SPECTROMETRY GROUP

Books/Book Chapters

Hettich, R. L. and Jin, C. "Laser Ablation and Laser Desorption Techniques with Fourier Transform Mass Spectrometry," in *Principles and Applications of Laser Ablation*, J. C. Miller, ed., Springer Series in Materials Science 28, Springer Verlag Publishers, Berlin (1994), pp. 135-154.

Journal Articles

Buchanan, M. V. and Hettich, R. L. "The Characterization of Large Biomolecules by Fourier Transform Mass Spectrometry of High Mass Biomolecules," *Anal. Chem.* (1993) **65**, 245A-259A.

Caton, J., Hazen, K., Griest, W., Watson, A. and Buchanan, M. "Rapid Method for Isolating Targeted Organic Chemicals from Biological Matrices," *Anal. Lett.* (1994) **27**, 351-362.

Chillier, X. F. D., Van Berkel, G. J., Gulacar, F. O. and Buchs, A. "Characterization of Chlorins Within a Natural Chlorin Mixture Using Electrospray/Ion Trap Mass Spectrometry," *Org. Mass Spectrom.* (1994) **29**, 672-678.

Dunphy, J. C., Busch, K. L., Hettich, R. L. and Buchanan, M. V. "Rapid Extraction and Structural Characterization of Biomolecules in Agarose Gels by Laser Desorption Fourier Transform Mass Spectrometry," *Anal. Chem.* (1993) **65**, 1329.

Goeringer, D. E., Asano, K. G., McLuckey, S. A., Hoekman, D. and Stiller, S. W. "Filtered-Noise-Field Signals for Mass-Selective Accumulation of Externally Formed Ions in a Quadrupole Ion Trap," *Anal. Chem.* (1994) **66**(3), 313-318.

Goeringer, D. E., Chambers, D. M., McLuckey, S. A. and Glish, G. L. "Matrix-Assisted Laser Desorption of Peptides Couples with CID in a Quadrupole Ion Trap," *Anal. Chem.* (1993) **65**, 14-20.

- Hettich, R., Jin, C. and Compton, R. "Determination of the Electron Affinities of Fluorinated Fullerenes ($C_{60}F_{44,46}$, $C_{70}F_{52,54}$) by Fourier Transform Mass Spectrometry," *Int. J. Mass Spectrom. Ion Proc.* (1994) **138**, 263-274.
- Hettich, R., Hurst, G., Buchanan, M. and Stemmler, E. "Characterization of Polycyclic Aromatic Hydrocarbon Dihydrodiol Epoxide DNA Adducts Using Matrix Assisted Laser Desorption Mass Spectrometry," *Polycycl. Arom. Compounds* (1994) **6**, 95-102.
- Jacobson, K. B. and Hettich, R. L. "Characterization of Underivatized Pterins by Laser Desorption Fourier Transform Mass Spectrometry," *Pteridines* (1993) **4**, 72-75.
- Jenkins, R., Buchanan, M., Merriweather, R., Ilgner, R., Gayle, T. and Watson, A. "Movement of Chemical Warfare Agent Simulants Through Porous Media," *J. Hazard. Mater.* (1994).
- Jin, C., Hettich, R. L., Compton, R. N., Joyce, D. B., Blencoe, J. G. and Burch, T. E. "Direct Solid Phase Hydrogenation of Fullerenes," *J. Phys. Chem.* (1994) **98**, 4215-4217.
- Jin, C., Hettich, R., Compton, R. and Tuinman, A. "Attachment of Two Electrons to $C_{60}F_{46,48}$: Shape Resonances in Multiply Charged Anions," *Phys. Rev. Lett.* (1994) **73**, 2821.
- Jin, Y., Xenopoulos, A., Cheng, J., Chen, W., Wunderlich, B., Diack, M., Jin, C., Hettich, R. L., Compton, R. N. and Guiochon, G. "Thermodynamic Characterization of the Plastic Crystal and Non-Plastic Crystal Phases of C_{70} ," *Mol. Cryst. Liq. Cryst.* (1994) **257**, 235-250.
- Jin, C., Haufler, R. E., Hettich, R. L., Compton, R. N., Puretzky, A. A. and Dem'yanenko, A. V. "Synthesis and Characterization of Molybdenum Carbide Clusters: MO_nC_{4n} ($n=1-4$)," *Science* (1994) **263**, 68-71.
- McLuckey, S. A., Van Berkel, G. J., Goeringer, D. E. and Glish, G. L. "Ion Trap Mass Spectrometry of Externally Generated Ions," *Anal. Chem.* (1994) **66**, 689A-696A.
- McLuckey, S. A., Van Berkel, G. J., Goeringer, D. E. and Glish, G. L. "Ion Trap Mass Spectrometry Using High Pressure Ionization," *Anal. Chem.* (1994) **66**, 737A-743A.
- McLuckey, S. A. and Ramsey, R. S. "Gaseous Myoglobin Ions Stored at Greater than 300 K," *J. Am. Soc. Mass Spectrom.* (1994) **5**, 324.
- Nourse, B. D., Hettich, R. L. and Buchanan, M. V. "Methyl Guanine Isomer Distinction by Hydrogen/Deuterium Exchange Using a Fourier Transform Mass Spectrometer," *J. Am. Soc. Mass Spectrom.* (1993) **4**, 296.
- Quirke, J. M. E., Adams, C. L. and Van Berkel, G. J. "Chemical Derivatization for Electrospray Ionization-Mass Spectrometry-I. Alkyl Halides, Alcohols, Phenols, Thiols, and Amines," *Anal. Chem.* (1994) **66**, 1302-1315.

- Ramsey, R. S., Kerchner, G. A. and Cadet, J. "Micellar Electrokinetic Capillary Chromatography of Nucleic Acid Constituents and Dinucleoside Monophosphate Photoproducts," *J. High Resol. Chromatogr.* (1994) 17, 4.
- Ramsey, R. S., Goeringer, D. E. and McLuckey, S. A. "Active Chemical Background and Noise Reduction in Capillary Electrophoresis/Ion Trap Mass Spectrometry," *Anal. Chem.* (1993) 65, 3521.
- Stemmler, E. A., Hettich, R. L., Hurst, G. B. and Buchanan, M. V. "Matrix-Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry of Oligodeoxyribonucleotides," *Rapid Commun. Mass Spectrom.* (1993) 7, 828-836.
- Stemmler, E. A. and Buchanan, M. V. "Negative and Positive Chemical Ionization Mass Spectra of Aromatic Amines: Surface-Assisted Reactions Involving Oxygen," *Org. Mass Spectrom.* (1993) 28, 953-962.
- Stemmler, E. A., Buchanan, M. V., Hurst, G. B. and Hettich, R. L. "The Structural Characterization of Polycyclic Aromatic Hydrocarbon Dihydodiols Epoxide DNA Adducts Using Matrix-Assisted Laser Desorption/Ionization Fourier Transform Mass Spectrometry," *Anal. Chem.* (1994) 66(8), 1274-1285.
- Van Berkel, G. J. and Goeringer, D. E. "Gas Chromatography-Tandem Mass Spectrometry Implemented on a Benchtop Quadrupole Ion Trap-Based Instrument Using Radar Noise to Effect Collision-Induced Dissociation," *Anal. Chim. Acta* (1993) 227, 41-54.
- Van Berkel, G. J., Quinones, M. A. and Quirke, J. M. E. "Geoporphyrin Analysis Using Electrospray Ionization-Mass Spectrometry," *Energy & Fuels* (1993) 7, 411.
- Van Berkel, G. J. and Zhou, F. "Chemical Electron-Transfer Reactions in Electrospray-Mass Spectrometry: Effective Oxidation Potentials of Electron-Transfer Reagents in Methylene Chloride," *Anal. Chem.* (1994) 66, 3408-3415.
- Van Berkel, G. J. and Asano, K. G. "Chemical Derivatization for Electrospray Ionization-Mass Spectrometry-II: Aromatic, Heteroaromatic, and Other Highly-Conjugated Systems," *Anal. Chem.* (1994) 66, 2096-2102.
- Van Berkel, G. J., Asano, K. G. and McLuckey, S. A. "Observation of Gas-Phase Molecular Dications Formed from Neutral Organics in Solution via Chemical Electron-Transfer Reactions Using Electrospray Ionization Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* (1994) 5, 689-692.
- Wise, M., Thompson, C. V., Buchanan, M. V., Guerin, M. R. and Merriweather, R. "Direct Sampling Ion Trap Mass Spectrometry," *Spectrosc.* (June, 1993).
- Yoshida, H. and Hettich, R. L. "Characterization and Identification of Radiation-Induced Products of Thymidine-3'-Monophosphate and Thymidylyl (3'->5') Thymidine by Laser Desorption Fourier Transform Mass Spectrometry," *Radiat. Res.* (1994) 139, 271-279.

Zhou, F., Van Berkel, G. J. and Donovan, B. T. "Electron Transfer Reactions of $C_{60}F_{48}$," *J. Am. Chem. Soc.* (1994) 116, 5485-5486.

Presentations/Conference Proceedings

Asano, K. G., Goeringer, D. E., McLuckey, S. A., Hoekman, D. and Stiller, S. W. "Mass-Selective Ion Accumulation in the Ion Trap: Ion Injection Using Filtered Noise Fields," 41st American Society of Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Asano, K. G. and Van Berkel, G. J. "Ionization of Aromatic Hydrocarbons in Solution for Analysis by Electrospray Ionization-Mass Spectrometry," 41st American Society of Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Asano, K. G., Goeringer, D. E. and McLuckey, S. A. "Pressure and Residence Time Effects in Atmospheric Sampling Glow Discharge Ionization," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Barshick, S. A., Smith, S. M., Buchanan, M. V. and Guerin, M. R. "Determination of Benzene in Food by Direct Sampling Ion Trap Mass Spectrometry," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Barshick, S. A. and Buchanan, M. V. "Novel Sampling Methods for Use with Thermal Desorption Ion Trap Mass Spectrometry," American Society of Mass Spectrometry (ASMS), Chicago, IL, May 30-June 3, 1994.

Barshick, S. A., Smith, S. M. and Buchanan, M. V. "Determination of Volatile Organic Compounds in Food Using a Novel Blender-Purge and Trap Device," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Britt, P. F., Hurst, G. B. and Buchanan, M. V. "Electrophore-Labeled DNA for Enhanced Sensitivity in Matrix-Assisted Laser Desorption Mass Spectrometry," DOE Contractor and Grantee Workshop of the Human Genome Program, Santa Fe, NM, Nov. 13-17, 1994.

Buchanan, M. V. "Rapid Detection of Trace Drugs in Physiological Media by Ion Trap Mass Spectrometry," Midwest Regional Meeting of American Association of Pharmaceutical Scientists, Chicago, IL, May 17, 1993.

Buchanan, M. V. and Barshick, S. A. "Direct Sampling Mass Spectrometry," Pittcon '93, Atlanta, GA, March 8-12, 1993.

Buchanan, M. V., Shahgholi, M. and Cook, K. D. "Effects of Surface Tension and Surface Activity on Electrospray Response," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Buchanan, M. V., Shahgholi, M. and Cook, K. D. "The Effect of Physical Parameters on Electrospray Response," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Buchanan, M. V., Wise, M. B. and Guerin, M. R. "Rapid Detection of Trace Organics with Direct Sampling Ion Trap Mass Spectrometry," Southeast Regional Meeting of the American Chemical Society, Johnson City, TN, Oct. 17-20, 1993.

Buchanan, M. V. "Probing Molecular Structure with Mass Spectrometry," Middle Atlantic Mass Spectrometry Discussion Group, Nov. 1993.

Buchanan, M. V. "Probing Molecular Structure with Fourier Transform Mass Spectrometry," SERS Lecture, Oak Ridge, TN, April 1993.

Buchanan, M. V. "Multi-Threat Analyzer," DOE EXPO, Oak Ridge, TN, May 1993.

Buchanan, M. V. Graduate Lecture on FTICR, Department of Chemistry, University of Tennessee, Nov. 1, 1993.

Buchanan, M. V. "Modern Mass Spectrometry: Solving Problems in Many Areas of Science," SERS Lecture to Undergraduates, Feb. 23, 1994.

Buchanan, M. V. "Advances in the Analysis of Oligonucleotides with Mass Spectrometry," Department of Chemistry, University of Illinois, Nov. 4, 1994.

Buchanan, M. V. "Characterization of Normal and Modified Oligonucleotides with FT ICR," Department of Chemistry, Ohio State University, March 30, 1994.

Goeringer, D. E., Ramsey, J. M., Dale, J. M., Wise, M. B., Buchanan, M. V. and McLuckey, S. A. "Advanced Chemical Analysis Instrumentation for Treaty Verification: Ion Trap Mass Spectrometry," Chemical Weapons Convention Verification Technology Research and Development Conference, Washington, DC, Mar. 2-3, 1993.

Goeringer, D. E. and McLuckey, S. A. "Advances in the Detection of Explosives Vapors via Ion Trap Tandem," 10th Annual ADPA Symposium and Exhibition on Security Technology, Williamsburg, VA, June 20-23, 1993.

Goeringer, D. E., Asano, K. G., McLuckey, S. A., Stiller, S. W. and Hoekman, D. "MS_n in the Quadrupole Ion Trap Using Filtered Noise Fields," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 31-June 4, 1993.

Goeringer, D. E. and McLuckey, S. A. "Ion Trap Collisional Activation: Shake and Bake," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Goeringer, D. E. and McLuckey, S. A. "A Theoretical Model for the Kinetics of Collision-Induced Dissociation in a Quadrupole Ion Trap," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Hart, K. J. and Buchanan, M. V. "Software Development for a Field Portable Ion Trap Mass Spectrometer," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Herron, W. J., Goeringer, D. E. and McLuckey, S. A. "Quadrupole Ion Trap Instrumentation for the Study of Multiply-Charged Ion Reactions," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Hettich, R. L., Stemmler, E., Hurst, G. and Buchanan, M. "Matrix-Assisted Laser Desorption FTMS for the Examination of Normal and Modified Oligonucleotides," W. Hancock visit to ORNL, Oak Ridge, TN, Aug. 30, 1993.

Hettich, R. L., Stemmler, E., Hurst, G. and Buchanan, M. "Structural Characterization of Normal and Modified Oligonucleotides by FTMS," Science Innovation '93, Boston, MA, Aug. 9, 1993.

Hettich, R. L., Jin, C., Thomas, R., Compton, R. N., Buseck, P. and Tsipursky, S. "Characterization of Naturally-Occurring and Modified Fullerenes by Fourier Transform Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Hettich, R. L., Jin, C., Britt, P. F., Hauffler, R. and Compton, R. N. "Preparation and Structural Characterization of Modified Fullerenes," Fullerenes '93 Meeting, Santa Barbara, CA, June 28-July 1, 1993.

Hettich, R. L., Jin, C., Compton, R., Buseck, P. and Tsipursky, S. "Characterization of Naturally-Occurring and Modified Fullerenes by Fourier Transform Mass Spectrometry," Second International Conference on Laser Ablation (COLA '93), Knoxville, TN, April 19-22, 1993.

Hettich, R. L., Hurst, G. B., Stemmler, E. and Buchanan, M. V. "MALDI Matrices for the FTMS Detection of Normal and Modified Oligonucleotides," Workshop on MALDI Matrices for Biomolecules, 41st ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, June 1, 1993.

Hettich, R. L., Hurst, G. B., Stemmler, E. and Buchanan, M. V. "Characterization of Modified Nucleic Acid Constituents by Matrix-Assisted Laser Desorption FTMS," 14th International Symposium on Polycyclic Aromatic Compounds, Osage Beach, Missouri, Sept. 8, 1993.

Hettich, R. L., Hurst, G. B. and Buchanan, M. V. "Matrix-Assisted Laser Desorption Mass Spectrometry for the Structural Characterization of Oligonucleotides," Human Genome Workshop, Santa Fe, NM, Feb. 7-11, 1993.

Hettich, R. L., Jin, C. and Stemmler, E. "Considerations for High Resolution Mass Detection with FTMS," Workshop on Detection of High Mass Ions at High Resolution, 41st ASMS Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, June 1, 1993.

Hettich, R. L. and Yoshida, H. "MALDI-FTMS for the Characterization of Ultraviolet and X-Ray Damage to Nucleic Acid Constituents," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Hettich, R. L., Jin, C., Compton, R., Buseck, P. and Tsipursky, S. "Characterization of Naturally-Occurring and Modified Fullerenes by Fourier Transform Mass Spectrometry," in *Proc., American Institute of Physics Conference*, J. C. Miller and D. B. Goehagan, eds., AIP Press, New York, Vol. 288, pp. 94-99 (1994).

Hettich, R. L. "Combining Laser Technology with FTMS for the Characterization of Non-Volatile Compounds," South Dakota School of Mines and Technology, Rapid City, South Dakota, Feb. 15, 1994.

Hettich, R. L., Jin, C., Compton, R. N. and Tuinman, A. A. "Electronic Properties of Modified Fullerenes: FTMS Charge Exchange Reactions of Hydrogenated Fullerene Cations and Fluorinated Fullerene Doubly-Charged Negative Ions," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Hettich, R. L. "Combining Laser Technology with FTMS for the Characterization of Non-Volatile Compounds," Montana State University, Bozeman, Montana, Feb. 16, 1994.

Hettich, R. L. and Compton, R. N. "FTMS for Determining Structures and Thermochemical Properties of Fullerenes and Fullerene Derivatives," Exxon Engineering and Research Division, Annandale, NJ, March 3, 1994.

Hettich, R. L., Jin, C., Britt, P. F., Tuinmann, A. A. and Compton, R. N. "Ionic Properties of Hydrogenated and Fluorinated Fullerenes," in *Proc., Materials Research Society Symposium*, Vol. 349, p. 133 (1994).

Hettich, R. L., Stemmler, E. A., Hurst, G. B. and Buchanan, M. V. "Identification and Structural Characterization of Modified Nucleotides and Oligonucleotides by MALDI-FTMS," 3rd International Symposium on Mass Spectrometry in the Health and Life Sciences, San Francisco, CA, Sept. 13-18, 1994.

Hettich, R. L., Stemmler, E. A., Hurst, G. B. and Buchanan, M. V. "Matrix-Assisted Laser Desorption FTMS for the Structural Examination of Modified Nucleotides and Oligonucleotides," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Hurst, G. B. "Fundamental Studies of Matrix-Assisted Laser Desorption/Ionization," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Hurst, G. B., Czartoski, T. J. and Buchanan, M. V. "Alternative Sample Preparation Methods for MALDI-MS," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Hurst, G. B., Hettich, R. L., Buchanan, M. V. and Stemmler, E. "Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry for the Structural Characterization of Modified Oligonucleotides," in *Proc., American Institute of Physics Conference*, J. C. Miller and D. B. Goehagan, eds., AIP Press, New York, Vol. 288, pp. 365-374 (1994).

Hurst, G. B., Hettich, R. L., Buchanan, M. V. and Stemmler, E. A. "Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry for the Structural Characterization of Modified Oligonucleotides," 2nd International Conference on Laser Ablation, Knoxville, TN, Apr. 19-22, 1993.

Jacobson, K. B., Buchanan, M. V., Chen, C. H., Doktycz, M. J., McLuckey, S. A. and Arlinghaus, H. F. "Application of Mass Spectrometry to DNA Fingerprinting and DNA Sequencing," in *Proc., Second International Symposium on the Forensic Aspects of DNA Analysis*, Federal Bureau of Investigation, Quantico, VA, March 29-April 2, 1993 (in press).

Jin, C., Hettich, R. L., Puretzky, A. A., Ying, C., Haufler, R. E. and Compton, R. N. "Electronic Structures of Endohedral Fullerenes," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Jin, C., Haufler, R. E., Hettich, R. L., Barshick, C. M., Compton, R. N., Puretzky, A. A., Dem'yanenko, A. V. and Tuinman, A. A. "Novel Metal Carbide Clusters MnC_4n , ($n=1-8$)," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Jin, C., Hettich, R. L. and Compton, R. N. "Laser Desorption Fourier Transform Mass Spectrometry Studies of Modified Fullerenes," in *Proc., Second International Conference on Laser Ablation (COLA '93)*, Knoxville, TN, April 19-22, 1993, J. C. Miller and D. B. Goehagan, eds., AIP Press, New York, Vol. 288, pp. 141-147 (1994).

Jin, C., Hettich, R. L. and Compton, R. N. "Generation of Fullerene-Based Compounds and Characterization by FTMS," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Jin, C., Hettich, R. L. and Compton, R. N. "Ionic Properties of Hydrogenated and Fluorinated Fullerenes," Materials Research Society Annual Meeting, Boston, MA, Nov. 29-Dec. 2, 1993.

Jin, C. and Hettich, R. L. "Examination of Fullerene Coalescence and Hydrogenation by Fourier Transform Mass Spectrometry," Recipient of Student Travel Award to ASMS Sponsored by the East Tennessee Mass Spectrometry Discussion Group, ETMSDG Meeting, Knoxville, TN, May 11, 1993.

Kruger, M. S., Cook, K. D. and Ramsey, R. S. "Evaluation of a Sheathless Capillary Electrophoresis/Electrospray Ionization Interface on an Ion Trap Mass Spectrometer," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Lammert, S. A. and Buchanan, M. V. "Modification of a Finnigan-MAT ITS-40 to Perform Selective Isolation and MS/MS Functions," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Limbach, P. A., Marshall, A. G., Duckworth, D. C. and Buchanan, M. V. "RF Glow Discharge Ionization with FT/ICR/MS Detection," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

McLuckey, S. A., Goeringer, D. E. and Hart, K. J. "Collisional Activation for the Study of Energetics and Structure," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

McLuckey, S. A. and Goeringer, D. E. "Explosives Vapor Detection by Ion Trap Tandem Mass Spectrometry," 9th Annual Joint Government-Industry Symposium and Exhibition on Security Technology, Virginia Beach, VA, June 21-24, 1993.

McLuckey, S. A., Goeringer, D. E. and Hart, K. J. "Ion Trap Collisional Activation," 6th Lake Louise Workshop on Tandem Mass Spectrometry, Calgary, Canada, Nov. 17-20, 1993.

McLuckey, S. A., Van Berkel, G. J., Hart, K. J., Habibi-Goudarzi, S., Ramsey, R. S. and Quirke, J. M. E. "Electrospray Ionization and the Quadrupole Ion Trap Mass Spectrometer," Pittsburgh Conference, Atlanta, GA, Mar. 10, 1993.

McLuckey, S. A. and Goeringer, D. "Cooking Ions in a Radio-wave Oven," Baltimore/Washington Area Mass Spectrometry Discussion Group Meeting, Washington, DC, Jan. 24, 1994.

Morton, S. J., Van Berkel, G. J., Duckworth, D. C., Keller, J. M. and Smith, D. H. "Development of Electrochemical Sample Pretreatment for Inductively Coupled Plasma Mass Spectrometry," American Society for Testing and Materials Symposium on Applications of ICP/MS to Radionuclide Determinations, Gatlinburg, TN, Oct. 13-14, 1994.

Puretzky, A. A., Goehagan, D. B., Haulfer, R. E., Hettich, R. L., Zheng, X-Y. and Compton, R. N. "Laser Ablation of Graphite in Different Buffer Gases," in *Proc., American Institute of Physics Conference*, J. C. Miller and D. B. Goehagan, eds., AIP Press, New York, Vol. 288, pp. 365-374 (1994).

Quirke, J. M. E., Adams, C. L., Van Berkel, G. J. and Asano, K. G. "Chemical Derivatization for Selective Detection by Electrospray Mass Spectrometry," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Ramsey, R. S., Goeringer, D. E. and McLuckey, S. A. "Target Effects on Resonance Ejection of High Mass Ions from the Quadrupole Ion Trap," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Ramsey, R. S., Goeringer, D. E., Van Berkel, G. J. and McLuckey, S. A. "Capillary Electrophoresis/Electrospray Ionization/Ion Trap Mass Spectrometry," 6th International Symposium on High Performance Capillary Electrophoresis, San Diego, CA, Jan. 31-Feb. 3, 1994.

Ramsey, R. S., Asano, K. G., Goeringer, D. E., Van Berkel, G. J., Hart, K. J. and McLuckey, S. A. "The Ion Trap Mass Spectrometer as a Chromatographic and Electrophoretic Detector," 15th International Symposium on Capillary Chromatography, Riva del Garda, Italy, May 24-28, 1993.

Ramsey, R. S., Asano, K. G., Hart, K. J., Goeringer, D. E., Van Berkel, G. J. and McLuckey, S. A. "Combining Capillary Electrophoresis with Electrospray Ionization/Ion Trap Mass Spectrometry for Biopolymer Analysis," 41st American Society of Mass Spectrometry Conference for Mass Spectrometry and Allied Topics, San Francisco, CA, May 31-June 4, 1993.

Ramsey, R. S., Goeringer, D. E., Asano, K. G., Van Berkel, G. J. and McLuckey, S. A. "On-Line Capillary Electrophoresis/Electrospray Ionization/Ion Trap Mass Spectrometry," 4th Annual Frederick Conference on Capillary Electrophoresis, Frederick, MD, Oct. 19-20, 1993.

Ramsey, R. S., Kerchner, G. A., Cadet, J., Habibi, S., Van Berkel, G. J. and McLuckey, S. A. "Micellar Electrokinetic Capillary Chromatography of DNA Photoproducts Using Cationic Surfactants," Fifth International Symposium on High Performance Capillary Electrophoresis, Orlando, FL, Jan. 25-28, 1993.

Shahgholi, M., Cook, K. D. and Buchanan, M. V. "Basicity and Solvation Effects in Electrospray Mass Spectrometry," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Shahgholi, M., Cook, K. D. and Buchanan, M. V. "The Roles of Solvation and Surface Chemistry in Ion Desorption," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Shahgholi, M., Cook, K. D. and Buchanan, M. V. "The Roles of Solvation, Basicity and Hydrophobicity in the Electrospray Mass Spectrometry of Amines and Amino Acids," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Stemmler, E. A., Hettich, R. L., Hurst, G. B. and Buchanan, M. V. "Experimental Conditions for the Matrix-Assisted Laser Desorption FTMS Analysis of Modified Oligonucleotides," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Thompson, C. V., Wise, M. B., Buchanan, M. V. and Guerin, M. R. "Direct Sampling Ion Trap Mass Spectrometry," Mobile Analytical Laboratory Workshop, Los Alamos, NM, July 20-21, 1993.

Van Berkel, G. J. "Interfacing Condensed-Phase Separations with an Ion Trap Mass Spectrometer: Current Capabilities and Expectations," International Mass Spectrometry Symposium, Helsinki, Finland, Sept. 9-10, 1993.

Van Berkel, G. J. and Goeringer, D. E. "Gas Chromatograph-Tandem Mass Spectrometry Implemented on a Bench-Top Quadrupole Ion Trap-Based Instrument Using Random Noise to Effect Collision-Induced Dissociation," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Van Berkel, G. J., McLuckey, S. A. and Ramsey, R. S. "Interfacing Condensed-Phase Separations with the Ion Trap Mass Spectrometer Circa 1993: Current Capabilities, Compromises and Expectations," 10th Symposium on Liquid Chromatography/Mass Spectrometry, Ithaca, NY, July 21-23, 1993.

Van Berkel, G. J., Quinones, M. A. and Quirke, J. M. E. "Geoporphyrin Analysis Using Electrospray Ionization-Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Van Berkel, G. J. and Quirke, J. M. E. "Chemical Derivatization for Electrospray Ionization-Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Van Berkel, G. J., Zhou, F., Morton, S. J. and Duckworth, D. C. "Electrochemical Preconcentration/Cleanup Techniques Coupled On-line with Inductively Coupled Plasma-Mass Spectrometry and Electrospray-Mass Spectrometry for Enhanced Trace Element Determination," 35th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 11-13, 1994.

Van Berkel, G. J., Quirke, J. M. and Adams, C. L. "Chemical Derivatization for Electrospray Ionization-Mass Spectrometry: Alkyl Halides, Alcohols, Phenols, Thiols, and Amines," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Van Berkel, G. J., Asano, K. G., Zhou, F. and McLuckey, S. A. "Chemical Derivatization for Electrospray Ionization-Mass Spectrometry: Aromatic, Heteroaromatic and Other Highly-Conjugated Systems," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Wise, M. B., Buchanan, M. V., Thompson, C. V., Goeringer, D. E., McLuckey, S. A., Crutcher, R. I., Hileman, M. S., Emery, M. L. and Alley, G. T. "Considerations for the Size and Power Reduction of a Field Transportable Ion Trap Mass Spectrometer," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Wise, M. B., Guerin, M. R., Thompson, C. V. and Buchanan, M. V. "Direct Sampling Ion Trap Mass Spectrometry for Rapid Environmental Analysis," National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Wise, M. B., Buchanan, M. V., Guerin, M. R., Merriweather, R. and Bayne, C. K. "Development of a Method for the Direct Purge Analysis of Volatile Organics in Water," in *Proc., 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics*, San Francisco, CA, May 30-June 4, 1993.

Wise, M., Buchanan, M. and Ilgner, R. "Rapid Detection of Chemical Warfare Agents Using Direct Sampling Ion Trap Mass Spectrometry," in *Proc., Analytical Methods for Environmental Sampling of Warfare Agents in Their Breakdown Products Conference*, Aberdeen, MD, Sept. 20-21, 1994 (in press).

Yang, M., Dale, J. M., Whitten, W. B. and Ramsey, J. M. "Optical and Mass Spectrometry of Individual Microparticles in Electrodynamical Traps," American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Yang, M. and Ramsey, J. M. "Nitrocellulose Destruction by Laser," U.S. Army Construction Engineering Laboratory Workshop on Nitrocellulose Research, W. Lafayette, IN, Nov. 4-5, 1993.

Ying, Z. C., Jin, C., Hettich, R. L., Paretzky, A. A., Haufler, R. E. and Compton, R. N. "Production and Characterization of Metallofullerene Superatoms," in *Proc., Electrochemical Society Meeting*, San Francisco, CA, May 22-26, 1994.

Zhou, F. and Van Berkel, G. J. "Electrochemically-Enhanced Electrospray Ionization-Mass Spectrometry," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Zhou, F., Van Berkel, G. J., Duckworth, D. C. and Morton, S. J. "Electrochemical Stripping Analysis Combined On-Line with Inductively Coupled Plasma-Mass Spectrometry for Enhanced Trace Metal Determination," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Zhou, F., Van Berkel, G. J., Duckworth, D. C. and Morton, S. J. "Stripping Analysis Combined On-line with Inductively Coupled Plasma-Mass Spectrometry for Enhanced Trace Metal Determination," 21st Annual Federation of Analytical Chemistry and Spectroscopy Societies Conference, St. Louis, MO, Oct. 2-7, 1994.

SECONDARY ION MASS SPECTROMETRY GROUP

Journal Articles

Bu, H., Chen, E., Xu, S., Guo, K. and Wunderlich, B. "Single Molecule Single Crystals of Isotactic Polystyrene," *J. Polym. Sci. B Polym. Phys.* (1994) 32, 1351-1357.

Short, R. T. and Todd, P. J. "Improved Energy Compensation for Time-of-Flight Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* (1994) 5, 779-787.

Short, R. T., McMahon, J. M., Holland, W. M. and Todd, P. J. "Charge Compensation for Imaging Large Insulating Samples by Using Secondary Ion Tandem Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* (1994) 5, 37-43.

Presentations/Conference Proceedings

McMahon, J. M., Short, R. T., Holland, W. B. and Todd, P. J. "Spatial Distribution of Nucleic Bases Using SIMS," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

McMahon, J. M., Short, R. T. and Todd, P. J. "Secondary Ion Emission from Solids and Liquids," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Short, R. T., McMahon, J. M. and Todd, P. J. "Sample Charge Compensation on a Large Sample Ion Microprobe," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Short, R. T., Todd, P. J., McMahon, J. M. and Holland, W. M. "Imaging of Organic Surfaces Using SIMS/MS," 6th East Coast Workshop on Secondary Ion Mass Spectrometry, Fishkill, NY, May 19-21, 1993.

Short, R. T. "Electrostatic Energy Compensation for the Acceleration Region of Time-of-Flight Mass Spectrometers," 10th Asilomar Conference on Mass Spectrometry, Estes Park, CO, Oct. 3-7, 1993.

Short, R. T. and Todd, P. J. "Isotope Ratios Using Time-of-Flight Secondary Ion Mass Spectrometry," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Todd, P. J., Short, R. T., McMahon, J. M., Brenna, J. T. and Markey, S. P. "Biological Sample Preparation for Imaging Organic SIMS," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Todd, P. J., Short, R. T., McMahon, J. M. and Holland, W. M. "Biologic Tissue Imaging with a Secondary Ion MS/MS Microprobe," 42nd American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Other

Todd, P. J. and Short, R. T. "Method for Improved Accuracy of Isotope Ratio Measurements Using Secondary Ion Mass Spectrometry," Patent Disclosure submitted to DOE by ORNL, 1994.

SURFACE CHEMISTRY AND HETEROGENEOUS CATALYSIS GROUP

Journal Articles

Grimm, F. A. and Huntley, D. R. "A Theoretical Study of the Binding Energy and Bonding of Benzene to the Ni(111), (100) and (110) Surfaces," *J. Phys. Chem.* (1993) **97**, 3800.

Hughes, I. G., Burgdorfer, J., Folkerts, L., Havener, C. C., Overbury, S. H., Robinson, M. T., Zehner, D. M., Zeijlmans van Emmichoven, P. A. and Meyer, F. W. "Separation of Kinetic and Potential Electron Emission Arising from Slow Multicharged Ion-Surface Interactions," *Phys. Rev. Lett.* (1993) **71**, 291.

Hulett, L. D., Donohue, D. L., Xu, J., Lewis, T. A., McLuckey, S. A. and Glish, G. L., "Mass Spectrometry Studies of the Ionization of Large Organic Molecules by Low Energy Positrons," *Chem. Phys. Lett.* (1993) **216**, 236-240.

Hulett, L. D., Gonzalez, R., Brown, B. L., Denison, A. L., Howell, R. H., Jean, Y. C., Jones, P. L., Kossler, W. J., Lynn, K. G., Mills, A. P., Okada, S., Schrader, D. M., Weiss, A. H., West, R. N. and Chen, Y. O. "Workshop Report on the Application of Positron Spectroscopy to Materials Science," *Appl. Phys. Rev.* (1993).

Hulett, L. D., Wallace, S., Xu, J., Nielsen, B., Szeles, C., Lynn, K. G., Pfau, J. and Schaub, A. "Labs Cooperate, Collaborate with Industrial Client," *ER News* (December 1993).

Mullins, D. R. and Lyman, P. F. "Sulfur Induced Changes in the W(001) Surface Core Level Shift," *Surface Science* (1993) **285**, L473.

Mullins, D. R. and Lyman, P. F. "The Adsorption and Reaction of Methanethiol on Ru(0001)," *J. Phys. Chem.* (1993) **97**, 12008-12013.

Mullins, D. R. and Lyman, P. F. "The Adsorption and Reaction of Methanethiol on W(001)," *J. Phys. Chem.* (1993) **97**, 9226-9232.

Overbury, S. H. and van den Oetelaar, R. J. A. "Surface Segregation in $\text{Mo}_{0.75}\text{Re}_{0.25}$ (001) Studied by Low Energy Alkali Ion Scattering," *Phys. Rev. B* (1993) **48**(3), 1718-1725.

Overbury, S. H., van den Oetelaar, R. J. A. and Mullins, D. R. "Sulfidation of W(001) Studied by Low Energy Ion Scattering," *Surf. Sci.* (1994) **317**, 341-352.

Overbury, S. H. "Comparison of Experimental and Simulated Low Energy Alkali Ion Scattering," *Nucl. Instrum. Meth.* (1994) **90**, 286.

Overbury, S. H. and van den Oetelaar, R. J. A. "Structure of the $\text{p}(2\times 1)\text{-O}/\text{Mo}_{0.75}\text{Re}_{0.25}$ (001) Surface Studied by Low Energy Li^+ Ion Scattering," *Surf. Sci.* (1994) **301**, 313-325.

Rufael, T. S., Gland, J. L., Huntley, D. R. and Mullins, D. R. "Adsorption and Reaction of Benzethiol on the Ni(111) Surface," *J. Phys. Chem.* (1994) **90**, 13022.

Xu, J., Hulett, L. D., Lewis, T. A., Donohue, D. L., Glush, G. L. and McLuckey, S. A. "Positron-Induced Dissociation of Organic Molecules," *Phys. Rev. A* (1993) **47**(2), 1023-1030.

Xu, J., Hulett, L. D., Lewis, T. A. and McLuckey, S. A. "Internal Energy Deposition into Molecules upon Positron-Electron Annihilation," *Phys. Rev. A*, (1994) **49**, R3151.

Yang, H., Caves, T. C., Whitten, J. L. and Huntley, D. R. "Chemisorption Studies of CH₃S on Ni(111)," *J. Am. Chem. Soc.* (1994) **116**, 8200.

Presentations/Conference Proceedings

Hulett, L. D. "Applications of Slow Positron Spectroscopy," ORNL Engineering Physics and Mathematics Division Information Meeting, Oak Ridge, TN, June 10, 1993.

Hulett, L. D. "Mass Spectrometry Studies of the Ionization of Large Organic Molecules by Low Energy Positrons," Traveling Lecture Series Seminar at the University of Missouri, Kansas City, MO, Jan. 27, 1993.

Huntley, D. R. "Controlling Reaction Selectivity: Effects of Co-Adsorbed H and O on Ethanethiol Reactions on Ni(110)," 13th North American Meeting of the Catalysis Society, Pittsburgh, PA, May 2-7, 1993.

Huntley, D. R. "Patterns of Reactivity for Ni(110) with Organosulfur Compounds," in *Proc., 206th National American Chemical Society Meeting, Division of Petroleum Chemistry*, Chicago, IL, Aug. 22-27, 1993, Vol. 38, p. 684 (1993).

Huntley, D. R. and Mullins, D. R. "The Kinetics of Carbon-Sulfur Bond Scission: Methanethiol on Ni(111)," 40th National American Vacuum Society Symposium and Topical Conference, Orlando, FL, Nov. 15-19, 1993.

Lyman, P. F. and Mullins, D. R. "Effect of C Adsorption on the W(100) Surface Environment as Studied by Core Level Spectroscopy," American Physical Society Meeting, Seattle, WA, Mar. 22-26, 1993.

Mullins, D. R. and Lyman, P. F. "The Adsorption and Reaction of Methanethiol on Clean and Modified W(001) and Ru(001)," in *Proc., 206th National American Chemical Society Meeting, Division of Petroleum Chemistry*, Chicago, IL, Aug. 22-27, 1993, Vol. 38, p. 688 (1993).

Overbury, S. H. "Comparison of Experimental and Simulated Low Energy Alkali Ion Scattering Distributions," International Conference on Atomic Collisions in Solids, London, Ontario, Canada, July 26-30, 1993.

Overbury, S. H., van den Oetelaar, R. J. A. and Mullins, D. R. "Ion Scattering Study of Structure of Sulfided W(001)," International Conference on Atomic Collisions in Solids, London, Ontario, Canada, July 26-30, 1993.

Overbury, S. H., van den Oetelaar, R. J. A. and Mullins, D. R. "Sulfidation of W(001) Studied by Low Energy Alkali Ion Scattering," 40th National American Vacuum Society Symposium and Topical Conference, Orlando, FL, Nov. 15-19, 1993.

Xu, J. and Hulett, L. D. "Fragmentation of Organic Molecules by Slow Positrons," American Physical Society Meeting, Mar. 22-26, 1993.

Hulett, L. D. "Positron Microscopy," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Hulett, L. D. "Positron Spectroscopy and Its Applications," Seminar at Fisk University, Department of Physics, Nashville, TN, Oct. 31, 1994.

Hulett, L. D. and Eberle, C. C. "A Design for a High Intensity Positron Facility to be Incorporated as Part of the Advanced Neutron Source," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Hulett, L. D. and Eberle, C. C. "A High Intensity Slow Positron Facility for the Advanced Neutron Source," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Hulett, L. D. and Eberle, C. C. "A High Intensity Slow Positron Facility for the Advanced Neutron Source," NJ/A 13th International Conference on Application of Accelerators in Research and Industry, Denton, TX, Nov. 7-10, 1994.

Hulett, L. D., Wallace, S., Xu, J., Nielsen, B., Szeles, C., Lynn, K. G., Pfau, J. and Schaub, A. "Assay of Weathering Effects on Protective Polymer Coatings Using Positron Annihilation Spectroscopy," 1995 6th International Workshop on Slow-Positron Beam Techniques for Solids and Surfaces (*Appl. Surf. Sci.* **85**), Makuhari, Japan, May 18-22, 1994.

Hulett, L. D., Wallace S., Xu, J., Nielsen B., Szeles, C., Lynn, K. G., Pfau, J. and Schaub, A. "The Monitoring of Paint Weathering by Positron Annihilation Spectroscopy," Annual Meeting of the Federation of Societies for Coatings Technology, New Orleans, LA, Oct. 12, 1994.

Hulett, L. D., Xu, J., Lewis, T. A. and Crawford, O. H. "Mass Spectrometry Studies of the Ionization of Organic Molecules by Slow Positrons," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Hulett, L. D., Xu, J., Lewis, T. A. and McLuckey, S. A. "The Generation of Slow Positrons with an Electron Linac and Studies of the Kinetics of Their Interactions with Organic Molecules," 13th International Conference on Application of Accelerators in Research and Industry, Denton, TX, Nov. 7-10, 1994.

Huntley, D. R. "Kinetics of C-S Bond Scission in Phenyl Thiolate and Methyl Thiolate on Ni(111)," National American Chemical Society Meeting, San Diego, CA, March 1994.

Huntley, D. R. "Mechanisms and Kinetics of Desulfurization Reactions on Ni Surfaces," DOE Conference on Surface and Catalysis, Okonomowoc, WI, May 1994.

Huntley, D. R. "Structure and Stability of Methyl Thiolate on Ni(111)," National American Vacuum Society Meeting, Denver, CO, Nov. 1994.

Huntley, D. R., Mullins, D. R. and Overbury, S. H. "The Structure and Stability of Methyl Thiolate on Ni(111)," 41st National AVS Symposium and Topical Conference, Denver, CO, Oct. 24-28, 1994.

Mullins, D. R. "Applications of SXPS for Studying Surface Structure, Reaction Mechanisms and Kinetics," 1994 Fall Meeting of Materials Research Society, Boston, MA, Nov. 28- Dec. 2, 1994 (in press).

Mullins, D. R., Huntley, D. R. and Overbury, S. H. "The Nature of the Sulfur Induced Surface Reconstruction on Ni(111)," 54th Annual Conference on Physical Electronics at The University of Tennessee, Knoxville, TN, June 13-15, 1994.

Overbury, S. H. "Structure of Sulfided Ultra-Thin Ni Films on W(001)," 41st National Symposium of the American Vacuum Society and NANO 3, Denver, CO, Oct. 24-28, 1994.

Overbury, S. H., Mullins, D. R., Lyman, P. F. and Shinn, N. D. "Ni Adsorption on W(001) Studied by Low Energy Alkali Scattering and W 4f Core Level Spectroscopy," 54th Annual Conference on Physical Electronics at The University of Tennessee, Knoxville, TN, June 13-15, 1994.

Overbury, S. H., Mullins, D. R., Lyman, P. F. and Shinn, N. D. "Substrate Core-Level Response to Nucleation and Growth of Ultra-Thin Ni Films on W(001)," 41st National Symposium of the American Vacuum Society and NANO 3, Denver, CO, Oct. 24-28, 1994.

Xu, J., Hulett, L. D., Lewis, T. A. and Tolk, N. "Light Emission from Polymers under Slow Positron Bombardment," 6th International Workshop on Slow-Positron Beam Techniques for Solids and Surfaces, Makuhara, Japan, May 18-22, 1994.

Xu, J., Hulett, L. D., Lewis, T. A. and Tolk, N. "Positron Induced Luminescence Studies from Polymers," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Xu, J., Hulett, L. D., Lewis, T. A. and Tolk, N. H. "Studies of Positron Induced Luminescence from Polymers," 10th International Conference on Positron Annihilation, Beijing, China, May 23-29, 1994.

Reports

Mullins, D. R. and Huntley, D. R. "Adsorption and Reaction of Methylthiolate on Ni(111)," *Contribution to National Synchrotron Light Source Annual Report* (November 1994).

Mullins, D. R. and Huntley, D. R. "Reaction Kinetics of Thiolate Intermediates on Ni(111)," *Contribution to National Synchrotron Light Source Annual Report* (November 1994).

Mullins, D. R. "The Reconstruction of Ni(111) Induced by the Adsorption of Atomic Sulfur," *Contribution to National Synchrotron Light Source Annual Report* (published and distributed to NSLS users) (1993).

Mullins, D. R. and Lyman, P. F. "Adsorption and Reaction of CH_3SH on Sulfur and Carbon Covered W(001)," *Contribution to National Synchrotron Light Source Annual Report* (published and distributed to NSLS users) (1993).

Overbury, S. H., Mullins, D. R., Lyman, P. F. and Shinn, N. D. "Ni Adsorption on W(001) Studied by W 4f Core Level Spectroscopy," *Contribution to National Synchrotron Light Source Annual Report* (published and distributed to NSLS users) (1993).

NUCLEAR AND RADIOCHEMISTRY SECTION

NEUTRON ACTIVATION ANALYSIS GROUP

Journal Articles

Glasgow, D. C. and Robinson, L. "Neutron Activation Analysis of Mercury in Air Monitors," *Trans. Am. Nucl. Soc.* (1994) **71**, 154-155.

Glasgow, D. C., Dyer, F. F. and Robinson, L. "Methods for Preparing Comparative Standards and Field Samples for Neutron Activation Analysis of Soil," *J. Radioanal. Nucl. Chem.* (1995) **192**.

Robinson, L., Dyer, F. F., Phillips, K. and Glasgow, D. C. "Neutron Activation Analysis of Background Soils at the ORNL Site," *Trans. Am. Nucl. Soc.* (1993) **68A**, 175-176.

Robinson, L., Dyer, F. F., Combs, D. W., Wade, J. W., Carlton, J. E., Ondracek, A. L. and Stokely, J. R. "Determination of Hg and Other Trace Elements in Soil Using Neutron Activation Analysis," *J. Radioanal. Nucl. Chem.* (1994) **179**(2), 305-313.

Robinson, L. and Brown, D. H. "Research and Learning Opportunities in a Reactor Based Nuclear Analytical Laboratory," *J. Chem. Ed.* (1994) **71**, 824-826.

Snyder, G. A., Taylor, L. A., Jerde, E. A., Sharkov, Y., Laz'ko, Y. and Hanna, S., "Petrogenesis of Garnet Pyroxenite and Spinel Peridotite Xenoliths of the Tell-Danun Alkali Basalt Volcano Harrat As Shamah, Syria," *Intl. Geol. Rev.* (1993) **35**, 1104-1120.

Van Dalsem, D. J., Robinson, L. and Ehmann, W. D. "A Novel Approach to Aluminum Determination in Biological Tissues Using a Pair of Pneumatic Tube Irradiation Facilities," *J. Radioanal. Nucl. Chem.* (1995) **192**, 131-138.

Van Dalsem, D. J., Robinson, L. and Ehmann, W. D. "Determination of Phosphorus Using (n, α) Nuclear Reactions," *Am. Nucl. Soc.* (1994) 71, 50-51.

Vance, D. E. and Robinson, L. "Validation of NAA Data for a Background Soil Characterization Project," *J. Radioanal. Nucl. Chem.* (1995) 192.

Presentations/Conference Proceedings

Brown, D. H., Robinson, L. and Dyer, F. F. "Automation of a Gamma Ray Spectroscopy System Using Laboratory Robotics," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Dyer, F. F. "From Hevesy to the Advanced Neutron Source. The Past and Final Frontier of Neutron Activation Analysis," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Dyer, F. F. "The Use of Standards in Nuclear Analytical Chemistry at Oak Ridge National Laboratory -- A Historical Perspective," 1994 Winter Meeting of the American Nuclear Society, Washington, DC, Nov. 13-17, 1994.

Fraracci, K. N., Taylor, L. A., Jerde, E. A., Snyder, G. A., Clayton, R. N., Mayeda, T. K., Riciputi, L. R. and Sobolev, N. V. "Two Unusual Diamondiferous Eclogite Xenoliths from the MIR Kimberlite in Yakutia, Siberia," Geological Society of American Meeting, Boston, MA, Oct. 25-29, 1993.

Glasgow, D. C., Dyer, F. F. and Robinson, L. "Methods for Preparing Comparative Standards and Field Samples for Neutron Activation Analysis of Soil," Methods and Applications of Radio-analytical Chemistry Meeting, Kona, HI, Apr. 10-16, 1994.

Glasgow, D. C. and Robinson, L. "Neutron Activation Analysis of Mercury in Air Monitors," American Nuclear Society Winter Meeting, Washington, DC, Nov. 13-17, 1994.

Glasgow, D. C., Dyer, F. F. and Robinson, L. "Neutron Activation Analysis for Large-Scale Environmental Studies," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Robinson, L., Johnson, E. and Robles, L. D., "Maximizing the Cold Neutron Flux from a Cf-252 Source," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, October 5-7, 1993.

Robinson, L., Dyer, F. F., Phillips, K. and Glasgow, G. C. "Neutron Activation Analysis of Background Soils at the ORNL Site," Annual Meeting of the American Nuclear Society, San Diego, CA, June 20-24, 1993.

Robinson, L., Dyer, F. F. and Nichols, G. R. "A Search for Arsenic in Hair and Nail Remains of Former President Zachary Taylor by Neutron Activation Analysis (A Historical Perspective)," ORAU Traveling Lecture Program, The University of Tennessee, Chattanooga, TN, Jan. 25, 1993.

Robinson, L. "Neutron Activation Analysis: An Overview," DOE Nuclear Waste Round Robin 7, Colorado Springs, CO, August 30-31, 1993.

Robinson, L. "Neutron Activation Analysis of High Purity Aluminum and Applications to On-Line Sorting of Aluminum Alloys," American Society of Mechanical Engineers Aluminum Industry Workshop, Colorado Springs, CO, Aug. 2-4, 1994.

Robinson, L. "Standardization Problems in NAA Facilities Proposed for the ANS," 1994 Winter Meeting of the American Nuclear Society, Washington, DC, Nov. 13-17, 1994.

Robinson, L. and Dyer, F. F. "Nuclear Methods of Analysis in the Advanced Neutron Source," 21st Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies, St. Louis, MO, Oct. 2-7, 1994.

Snyder, G. A., Taylor, L. A., Jerde, E. A. and Riciputi, L. R. "Evolved QMD-Melt Parentage for Lunar Highlands Alkali Suite Cumulates: Evidence from Ion Probe-Rare-Earth Element Analyses of Individual Minerals," 25th Lunar and Planetary Science Conference, Houston, TX, Mar. 14-17, 1994.

Van Dalsem, D. J., Robinson, L. and Ehmann, W. D. "A Novel Approach to Aluminum Determination in Biological Tissues Using a Pair of Pneumatic Tube Irradiation Facilities," 3rd International Conference on Methods and Applications of Radioanalytical Chemistry (MARC-III), Kona, Hawaii, April 10-15, 1994.

Van Dalsem, D. J., Robinson, L. and Ehmann, W. D. "Determination of Phosphorus Using (n, α) Nuclear Reactions," American Nuclear Society 1994 Winter Meeting, Washington, D.C, Nov. 13-17, 1994.

Reports

Farrell, K., Kam, F. B., Baldwin, C. A., Pace, J. V., Corwin, W. R., Robinson, L., Dyer, F. F., Haggag, F. M., Stallman, F. W., Oliver, B. M. and Greenwood, L. R. "The DOS 1 Neutron Dosimetry Experiment at the HB-4-A Key 7 Surveillance Site on the HFIR Pressure Vessel," ORNL/TM-12511 (1994).

RADIOACTIVE MATERIALS ANALYSIS GROUP

Journal Articles

Zhou, F., Van Berkel, G. J., Morton, S. J., Duckworth, D. C., Adeniyi, W. K. and Keller, J. M. "Development of On-line Electrochemical Sample Pretreatment Methods for ICP-MS," *American Society for Testing and Materials, Special Technical Publication* (1994).

Presentations/Conference Proceedings

Giaquinto, J. M. and Ross, T. "Comparison of Nitric Acid vs Total Dissolution of Radioactive Waste Tank Sludge Using Microwave Technology," American Society for Testing and Materials Symposium on Applications of ICP/MS to Radionuclide Determinations, Gatlinburg, TN, Oct. 13-14, 1994.

Kay, C. L., Stump, N. A., Gibson, J. K. and Peterson, J. R. "Luminescence Lifetime Study of the Thermal Decomposition of Eu^{3+} -Doped $\text{La}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$," International Conference on Luminescence, CT, Aug. 9-13, 1993.

Meeks, A. S. and Keller, J. M. "Improved Separation Techniques for the Characterization of Mixed Waste Samples," National American Chemical Society Meeting on the Characterization and Treatment of High-Level Nuclear Waste, Washington, DC, Aug. 21-24, 1994.

Morton, S. J., Van Berkel, G. J., Duckworth, D. C., Keller, J. M. and Smith, D. H. "Development of Electrochemical Sample Pretreatment for Inductively Coupled Plasma Mass Spectrometry," American Society for Testing and Materials Symposium on Applications of ICP/MS to Radionuclide Determinations, Gatlinburg, TN, Oct. 13-14, 1994.

Robinson, L., Dyer, F. F., Combs, D. W., Wade, J. W., Teasley, N. A., Carlton, J. E., Ondracek, A. L. and Stokely, J. R. "The Determination of Hg and Other Trace Elements in Soil Using Neutron Activation Analysis," 33rd ORNL/DOE Conference on Analytical Chemistry, Gatlinburg, TN, Oct. 6-8, 1992.

Swafford, A. M. and Keller, J. M. "Sample Clean-up of Radioactive Mixed Waste for ICP/ICP-MS Analysis," The Pittsburgh Conference, Atlanta, GA, Mar. 7-10, 1993.

Reports

Swafford, A. M. and Keller, J. M. *Separation Techniques for the Clean-up of Radioactive Mixed Waste for ICP AES/ICP-MS Analysis*, ORNL/TM-12329 (1994).

Thesis

Kay, C. L. "A Luminescence Spectral and Lifetime Study of Selected Europium and Europium-Doped Inorganic Salts," *M.S. Thesis*, The University of Tennessee, Knoxville, TN (1994).

TRANSURANIUM ELEMENT CHEMISTRY GROUP

Books/Book Chapters

Haire, R. G. and Eyring, L. "Comparisons of the Binary Oxides of the Lanthanides and Actinides," in *Handbook on the Physics and Chemistry of Rare Earths, Lanthanides/Actinides: Chemistry*, Chapter 125, K. Gschneider, Jr., L. Eyring, G. R. Choppin, and G. H. Lander, eds., Elsevier Science, Amsterdam (1994) 18, 413-505.

Journal Articles

- Bamberger, C. E., Haverlock, T. J., Shoup, S. S., Kopp, O. C. and Stump, N. A. "Compounds of Cerium, Titanium and Oxygen," *J. Alloys and Compounds* (1994) **204**, 101-107.
- Caldwell, C. D. and Krause, M. O. "K-Shell Auger Spectrum of Atomic Oxygen," *Phys. Rev.* (1993) **A47**, R759.
- Caldwell, C. D. and Krause, M. O. "Electron-Emission Analysis of the $2p^4(^1D)$ ns, nd Rydberg Excitations in Atomic Fluorine," *J. Phys. B.* (1994) **27**, 4891-4896.
- Caldwell, C. D., Schaphorst, S. J., Krause, M. O. and Jimenez-Mier, J. "Photoexcited K Auger Spectra of Atomic and Molecular Oxygen," *J. Electron Spectrosc. Rel. Phenom.* (1994) **67**, 243-259.
- Chen, G., Haire, R. G. and Peterson, J. R. "Effect of Temperature on the Luminescence from Eu_2O_3 ," *J. Solid State Chem.* (1993) **102**, 126.
- Chen, G., Burns, J. B., Stump, N. A., Haire, R. G. and Peterson, J. R. "Pressure-Induced Phase Transition in B-Type Eu_2O_3 : A Luminescence Study at High Pressure," *Bull. Am Phys. Soc* (1993) **38**, 1545.
- Chen, G., Wang, S., Haire, R. G. and Peterson, J. R. "Pressure-Induced d- to f-Orbital Energy Cross-over in Sm^{2+} Ion in CsCmI_3 : A Luminescence Study," *Appl. Spectrosc.* (1994) **48**, 1026.
- Chen, G., Stump, N. A., Haire, R. G. and Peterson, J. R. "Pressure-Induced Amorphization in $\text{Eu}(\text{OH})_3$: A Luminescence Study," *Solid State Commun.* (1994) **89**, 83.
- Chen, G., Stump, N. A., Haire, R. G., Burns, J. B. and Peterson, J. R. "A Luminescence Study of B-Type Eu_2O_3 under Pressure," *High Pressure Res.* (1994) **12**, 83.
- Chen, G., Peterson, J. R. and Brister, K. E. "An Energy-Dispersive Chemistry X-Ray Diffraction Study of Monoclinic Eu_2O_3 under Pressure," *J. Solid State Chem.* (1994) **111** 437.
- Chen, G., Haire, R. G., Peterson, J. R. and Abraham, M. M. "A Luminescence Study of EuVO_4 at High Pressure," *J. Phys. Chem. Solids* (1994) **55**, 313.
- Del Cul, G. D., Nave, S. E. and Peterson, J. R. "Polarized Raman Spectra of Single-Crystal Lanthanide Oxychlorides," *J. Alloys and Compounds* (1993) **193**, 194-196.
- Fricke, B., Johnson, E. and Martinez, G. "Ionization Potentials and Radii of Atoms and Ions of Element 105 (ununpentium) and Ions of Tantalum Derived from Multiconfiguration Dirac-Fock Calculations," *Radiochim. Acta* (1993) **62**, 17.
- Fuger, J. J., Haire, R. G. and Peterson, J. R. "Molar Enthalpies of Formation of BaCmO_3 and BaCfO_3 ," *J. Alloys and Compounds* (1993) **200**, 181.

- Gensini, M. M., Haire, R. G., Benedict, G. U. and Hulliger, F. "High-Pressure Behavior of CmBi, UBi," *Phys. B* (1993) **190**, 75.
- Gensini, M. M., Haire, R. G. and Gibson, J. K. "Investigation of the Np-Zr and Am-Np Systems by X-ray Diffraction," *J. Alloys and Compounds* (1994) **213/214**, 402.
- Gibson, J. K., Haire, R. G., Gensini, M. M. and Ogawa, T. "Alloying Behavior in Selected Neptunium Binary Systems: The Role of 5f-Bonding," *J. Alloys and Compounds* (1994) **213/214**, 106-110.
- Gibson, J. K. "Lanthanide Oxide Cluster Ions Generated by Vacuum Laser Ablation: Metal Valence Effects on Cluster Compositions," *J. Phys. Chem.* (1994) **98(44)**, 11321-11330.
- Gibson, J. K. "Clusters Formed Directly from Laser Ablation of Ytterbium Oxide: Yb_3O_4^+ and Yb_6O_8^+ ," *J. Phys. Chem.* (1994) **98**, 6063.
- Gibson, J. K. "Mass Spectrometric Identification of Gaseous Uranium(IV) Fluoride Chlorides: $\text{UF}_3\text{Cl}(\text{g})$ and $\text{UF}_2\text{Cl}_2(\text{g})$," *Radiochim. Acta* (1994) **65**, 227-231.
- Gibson, J. K. "High-Temperature Oxide and Hydroxide Vapor Species of Technetium," *Radiochim. Acta* (1993) **60**, 121-126.
- Gibson, J. K., Haire, R. G., Beahm, E. C., Gensini, M. M., Maeda, A. and Ogawa, T. "The Neptunium-Iron Phase Diagram," *J. Nucl. Mater.* (1994) **211**, 215.
- Gibson, J. K. "Mass Spectroscopic Investigation of Gaseous Technetium Oxide Halides: TcO_3Br and TcO_3I ," *Radiochim. Acta* (1994) **64**, 185-189.
- Gibson, J. K. and Stump, N. A. "Spectroscopic Investigation of the Thermal Decomposition of Europium Oxalate," *Thermochem. Acta* (1993) **226**, 301-310.
- Gibson, J. K. and Haire, R. G. "Investigation of the Neptunium-Zirconium Phase Diagram by Differential Thermal Analysis," *J. Nucl. Mater.* (1993) **201**, 225-230.
- Gibson, J. K. "Mass Spectrometric Identification of Gaseous Potassium and Cesium Pertechnetates and Bimetallic Technetium Rhenium Oxide Dimers," *Radiochim. Acta* (1993) **62**, 127-132.
- Haire, R. G. "High-Temperature Vaporization of Transplutonium Oxides," *J. Alloys and Compounds* (1994) **213/214**, 185-190.
- Hermesmeier, B. D., Fadley, C. S., Sinkovic, B., Krause, M. O., Jimenez-Mier, Gerard, P., Carlson, T. A., Manson, S. T. and Bhattacharya, S. K. "Energy Dependence of the Outer Core-Level Multiplet Structures in Atomic Mn and Mn-Containing Compounds," *Phys. Rev.* (1993) **B48**, 12425.
- Krause, M. O., Caldwell, C. D., Whitfield, S. B., de Lange, C. A. and van der Meulen, P. "Population of the $^3\text{P}_{2,1,0}$ Fine-Structure States in the 3s and 3p Photoionization of Atomic Chlorine," *Phys. Rev.* (1993) **A47**, 3015-3019.

- Krause, M. O. "Electron Spectrometry of Open-Shell Atoms," *Nucl. Instrum. Meth. Phys. Res. B* (1994) **B87**, 178-182.
- Link, P., Braithwaite, K., Benedict, U., Wittig, J. and Haire, R. G. "Americium Is a Good Superconductor under Pressure," *J. Alloys and Compounds* (1994) **213/214**, 153.
- Martin, N. L. S., Thompson, D. B., Bauman, R. P., Wilson, M., Jimenez-Mier, J., Caldwell, C. D. and Krause, M. O. "Photoelectron Spectra in Cadmium: Comparison with Theory and (e, 2e) Spectra," *J. Phys. B* (1994) **1327**, 3945.
- Pahler, M., Caldwell, C. D., Schaphorst, S. J. and Krause, M. O. "Intrinsic Line Widths of Neon $2s2p^5(^1\text{^}^3\text{P})nl^2\text{L}$ Correlation Satellites," *J. Phys. B* (1993) **26**, 1617.
- Pershina, V., Fricke, B., Ionova, G. V. and Johnson, E. "Thermodynamic Functions of Element 105 in Neutral and Ionized States," *J. Phys. Chem.* (1994) **98**, 1482.
- Peterson, J. R., Heathman, S. P. and Benedict, G. U. "Energy Dispersive X-Ray Diffraction Analysis of NdBr_3 at Pressures Up to 52 GPa," *J. Alloys and Compounds* (1993) **193**, 306-308.
- Peterson, J. R. "Some Experiences with Absorption, Phonon Raman, and Luminescence Spectroscopic Probes of Crystal Structure of f-Element Compounds," *J. Alloys and Compounds* (1993) **193**, 165-169.
- Peterson, J. R. "Phase Behavior of Actinide Trihalides Under Pressure," *J. Alloys and Compounds* (1994) **213/214**, 394.
- Schaphorst, S. J., Caldwell, C. D., Krause, M. O. and Jimenez-Mier, J. "Evidence for Atomic Features in the Decay of Resonantly Excited Molecular Oxygen," *Chem. Phys. Lett.* (1993) **213(3,4)**, 315-320.
- Stewart, G. and Haire, R. G. "Specific Heat of Some Transuranic Intermetallic Compounds for Heavy Fermions," *J. Alloys and Compounds* (1994) **213/214**, 111.
- Stump, N. A., Burns, J. B., Dai, S., Mamantov, G., Young, J. P. and Peterson, J. R. "Europium Oxichloride Absorption Spectroscopy as an Optical Probe of Temperature," *Spectrosc. Lett.* (1993) **26**, 1073.
- Stump, N. A., Chen, G., Haire, R. G. and Peterson, J. R. "Lanthanide Luminescence Spectroscopy as a Monitor of Crystal Structure," *J. Appl. Spectrosc.* (1993) **47(11)**, 1951-1952.
- Stump, N. A., Chen, G. and Peterson, J. R. "Some Uses of Emission Spectroscopy in Studies of the f-Elements," *Trends Appl. Spectrosc.* (1993) **1**, 217-229.
- Stump, N. A., Murray, G. M., Del Cul, G. D., Haire, R. G. and Peterson, J. R. "Stokes and Anti-Stokes Luminescence from the Trihalides of Cm-248," *Radiochim. Acta* (1993) **61**, 129-136.

Stump, N. A., Chen, G., Haire, R. G. and Peterson, J. R. "Temperature Dependence of the Eu^{3+} Ion Luminescence Lifetime Exhibited by Anhydrous EuCl_3 ," *Appl. Spectrosc.* (1994) **48**, 1174-1176.

Stump, N. A., Schweitzer, G. K., Gibson, J. K., Haire, R. G. and Peterson, J. R. "Luminescence Study of the Thermal Decomposition of Europium Trichloride Hexahydrate, $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$," *Appl. Spectrosc.* (1994) **48**, 937.

Stump, N. A., Schweitzer, G. K., Murray, G. M. and Peterson, J. R. "Luminescence Detection of Cation Exchange in $\text{Na}_3[\text{Eu}(\text{2,6-Pyridinedicarboxylato})_3]$," *J. Luminesc.* (1994) **60&61**, 104-107.

Whitfield, S. B., Krause, M. O., van der Meulen, P. and Caldwell, C. D. "High-Resolution Photoelectron Spectrometry of Atomic Manganese from the Region of the 3p 3d Giant Resonance to 120 eV," *Phys. Rev. A* (1994) **50(2)**, 1269-1286.

Xu, W., Chen, G. and Peterson, J. R. "The Blue Up-Conversion Emission of Glass Ceramics Doped with Er^{3+} Ion Upon Green Line (19436 cm^{-1}) Excitation," *Chem. Phys. Lett.* (1994) **224**, 56.

Presentations/Conference Proceedings

Caldwell, C. D., Pahler, M., Schaphorst, S. J. and Krause, M. O. "Line Widths of Neon $2s2p^5(^1,^3\text{P})nl$ Correlation Satellites," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Oct. 18-19, 1993.

Caldwell, C. D., Schaphorst, S. J., Jimenez-Mier, J. and Krause, M. O. "Resonance Auger Decay of K-Shell Excitations in Atomic and Molecular Oxygen," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Oct. 18-19, 1993.

Caldwell, C. D., Schaphorst, S. J., Jimenez-Mier, J. and Krause, M. O. "Resonance Auger Spectra of Atomic Oxygen," 16th International Conference on X-Ray and Inner-Shell Processes, Debrecen, Hungary, July 12-16, 1993.

Caldwell, C. D. and Krause, M. O. "The $2p^5(^2\text{P}^o) \rightarrow 2p^4(^1\text{D}_2)ns,nd$ Rydberg Excitations in Atomic Fluorine," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Sept. 15-16, 1994.

Caldwell, C. D. and Krause, M. O. "AMO Physics at the ALS: Electron-Electron Coincidence," American Physical Society DAMOP Meeting, Washington, DC, Apr. 18-21, 1994.

Caldwell, C. D., Schaphorst, S. J. and Krause, M. O. "Resonance Auger Spectra of Atomic and Molecular Oxygen," American Physical Society DAMOP Meeting, Washington, DC, Apr. 18-21, 1994.

Chen, G., Haire, R. G., Peterson, J. R. and Abraham, M. M. "A Luminescence Study of EuVO_4 at High Pressure," International Conference on Luminescence, Storrs, CT, Aug. 9-13, 1993.

Chen, G., Burns, J. B., Stump, N. A., Haire, R. G. and Peterson, J. R. "Pressure-Induced Phase Transition in B-Type Eu_2O_3 : A Luminescence Study at High Pressure," Joint AIRAPT/American Physical Society Conference, Colorado Springs, CO, June 28-July 2, 1993.

Chen, G., Haire, R. G. and Peterson, J. R. "Effect of Pressure on Amorphous $\text{Eu}(\text{OH})_3$: A Luminescence Study," American Physical Society Meeting, San Diego, CA, March 13-17, 1994.

Chen, G., Stump, N. A., Haire, R. G., Burns, J. B. and Peterson, J. R. "A Luminescence Study of B-Type Eu_2O_3 Under Pressure," in *Proc., High Pressure Science and Technology Meeting*, 1993, S. C. Schmidt, J. W. Shaner, G. A. Samara and M. Ross, eds., AIP Conference Proceedings 309, American Institute of Physics Press, New York (1994) Part I, 359-361.

Cort, B., Ward, J. and Haire, R. G. "Low-Temperature Electrical Resistivity Study of Cubic Americium Hydrides," Actinides-93 International Conference, Santa Fe, NM, Sept. 19-24, 1993.

Gensini, M. M., Haire, R. G., Gibson, J. K. and Maeda, A. "Probing Selected Binary Actinide Alloy Systems by Room-Temperature X-Ray Diffraction Studies," American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1993.

Gensini, M. M., Haire, R. G. and Gibson, J. K. "Investigation of NpZr and Np-Am Systems by X-ray Diffraction," International Actinides '93 Conference, Santa Fe, NM, Sept. 19-24, 1993.

Gibson, J. K., Haire, R. G. and Gensini, M. M. "Alloying Behavior in Selected Neptunium Binary Systems," Actinides-93 International Conference, Santa Fe, NM, Sept. 19-24, 1993.

Gibson, J. K. "Mass Spectrometric Study of Alkali Pertechnetate Vapor Species," 205th National American Chemical Society Meeting, Denver, CO, Mar. 28-Apr. 2, 1993.

Gibson, J. K. "Lanthanide Oxide Cluster Ions Generated by Vacuum Laser Ablation," 46th Southeast Regional American Chemical Society Meeting, Birmingham, AL, Oct. 16-19, 1994.

Gibson, J. K., Haire, R. G., Gensini, M. M. and Ogawa, T. "Characterization of Actinide Alloy Phase Diagrams," American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Haire, R. G. "High-Temperature Vaporization of the Actinides and Their Oxides," International Actinides-93 Conference, Santa Fe, NM, Sept. 19-24, 1993.

Haire, R. G. "Exploring the Chemistry of Transplutonium Elements by Solid and Vapor State Studies," American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1993.

Haire, R. G. "High-Temperature Vaporization of Transplutonium Oxides," 2nd International Conference on f-Elements, Helsinki, Finland, Aug. 1-6, 1994.

Haire, R. G. "High-Temperature High-Pressure Chemistry of the Heavy Actinides, 207th National American Chemical Society Meeting, San Diego, CA, March 13-18, 1994.

Haire, R. G. "Exploring Actinide Chemistry by Systematic High-Temperature and High-Pressure Studies," DOE/OPA Peer Review of BES Heavy Element Chemistry Research Program, Washington, DC, Oct. 6, 1994.

Haire, R. G. "Dependence of the Vaporization Behaviors of Actinide Oxides on the Electronic Nature of the Actinide Atoms," 2nd International Conference on f-Elements, Helsinki, Finland, Aug. 1-6, 1994.

Haire, R. G. "Comparison of the Physical and Chemical Properties of f-Element Metals and Oxides and Their Dependence on Electronics," 1st Workshop on Comparative Science of the f-Elements, Buhlerhohe, Germany, July 28-30, 1994.

Jimenez-Mier, J., Caldwell, C. D., Schaphorst, S. and Krause, M. O. "Decaimiento Auger de las Resonancias $1s \rightarrow np$ en Oxigeno y Berilio Atomicos," XXXVI Congreso Nacional de Fisica, Acapulco, Mexico, Oct. 19, 1993.

Kay, C. L., Stump, N. A., Gibson, J. K. and Peterson, J. R. "Luminescence Lifetime Study of the Thermal Decomposition of Eu^{3+} -Doped $\text{La}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$," International Conference on Luminescence, Storrs, CT, Aug. 9-13, 1993.

Krause, M. O. "Synchrotron Radiation in Atomic and Molecular Physics," American Physical Society Meeting, Washington, DC, Apr. 12-15, 1993.

Krause, M. O. "Photoelectron Angular Distributions: From the Past into the Future," *Proc., International Workshop on Photoionization 1992*, U. Becker and U. Heinzmann, eds., AMS Press, Inc., New York, p. 41 (1993).

Krause, M. O. "High Resolution Electron Spectrometry of Atomic Processes with the Use of Synchrotron Radiation: Status and Prospects," Excited State Spectrometry and Dynamics, Very High Resolution Spectroscopy with Photoelectrons Meeting, Giens, France, Sept. 18-23, 1993.

Krause, M. O. "Electron Spectrometry of Open-Shell Atoms," 16th International Conference on X-Ray and Inner-Shell Processes, Debrecen, Hungary, July 12-16, 1993.

Krause, M. O. "Auger Electron Spectrometry of Atomic Processes with the Use of Synchrotron Radiation: Status and Prospects," American Physical Society Workshop on Atomic Physics, Argonne, IL, Apr. 23-24, 1994.

Krause, M. O. "Auger Electron Spectrometry of Atoms and Molecules with the Use of Synchrotron Radiation," Seminar at National Renewable Energy Laboratory (NREL), Surface Analysis Lab., Golden, CO, Aug. 5, 1994.

Krause, M. O., Schaphorst, S. J. and Caldwell, C. D. "Photoionization of Atomic Oxygen: Branching Ratios and Subshell Cross Sections," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Sept. 15-16, 1994.

Link, P., Braithwaite, D., Benedict, U., Wittig, J. and Haire, R. G. "Americium Is a Good Superconductor under Pressure," Actinide-93 International Conference, Santa Fe, NM, Sept. 19-24, 1993.

Pesterfield, L. L., Pan, W. P., Dieckmann, C. M., Peterson, J. R., Schweitzer, G. K. and Stump, N. A. "Thermogravimetric and Luminescence Studies of Ethylenediaminetetraacetatoeuropate(III)," Inorganic Chemistry Session, National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Pesterfield, L. L., Schweitzer, G. K., Peterson, J. R. and Stump, N. A. "Synthesis and Spectral Characterization of Silver Diethylenetriaminepenta- acetatoeuropate(III)," Inorganic Chemistry Session, National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Peterson, J. R. "Einsteinium: The Heaviest Element Amenable to Bulk-Phase Chemical Study," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Peterson, J. R. "Phase Behavior of Actinide Trihalides Under Pressure," Actinides '93 Meeting, Santa Fe, NM, Sept. 19-24, 1993.

Peterson, J. R. "Microchemical Techniques Used to Study the Properties of the Transplutonium Elements; Physical and Chemical Consequences of Radioactive Decay in the Solid State," Ecole Europeenne des Hautes Etudes des Industries Chimiques de Strasbourg, France, May 29, 1993.

Peterson, J. R. "Introduction to the Symposium Comparative Aspects (Similarities and Differences) of Lanthanide and Actinide Behavior," 20th Rare Earth Research Conference, Monterey, CA, Sept. 12-17, 1993.

Peterson, J. R. "Fundamentals of Radioactivity and the Discovery and Placement of the Transuranium Elements in the Periodic Chart of the Elements," Ecole Europeenne des Hautes Etudes des Industries Chimiques de Strasbourg, Strasbourg, France, May 28, 1993.

Peterson, J. R. "Bulk Phase Chemical Studies on the Edge of Matter: The Transcurium Elements," Indiana State University, Terre Haute, IN, Nov. 2, 1993.

Peterson, J. R. "Bulk Phase Studies on the Edge of Matter: The Transcurium Elements," The University of Tennessee, Knoxville, TN, July 15, 1993.

Peterson, J. R. "Bulk Phase Chemical Studies on the Edge of Matter: Lessons Learned About the Consequences of α and β Decay," San Jose State University, San Jose, CA, July 2, 1993.

Peterson, J. R. "Comparative Science of the Lanthanide and Actinide (Lanact) Halides," 1st Workshop on Comparative Science of the f-Elements, Buhlerhohe, Germany, July 28-30, 1994.

Peterson, J. R. "Consequences of Alpha and Beta Decay in the Solid State," Cincinnati Section American Chemical Society Meeting, Sept. 15, 1994.

Peterson, J. R. "Some Recent Advances in the Study and Characterization of f-Element Materials via Optical Spectroscopy," 2nd International Conference on f-Elements, Helsinki, Finland, Aug. 1-5, 1994.

Peterson, J. R. "Using Diamonds for Materials Research at High Pressure," Carson-Newman College, Jefferson City, TN, Feb. 9, 1994.

Peterson, J. R. "Chemistry of Some Exotic Radioactive Elements," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Peterson, J. R. "Chemical Studies on the Edge of Matter," Juniata College, Huntingdon, PA, Dec. 7, 1994.

Peterson, J. R. "Bulk Phase Chemical Studies on the Edge of Matter: Lessons Learned About the Consequences of α and β Decay," San Jose State University, San Jose, CA, June 29, 1994.

Robinson, L., Johnson, E. and Robles, L. D. "Maximizing the Cold Neutron Flux from a Californium-252 Source," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, Oct. 5-7, 1993.

Schaphorst, S. C., Caldwell, C. D., Krause, M. O. and Jimenez-Mier, J. "Atomic Features in the Decay of Resonantly Excited Molecular Oxygen," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Oct. 18-19, 1993.

Schaphorst, S. J., Caldwell, C. D., Saha, H. P. and Krause, M. O. "Partial Photoionization Cross Section for Atomic Oxygen," American Physical Society DAMOP Meeting, Washington, DC, Apr. 18-21, 1994.

Shoup, S. S., Haverlock, T. J. and Bamberger, C. E. "Solid Solutions within Selected $\text{SrO-LnO}_{1.5}\text{-TiO}_2$ Systems," Southeast Regional American Chemical Society Meeting, Birmingham, AL, Oct. 19, 1994.

Stewart, G. and Haire, R. G. "Specific Heat of Some Transplutonium Intermetallic Compounds for Heavy Fermion Behavior," Actinides-93 Internal Conference, Santa Fe, NM, Sept. 19-24, 1993.

Stump, N. A. and Peterson, J. R. "Luminescence Study of the Thermal Decomposition of Europium Trichloride Hexahydrate," 44th Pittsburgh Conference and Exposition, Atlanta, GA, Mar. 8-12, 1993.

Stump, N. A., Schweitzer, G. K., Murray, G. M. and Peterson, J. R. "Luminescence Detection of Cation Exchange in $\text{Na}_3[\text{Eu}(\text{2,6-Pyridinedicarboxylate})_3]$," International Conference on Luminescence, Storrs, CT, Aug. 9-14, 1993.

Whitfield, S. B., Caldwell, C. D., van der Meulen, P. and Krause, M. O. "High-Resolution Photoelectron Spectroscopy of Atomic Mn in the Vicinity of the $3p \rightarrow 3d$ Giant Resonance," 16th International Conference on X-Ray and Inner-Shell Processes, Debrecen, Hungary, July 12-16, 1993.

Whitfield, S. B., Caldwell, C. D., van der Meulen, P. and Krause, M. O. "High-Resolution Photoelectron Spectrometry of Atomic Manganese in the Vicinity of the 3p $\rightarrow$ 3d Resonance," Synchrotron Radiation Center Users Group Meeting, Madison, WI, Oct. 18-19, 1993.

ORGANIC CHEMISTRY SECTION

ANALYTICAL METHODS GROUP

Journal Articles

Barshick, S. A. and Buchanan, M. V., "Rapid Analysis of Animal Drug Residues Using Microcolumn Solid Phase Extraction and Thermal Desorption Ion Trap Mass Spectrometry," *J. Assoc. Off. Anal. Chem.* (1994) 77, 1428-1434.

Caton, J. E., Ho, C-h., Williams, R. T. and Griest, W. H. "Characterization of Insoluble Fractions of TNT Transformed by Composting," *J. Environ. Sci. Health. A Environ. Sci. Eng.* (1994) A29, 659-670.

Caton, J. E., Hazen, K. H., Griest, W. H., Watson, A. P. and Buchanan, M. V. "Rapid Method for Isolating Targeted Organic Chemicals from Biological Matrices," *Anal. Lett.* (1994) 27, 351-362.

Griest, W. H., Stewart, A. J., Tyndall, R. L., Caton, J. E., Ho, C-h., Ironside, K. S., Caldwell, W. M. and Tan, E. "Chemical and Toxicological Testing of Composted Explosives-Contaminated Soil," *Environ. Toxicol. Chem.* (1993) 12, 1105-1116.

Ma, C. Y. and Bayne, C. K. "Differentiation of Aroclors Using Linear Discrimination for Environmental Samples Analyzed by Electron Capture Negative Ion Chemical Ionization Mass Spectrometry," *Anal. Chem.* (1993) 65, 772-777.

Rossi, S. A., Johnson, J. V. and Yost, R. A. "Short-Column Gas Chromatography/Tandem Mass Spectrometry for the Detection of Underivatized Anabolic Steroids in Urine," *Biol. Mass. Spectrom.* (1994) 23, 131-139.

Tomkins, B. A. "Screening Procedure for Sodium Fluoroacetate (Compound 1080) at Sub-microgram/gram Concentrations in Soils," *Anal. Lett.* (1994) 27(14), 2703-2718.

Presentations/Conference Proceedings

Barshick, S. A., Buchanan, M. V. and Guerin, M. R., "Survey of Priority Semivolatile Organic Compounds by Direct Sampling Ion Trap Mass Spectrometry," 34th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN, October 5-7, 1993.

Barshick, S. A., Smith, S. M., Buchanan, M. V. and Guerin, M. R. "Determination of Benzene in Food by Direct Sampling Ion Trap Mass Spectrometry," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Barshick, S. A. and Buchanan, M. V. "Novel Sampling Methods for Use with Thermal Desorption Ion Trap Mass Spectrometry," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Barshick, S. A., Grimm, C. C., Lloyd, S. W. and Johnsen, P. "Rapid Screening for Methylisoborneol in Catfish using Purge and Trap DSITMS," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Barshick, S. A., Smith, S. M., Buchanan, M. V. and Thayer, D. W. "Determination of Volatile Organic Compounds in Food Using a Novel Blender-Purge and Trap Device," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, St. Louis, MO, Oct. 2-7, 1994.

Buchanan, M. V. and Barshick, S. A. "Direct Sampling Ion Trap Mass Spectrometry," 44th Pittsburgh Conference and Exhibition, Atlanta, GA, March 8-12, 1993.

Caton, J. E., Griest, W. H. and Guerin, M. R. "Technique for Introducing Intractable Samples into a Liquid Chromatograph," ALEX'93, The Analytical Laboratory Exposition and Conference, San Francisco, CA, Oct. 5-7, 1993.

Greenbaum, E., Tevault, C. V. and Ma, C. Y. "One-Step Photoconversion of Biomass to Volatile Hydrocarbons and Molecular Oxygen," Fifteenth Symposium on Biotechnology for Fuels and Chemicals, Colorado Springs, CO, May 10-14, 1993.

Greenbaum, E., Tevault, C. V. and Ma, C. Y., "Direct Photoconversion of Biomass to Volatile Hydrocarbons," Sixteenth Symposium on Biotechnology for Fuels and Chemicals, Gatlinburg, TN, May 9-13, 1994.

Greenbaum, E., Tevault, C. V. and Ma, C. Y. "Fundamental Studies in Photosynthesis for the Production of Fuels and Chemicals from Renewable Resources," Eighteenth DOE Solar Photochemistry Research Conference, Tahoe City, CA, June 5-9, 1994.

Greenbaum, E., Tevault, C. V. and Ma, C. Y. "Direct Photoconversion of Lignocellulosic Substrates to Fuels and Chemicals," American Chemical Society Spring National Meeting, San Diego, CA, March 13-18, 1994.

Griest, W. H., Tyndall, R. L., Stewart, A. J., Ho, C-h., Caton, J. E. and Caldwell, W. M. "Chemical/Toxicological Evaluation of Windrow Composting of Explosives-Contaminated Sediments," 35th Rocky Mountain Conference on Analytical Chemistry, Denver, CO, July 25-29, 1993.

Griest, W. H., Ho, C-h., Ramsey, R. S. and Caldwell, W. M. "Supercritical Fluid and Microsolvent Extraction of Chemical Warfare Agent Simulants from Soil," in *Proc., 1991 U.S. Army Chemical Research, Development and Engineering Center Scientific Conference on Chemical Defense Research*, ERDEC-SP-002, U.S. Army Chemical Research, Development and Engineering Center, Aberdeen Proving Ground, MD, pp. 257-263 (June 1993).

Griest, W. H. "A Proposal for the Analysis of Nitrocellulose in Soil or Compost," in *Proc., U.S. Army-Purdue University Workshop on Nitrocellulose Fines Separation and Treatment*, W. Lafayette, IN, Nov. 4-5, 1993.

Griest, W. H., Ho, C-h., Moneyhun, J. H., Agouridis, D. C., Gayle, T. M. and Bates, B. E. "Indicator Strip and Portable Instrument Technologies for Determining Nitroesters or Moisture in Combustible Cartridge Cases," in *Proc., The Predictive Technology Symposium '93, American Defense Preparedness Association*, New Jersey, pp. 223-237 (1993).

Griest, W. H., Schenley, R. L., Caton, J. E. and Wolfe, P. F. "Adaptation of the TCLP and SW-846 Methods to Radioactive Mixed Waste," in *Proc., International Topical Meeting on Nuclear and Hazardous Waste Management, Spectrum '94, American Nuclear Society*, La Grange Park, IL, pp. 634-639 (1994).

Griest, W. H., Schenley, R. L., Caton, J. E. and Wolfe, P. F. "Adaptation of the TCLP and SW-846 Methods to Radioactive Mixed Waste," *Spectrum '94*, Atlanta, GA, Aug. 14-18, 1994.

Jenkins, R. A., Bayne, C. K., Maskarinec, M. P., Johnson, L. H., Holladay, S. K. and Tomkins, B. A. "Experimental Determination of Maximum Pre-Analytical Holding Times for Volatile Organics in Selected Soils," *National Symposium on Measuring and Interpreting VOCs in Soils: State of the Art and Research Needs*, Las Vegas, NV, January 12-14, 1993.

Ma, C. Y., Skeen, J. T., Dindal, A. B., Higgins, C. E. and Jenkins, R. A. "Triple Sorbent Thermal Desorption/Gas Chromatography/Mass Spectrometry Determination of Vapor Phase Organic Contaminants," in *Proc., 1994 USEPA/A&WMA International Specialty Conference on Measurement of Toxic and Related Air Pollutants*, Durham, NC, May 3-6, 1994, pp. 30-42.

Maskarinec, M. P. and Bayne, C. K. "Development of Stability Data for Organics in Environmental Samples," *National American Chemical Society Meeting*, San Diego, CA, Mar. 13-18, 1994.

Schenley, R. L., Caton, J. E. and Griest, W. H. "Direct Determination of TCLP Phenols and Herbicides by HPLC," *9th Annual Waste Testing and Quality Assurance Symposium*, Arlington, VA, July 12-16, 1993.

Schenley, R. L., Wolfe, P. F., Caton, J. E. and Griest, W. H. "Adaptation of TCLP Extraction and Analytical Methods for Radioactive Mixed Waste," *48th Northwest Regional American Chemical Society Meeting*, Laramie, WY, June 17-19, 1993.

Smith, S. M., Ma, C. Y., Bayne, C. K. and Laing, W. R. "Detection Limit Determination for Polychlorinated Biphenyls Analyzed by Gas Chromatography and Electron Capture Negative Ion Chemical Ionization Mass Spectrometry," *35th ORNL/DOE Conference on Analytical Chemistry in Energy Technology*, Gatlinburg, TN, October 11-13, 1994.

Tomkins, B. A. "Challenge of Quantitating Ultratrace Concentrations of Water-Miscible Polar Neutrals in Groundwaters," *35th ORNL/DOE Conference on Analytical Chemistry in Energy Technology*, Gatlinburg, TN, Oct. 11-13, 1994.

Vaas, A. A., Tyndall, R. L., Stewart, A. J., Ho, C.-h., Caton, J. E., Caldwell, W. M. and Griest, W. H. "Evaluation of Windrow Composting for Detoxifying Explosives-Contaminated Sediments," 17th Annual Army Environmental R&D Symposium and 3rd U.S. Army Corps of Engineers Innovative Technology Transfer Workshop, Williamsburg, VA, June 22-24, 1993.

Reports

Agouridis, D. C., Gayle, T. M. and Griest, W. H. *Development of the Prototype Munitions Case Moisture Meter Model ORNL-1*, ORNL/TM-12334 (February 24, 1993).

Bates, B. and Griest, W. H. *Prototype Indicator Strip for Tank Ammunition*, ORNL/TM-12405 (October, 31, 1993).

Counts, H. W., Bayne, C. K. and Griest, W. H. *Predictive Modelling of Adhesive Joint Deterioration and Nitroester Migration in the M829 APFSDS Kinetic Energy Round*, ORNL/TM-12659 (December 15, 1993).

Griest, W. H. and Stokely, J. R. "Characterization of Mixed Wastes: Scientific Perspective," in *Environmental Monitoring Issues, Results of Workshops Held in July 1992 as part of EPA's Eighth Annual Waste Testing and Quality Assurance Symposium*, EPA/600R-93/033, U.S. Environmental Protection Agency, Office of Research and Development, Washington, D.C., pp. D-20-D36 (March 1993).

Griest, W. H. [Characterization Team Leader and Section Editor for] *Oak Ridge National Laboratory Technology Logic Diagram*, Volumes 1 and 2, ORNL/M-2751 (September 1993).

Griest, W. H., Stewart, A. J., Ho, C.-h., Tyndall, R. L., Vass, A. A., Caton, J. E. and Caldwell, W. M. *Characterization of Explosives Processing Waste Decomposition Due to Composting*, ORNL/TM-12812 (September 1994).

Other

Griest, W. H. [Author or coauthor of 8 method protocols published in] "DOE Methods for Evaluating Environmental and Waste Management Samples," DOE/EM-0089T, Rev. 1, Addendum 1, U.S. Department of Energy, Assistant Secretary for Environmental Restoration and Waste Management, Washington, D.C., October, 1993.

ENVIRONMENTAL MONITORING GROUP

Journal Articles

Bayne, C. K., Schmoyer, D. D. and Jenkins, R. A. "Practical Reporting Times for Environmental Samples," *Environ. Sci. Technol.* (1994) **28**, 1430-1436.

Jenkins, R. A., Buchanan, M. V., Merriweather, R., Ilgner, R. H., Gayle, T. M. and Watson, A. P. "Movement of Chemical Warfare Simulants Through Porous Media," *J. Hazard. Mater.* (1994) 37, 303-325.

Teague, S. V., Pinkerton, K. E., Goldsmith, M., Gebremichael, A., Chang, S., Jenkins, R. A. and Moneyhun, J. H. "Sidestream Cigarette Smoke Generation and Exposure System for Environmental Tobacco Smoke Studies," *Inhalat. Toxicol.* (1994) 6, 79-93.

Waters, L. C., Counts, R. W., Palausky, A. and Jenkins, R. A. "Colorimetric Strips Test: A Comparison of Visual and Reflectometric Measurements for Quantitative Applications," *J. Hazard. Mater. (Special Issue)* (1994)

Waters, L. C., Smith, R. R., Stewart, J. H. and Jenkins, R. A. "Evaluation of Two Field Screening Test Kits for the Detection of PCBs in Soil by Immunoassay," *J. AOAC International* (1994) 77(6), 1664-1671.

Presentations/Conference Proceedings

Higgins, C. E. and Dindal, A. B. "Evaluation of Purge and Trap/Thermal Desorption Gas Chromatography for the Determination of Nicotine and Cotinine in Aqueous Solutions," 48th Tobacco Chemists' Research Conference, Greensboro, NC, Sept. 25-28, 1994.

Jenkins, R. A., Higgins, C. E., Gayle, T. M., Allin, G. W. and Smith, R. R. "Field Experiences with a Multisorbent Arrayed Sampler for the In-Situ Collection of Vadose Zone Volatile Organic Compounds," 3rd International Symposium for Field Screening Methods for Hazardous Wastes and Toxic Chemicals, Las Vegas, NV, Feb. 24-26, 1993.

Jenkins, R. A., Bayne, C. K., Maskarinec, M. P., Johnson, L. H., Holladay, S. K. and Tomkins, B. A. "Experimental Determination of Maximum Pre-Analytical Holding Times for Volatile Organics in Selected Soils," National Symposium on Measuring and Interpreting VOCs in Soils: State of the Art and Research Needs, Las Vegas, NV, Jan. 12-14, 1993.

Jenkins, R. A., Palausky, A., Counts, R. W., Guerin, M. R., Dindal, A. B. and Bayne, C. K. "Determination of Personal Exposure of Non-Smokers to Environmental Tobacco Smoke in the United States," International Symposium on Lifestyle Factors and Human Lung Cancer, Guangzhou, PRC, Dec. 12-16, 1994.

Jenkins, R. A. "Adventures in Workplace Air Sampling: From the Ordinary to the Unconventional," Cincinnati Milacron Technical Seminar, Cincinnati, OH, Oct. 27, 1994.

Jenkins, R. A. and Fancher, J. "A Deep Subsurface Multisorbent Soil Gas Sampler for Collection of Volatile Organic Compounds," U.S. DOE Technology Information Exchange Meeting, Seattle, WA, Jan. 1994.

Jenkins, R. A., Palausky, A., Counts, R. W., Guerin, M. R., Dindal, A. B. and Bayne, C. K. "Determination of Personal Exposure of Non-Smokers to Environmental Tobacco Smoke," 48th Tobacco Chemists' Research Conference, Greensboro, NC, Sept. 28-30, 1994.

Ma, C. Y., Skeen, J. T., Dindal, A. B., Higgins, C. E. and Jenkins, R. A. "Triple Sorbent Desorption/ Gas Chromatography/Mass Spectrometry Determination of Vapor Phase Organic Contaminants," Measurement of Toxic and Related Air Pollutants Meeting, Durham, NC, May 3-6, 1994.

Waters, L. C., Smith, R. R., Counts, R., Stewart, J. and Jenkins, R. A. "Evaluation of Field Test Kits Including Immunoassays for the Detection of Contaminants in Soil and Water," 3rd International Symposium on Field Screening Methods for Hazardous Wastes and Toxic Chemicals, Las Vegas, NV, Feb. 24-26, 1993.

Reports

Compere, A. L., Griffith, W. L., Huxtable, W. P. and Googin, J. M. *Rapid Nitrate Micromethod*, ORNL Report (1993).

Compere, A. L., Griffith, W. L., Hayden, H. W., Johnson, J. S. and Wilson, D. F. *Contaminated Nickel Scrap Processing*, ORNL/TM-12900 (1994).

Griffith, W. L., Compere, A. L., Huxtable, W. P. and Googin, J. M. *Decreasing Raffinate Overflow*, ORNL Report (1993).

Huxtable, W. P., Compere, A. L., Griffith, W. L. and Googin, J. M. *Process Waste Minimization Opportunities at the Y-12 Plant*, Martin Marietta Energy Systems Report Y/EN-4841 (1993).

Waters, L. C., Jenkins, R. A., Counts, R. W. and Hernandez, L. J. "A Photoacoustic Infra-red Method for the Detection of Selected Chlorinated Volatile Organic Chemicals (VOCs) in Water," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Waters, L. C., Jenkins, R. A. and Hernandez, L. J. "Immunoassay for Mercury in Soils: A Modification of MB 100 to Use Test Tubes Instead of Microplates," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Waters, L. C., Jenkins, R. A., Smith, R. R., Counts, R. W. and Stewart, J. H. "Immunoassay for PCBs in Soils," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Waters, L. C., Jenkins, R. A., Smith, R. R., Counts, R. W. and Stewart, J. H. "An Indicator Strip-based Colorimetric Test for Nitrate in Water and Soil," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Waters, L. C., Jenkins, R. A., Smith, R. R., Counts, R. W. and Stewart, J. H. "An Indicator-Strip-based Colorimetric Test for Lead in Water," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1, Mar. 1993.

Waters, L. C., Jenkins, R. A., Smith, R. R., Stewart, J. H. and Counts, R. W. "Immunoassay for Mercury in Soils," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Waters, L. C. and Jenkins, R. A. "An Indicator Strip-Based Colorimetric Test for Chromate Ions (CrO_4^{2-}) in Aqueous Samples," Chapter in *DOE Methods for Evaluating Environmental and Waste Management Samples*, DOE/EM-0089T, Rev. 1 (Mar. 1993).

Other

Bauer, M. L., Compere, A. L., Googin, J. M. and Griffith, W. L. "RF/Microwave Enhanced Reaction and Physical Extraction," ESID 1562-X, Jan. 1994.

Bigelow, T. S., Compere, A. L., Gardner, W. L. and Griffith, W. L. "Microwave Pretreatment of Wood," *Videotape* (1994).

Compere, A. L. and Griffith, W. L. "Low Emissions Fuels," ESID 1230-X, DOE Case S-77, 502 March 25, 1994.

Compere, A. L., Dorsey, G. F., Googin, J. M., Griffith, W. L. and West, B. H. "Low Emission Diesel Fuels Containing Melamine Cyanurate," ESID 1531-X, May 1994.

INSTRUMENTATION GROUP

Journal Articles

Hart, K. J. and McLuckey, S. A. "Relative Dissociation Energy Measurements Using Ion Trap Collisional Activation," *J. Am. Soc. Mass Spectrom.* (1994) 5, 250-259.

Lammert, S. A. "1994 Directory of Mass Spectrometry Manufacturers and Suppliers," *Rapid Commun. Mass Spectrom.*

Wise, M. B., Thompson, C. V., Buchanan, M. V. and Guerin, M. R. "Direct Sampling Ion Trap Mass Spectrometry," *Spectrosc.* (1993) 8(5), 14-22.

Presentations/Conference Proceedings

Buchanan, M. V., Wise, M. B. And Guerin, M. R. "Rapid Detection of Trace Organics with Direct Sampling Ion Trap Mass Spectrometry," Southeast Regional Meeting of the American Chemical Society, Johnson City, TN, Oct. 17-20, 1993.

Goeringer, D. E., Ramsey, J. M., Dale, J. M., Wise, M. B., Buchanan, M. V. and McLuckey, S. A. "Advanced Chemical Analysis Instrumentation for Treaty Verification: Ion Trap Mass Spectrometry," Chemical Weapons Convention Verification Technology Research and Development Conference, Washington, DC, Mar. 2-3, 1993.

Habibi-Goudarzi, S., Hart, K. J. and McLuckey, S. A. "The Effect of Charge on Ion Stability: A Quantitative Comparison," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Hart, K. J., Habibi-Goudarzi, S. and McLuckey, S. A. "Computer-Assisted Interpretation of Electrospray-Tandem Mass Spectra of Oligonucleotides," 41st American Society of Mass Spectrometry Conference, San Francisco, CA, May 30-June 4, 1993.

Hart, K. J., Habibi-Goudarzi, S. and McLuckey, S. A. "Determination of Relative Dissociation Energies in an Ion Trap Mass Spectrometer," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Hart, K. J. and Buchanan, M. V. "Software Development for a Field Portable Ion Trap Mass Spectrometer," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 30-June 3, 1994.

Lammert, S. A. and Buchanan, M. V. "Modification of a Finnigan ITS 40 to Perform Selective Isolation and MS/MS Functions," American Society for Mass Spectrometry Meeting, Chicago, IL, May 30-June 3, 1994.

Lammert, S. A., Merriweather, R., Sarver, E. W. and Wasserman, M. B. "Detection of Chemical Agents, Precursors and By-Products Using Ion Trap Technology," Scientific Conference on Chemical and Biological Defense Research, Baltimore, MD, Nov. 15-18, 1994.

Lammert, S. A., Merriweather, R. and Wasserman, M. B. "Analysis of Chemical Weapons Convention Treaty Compounds Using a Field-portable Ion Trap Mass Spectrometer," 3rd International On-Site Analysis-Field Portable Instrumentation...The Lab Comes to the FieldSM, Houston (Montgomery), TX, Jan. 22-25, 1995.

McLuckey, S. A., Van Berkel, G. J., Hart, K. J., Habibi-Goudarzi, S., Ramsey, R. S. and Quirke, J. M. E. "Electrospray Ionization and the Quadrupole Ion Trap Mass Spectrometer," Pittsburgh Conference, Atlanta, GA, Mar. 10, 1993.

McLuckey, S. A., Goeringer, D. E. and Hart, K. J. "Ion Trap Collisional Activation," 6th Lake Louise Workshop on Tandem Mass Spectrometry, Calgary, Canada, Nov. 17-20, 1993.

McLuckey, S. A., Goeringer, D. E. and Hart, K. J. "Collisional Activation for the Study of Energetics and Structure," Federation of Analytical Chemistry and Spectroscopy Societies Meeting, Detroit, MI, Oct. 17-22, 1993.

Ramsey, R. S., Asano, K. G., Hart, K. J., Goeringer, D. E., Van Berkel, G. J. and McLuckey, S. A. "Combining Capillary Electrophoresis with Electrospray Ionization/Ion Trap Mass Spectrometry for Biopolymer Analysis," 41st American Society of Mass Spectrometry Conference for Mass Spectrometry and Allied Topics, San Francisco, CA, May 31-June 4, 1993.

Ramsey, R. S., Asano, K. G., Goeringer, D. E., Van Berkel, G. J., Hart, K. J. and McLuckey, S. A. "The Ion Trap Mass Spectrometer as a Chromatographic and Electrophoretic Detector," 15th International Symposium on Capillary Chromatography, Riva del Garda, Italy, May 24-28, 1993.

Sarver, E. W., Wasser, M. B., Merriweather, R. and Lammert, S. A. "Detection of Chemical Agents, Precursors and By-Products Using Ion Trap Technology," Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, New Orleans, LA, Mar. 5-10, 1995.

Thompson, C. V., Wise, M. B., Buchanan, M. V. and Guerin, M. R. "Direct Sampling Ion Trap Mass Spectrometry," Mobile Analytical Laboratory Workshop, Los Alamos, NM, July 20-21, 1993.

Wasserman, M. B. and Lammert, S. A. "Detection of Chemical Weapons Precursors and By-Products Using Ion Trap Mass Technology," 2nd International On-Site Analysis: Field Portable Instrumentation...The Lab Comes to the Field, Houston, TX, Jan. 24-26, 1994.

Wise, M. B. "A Direct Approach to Environmental Analysis," ORNL Showcase Lecture Series, Oak Ridge, TN, September 10, 1993.

Wise, M. B., Thompson, C. V. and Guerin, M. R. "Development and Testing of a Field Transportable Direct Sampling Ion Trap," 3rd International Symposium on Field Screening, Las Vegas, NV, Feb. 24-26, 1993.

Wise, M. B., Guerin, M. R., Thompson, C. V. and Buchanan, M. V. "Direct Sampling Ion Trap Mass Spectrometry for Rapid Environmental Analysis," National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Wise, M. B., Buchanan, M. V., Thompson, C. V., Goeringer, D. E., McLuckey, S. A., Crutcher, R. I., Hileman, M. S., Emery, M. L. and Alley, G. T. "Considerations for the Size and Power Reduction of a Field Transportable Ion Trap Mass Spectrometer," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Wise, M. B., Buchanan, M. V., Guerin, M. R., Merriweather, R. and Bayne, C. K. "Development of a Method for the Direct Purge Analysis of Volatile Organics in Water," 41st American Society of Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, May 30-June 4, 1993.

Wise, M. B., Guerin, M. R. and Merriweather, R. "Direct Sampling Ion Trap Mass Spectrometry for Rapid Environmental Analysis," EPA Region IV Laboratory, Athens, GA, August 16, 1994.

Wise, M. B., Ilgner, R. and Buchanan, M. V. "Rapid Detection of Chemical Warfare Agents Using Direct Sampling Ion Trap Mass Spectrometry," Conference on Analytical Methods for Environmental

Sampling of Chemical Warfare Agents and Their Breakdown Products, Aberdeen, MD, September 20-21, 1994.

Wise, M. B., Thompson, C. V. and Guerin, M. R. "Enhanced Sensitivity Real-Time Monitoring of VOCs in Air and Water Using Filtered Noise Field in Conjunction with a Direct Sampling Ion Trap Mass Spectrometer," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Wise, M. B., Thompson, C. V. and Guerin, M. R. "Real-Time Determination of Volatile Organic Compounds in Air and Water Using Direct Sampling Ion Trap Mass Spectrometry," 42nd American Society for Mass Spectrometry Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 29-June 3, 1994.

Wise, M. B., Thompson, C. V., Guerin, M. R. and Jenkins, R. A. "Field Transportable Ion Trap Mass Spectrometer," International Forum on Process Analytical Chemistry '94 On-Site Conference, Houston, TX, January 26, 1994.

Other

Wise, M. B. and Guerin, M. R. Participation in the EPA Office of Solid Waste Organic Methods Review of DSITMS Method, Washington, D.C., July 11, 1994.

PHYSICAL ORGANIC CHEMISTRY GROUP

Books/Book Chapters

Sigman, M. E. and Zingg, S. P. "Anthracene Photochemistry in Aqueous and Heterogeneous Media," in *Environmental Aspects of Surface and Aquatic Photochemistry*, D. Helz and R. G. Zepp, eds., Lewis Publishers, Boca Raton, FL (1994) p. 197.

Journal Articles

Barbas, J. T., Sigman, M. E., Buchanan, A. C. and Chevis, E. A. "Photolysis of Substituted Naphthalenes on SiO_2 and Al_2O_3 ," *Photochem. Photobiol.* (1993) **58**(2), 155-158.

Barbas, J. T., Dabestani, R. T. and Sigman, M. E. "A Mechanistic Study of Photodecomposition of Acenaphthylene on a Dry Silica Surface," *J. Photochem. Photobiol. A Chem.* (1994) **80**, 103.

Bilski, P., Dabestani, R. and Chignell, C. F. "Photoprocesses of Eosine and Rose Bengal Ion Pairs With Cationic Surfactant in Non-Polar Solvents: Application in Photosensitization Studies." *J. Photochem. Photobiol. A Chem.* (1994) **79**, 121.

Britt, P. F., Buchanan, A. C., Malcolm, E. A. and Biggs, C. A. "Effect of Cross-Linking on the Pyrolysis of Diphenylalkanes," *J. Anal. Appl. Pyrol.* (1993) **25**, 407-417.

Buchanan, A. C., Britt, P. F., Thomas, K. B. and Biggs, C. A. "A Surface-Immobilized Model Compound Investigation of Catalytic Reactions in Dispersed Solids," *Energy and Fuels* (1993) 7, 373-379.

Burns, J. H. and Hagaman, E. W. "Three Monofluorinated Small Molecules: Ortho-Fluorophenylglycine, Methyl 4-(Fluorocarbonyl)benzoate, and 16 α -Fluoro-*a*-estradiol 3-Methyl Ether," *Acta Cryst.* (1993) C49, 1393-1396.

Cox, D. M., Cameron, S. D., Tuinman, A., Gakh, A., Adcock, J. L., Compton, R. N., Hagaman, E. W., Kniaz, K., Fischer, J. E., Strongin, R. M., Cichy, M. A. and Smith, A. B. "X-Ray Photoelectron and NMR Studies of Perfluorinated C₆₀: Evidence That C-C Bonds Are Broken," *J. Am. Chem. Soc.* (1994) 116, 1115-1120.

Dabestani, R., Sik, R.H., Davis, D.G., Dubay, G. and Chignell, C.F. "Spectroscopic Studies of Cutaneous Photosensitizing Agents. XVIII. Indomethacin," *Photochem. Photobiol.* (1993) 58, 367.

Hagaman, E. W. "¹³C-¹⁹F Dipolar Dephasing in the Monofluorinated Organic Substances: Characterization by ¹H-¹³C-¹⁹F Triple Resonance ¹³C CP/MAS and ¹⁹F MAS NMR," *J. Magn. Reson.* (1993) A104, 125-131.

Hagaman, E. W. and Burns, J. H. "The Determination of Local Structure in Organofluorides Using Fluorine-19 Carbon-13 Dipolar Coupling," *Fuel*, (1993) 72, 1239.

Mitchell, S. C., Lafferty, C. J., Garcia, R., Snape, C. E., Buchanan, A. C., Britt, P. F. and Klavetter, E. "Silica-Immobilized Compounds as Models for Probing Coal Pyrolysis and Hydropyrolysis Phenomena," *Energy and Fuels* (1993) 7, 331-333.

Rives, S. and Sigman, M. E. "Prediction of Atomic Ionization Potentials I-III Using an Artificial Neural Network," *J. Chem. Info. Comput. Sci.* (1994) 34, 617.

Zingg, S. P. and Sigman, M. E. "Influence of a SiO₂/Cyclohexane Interface on the Photochemistry of Anthracene," *Photochem. Photobiol.* (1993) 57(3), 453-459.

Presentations/Conference Proceedings

Barbas, J. T., Sigman, M. E. and Dabestani, R. T. "The Photo-Oxidation of Aromatic Compounds on Silica Surfaces," Georgia Academy of Science, Atlanta, GA, Apr. 29-30, 1994.

Barbas, J. T., Sigman, M. E. and Dabestani, R. T. "The Photo-oxidation of Naphthalenes on Silica Surfaces," VI Inter-American Photochemical Society Winter Conference, Clearwater Beach, FL, Jan. 1-5, 1994.

Barbas, J. T., Sigman, M. E. and Dabestani, R. T. "The Photolysis of Naphthalenes on Silica Surfaces," Georgia Academy of Sciences, Atlanta, GA, Apr. 29-30, 1994.

- Britt, P. F., Buchanan, A. C. and Malcolm, E. A. "Model Compound Studies of the Thermolysis of Lignin," National American Chemical Society Meeting, Denver, CO, March 28-April 2, 1993.
- Britt, P. F. and Buchanan, A. C. "Pyrolysis of Polymer Models of Coal," in *Proc., 7th International Conference on Coal Science*, Banff, Alberta, Canada, September 12-17, 1993, Vol. 2, 297 (1993).
- Britt, P. F. "Fundamental Investigations of Pyrolysis Mechanisms for Biopolymers", Gordon Research Conference on Analytical Pyrolysis and Oxidative Degradation of Materials, Plymouth, NH, June 13-18, 1993.
- Britt, P. F., Buchanan, A. C. and Malcolm, E. A. "Thermolysis of Phenethyl Phenyl Ether. A Model of Ether Linkages in Low Rank Coal," in *Preprints, Div. Fuel Chem., American Chemical Society*, Washington, DC, Aug. 21-25, 1994, **39(3)**, 678 (1994).
- Britt, P. F., Buchanan, A. C., Thomas, K. B. and Lee, S-K. "Pyrolysis Mechanisms of Lignin," 11th International Symposium on Analytical and Applied Pyrolysis, Nagoya, Japan, May 30-June 3, 1994.
- Britt, P. F., Hurst, G. B. and Buchanan, M. V. "Electrophore-Labeled DNA for Enhanced Sensitivity in Matrix-Assisted Laser Desorption Mass Spectrometry," DOE Contractor and Grantee Workshop of the Human Genome Program, Santa Fe, NM, Nov. 13-17, 1994.
- Brown, S. D., Sirkecioglu, O., Ismail, K., Andersen, J., Snape, C. E., Buchanan, A. C. and Britt, P. F. "Use of Hydropyrolysis-MS to Probe the Hydrocracking of Diphenylalkane Linkages in the Solid State," in *Preprints, Div. Fuel Chem., National American Chemical Society Meeting*, Washington, DC, Aug. 21-25, 1994, **39(3)** 801 (1994).
- Buchanan, A. C. and Britt, P. F. "The Role of Model Compound Studies in Coal Research," in *Preprints, Div. Fuel Chem., American Chemical Society Meeting*, San Diego, CA, Mar. 13-17, 1994, **39(1)**, 22 (1994).
- Buchanan, A. C., Britt, P. F. and Thomas, K. B. "Restricted Mass Transport Effects on Free Radical Reactions," in *Preprints, National American Chemical Society Meeting*, Washington, DC, Aug. 21-25, 1994, **39(3)**, 684 (1994).
- Buchanan, A. C., Britt, P. F. and Thomas, K. B. "Influence of Restricted Diffusion on Retrogressive Free Radical Reactions," in *Proc., 7th International Conference on Coal Science*, Banff, Alberta, Canada, Sept. 12-17, 1993, Vol. 1, p. 627 (1993).
- Buchanan, A. C., Britt, P. F. and Thomas, K. B. "Acid-Catalyzed Reactions in Dispersed Solids," American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.
- Buchanan, A. C. and Britt, P. F. "Exploration of High Temperature, Organic Reactions on Surfaces," Seminar at The University of Tennessee, Knoxville, TN, Apr. 15, 1993.

Dabestani, R. T., Barbas, J. T. and Sigman, M. E. "Photochemistry of Acenaphthylene on Silica Surface: Mechanism and Products," XVI International Conference on Photochemistry, Vancouver, Canada, Aug. 1-6, 1993.

Dabestani, R. T., Barbas, J. T. and Sigman, M. E. "Photodecomposition of Acenaphthylene on the Surface of SiO₂," American Society for Photobiology Meeting, Chicago, IL, June 26-30, 1993.

Dabestani, R. T., Ellis, K. J. and Sigman, M. E. "Photochemistry of Anthracene on a Dry Silica Surface: Products and Mechanism," VI Inter-American Photochemical Society Winter Conference, Clearwater, FL, Jan. 1-5, 1994.

Dabestani, R. T., Ellis, K. J. and Sigman, M. E. "Photochemistry of Anthracene on Dry Surfaces: Products and Mechanism," National Meeting of the American Chemical Society, San Diego, CA, Mar. 13-18, 1994.

Guthrie, R. D., Ramakrishnan, S., Britt, P. F., Buchanan, A. C. and Davis, B. H. "Thermolysis of Silica-Immobilized 4'-Hydroxy-1,2-Diphenylethane under D₂. A Coal Hydroliquefaction Model," in *Preprints, American Chemical Society Meeting*, Washington, DC, Aug. 21-26, 1994, **39(3)**, 668 (1994).

Hagaman, E. W. and Vierkotter, S. A. "The Block-Siegert Shift in Solid State ¹H Decoupled ¹⁹F MAS NMR: Correct Chemical Shift Referencing and Determination of the Strength and Homogeneity of Proton H₁ Fields," 26th Southeastern Magnetic Resonance Conference, Chapel Hill, NC, Oct. 23-35, 1994.

Hagaman, E. W. and Lee, S-K. "Investigation of Oxygen Functional Groups in Low Rank Coal," in *Proc., 7th International Conference on Coal Science*, Banff, Alberta, Canada, Sept. 12-17, 1993, p. 481.

Hagaman, E. W. and Lee, S-K. "Introduction of Fluorine into Coals Using N-Fluorobenzene-sulfonimide," American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Hagaman, E. W. and Lee, S-K. "A Chemical And Solid State ¹⁹F NMR Study of the Fluorination of Poly(methacrylic Acid) and Poly(4-Vinylbenzoic Acid)" 11th Winter Fluorine Conference, St. Petersburg Beach, Florida, January 25-30, 1993.

Hagaman, E. W. "Structure Analysis of Fluorinated Organic Solids Using the ¹⁹F-¹³C Dipolar Interaction: Ramifications of ¹⁹F Magnetization Diffusion," 25th Southeastern Magnetic Resonance Conference, Gainesville, FL, Oct. 29-30, 1993.

Hagaman, E. W. "Substructure Analysis by Solid State ¹H-¹³C-¹⁹F Double Cross Polarization ¹³C CP/MAS NMR," National American Chemical Society Meeting, Chicago, Illinois, August 22-26, 1993.

Hagaman, E. W. "¹³C-¹⁹F Dipolar Dephasing in Monofluorinated Organic Substances," 35th Rocky Mountain Conference on Analytical Chemistry, Denver, CO, July 25-29, 1993.

Hagaman, E. W. and Gakh, A. "Solid State ^{19}F - ^{13}C CP/MAS ^{13}C NMR Study of Polyfluorinated C_{60} ," 36th Rocky Mountain Conference on Analytical Spectroscopy, Denver, Colorado, July 3, 1994.

Hettich, R. L., Jin, C., Britt, P. F., Hauffler, R. and Compton, R. N. "Preparation and Structural Characterization of Modified Fullerenes," Fullerenes '93 Meeting, Santa Barbara, CA, June 28-July 1, 1993.

Hettich, R. L., Jin, C., Britt, P. F., Tuinman, A. A. and Compton, R. N. "Ionic Properties of Hydrogenated and Fluorinated Fullerenes" in *Proc., Materials Research Society Symposium* (1994) **349**, 133.

Ismail, K., Garcia, R., Mitchell, S. C., Snape, C. E., Buchanan, A. C., Britt, P. F., Franco, D. and Yperman, J. "Immobilized Sulphur Compounds as Solid Calibrants for TPR," in *Proc., 7th International Conference on Coal Science*, Banff, Alberta, Canada, Sept. 12-17, 1993, Vol. 2, p. 3 (1993).

Lee, S.-K. and Hagaman, E. W. "The Acid-Catalyzed Reactions of Pentamethylbenzyl Fluoride," National American Chemical Society Meeting, Washington, DC, Aug. 21-25, 1994.

Sigman, M. E. and Barbas, J. T. "Photochemistry of Substituted Naphthalenes at an SiO_2 Air Interface," Inter-American Photochemical Society Winter Conference, Clearwater Beach, FL, Jan. 2-6, 1993.

Sigman, M. E. and Dabestani, R. T. "Polynuclear Aromatic Hydrocarbon Aqueous Photochemistry: Mechanisms and Products," XVI International Conference on Photochemistry, Vancouver, Canada, Aug. 1-6, 1993.

Sigman, M. E., Barbas, J. T. and Dabestani, R. T. "Photodecomposition of Substituted Naphthalenes at Inorganic-Oxide/Air Interfaces," American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Sigman, M. E. and Dabestani, R. T. "Direct Photolysis of Polycyclic Aromatic Hydrocarbons in Dilute Aqueous Solutions," VI Emerging Technologies in Hazardous Waste Management Meeting, Atlanta, GA, Sept. 19-21, 1994.

Sigman, M. E., Dabestani, R. T. and Barbas, J. T. "Aqueous Photochemistry of Acenaphthylene: The Role of the Hydrophobic Effect," VI Inter-American Photochemical Society Meeting, Clearwater Beach, FL, Jan. 1-5, 1994.

ORNL/UTK RESEARCH PROGRAM GROUP

Books

Guiochon, G., Shirazi, S. G. and Katti, A. M. *Fundamentals of Preparative and Nonlinear Chromatography*, Academic Press, Boston, MA, (May 1994), 709 p.

Journal Articles

Charton, F. and Guiochon, G. "Modeling of the Adsorption Behavior and the Chromatographic Band Profiles of Enantiomers on Immobilized Cellulose," *J. Chromatogr.* (1993) **630**, 21-35.

Charton, F., Bailly, M. and Guiochon, G. "Recycling in Preparative Liquid Chromatography," *J. Chromatogr. A* (1994) **687**, 13-31.

Cheng, J., Jin, Y., Xenopoulos, A., Chen, W., Wunderlich, B., Diack, M., Compton, R. N. and Guiochon, G. "Motion and Disorder in the Plastic Crystal of the C₇₀ Complex with Toluene by Solid State NMR and Thermal Analysis," *Mol. Cryst. Liq. Cryst.* (1994) **250**, 359-371.

Comel, A. and Guiochon, G. "The Chemical Composition of Mixed Wastes Analysis of the Photolysis Products of Organic Ligands," *J. Radiolog. Nucl. Chem.* (1994) **181**, 373-384.

Diack, M., Compton, R. N. and Guiochon, G. "Evaluation of Stationary Phases for the Separation of the Buckminster Fullerenes by High Performance Liquid Chromatography," *J. Chromatogr.* (1993) **639**, 129-140.

Diack, M. and Guiochon, G. "The Separation and Purification of Fullerenes by Liquid Chromatography," *Quim. Anal.* (1993) **12**, 75-82.

Dose, E. V. and Guiochon, G. "Timescales of Transient Processes in Capillary Electrophoresis," *J. Chromatogr.* (1993) **652**, 263-275.

Farkas, T., Chambers, J. Q. and Guiochon, G. "Column Efficiency and Radial Homogeneity in Liquid Chromatography," *J. Chromatogr.* (1994) **679**, 231-245.

Felinger, A. and Guiochon, G. "The Change of Pressure Drop During Large-Scale Chromatography of Viscous Samples," *Biotechnol. Progr.* (1993) **9**, 450-455.

Felinger, A. and Guiochon, G. "Comparison of Maximum Production Rates and Optimum Operating/Design Parameters in Overloaded Elution and Displacement Chromatography," *Biotechnol. Bioeng.* (1993) **41**, 134-147.

Felinger, A. and Guiochon, G. "Optimization of Economical Experimental Conditions in Preparative Chromatography," *J. Am. Inst. Chem. Eng.* (1994) **40**, 594-605.

Fornstedt, T. and Guiochon, G. "Comparison Between Experimental and Theoretical Profiles of High Concentration Elution Bands and Large System Peaks in Non-Linear Chromatography," *Anal. Chem.* (1994) **66**, 2686-93.

Fornstedt, T. and Guiochon, G. "Theoretical Study of High Concentration Elution Profiles and Large System Peaks in Nonlinear Chromatography," *Anal. Chem.* (1994) **66**, 2116-2128.

Golshan-Shirazi and Guiochon, G. "Comparative Evaluation of the Adsorption Energy Distribution Functions Obtained by Analytical and Numerical Methods," *J. Chromatogr.* (1994) **670**, 1-14.

Golshan-Shirazi, S. and Guiochon, G. "The Modeling of Preparative Liquid Chromatography," *J. Chromatogr. A* (1994) **658**, 149-172.

Guan, H. and Guiochon, G. "Study of the Overloading Properties of some C18 Silica Adsorbents in Reversed Phase Liquid Chromatography. Part II. Column Efficiency," *J. Chromatogr. A* (1994) **687**, 201-212.

Guan, H., Stanley, B. J. and Guiochon, G. "Theoretical Study of the Accuracy and Precision of the Measurement of Single Component Isotherms by the Elution by Characteristic Point (ECP) Method," *J. Chromatogr. A* (1994) **659**, 27-41.

Guan, H. and Guiochon, G. "Study of the Overloading Properties of Some C18 Silica Adsorbents in Reversed Phase Liquid Chromatography. Part I. Isotherm Study," *J. Chromatogr. A* (1994) **687**, 179-200.

Guiochon, G. "Chromatography, Today and Tomorrow," *Anal. Chim. Acta* (1993) **283**, 309-319.

Guiochon, G. and Golshan-Shirazi, S. "Retrospective on the Solution of the Ideal Model of Chromatography," *J. Chromatogr. A* (1994) **658**, 173-178.

Jacobson, S. C., Andersson, S., Allenmark, S. G. and Guiochon, G. "Estimation of the Number of Enantioselective Sites of Bovine Serum Albumin Using Frontal Chromatography," *Chirality* (1993) **5**, 513-515.

Jacobson, S. C., Felinger, A. and Guiochon, G. "Optimizing the Sample Size and the Retention Parameters to Achieve Maximum Production Rates for Enantiomers in Chromatography," *Biotechnol. Bioeng.* (1993) **40**, 1210-1217.

Jacobson, S. C., Felinger, A. and Guiochon, G. "Optimizing the Sample Size and the Reduced Velocity to Achieve Maximum Production Rates for Enantiomers," *Biotechnol. Progr.* (1993) **8**, 533-539.

Jacobson, S. C., Seidel-Morgenstern, A. and Guiochon, G. "The Study of Band Broadening in Enantio-selective Separations using Microcrystalline Cellulose Triacetate. I. The Linear Case," *J. Chromatogr.* (1993) **637**, 13-18.

Jin, Y., Xenopoulos, A., Cheng, J., Chen, W., Wunderlich, B., Diack, M., Jin, C., Hettich, R. L., Compton, R. N. and Guiochon, G. "Thermodynamic Characterization of the Plastic Crystal and Non-Plastic Crystal Phases of C₇₀," *Mol. Cryst. Liq. Cryst.* (1994) **257**, 235-250.

Levin, S., Abu-Lafi, S., Golshan-Shirazi, S. and Guiochon, G. "The Use of System Peaks for the Determination of the Distribution of Resorcinol, Catechol and Phenol in Liquid Chromatography," *J. Chromatogr. A* (1994) **679**, 213-229.

- Newburger, J., DeLange, B. and Guiochon, G. "A New Hybrid Displacement Technique for Preparative Chromatography," *J. Chromatogr. A* (1994) **684**, 1-11.
- Pyda, M., Stanley, B. J., Xie, M. and Guiochon, G. "Analysis of the Surface Heterogeneity of Unmodified and Modified Silica by Capillary Inverse Gas-Solid Chromatography at Finite Dilution," *Langmuir* (1994) **10**, 1573-1579.
- Sarker, M. and Guiochon, G. "Study of the Packing Behavior of Radial Compression Columns for Preparative Chromatography," *J. Chromatogr. A* (1994) **683**, 293-309.
- Sarker, M. and Guiochon, G. "The Packing Stability of Dynamically Compressed Preparative Chromatographic Columns," *LC-GC* (1994) **12**, 300-306.
- Seidel-Morgenstern, A. and Guiochon, G. "Thermodynamics of the Adsorption of Tröger's Base Enantiomers from Ethanol on Cellulose Triacetate," *J. Chromatogr.* (1993) **631**, 37-47.
- Seidel-Morgenstern A, Jacobson, S. C. and Guiochon, G. "The Study of Band Broadening in Enantio-selective Separations Using Microcrystalline Cellulose Triacetate. II. Frontal Analysis," *J. Chromatogr.* (1993) **637**, 19-28.
- Seidel-Morgenstern, A. and Guiochon, G. "Theoretical Study of Recycling in Preparative Chromatography," *J. Am. Inst. Chem. Eng.* (1993) **39**, 809-819.
- Seidel-Morgenstern, A. and Guiochon, G. "Determination of Adsorption Isotherms and Calculation of Elution Profiles for the Enantiomers of Troeger's Base on Microcrystalline Cellulose Triacetate," *Chem. Eng. Sci.* (1993) **48**, 2787.
- Stanley, B. J. and Guiochon, G. "Numerical Estimation of Adsorption Energy Distributions from Adsorption Isotherm Data with the Expectation-Maximization Method," *J. Phys. Chem.* (1993) **97**, 8098-8104.
- Stanley, B. J. and Guiochon, G. "Importance of the Accuracy of Experimental Data in the Nonlinear Chromatographic Determination of Adsorption Energy Distributions," *Langmuir* (1994) **10**, 4278-85.
- Yun, T. and Guiochon, G. "The Modeling of Radial Heterogeneity in Chromatographic Columns. Cylindrical Column and Ideal Model," *J. Chromatogr. A* (1994) **672**, 1-10.
- Zhong, G., Meunier, F. and Guiochon, G. "Interference Theory: Moment Solution for Two Components in Non-Equilibrium Adsorption Chromatography," *Chromatogr.* (1993) **36**, 289-292.
- Zhong, G., Meunier, F. and Guiochon, G. "Interference and Heat Effects: Moment Analysis for Two-Component Chromatography," *J. Chromatogr. A* (1994) **658**, 355-360.
- Zhong, G. and Guiochon, G. "Theoretical Analysis of Band Profiles in Nonlinear Ideal Countercurrent Chromatography," *J. Chromatogr. A* (1994) **688**, 1-23.

Zhu, J. and Guiochon, G. "The Shock Layer Thickness, A New Approach to the Study of Column Performance in Non-linear Chromatography. I. Optimum Linear Velocity in Frontal Analysis," *J. Chromatogr.* (1993) **636**, 189.

Zhu, J., Ma, Z. and Guiochon, G. "The Thickness of Shock Layers in Liquid Chromatography," *Biotechnol. Progr.* (1993) **9**, 421.

Zhu, J. and Guiochon, G. "Shock Layer Thickness and Optimum Linear Velocity in Displacement Chromatography," *J. Chromatogr. A* (1994) **659**, 15-25.

Presentations/Conference Proceedings

Jin, Y., Xenopoulos, A., Wunderlich, B., Diack, M., Guiochon, G. A. and Compton, R. N. "Thermodynamic Properties of C₇₀," American Physical Society Meeting, Seattle, WA, Mar. 22-26, 1993.

PHYSICAL AND MATERIALS CHEMISTRY SECTION

CHEMICAL SEPARATIONS GROUP

Journal Articles

Baes, C. F., Reardon, E. J. and Moyer, B. A. "Ion Interaction Model Applied to the CuSO₄-H₂SO₄-H₂O System at 25°C," *J. Phys. Chem.* (1993) **97**, 12343-12348.

Burns, J. H., Sachleben, R. A. and Davis, M. C. "Structures of Isomeric Substituted 14-Crown-4 Ethers," *Inorg. Chim. Acta* (1994) **223**, 125-130.

Chen, Z. and Sachleben, R. A. "Conformational Analysis of Substituted Dibenzo-14-Crown-4 Ethers in Solution by 1D and 2D NMR," *J. Inclusion Phenom. Mol. Recogn. Chem.* (1993) **16**, 91-95.

Chen, Z., Sachleben, R. A. and Moyer, B. A. "Dimerization Behavior of Substituted Dibenzo-14-Crown-4 Alcohols Studied by NMR Spectroscopy," *Supramolecular Chem.* (1994) **3**, 219-222.

Chen, Z. and Sachleben, R. A. "¹H and ¹³C NMR of Substituted Dibenzo-14-Crown-4 Ethers," *Magn. Reson. Chem.* (1994) **32**, 375-378.

Chen, Z. and Sachleben, R. A. "Conformational Studies of Substituted Dibenzo-14-Crown-4 Ethers: A 1-D and 2-D ¹H and ¹³C NMR Investigation," *J. Chem. Soc. Perkins Trans. 2* (1994) 537-541.

Garritty, M. L., Brown, G. M., Elbert, J. E. and Sachleben, R. A. "A New Synthetic Route to 2-(p-Nitrobenzyl)-1,4,7,10-Tetraazacyclododecane," *Tetrahedron Lett.* (1993) **34(35)**, 5531-5534.

Kruger, A. A., Alexandratos, S. D., Ciaccio, C. G. and Moyer, B. A. "Synergistic Complexation of Metal Ions with Bifunctional Interpenetrating Polymer Networks," *React. Polym.* (1994) **24**, 35-39.

Moyer, B. A., Delmau, L. H., Lumetta, G. J. and Baes, C. F. "Extraction of Mn(II) from Nitric Acid by Crown Ether-Synergized Cation Exchange: Extended Equilibrium and Infrared Analysis," *Solv. Extr. Ion Exch.* (1993) **11**, 889-922.

Moyer, B. A., Case, G. N., Alexandratos, S. D. and Kriger, A. A. "Extraction of Cu(II) from Sulfuric Acid by Macrocyclic-Synergized Cation Exchange: Comparing a Novel Impregnated Resin with Its Solvent-Extraction Analog," *Anal. Chem.* (1993) **65**, 3389-3395.

Moyer, B. A., Baes, C. F. Jr., Case, G. N., Lumetta, G. J. and Wilson, N. M. "Equilibrium Analysis of Aggregation Behavior in the Solvent Extraction of Cu(II) from Sulfuric Acid by Didodecylphthalene Sulfonic Acid," *Sep. Sci. Technol.* (1993) **28**(1-3), 81-113.

Sachleben, R. A., Davis, M. C., Bruce, J. J., Ripple, E. J., Driver, J. L. and Moyer, B. A. "An Efficient Synthesis of Lithium-Selective Extractants: Tertiary-Alkyl-14-Crown-4 Ethers," *Tetrahedron Lett.* (1993) **34**, 5373-5376.

Sloop, F. V., Brown, G. M., Foote, R. S., Jacobson, K. B. and Sachleben, R. A. "Synthesis of TESPA: An Organotin Mass Label for DNA," *Bioconjug. Chem.* (1993) **4**, 406-409.

Sloop, F. V., Brown, G. M., Sachleben, R. A., Jacobson, K. B., Garrity, M. L. and Elbert, J. E. "Metal-lurgical Labels for DNA Sequencing and Mapping," *New J. Chem.* (1994) **18**, 317-326.

Thundat, T., Allison, D. P., Warmack, R. J., Doktycz, M. J., Jacobson, K. B. and Brown, G. M. "Atomic Force Microscopy of Single- and Double-Stranded Deoxyribonucleic Acid," *J. Vac. Sci. Technol. A* (1993) **11**(4), 824.

Presentations/Conference Proceedings

Baes, C. F., Reardon, E. J. and Moyer, B. A. "Ion interaction Model Applied to the $\text{CuSO}_4\text{-H}_2\text{SO}_4\text{-H}_2\text{O}$ Systems at 25°C," 48th Annual Calorimetry Conference, Durham, NC, July 18-23, 1993.

Bonnesen, P. V., Moyer, B. A., Armstrong, V. S., Haverlock, T. J., Sachleben, R. A. and Sloop, F. V. "Removal of Technetium from Alkaline Waste Media by a New Solvent Extraction Process," Emerging Technologies in Hazardous Waste Management IV Meeting, Atlanta, GA, Sept. 19-21, 1994.

Brown, G. M., Elbert, J. E., Sloop, F. V., Doktycz, M. J., Sachleben, R. A. and Jacobson, K. B. "Luminescent Lanthanide Ions as Labels for DNA Sequencing and Mapping," Contractor-Grantee Workshop, Human Genome Program, Santa Fe, NM, Nov. 13-17, 1994.

Brown, G. M., Garrity, M. L., Elbert, J. E., Sachleben, R. A., Sloop, F. V. and Jacobson, K. B. "Luminescent Lanthanide Ion Complexes as Labels for DNA Sequencing," Human Genome Program Contractor-Grantee Workshop, Santa Fe, NM, Feb. 7-11, 1993.

Burns, J. H., Sachleben, R. A. and Moyer, B. A., "Crown Ethers as Extractants for Metal Ions: Neutral, Substituted 14-Crown-4 Ligands," First BES/DOE Separations Research Conf., Seattle, WA, Oct. 14-15, 1993.

Cavanaugh, K. L., Chen, Z., Sachleben, R. A. and Moyer, B. A. "Solvent Extraction of Li^+ Ions by Substituted 14-Crown-4 Ethers Studied by ^7Li Nuclear Magnetic Resonance Spectroscopy," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Chen, Z., Sachleben, R. A., Cavanaugh, K. L. and Moyer, B. A. "Multinuclear and Dynamic NMR Study of Li^+ and Na^+ Ion Complexation by Substituted 14-Crown-4 Ethers," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Chen, Z. and Sachleben, R. A. "Stereochemistry of Substituted Dibenzo-14-crown-4 Ethers and Their Complexes of Li^+ and Na^+ . A 1D and 2D NMR Investigation," National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Deng, Y., Burns, J. H., Sachleben, R. A. and Moyer, B. A. "Selective Solvent Extraction of Metal Ions by Crown Ethers and Beyond," Seminar at the Chinese Academy of Sciences, Beijing, China, Nov. 12, 1994.

Deng, Y., Burns, J. H., Sachleben, R. A. and Moyer, B. A. "Selective Solvent Extraction of Metal Ions by Crown Ethers and Beyond," Dalian Institute of Chemical Physics, Dalian, China, Nov. 21, 1994.

Deng, Y., Burns, J. H. and Moyer, B. A., "Interaction of a Crown Ether with Divalent First-Row Transition Metal Ions: Calorimetric, Spectroscopic, and X-ray Crystallographic Investigation," 206th American Chemical Society National Meeting, Chicago, IL, August 22-27, 1993.

Deng, Y., Burns, J. H., Sachleben, R. A. and Moyer, B. A. "Selective Solvent Extraction of Metal Ions by Crown Ethers and Beyond," Nankai University, Tianjing, China, Nov. 14, 1994.

Elbert, J. E., Brown, G. M., Garrity, M. L., Sachleben, R. A. and Sloop, F. V. "Lanthanide Complexes as Reporter Groups for DNA Sequencing," National American Chemical Society Meeting, Chicago, IL, Aug. 22-27, 1993.

Jacobson, K. B., Sachleben, R. A., Brown, G. M., Sloop, F. V., Garrity, M. L., Doktycz, M. J., Arlinghaus, H. F., Foote, R. S., Larimer, F. W., Woychik, R. P. and Thonnard, N., "Analysis of Iron, Tin and Lanthanide Labeled DNA by Resonance Ionization Spectroscopy (RIS) for Genome Mapping and Sequencing," DOE Contractor-Grantee Workshop III, Human Genome Program, Santa Fe, NM, Feb. 7-13, 1993.

Moyer, B. A., Baes, C. F., Bryan, S. A., Burns, J. H., Case, G. N., Lumetta, G. J., McDowell, W. J. and Sachleben, R. A. "Developing New Chemical Tools for Solvent Extraction," in *Proc., 1st Hanford Separation Science Workshop*, Richland, WA, July 23-25, 1991; Report PNL-SA-21775, Pacific Northwest Laboratory, Richland, WA (May 1993) pp. II.39-II.45.

Moyer, B. A., Case, G. N., Delmau, L. H., Bajo, S. and Baes, C. F. "Comprehensive Equilibrium Analysis of the Complexation of Cu(II) by Tetrathia-14-Crown-4 in a Synergistic Extraction System Employing Didodecyl-naphthalene Sulfonic Acid," 8th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN, Oct. 24-28, 1993.

Moyer, B. A., Sachleben, R. A. and Case, G. N. "Synergism in the Extraction of Cu(II) by Polydentate Thia Ligands Combined with Didodecyl-naphthalene Sulfonic Acid," in *Proc., International Solvent Extraction Conference*, York, England, Sept. 9-12, 1993, D. H. Logsdail and M. J. Slater, eds., Vol. 1, pp. 525-532, Society for Chemical Industry, London (1993).

Moyer, B. A., Burns, J. H. and Sachleben, R. A. "Understanding the Behavior of Crown Ethers in Solvent Extraction," 1st BES/DOE Separations Conference, Seattle, WA, Oct. 14-15, 1993.

Moyer, B. A. and Baes, C. F. "Understanding Solvent Extraction of Metal Ions with the Aid of a Computer: Equilibrium Analysis of Two Illustrative Systems," International Symposium on Metal Ions in Solution, Malelane, South Africa, Apr. 21-23, 1993.

Moyer, B. A. "Oak Ridge National Laboratory: Past, Present, and Future Directions in Technology," Atomic Energy Corporation of South Africa, Pretoria, South Africa, April 14, 1993.

Moyer, B. A. "Investigating Crown Ethers as Selective Extractants for Metal Ions," Department of Chemistry, University of Natal, Durban, Republic of South Africa, Apr. 28, 1993.

Moyer, B. A. "Investigating Crown Ethers as Selective Extractants for Metal Ions," Department of Chemistry, University of Port Elizabeth, Port Elizabeth, South Africa, Apr. 27, 1993.

Moyer, B. A. "Investigating Crown Ethers as Selective Extractants for Metal Ions," JCI Minerals Processing Research Laboratories, Randburg, South Africa, April 16, 1993.

Moyer, B. A., Sachleben, R. A. and Burns, J. H. "Binding and Extraction of Alkali Metal Cations by Neutral and Ionizable Crown Ethers," Department of Chemistry, University of the Witwatersrand, Johannesburg, South Africa, April 15, 1993.

Moyer, B. A., Sachleben, R. A., Sun, Y., Driver, J. L., Chen, Z. and Cavanaugh, K. L. "Thermodynamic Aspects of the Solvent Extractions of Lithium Salts by Highly Alkylated 14-Crown-4 Ethers," XIX International Symposium on Macrocyclic Chemistry, Lawrence, KS, June 12-17, 1994.

Moyer, B. A., Bonnesen, P. V., Sachleben, R. A., Armstrong, V. S., Haverlock, T. J. and Sloop, F. V. "Exploring the Potential of Crown Ethers for Removing Technetium from Alkaline Waste," Separation Science and Technology Seminar, Battelle Pacific Northwest Laboratories, Richland, WA, July 15, 1994.

Moyer, B. A., Bonnesen, P. V. and Sachleben, R. A. "Alkaline-Side Extraction of Technetium from Tank Waste Using Crown Ethers and Other Extractants," Technical Exchange Meeting of the U.S. DOE Efficient Separations and Processes Integrated Program, Dallas/Fort Worth, TX, Jan. 10-11, 1994.

Moyer, B. A., Bonnesen, P. V., Haverlock, T. J., Armstrong, V. S., Sachleben, R. A. and Sloop, F. V. "Crown Ethers as Extractants for the Removal of Technetium from Alkaline Waste," Los Alamos National Laboratory, Nov. 18, 1994.

Moyer, B. A., Armstrong, V. S., Bonnesen, P. V., Burns, J. H., Delmau, L. H., Haverlock, T. J., Sachleben, R. A. and Sloop, F. V. "Investigating the Solvent Extraction of Technetium(VII) from Alkaline Sodium Nitrate by Crown Ethers," 3rd Nuclear Energy Agency International Information Exchange Meeting, Cadarache, France, Dec. 12-14, 1994.

Moyer, B. A., Armstrong, V. S., Bonnesen, P. V., Burns, J. H., Delmau, L. H., Haverlock, T. J., Sachleben, R. A. and Sloop, F. V. "Crown Ethers as Extractants for the Removal of Technetium from Alkaline Waste Solutions," Seminar at the Section d'Etudes et Applications des Technologies Nouvelles, Cadarache, France, Dec. 15, 1994.

Moyer, B. A. "Current Research at ORNL and Future Directions," U.S./Russian Crown Ether Workshop, Gatlinburg, TN, Aug. 19, 1994.

Moyer, B. A. "Research at ORNL on Crown Ethers," U.S./Russian Crown Ether Workshop, Gatlinburg, TN, Aug. 18, 1994.

Sachleben, R. A., Moyer, B. A., Case, F. I. and Garmon, S. A. "Alkylated Lariat Ethers As Solvent Extraction Reagents: Surveying the Extraction of Alkali Metals by Bis-(*t*-octylbenzo)-14-crown-4-acetic Acid by Potentiometric Two-Phase Titrimetry," in *Proc., 7th Symposium on Separation Science and Technology for Energy Applications*, Knoxville, TN, October 20-24, 1991, *Sep.Sci. Technol.* (1993) **28**, 1-23

Sachleben, R. A., Burns, J. H., Davis, M. C., Driver, J. L., Chen, Z., Deng, Y. and Moyer, B. A. "Recognition of Lithium Cation by Substituted 14-Crown-4 Macrocycles," National American Chemical Society Meeting, Denver, CO, Mar. 28-Apr. 2, 1993.

Sachleben, R. A., Burns, J. H. and Moyer, B. A. "Crown Ethers as Extractants for Metals Ions: Ionizable Lariat Ethers," 1st DOE/BES Separations Conference, Seattle, WA, Oct. 14-15, 1993.

Sachleben, R. A., Moyer, B. A., Case, F. I. and Driver, J. L. "Extraction of Alkali Metal Cations Using a Lipophilic Lariat Ether Having a C-pivot Carboxylic Acid Sidearm," in *Proc., International Solvent Extraction Conference*, York, England, Sept. 9-15, 1993, D. H. Logsdail and M. J. Slater, eds., Vol. 2, pp. 737-744, Society for Chemical Industry, London (1993).

Sachleben, R. A., Moyer, B. A. and Driver, J. L. "Extraction of Alkali Cations by Lipophilic Dibenzo-14-crown-4-Carboxylic Acids," 8th Symposium on Separations Science and Technology, Gatlinburg, TN, Oct. 17-21, 1993.

Sun, Y., Brown, G. M. and Moyer, B. A. "Application of Separation and TiO₂-Mediated Photodegradation to the Treatment of Waste Streams Containing Trichloroethylene," 8th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN, Oct. 24-28, 1993.

Sun, Y., Brown, G. M. and Moyer, B. A. "Semiconductor Catalyzed Photooxidation of Hazardous Chemicals in Mixed-Waste Streams," Science and Technology Alliance Solar Photocatalytic Detoxification Symposium, Sandia National Laboratory, Albuquerque, NM, Aug. 5, 1993.

Sun, Y., Brown, G. M. and Moyer, B. A. "Photodegradation of Trichloroethylene Using TiO_2 Suspended in Fluorocarbon Solvents," National American Chemical Society Meeting, San Diego, CA, Mar. 13-18, 1994.

Other

Moyer, B. A. and Sachleben, R. A. "Improved Method for Extracting Copper, Silver, and Related Metals," Patent Application, Martin Marietta Energy Systems, Inc., (March 28, 1993).

Moyer, B. A., Sachleben, R. A. and Bonnesen, P. V. "Process for Extracting Technetium from Alkaline Solutions," Patent Application, U.S. Department of Energy (July 1994).

GEOCHEMISTRY GROUP

Books/Book Chapters

Bell, J. L. S. and Palmer, D. A. "Experimental Studies of Organic Acid Decomposition," in *The Role of Organic Acids in Geological Processes*, M. D. Lewan and E. D. Pittman, eds., Springer-Verlag, (1994), pp. 226-269.

Journal Articles

Anovitz, L. M., Blencoe, J. G., Joyce, D. B. and Burch, T. E. "Thermodynamic Re-Analysis of the Dry Fusion of High Albite," *EOS* (1994) **75**, 693.

Bell, J. L. S., Wesolowski, D. J. and Palmer, D. A. "The Dissociation Quotient of Formic Acid in Sodium Chloride Solutions to 200°C," *J. Solution Chem.* (1993) **22**, 125-136.

Bell, J. L. S., Palmer, D. A., Barnes, H. L. and Drummond, S. E. "Thermal Decomposition of Acetate. Part III. Catalysis by Mineral Surfaces," *Geochim. Cosmochim. Acta* (1994) **58**, 4155-4177.

Blencoe, J. G. "Calculated Activities for Species in Albite-Water Melts," *Mineral Mag.*, (1994) **58A**, 97-98.

Blencoe, J. G., Anovitz, L. M., Joyce, D. B. and Burch, T. E. "A New Thermodynamic Model for Albite-Water Melts," *EOS* (1994) **75**, 693.

Blencoe, J. G., Guidotti, C. V. and Sassi, F. P. "The Paragonite-Muscovite Solvus: II. Numerical Geothermometers for Natural Quasibinary Paragonite-Muscovite Pairs," *Geochim. Cosmochim. Acta* (1994) **58**, 2277-2288.

- Burch, T. E. and Cole, D. R., "Stable Isotope Kinetics in the System Calcite $\pm$ CO₂ $\pm$ H₂O to 700°C, 1000 Bar: The Effect of Fluid Composition," *Min. Mag.* (1994) **58A**, 132-133.
- Cole, D. R. "Evidence for Oxygen Isotope Disequilibrium in Selected Geothermal and Hydrothermal Ore Deposit Systems," *Chem. Geol.* (1994) **111**, 283-296.
- Cole, D. R. "Oxygen Isotope Exchange Rates in Mineral-Fluid Systems: Correlations and Predictions," *Mineral Mag.* (1994) **58A**, 189-190.
- Cole, D. R. and Monger, H. C. "Influence of Atmospheric CO₂ on the Decline of C₄ Plants During the Last Deglaciation," *Nature* (1994) **368**, 533-536.
- Drummond, M. S., Allison, D. T. and Wesolowski, D. J. "Igneous Petrogenesis and Tectonic Setting of the Elkahatchee Quartz Diorite, Alabama Appalachians: Implications for Penobscotian Magmatism in the Eastern Blue Ridge," *Am. J. Sci.* (1994) **294**, 173-236.
- Dunbar, N. W., Riciputi, L. R., Jacobs, G. K., Naney, M. T. and Christie, W. H. "Generation of Rhyolitic Melt in a Man-Made Magma: Implications for Fractional Crystallization Processes in Natural Magmas," *J. Volcanol. Geotherm. Res.* (1993) **57**, 157-166.
- Feiss, P. G., Vance, R. K. and Wesolowski, D. J. "Volcanic Rock-Hosted Gold and Base-Metal Mineralization Associated with Neoproterozoic-Early Paleozoic Back-Arc Extension in the Carolina Terrane, Southern Appalachian Piedmont," *Geol.* (1993) **21**, 439-442.
- Guidotti, C. V., Sassi, F. P., Blencoe, J. G. and Selverstone, J. "The Paragonite-Muscovite Solvus: I. P-T-X Limits Derived from the Na-K Compositions of Natural, Quasibinary Paragonite-Muscovite Pairs," *Geochim. Cosmochim. Acta* (1994) **58**, 2269-2275.
- Horita, J. and Wesolowski, D. J. "Liquid-Vapor Fractionation of Oxygen and Hydrogen Isotopes of Water from the Freezing to the Critical Temperature," *Geochim. Cosmochim. Acta* (1994) **58**, 3425-3437.
- Horita, J., Cole, D. R. and Wesolowski, D. J. "The Activity-Composition Relationship of Oxygen and Hydrogen Isotopes in Aqueous Salt Solutions. II: Vapor-Liquid Water Equilibration of Mixed Salt Solutions from 50 to 100°C and Geochemical Implications," *Geochim. Cosmochim. Acta* (1993) **57**, 4703-4711.
- Horita, J., Wesolowski, D. J. and Cole, D. R. "The Activity-Composition Relationship of Oxygen and Hydrogen Isotopes in Aqueous Salt Solutions. I: Vapor-Liquid Water Equilibration of Single Salt Solutions from 50 to 100°C," *Geochim. Cosmochim. Acta* (1993) **57**, 2797-2817.
- Jin, C., Hettich, R. L., Compton, R. N., Joyce, D. B., Blencoe, J. G. and Burch, T. E. "Direct Solid Phase Hydrogenation of Fullerenes," *J. Phys. Chem.* (1994) **98**, 4215-4217.
- Joyce, D. B. and Blencoe, J. G. "Excess Molar Free Energies for {xH₂O + (1-x)CO₂} at Temperatures from 673 K to 973 K, at the Pressure 50 MPa," *J. Chem. Thermodynam.* (1994) **26**, 765-777.

- Joyce, D. B. and Holloway, J. R. "An Experimental Determination of the Thermodynamic Properties of $\text{H}_2\text{O}-\text{CO}_2-\text{NaCl}$ Fluids at High Pressures and Temperatures," *Geochim. Cosmochim. Acta* (1993) **57**, 733-746.
- Joyce, D. B. and Voigt, D. E. "A Phase Equilibrium Study in the System $\text{KA1Si}_3\text{O}_8-\text{SiO}_2-\text{Al}_2\text{SiO}_5-\text{H}_2\text{O}$ at 2 kbar and Petrogenetic Implications," *Am. Mineral.* (1994) **79**, 504-512.
- Machesky, M. L., Palmer, D. A. and Wesolowski, D. J. "Hydrogen Ion Adsorption at the Rutile-Water Interface to 250°C," *Geochim. Cosmochim. Acta* (1994) **58**, 5627-5632.
- Mack, G. H., Cole, D. R., James, W. C., Giordano, T. H. and Salyards, S. "Stable Oxygen and Carbon Isotopes of Pedogenic Carbonate as Indicators of Plio-Pleistocene Paleoclimate in the Southern Rio Grande Rift, South-Central New Mexico," *Am. J. Sci.* (1994) **294**, 621-640.
- Monger, H. C. and Cole, D. R. "Stable Isotopes in Arid Paleosols of Southern New Mexico, as Indicators of Climate Change and the Effects of Atmospheric CO_2 on Plant Communities," *Trans., 15th World Congress of Soil Science 5b, International Society of Soil Science* (1994) 224-225.
- Monger, H. C. and Cole, D. R. "Climate, CO_2 and Plant Abundance-Reply," *Mineral Mag.* (1994) **58A**, 770-771.
- Palmer, D. A. and Wesolowski, D. J. "Aluminum Speciation and Equilibria in Aqueous Solution, Part III. Potentiometric Determination of the Formation Constants of $\text{Al}(\text{OH})^{2+}$ in 0-5 Molal NaCl Solutions from 25 to 125°C," *Geochim. Cosmochim. Acta* (1993) **57**, 2929-2938.
- Palmer, D. A. and Bell, J. L. S. "Aluminum Speciation and Equilibria in Aqueous Solution. Part IV. A Potentiometric Study of Aluminum Acetate Complexation in Acidic NaCl Brines to 150°C," *Geochim. Cosmochim. Acta* (1994) **58**, 651-659.
- Pasteris, J. D., Seitz, J. C., Morgan, G. B. and Wopenka, B. " CH_4 -rich Inclusions from Quartz Veins in the Valley and Ridge Province and Anthracite Fields of the Pennsylvania Appalachians--Discussion," *Am. Mineral.* (1993) **78**, 216-219.
- Riciputi, L. R., Christie, W. H., Cole, D. R. and Rosseel, T. M. "Analysis of Rare Earth Elements in Silicates by Ion Microprobe Using Doubly-Charged Ions," *Anal. Chem.* (1993) **65**, 1186-1191.
- Riciputi, L. R. and Paterson, B. A. "High Spatial-Resolution Measurement of O Isotope Ratios in Silicates and Carbonates by Ion Microprobe," *Am. Mineral.* (1994) **79**, 1227-1230.
- Riciputi, L. R. and Paterson, B. A. "In-situ Analysis of Oxygen Isotope Ratios in Silicates and Carbonates by Ion Microprobe," *Mineral Mag.* (1994) **58A**, 770-771.
- Riciputi, L. R., Machel, H. G. and Cole, D. R. "Ion Microprobe Studies of Diagenetic Carbonates in the Devonian Nisku Formation of Alberta, Canada," *J. Sediment. Petrol.* (1994) **A64**, 115-127.

Riciputi, L. R., McSween, H. Y., Johnson, C. A. and Prinz, M. "Minor and Trace Element Concentrations in Carbonates of Carbonaceous Chondrites, and Implications for the Compositions of Coexisting Fluids," *Geochim. Cosmochim. Acta* (1994) **58**, 1343-1351.

Seitz, J. C., Pasteris, J. D. and Morgan, G. B. "Quantitative Analysis of Mixed Volatile Fluids by Raman Microprobe Spectroscopy: A Cautionary Note on Spectral Resolution and Peak Shape," *Appl. Spectrosc.* (1993) **47**, 816-820.

Seitz, J. C., Blencoe, J. G. and Bodnar, R. J. "Experimentally Determined Volumetric Properties of CO₂-CH₄ Mixtures at 100-1000 Bars and 50-300°C," *Geol. Soc. Amer. Abstracts with Programs* (1993) **25**, A-212—A-213.

Seitz, J. C., Pasteris, J. D. and Chou, I-M. "Raman Spectroscopic Characterization of Gas Mixtures. I. Quantitative Composition and Pressure Determination of CH₄, N₂, and Their Mixtures," *Am. J. Sci.* (1993) **293**, 297-321.

Seitz, J. C., Blencoe, J. G. and Bodnar, R. J. "Experimentally Determined Volumetric Properties of CO₂-CH₄, CO₂-N₂, and CH₄-N₂ Mixtures at 100-1000 Bars and 50-300°C," *EOS, Trans. Am. Geophys. Union* (1994) **75**, 136-137.

Seitz, J. C., Blencoe, J. G., Joyce, D. B. and Bodnar, R. J. "Volumetric Properties of CO₂-CH₄-N₂ Fluids at 200°C and 1000 Bars: A Comparison of Equations of State and Experimental Data," *Geochim. Cosmochim. Acta* (1994) **58**, 1065-1071.

Wesolowski, D. J. and Palmer, D. A. "Aluminum Speciation and Equilibria in Aqueous Solution. Part V. Gibbsite Solubility at 50°C and pH 3 to 9 in 0.1 molal NaCl Solutions, A General Model for Aluminum Speciation, and Analytical Methods," *Geochim. Cosmochim. Acta* (1994) **58**, 2947-2969.

Presentations/Conference Proceedings

Blencoe, J. G. and Joyce, D. B. "Thermodynamic Analysis of Volumetric Data for Near-Critical and Supercritical H₂O-CO₂ Fluids," *EOS, Trans., American Geophysical Union, Spring American Geophysical Union Meeting*, Baltimore, MD, May 23-26, 1994, Vol. 75, p. 135 (1994).

Blencoe, J. G., Drummond, S. E., Seitz, J. C. and Nesbitt, B. E. "A Vibrating-Tube Densimeter for Fluids at High Pressures and Temperatures," *Program, 12th Symposium on Thermophysical Properties* (1994).

Burch, T. E. and Cole, D. R. "Stable Isotope Exchange Kinetics in the System Calcite±CO₂±H₂O to 700°C, 1000 Bars: The Effect of Fluid Composition," V. M. Goldschmidt Conference, Edinburgh, Scotland, *Mineral Mag.* (1994) **58A**, 132.

Cole, D. R., Riciputi, L. R. and Machel, H. G. "Stable Isotope Systematics During Burial Diagenesis in the Alberta Deep Basin: An Ion Microprobe Study," DOE/BES/Geosciences Program Workshop on Experimental and Analytical Geochemistry, California Institute of Technology, Jan. 14-15, 1993.

Cole, D. R., Riciputi, L. R. and Machel, H. G. "An Ion Microprobe Study of Sulfur Isotope Variability in Pyrites from Devonian Carbonates, Western Canada Sedimentary Basin, Alberta, Canada," in *Proc., Meeting of the European Union of Geosciences*, Strasbourg, France, Terra Nova, Vol. 5, p. 369 (1993).

Cole, D. R. "Applications of Stable Isotope Geothermometry and Speedometry to Hydrothermal Systems: Progress, Problems and Prospects," Gordon Research Conference on Inorganic Geochemistry of Hydrothermal Ore Deposits, Tilton School, Tilton, NH, Aug. 16-20, 1993.

Cole, D. R. "Stable Isotope Systematics of Fluid/Rock Interaction," DOE/BES/Geosciences Program Workshop on Sedimentary Systems, Aqueous and Organic Geochemistry, Lawrence Berkeley Laboratory, July 15-16, 1993.

Cole, D. R. "Oxygen Isotope Exchange Rates in Mineral-Fluid Systems: Correlations and Predictions," V. M. Goldschmidt Conference, Edinburgh, Scotland, *Mineral Mag.* (1994) 58A, 189.

Cole, D. R. "Ion Microprobe Studies of Diagenesis: Sulfur Isotope Variations in the Western Canada Sedimentary Basin," Gordon Research Conference on Inorganic Geochemistry of Hydrothermal Ore Deposits, Tilton School, Tilton, NH, Aug. 16-20, 1993.

Horita, J. and Wesolowski, D. J. "Liquid-Vapor Partitioning of Oxygen and Hydrogen Isotopes of Water to 350°C," Geological Society of America abstracts with program, Vol. 25, p. A438 (1993).

Horita, J., Wesolowski, D. J. and Cole, D. R. "D/H and $^{18}\text{O}/^{16}\text{O}$ Partitioning Between Water Liquid and Vapor in the System $\text{H}_2\text{O}-\text{Na}-\text{K}-\text{Ca}-\text{Mg}-\text{Cl}-\text{SO}_4$ from 0 to 350°C," in *Proc., 12th International Conference on the Properties of Water and Steam*, Orlando, FL, Sept. 11-16, 1994 (in press).

Horita, J., Cole, D. R. and Wesolowski, D. J. "Salt Effects on Stable Isotope Partitioning and Their Geochemical Implications for Geothermal Brines," in *Proc., 19th Workshop on Geothermal Reservoir Engineering*, Stanford, CA, Jan. 18-20, 1994, p. 285-290.

Horita, J., Cole, D. R. and Wesolowski, D. J. "Salt Effects on Stable Isotope Partitioning Between Brines, Vapor and Minerals at Elevated Temperatures," Abstracts of 8th International Conference on Geochronology, Cosmochronology, and Isotope Geology, Berkeley, CA, June 5-14, 1994, U.S. Geological Survey Circular 1107, M. A. Lanphere, G. B. Dalrymple and B. D. Turrin, eds., p. 143.

Joyce, D. B. and Blencoe, J. G. "Chemical Techniques for Measuring and Controlling the Thermodynamic Properties of Aqueous Fluids at High Pressures and Temperatures," *Program, 12th Symposium on Thermophysical Properties* (1994).

Joyce, D. B., Blencoe, J. G. and Burch, T. E. "A Least-Squares G^{ex} Model for $\text{H}_2\text{O}-\text{CO}_2$ Fluids at $1 < P < 10,000$ Bar and $T > 100^\circ\text{C}$," *EOS, Trans., American Geophysical Union Spring Meeting*, Baltimore, MD, May 23-26, 1994, Vol. 75, p. 135 (1994).

Joyce, D. B., Blencoe, J. G., Burch, T. E. and Holloway, J. R. "A Two-Parameter Margules Method for Modeling the Thermodynamic Mixing Properties of H_2O - CO_2 Fluids," in *Proc., Annual Geological Society of America Meeting*, Boston, MA, Oct. 25-28, 1993, Vol. 25, p. A-212 (1993).

Kettler, R. M., Palmer, D. A. and Wesolowski, D. J. "Dissociation Quotients of Malonic Acid in Aqueous Sodium Chloride Media to 100°C," in *Proc., 1991 Symposium on Chemistry in High Temperature Aqueous Solutions*, Palo Alto, California, Electric Power Research Institute (EPRI) Report TR-10276, B2g-1 to B2g-19, R. M. Izatt, J. L. Oscarson, and S. E. Gillespie, eds. (1993).

Land, L. S., Eustice, R. A., Mack, L. E. and Horita, J. "Reactivity of Evaporites During Burial: An Example from the Jurassic of Alabama," GSA abstract with program, Vol. 26, p. A-220 (1994).

Monger, H. C. and Cole, D. R. "Stable Carbon and Oxygen Isotopes of Carbonates as Paleoenvironmental Indicators in Arid Regions," Agronomy Abstracts, American Society of Agriculture, Madison, WI, Soil Sciences Society of America Meeting, Seattle, WA, 1994.

Monger, H. C., Cole, D. R. and Glish, J. W. "A Major Desertification Episode Beginning About 8,000 Years Ago in the Chihuahuan Desert of Southern New Mexico and West Texas," Abstracts of the International Symposium and Workshop on Desertification in Developed Countries: Why Can't We Control It? U.S. Bureau of Land Management, Tucson, AZ, Oct. 24-29, 1994.

Monger, H. C. and Cole, D. R. "Isotopic Evidence of Holocene and Pleistocene Paleoenvironments in the Chihuahuan Desert, USA," 8th International Conference on Geochronology, Cosmochronology and Isotope Geology, Berkeley, CA, June 5-14, U.S. Geological Survey Circular 1107, p. 223 (1994).

Monger, C. H. and Cole, D. R. "Paleosols as Indicators of Paleoclimatic Conditions," INQUA/ISSA Paleopedology Commission Newsletter No. 9, Illinois State Geological Survey, Champaign, IL, p. 24 (1993).

Palmer, D. A. and Wesolowski, D. J. "High Temperature Potentiometric Measurements of Hydrolysis and Metal Complexation Reactions," 4th International Symposium on Hydrothermal Reactions, Nancy, France, August 31-September 3, 1993.

Palmer, D. A. and Drummond, S. E. "An Experimental Study of the Solubility of Magnetite in Sodium Acetate Solutions," in *Proc., International Conference on Interaction of Iron Based Materials with Water and Steam*, EPRI Book TR-102101, B. Dooley and A. Bursik, eds., (1993).

Palmer, D. A., Wesolowski, D. J. and Bell, J. L. S. "EMF Measurements of Oxalic and Formic Acid Decomposition Kinetics and Interaction of Acetate with Aluminum(III) to High Temperatures," *EOS, Trans. American Geophysical Union Annual Meeting*, Baltimore, MD, May 23-27, 1993, Vol. 74, No. 16, pp. 327-328.

Palmer, D. A., Wesolowski, D. J. and Mesmer, R. E. "The Hydrogen-Electrode Concentration Cell as a Sensitive Tool in High Temperature Aqueous Chemistry," 208th American Chemical Society National Meeting, Washington, D.C., Aug. 1994.

Palmer, D. A., Wesolowski, D. J. and Bell, J. L. S. "High Temperature Potentiometric Measurements of Hydrolysis and Metal Complexation Reactions," Symposium on Properties of Aqueous Solutions, Theory and Applications, Annual Meeting of International Association for the Properties of Water and Steam, Milan, Italy, Sept. 15, 1993.

Paterson, B. A., McSween, H. Y. and Riciputi, L. R. "High Spatial Resolution Sulfur Isotopic Analysis of Troilite in Ordinary Chondrites by Ion Microprobe," in *Proc., 25th Lunar and Planetary Science Conference*, p. 1057-1058 (1994).

Riciputi, L. R., Cole, D. R. and Machel, H. G. "Sulfur Isotope Variations in Devonian Carbonates of the Western Canada Sedimentary Basin, Alberta, Canada: An Ion Microprobe Study," Geological Society Annual Meeting., Abstract with programs, Vol. 25, No. 6, p. A-162 (1993).

Riciputi, L. R., Paterson, B., Cole, D. R. and Machel, H. G. "Ion Microprobe Investigations of $\delta^{34}\text{S}$ Variability in Sulfides from the Obed Sour Gas Reservoir, Alberta, Canada," SEPM Symposium on Basin-Wide Diagenetic Patterns: Integrated Petrologic, Geochemical, and Hydrologic Considerations, Lake Ozark, MO, May 21-25, 1994.

Snyder, G. A., Taylor, L. A., Jerde, E. A. and Riciputi, L. R. "Evolved QMD Parentage for Lunar Highlands Alkali Suite Cumulates: Evidence from Ion-Probe Rare-Earth Element Analyses of Individual Minerals," in *Proc., 25th Lunar and Planetary Science Conference*, p. 1311-1312 (1994).

Wesolowski, D. J. "Fluid-Rock Interactions in the Earth's Crust: Geochemistry Related to Energy Technologies," Showcase Series Lecture, Oak Ridge, TN, Jan. 15, 1993.

Wesolowski, D. J. and Palmer, D. A. "EMF Measurements of the Hydrolysis of Mg^{2+} in 0.1 to 5.0 molal NaCl Solutions from 1 to 250°C," *EOS, Trans., American Geophysical Union Annual Meeting*, Baltimore, MD, May 23-27, 1993, Vol. 74, No. 16, p. 323.

Thesis

Seitz, J. C. "Experimental Determination of the Volumetric Properties for the System $\text{CO}_2\text{-CH}_4\text{-N}_2$ at 100-1000 Bars and 50-300°C," *Ph.D. Thesis*, Virginia Polytechnic Institute and State University (1994).

HIGH TEMPERATURE AQUEOUS CHEMISTRY GROUP

Books/Book Chapters

Bell, J. L. S. and Palmer, D. A. "Experimental Studies of Decomposition of Organic Acid Anions," in *The Role of Organic Acids in Geological Processes*, Chapter 9, M. D. Lewan and E. D. Pittman, eds., Springer-Verlag (1994) pp. 226-269.

Simonson, J. M. and Mesmer, R. E. "Calorimetry of Electrolyte Solutions at High Temperatures and Pressures," in *Experimental Thermodynamics*, K. N. Marsh and P. A. G. O'Hare, eds., Blackwell Publishers (1994).

Journal Articles

Bell, J. L. S., Wesolowski, D. J. and Palmer, D. A. "The Dissociation Quotients of Formic Acid in Sodium Chloride Solutions to 200°C," *J. Solution Chem.* (1993) **22**(2), 125-136.

Bell, J. L. S., Palmer, D. A., Barnes, H. B. and Drummond, S. E. "Thermal Decomposition of Acetate. Part III. Catalysis and Oxidation by Mineral Surfaces," *Geochim. Cosmochim. Acta* (1994) **58**, 4155-4177.

Ho, P. C., Palmer, D. A. and Mesmer, R. E. "Electrical Conductivity Measurements of Aqueous Sodium Chloride Solutions to 600°C and 300 MPa," *J. Solution Chem.* (1994) **23**, 997-1017.

Holmes, H. F., Busey, R. H., Simonson, J. M. and Mesmer, R. E. "CaCl₂(aq) at Elevated Temperatures, Enthalpies of Dilution, Isopiestic Molalities, and Thermodynamic Properties," *J. Chem. Thermodyn.* (1994) **26**, 271.

Holmes, H. F. and Mesmer, R. E. "An Isopiestic Study of {(1-y)NaHSO₄+yNa₂SO₄}(aq) at Elevated Temperatures," *J. Chem. Thermodyn.* (1994) **26**, 581.

Machesky, M. L., Palmer, D. A. and Wesolowski, D. J. "Hydrogen Ion Binding at the Rutile-Water Interface to 250°C," *Geochim. Cosmochim. Acta* (1994) **58**, 5627-5632.

Oakes, C. S., Bodnar, R. J., Simonson, J. M. and Pitzer, K. S. "Critical and Supercritical Properties of 0.3 to 3.0 mol·kg⁻¹ CaCl₂(aq)," *Geochim. Cosmochim. Acta* (1994) **58**, 2421.

Palmer, D. A. and Wesolowski, D. J. "Aluminum Speciation and Equilibria in Aqueous Solution. III. Potentiometric Determination of the First Hydrolysis Constant of Aluminum(III) in Sodium Chloride Solutions to 125°C," *Geochim. Cosmochim. Acta* (1993) **57**(13), 2929-2938.

Palmer, D. A. and Simonson, J. M. "The Volatility of Ammonium Chloride over Aqueous Solutions to High Temperatures," *J. Chem. Eng. Data* (1993) **38**, 465-474.

Palmer, D. A., Begun, G. M. and Ward, F. H. "A Micro-Raman Cell for Studying Aqueous Solutions at High Temperatures and Pressures," *Rev. Sci. Instrum.* (1993) **64**(7), 1994-1998.

Palmer, D. A. and Bell, J. L. S. "Aluminum Speciation and Equilibria in Aqueous Solution: IV. A Potentiometric Study of Aluminum Acetate Complexation in Acidic NaCl Brines to 150°C," *Geochim. Cosmochim. Acta* (1994) **58**, 651-659.

Simonson, J. M. and Palmer, D. A. "Vapor-Liquid Equilibrium of Chlorides in Aqueous Systems to High Temperatures: Application to the Geysers Geothermal Field," *Geothermal Resources Council Trans.* (1994) **18**, 347-352.

Simonson, J. M., Oakes, C. S. and Bodnar, R. J. "Densities of NaCl(aq) to 523 K and 40 MPa Measured with a New Vibrating-Tube Densimeter," *J. Chem. Thermodyn.* (1994) 26, 345.

Wesolowski, D. J. and Palmer, D. A. "Aluminum Speciation and Equilibria in Aqueous Solution. V. The Solubility of Gibbsite at 50°C in 0.1 Molal NaCl Solutions at Hydrogen Ion Concentrations of 10^{-3} to 10^{-9} Molal," *Geochim. Cosmochim. Acta* (1994) 58, 2947-2969.

Presentations/Conference Proceedings

Bell, J. L. S., Palmer, D. A., Barnes, H. L. and Drummond, S. E. "Decomposition to Acetic Acid on Iron Oxide Surfaces," National American Chemical Society Meeting, Denver, CO, Mar. 28-Apr. 2, 1993.

Bloomington, G. F., Simonson, J. M., Moore, R. C., Cochran, H. D. and Mesmer, R. E. "Aqueous Electrolyte Modeling of ASPEN PLUS," 12th International Conference on the Properties of Water and Steam, Orlando, FL, September 11-16, 1994.

Carter, R. W., Palmer, D. A. and Simonson, J. M. "Liquid-Vapor Partitioning of Aqueous Electrolytes," 48th Annual Calorimetry Conference, Durham, NC, July 18-23, 1993.

Corti, H. R. and Simonson, J. M. "Enthalpies of Dilution and the Thermodynamics of MgCl₂(aq) to High Temperatures," 48th Calorimetry Conference, Durham, NC, July 18-22, 1993.

Cummings, P. T., Cochran, H. D., Simonson, J. M., Mesmer, R. E. and Karaborni, S. "Simulation of Supercritical Water and of Supercritical Aqueous Solution," in *Proc., 2nd International Symposium on Chemistry in High Temperatures Aqueous Solutions*, EPRI TR-102706, B2a-1, August 1993.

Ho, P. C. and Palmer, D. A. "Electrical Conductivity Measurements of Dilute Aqueous Solutions at High Temperatures and High Pressures," in *Proc., 4th International Symposium on Hydrothermal Reactions*, Nancy, France, Aug. 31-Sept. 3, 1993, pp. 83-85.

Ho, P. C. and Palmer, D. A. "Electrical Conductivity Measurements of Aqueous Electrolyte Solutions at High Temperatures and High Pressures," 49th Calorimetry Conference, Santa Fe, New Mexico, July 1994.

Ho, P. C. and Palmer, D. A. "Electrical Conductivity Measurements of Aqueous Electrolyte Solutions at High Temperatures and High Pressures," 12th International Conference on the Properties of Water and Steam, Orlando, FL, Sept. 11-16, 1994.

Holmes, H. F. and Mesmer, R. E. "Mixing Effects in Aqueous Solutions at Elevated Temperatures," in *Journal Chem. and Proceedings, 2nd International Symposium on Chemistry in High Temperatures Aqueous Solutions*, EPRI TR-10276, August 1993.

Holmes, H. F. and Mesmer, R. E. "An Isopiestic Study of [Na(HSO₄,SO₄)](aq) at Elevated Temperatures," 48th Annual Calorimetry Conference, Duke University, Durham, NC, July 18-23, 1993.

Holmes, H. F. and Mesmer, R. E. "Thermodynamics of Aqueous Alkali Metal Bisulfates to 225°C by the Isopiestic Technique," 13th International Union of Pure and Applied Chemistry Conference on Chemical Thermodynamics, Clermond-Ferrand, France, July 17-22, 1994.

Holmes, H. F. and Mesmer, R. E. "Thermodynamics of Aqueous Electrolytes at High Temperatures by the Isopiestic Technique," 12th International Conference on the Properties of Water and Steam, Orlando, FL, Sept. 9-11, 1994.

Holmes, H. F. and Mesmer, R. E. "Thermodynamics of Aqueous Solutions of the Alkaline Earth Metal Chlorides to 250°C," 49th Annual Calorimetry Conference, Santa Fe, NM, July 31-Aug. 4, 1994.

Jensen, J. P., Palmer, D. A. and Simonson, J. M. "Measurements of the Volatilities of Solutes from Aqueous Solutions and their Application to Water/Steam Cycles," in *Proc., VGB Conference on Power Plant Chemistry 1994*, Essen, Germany, Oct. 26-27, 1994.

Kettler, R. M., Wesolowski, D. J. and Palmer, D. A. "Dissociation Quotients of Succinic and Benzoic Acid in Aqueous Sodium Chloride Solutions," Geological Society of America Annual Meeting, Seattle, WA, November 1994.

Mesmer, R. E. and Holmes, H. F. "pH, Definition and Measurement at High Temperatures and Pressures," in *Proc., 2nd International Symposium on Chemistry in High Temperature Aqueous Solutions*, EPRI Report, EPRI TR-10276, C36-1, August 1993.

Mesmer, R. E. "Research in High Temperature Aqueous Chemistry at ORNL," Bristol University, United Kingdom, August 13, 1993.

Mesmer, R. E., Ho, P. C., Holmes, H. F., Palmer, D. A. and Simonson, J. M. "Ion-Association: Data, Models, and Thermodynamics," National American Chemical Society Meeting, Washington, DC, Aug. 21-25, 1994.

Mesmer, R. E., Palmer, D. A. and Wesolowski, D. J. "Potentiometric Studies at ORNL with Hydrogen Electrode Concentration Cells," 12th International Conference on the Properties of Water and Steam, Orlando, FL, Sept. 11-16, 1994.

Mesmer, R. E. "Overview of Research in High Temperature Aqueous Chemistry at Oak Ridge National Laboratory," International Union of Pure and Applied Chemistry Conference on Solution Chemistry, Leicester University, United Kingdom, Aug. 15-21, 1993.

Mesmer, R. E. "Needs for Research in Aqueous Chemistry at High Temperatures and Pressures," *Proc., 2nd International Symposium on Aqueous Chemistry in High Temperature Aqueous Solutions*, EPRI TR-10276, E5a-1, August 1993.

Milioto, S. and Simonson, J. M. "Enthalpies of Dilution to High Temperatures in the System $\{(1-y)(\text{NH}_4)_2\text{SO}_4 + y \text{H}_2\text{SO}_4\}(\text{aq})$," 48th Calorimetry Conference, Durham, NC, July 18-22, 1993.

Narkhede, M. R. and Palmer, D. A. "Formation Constants of Zinc Chloride and Zinc Sulfate Complexes in Aqueous Solutions to 250°C: A Potentiometric Study," 49th Calorimetry Conference, Santa Fe, New Mexico, July 1994.

Nguyen-Trung, C., Palmer, D. A. and Begun, G.M. "Hydrolysis of the Uranyl Ion in Hydrothermal Solutions by Raman Spectroscopy and Potentiometric up to 225°C, 50 MPa," in *Proc., Fourth International Symposium on Hydrothermal Reactions*, Nancy, France, August 31-September 3, 1993, pp. 163-164.

Nguyen-Trung, C. and Palmer, D. A. "Hydrolysis of the Uranyl(VI) Ion in Aqueous Solutions up to 100°C, 0.1 MPa," 49th Calorimetry Conference, Santa Fe, New Mexico, July 1994.

Oakes, C. S., Simonson, J. M., Bodnar, R. J. and Pitzer, K. S. "[NaCl+CaCl₂](aq) Densities to 350°C and 400 Bars," 49th Calorimetry Conference, Santa Fe, NM, July 31-August 4, 1994.

Oakes, C. S., Pitzer, K. S., Simonson, J. M. and Bodnar, R. J. "CaCl₂-H₂O in the Supercritical and Two-Phase Ranges," 49th Calorimetry Conference, Santa Fe, NM, July 31-August 4, 1994.

Oakes, C. S., Bodnar, R. J., Simonson, J. M. and Pitzer, K. S. "CaCl₂-H₂O in the Supercritical and Two-Phase Ranges," 12th Symposium on Thermophysical Properties, Boulder, CO, June 19-24, 1994.

Oakes, C. S., Bodnar, R. J., Simonson, J. M. and Pitzer, K. S. "CaCl₂-H₂O in the Supercritical and Two-Phase Ranges," American Geophysical Union Meeting, Baltimore, MD, May 23-27, 1994.

Palmer, D. A. and Nguyen-Trung, C. "Potentiometric and Raman Studies of Aqueous Uranyl(VI) Chemistry," 4th International Conference on Chemistry and Migration Behavior of Actinide and Fission Products in the Geosphere, Charleston, SC, Dec. 12-17, 1993.

Palmer, D. A., Simonson, J. M. and Carter, R. W. "Experimental Measurements of the Volatilities of Inorganic Electrolytes in Aqueous Solutions to 350°C," 1993 Crevice Chemistry Workshop, Boston, MA, June 27-29, 1993.

Palmer, D. A., Wesolowski, D. J. and Bell, J. L. S. "EMF Measurements of Oxalic and Formic Acid Decomposition Kinetics and Interaction of Acetate with Aluminum(III) to High Temperatures," American Geophysical Union Annual Meeting, Baltimore, MD, May 23-27, 1993.

Palmer, D. A., Wesolowski, D. J. and Bell, J. L. S. "High Temperature Potentiometric Measurements of Hydrolysis and Metal Complexation Reactions," Symposium on Properties of Aqueous Solutions, Theory and Applications, International Association for the Properties of Water and Steam, Milan, Italy, Sept. 15, 1993.

Palmer, D. A. and Wesolowski, D. J. "High Temperature Potentiometric Measurements of Hydrolysis and Metal Complexation Reactions," in *Proc., 4th International Hydrothermal Reactions Symposium*, Nancy, France, Aug. 31-Sept. 3, 1993, pp. 173-176.

Palmer, D. A., Wesolowski, D. J. and Mesmer, R. E. "The Hydrogen-Electrode Concentration Cell as a Sensitive Tool in High Temperature Aqueous Chemistry," American Chemical Society Meeting, Washington, DC, Aug. 21-26, 1994.

Palmer, D. A., Simonson, J. M. and Jensen, J. P. "Measurements of the Volatilities of Electrolytes: Application to Water/Steam Cycles," 4th International Conference on Cycle Chemistry in Fossil Plants, EPRI, Atlanta, GA, Sept. 7-9, 1994.

Palmer, D. A. and Simonson, J. M. "Experimental Studies of the Volatility of Salts in the Water/Steam Cycle," International Collaboration on Steam, Chemistry, and Corrosion in the Phase Transition Zone of Steam Turbines, and ESKOM Power Plant Chemistry Symposium, Midrand, South Africa, June 6-9, 1994.

Palmer, D. A. "Aqueous Chemistry of Aluminum Under Moderate Conditions," IAEA-Sponsored Visit, CNEA, Buenos Aires, Argentina, March 16, 1994.

Palmer, D. A. "Experimental Studies of Aqueous Equilibria to High Temperatures, First Part. Volatility of Ionic Solutes and Electrical Conductivity of Electrolytes," IAEA-Sponsored Visit, CNEA, Buenos Aires, Argentina, March 15, 1994.

Palmer, D. A. "Experimental Studies of Aqueous Equilibria to High Temperatures, Second Part. Stability of Metal Complexes and Sorption of Ions on Oxides," IAEA-Sponsored Visit, CNEA, Buenos Aires, Argentina, March 17, 1994.

Palmer, D. A. and Nguyen-Trung, C. "A Potentiometric Study of the Hydrolysis of Ethylenediamine-tetraacetic Acid, EDTA, to 150°C," 12th International Conference on the Properties of Water and Steam, Orlando, FL, Sept. 11-16, 1994.

Simonson, J. M. "Thermodynamic Properties of Simple Aqueous Electrolytes to High Temperatures," 48th Calorimetry Conference, Durham, NC, July 18-22, 1993.

Simonson, J. M. and Palmer, D. A. "Distribution of Ammonium Salts Between Liquid and Vapor at High Temperatures," in *Proc., International Conference on Interaction of Iron-Based Materials with Water and Steam*, 1993.

Simonson, J. M., Palmer, D. A. and Carter, R. W. "Liquid-Vapor Partitioning of NaCl(aq) from Concentrated Brines at Temperatures to 350°C," 19th Stanford Geothermal Reservoir Engineering Workshop, Stanford, CA, Jan. 19-20, 1994.

Simonson, J. M. "Measurements and Estimation of Excess Thermodynamic Properties of Aqueous Electrolyte Solutions to High Temperatures," American Chemical Society Meeting, Washington, DC, Aug. 21-25, 1994.

Simonson, J. M. and Palmer, D. A. "Partitioning of Acid Chlorides Between Liquid and Steam at High Temperatures," Geysers Geothermal Research Update Meeting, San Francisco, CA, April 28, 1994.

Simonson, J. M. and Palmer, D. A. "Partitioning of Solutes Between Liquid Water and Steam in the System," 12th International Conference on the Properties of Water and Steam, Orlando, FL, Sept. 11-16, 1994.

Simonson, J. M. and Palmer, D. A. "Production and Mitigation of Acid Chlorides in Geothermal Steam," DOE Geothermal Program Research Workshop, San Francisco, CA, September 21-22, 1994.

Simonson, J. M. and Palmer, D. A. "Vapor-Liquid Equilibrium of Chlorides in Aqueous Systems to High Temperatures: Application to the Geysers Geothermal Field," Annual Geothermal Resources Council Meeting, Salt Lake City, UT, Oct. 2-5, 1994.

Simonson, J. M., Mesmer, R. E., Moore, R. C., Bloomingburg, G. F. and Cochran, H. D. "In Situ Neutralization and Solubility Studies in Supercritical Water Oxidation," DOE Supercritical Water Oxidation Technical Support Mid-Year Program Review, Denver, CO, February 28-March 1, 1994.

Simonson, J. M., Palmer, D. A. and Carter, R. W. "Liquid-vapor Partitioning of Chlorides from Concentrated Brines at High Temperatures," 49th Calorimetry Conference, Santa Fe, NM, July 31-August 4, 1994.

Wesolowski, D. J. and Palmer, D. A. "The Hydrolysis of Mg^{2+} in 0.5 Molal NaCl Brines from 0 to 250°C by Potentiometric Titration," American Geophysical Union Annual Meeting, Baltimore, MD, May 23-27, 1993.

Reports

Moore, R. C., Simonson, J. M. and Mesmer, R. E., *A Visual Cell for Measuring the Solubility of Prograde Soluble Salts in Water at High Temperatures and Pressures*, ORNL-6829 (Oct. 1994).

Palmer, D. A. and Simonson, J. M. *Behavior of Ammonium Salts in Steam Cycles*, Report EPRI TR-102377, Electric Power Research Institute, Palo Alto, CA (Dec. 1993).

Simonson, J. M., Moore, R. C., Holmes, H. F., Mesmer, R. E., Bloomingburg, G. and Cochran, H. D. *Interim Report for FY 1994. Supercritical Water Oxidation (SCWO) Technical Support*, Report to DOE Office of Technology Development (1994).

INORGANIC MATERIALS GROUP

Books/Book Chapters

Paranthaman M. and Hermann, A. M. "Thallium Based High- T_c Superconducting Oxides - A Summary," in *Organic Conductors: Fundamentals and Applications*, Jean-Pierre Farges, ed., Marcel Dekker, Inc., New York (1994) pp. 735-757.

Journal Articles

- Bamberger, C. E. and Alexander, K. B. "The Pseudomorphic Conversion of Platelets of Cr_2O_3 into CrN and Cr_3C_2 ," *J. Cryst. Growth* (1993) **126**, 525-529.
- Bamberger, C. E. and Kopp, O. C. "Acicular Crystals of Sodium Tungsten Bronzes," *J. Cryst. Growth* (1993) **131**, 473-480.
- Bamberger, C. E. "The Pseudomorphic Conversion of Acicular Crystals of Sodium Tungsten Bronze into WC/W," *J. Mater. Sci. Lett.* (1994) **12**(24), 1742-1745.
- Bamberger, C. E., Haverlock, T. J., Shoup, S. S., Kopp, O. C. and Stump, N. A. "Compounds of Cerium, Titanium and Oxygen," *J. Alloys and Compounds* (1994) **204**, 101-107.
- Chakoumakos, B. C. and Paranthaman, M. "Neutron Powder Diffraction Study of the Superconducting Quaternary Intermetallic Compound $\text{YNi}_2\text{B}_2\text{C}$," *Phys. C* (1994) **227**, 143-150.
- Hoffman, W., Breitzke, H., Baenitz, M., Luders, K., Buntkowsky, G., Limbach, H. H., Antipov, E. A., Gippius, A. A., Loebich, O., Khan, H. R., Paranthaman, M. and Thompson, J. R. "Application of ^{199}Hg Solid State NMR to Hg-based HTSC," *Phys. C* (1994) **227**, 225-229.
- Maya, L. "Paracyanogen Reexamined," *J. Polym. Sci. A Polym. Chem.* (1993) **31**, 2595.
- Maya, L. "Deposition of Crystalline Binary Nitride Films of Tin, Copper, and Nickel by Reactive Sputtering," *J. Vac. Sci. Technol. A* (1993) **11**(3), 604-608.
- Maya, L. "Deposition of Amorphous Hydrogenated Silicon Carbide Films Using Organosilanes in an Argon/Hydrogen Plasma," *J. Vac. Sci. Technol.* (1994) **12**, 754.
- Paranthaman, M., Thompson, J. R., Sun, Y. R., Brynestad, J. and Kroege, D. M. "Evidence for Phase Stability and Weak Links in Polycrystalline $\text{HgBa}_2\text{CuO}_{4+\delta}$," *Appl. Supercond.* (1994) **2**, 359-365.
- Paranthaman, M., Brynestad, J., Thompson, J. R. and Sun, Y. R. "Synthesis and Magnetic Characterization of High- T_c Superconducting Compound $\text{HgBa}_2\text{CuO}_{4+\delta}$," *Phys. C* (1993) **213**, 217-275.
- Paranthaman, M. "Single Step Synthesis of Bulk $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ Superconductors," *Phys. C* (1994) **222**, 7-12.
- Subramaniam, C. K., Paranthaman, M. and Kaiser, A. B. "Thermoelectric Power and Resistivity of Bulk $\text{HgBa}_2\text{CuO}_{4+y}$ Superconductors and the Effects of Annealing," *Phys. C* (1994) **222**, 47-51.
- Sun, Y. R., Thompson, J. R., Kerchner, H. R., Christen, D. K., Paranthaman, M. and Brynestad, J. "Strong Surface Pinning Effects in Polycrystalline $\text{Hg}_2\text{Ba}_2\text{Cu}_1\text{O}_{4+\delta}$ Superconductor," *Phys. Rev. B* (1994) **50**, 3330-3336.

Thompson, J. R., Ossandon, J. G., Christen, D. K., Chakoumakos, B. C., Sun, Y. R., Paranthaman, M. and Brynstad, J. "Vortex Fluctuation, Magnetic Penetration Depth, and H_{c2} in Hg- and Tl- Based High- T_c Superconductors," *Phys. Rev. B* (1993) **48**, 14031.

Vallet, C. E., Choudhury, A., Sobol, P. E. and White, C. W. "XPS Characterization of Anodic Layers Grown on Ir- and Rh-Implanted Titanium," *Electrochim. Acta* (1993) **38(10)**, 1313-1320.

Vallet, C. E. and White, C. W. "Electrochemical Surfaces Modelled by Ion Implantation," *Electrochim. Acta* (1994) **39**, 1537-1543.

Presentations/Conference Proceedings

Goyal, A., Paranthaman, M., Brynstad, J., Kroeger, D. M. and Haldar, P. "Fabrication, Processing and Superconducting Properties of Tl-1223 Powder-in-tube Conductors," 1994 Applied Superconductivity Conference, Boston, MA, Oct. 16-21, 1994.

Maya, L. "Deposition of a-SiC:H Using Organosilanes in an Argon/Hydrogen Plasma," in *Proc., Materials Research Society Symposium, Fall Materials Research Society Meeting*, Boston, MA, Nov. 29-Dec. 3, 1993, Vol. 327, p. 215 (1994).

Maya, L. "Covalent Nitrides for Maskless Laser Writing of Microscopic Metal Lines," in *Proc., Materials Research Society Symposium, Materials Research Society Fall Meeting*, Boston, MA, Nov. 30-Dec. 4, 1992, Vol. 282, p. 203 (1993).

Paranthaman, M., Sun, Y. R. and Thompson, J. R. "Synthesis and Magnetic Characterization of Bulk $HgBa_2CuO_{4+\delta}$, $HgBa_2CaCu_2O_{6+\delta}$ and $HgBa_2Ca_2Cu_3O_{8+\delta}$ Superconductors," American Physical Society Meeting, Pittsburgh, PA, Mar. 21-25, 1994.

Paranthaman, M. "Thallium Based High- T_c Superconducting Oxides -- An Overview," Midwest Superconductivity Consortium Workshop, Purdue University, West Lafayette, IN, Aug. 11-12, 1994.

Paranthaman, M., Goyal, A., Heatherly, D. E. and Kroeger, D. M. "Formation of Anisotropic Tl-1212, Tl-2212, Tl-1223 and Tl-2223 Particles Using Aerosol Flow Reacted Powders," 1994 Applied Superconductivity Conference, Boston, MA, Oct. 16-21, 1994.

Shoup, S. S., Haverlock, T. J. and Bamberger, C. E. "Solid Solutions within Selected $SrO-LnO_{1.5}-TiO_2$ Systems," Southeast Regional American Chemical Society Meeting, Birmingham, AL, Oct. 19, 1994.

Vallet, C. E., Choudhury, A., Sobol, P. E. and White, C. W. "XPS Characterization of Anodic Layers Grown on Ir- and Rh-Implanted Titanium," 44th International Society of Electrochemistry Meeting, Berlin, Germany, Sept. 5-10, 1993.

Vallet, C. E. and White, C. W. "Electrocatalyst Surfaces Modelled by Ion Implantation," Conference on Progress in Electrocatalysis -- Theory and Practice, Ferrara, Italy, Sept. 12-15, 1993.

Wang, Z. L., Brynestad, J., Kroeger, D. M., Sun, Y. R., Thompson, J. R. and Williams, R. K. "Nano-Probe Microanalysis of Grain Boundary Chemistry in $\text{YBa}_2\text{Cu}_3\text{O}_7$ and Its Relationship to Weak-Link Behavior," in *Proc., 51st Annual Meeting of the Microscopy Society of America*, G. W. Bailey and C. L. Rieder, eds., San Francisco Press, Inc. (1993) pp. 598-599.

POLYMER SCIENCE GROUP

Books/Book Chapters

Darsey, J. A., Sumpter, B. G. and Noid, D. W. "Correlating Physical Properties of Polymeric Materials and Organic Precursors of Polymers Using Artificial Neural Networks," in *Intelligent Engineering Systems Through Artificial Neural Networks*, Dagli, Fernandez, Ghosh and Kumara, eds., ASME Press (1994) 4, 875.

Getino, C., Sumpter, B. G. and Noid, D. W. "A Neural Network Approach to the Study of Dynamics and Structure of Molecular Systems," in *Intelligent Engineering Systems Through Artificial Neural Networks*, Dagli, Fernandez, Ghosh and Kumara, eds., ASME Press (1994) 4, 849.

Sumpter, B. G., Gakh, A. A. and Noid, D. W. "Predicting Materials Properties Using Neural Networks," in *Intelligent Engineering Systems Through Artificial Neural Networks*, Dagli, Fernandez, Ghosh and Kumara, eds., ASME Press (1994) 4, 863.

Wunderlich, B. "Thermal Analysis," in *Encyclopedia of Materials Science and Engineering*, Vol. 6, M. B. Bever, ed., Pergamon Press, Oxford, (1986) p. 2939; updated and reprinted as "Thermal Analysis: An Overview," in D. Bloor, R. J. Brook, M. C. Flemings and S. Mahajan, *Encyclopedia of Advanced Materials*, Vol. 4, Pergamon, Elsevier, Oxford, (1994) p. 2807.

Wunderlich, B., Sumpter, B. G., Noid, D. W. and Liang, G. L. "Computer Simulation of Macromolecular Crystals and Their Defects," in *Ordering in Macromolecular Systems*, A. Teramoto, M. Kobayashi, T. Norisuje, eds., Springer-Verlag, Berlin (1994) p. 35.

Journal Articles

Alamo, R. A., Londono, J. D., Mandelkern, L., Stehling, F. C. and Wignall, G. D. "The Phase Behavior of Blends of Linear and Branched Polyethylenes in the Molten and Solid States by SANS," *Macromols.* (1994) 27, 411.

Annis, B. K. and Pedraza, D. "Effect of Friction on Atomic Force Microscopy of Ion Implanted Highly Oriented Pyrolytic Graphite," *J. Vac. Technol.* (1993) B11, 1759.

Annis, B. K. and Wunderlich, B. "Atomic Force Microscopy of Extended Chain Crystals of Polyethylene," *J. Polym. Sci. B Polym. Phys.* (1993) 31, 93.

Annis, B. K., Pedraza, D. F. and Withrow, S. P. "Topographical Changes Induced by High Dose Carbon-bombardment of Graphite," *J. Mater. Res.* (1993) 8, 2587.

Boller, A. and Wunderlich, B. "Heat Capacity Measurement by Modulated DSC at Constant Temperature," *J. Thermal Anal.* (1994) **42**, 307-330.

Boller, A., Jin, Y., Cheng, J. and Wunderlich, B. "Analysis of the Thermal Properties and Motion in Crystalline trans-1,4-Poly(butadiene)," *Thermochim. Acta* (1994) **234**, 95.

Bu, H., Chen, E., Xu, S., Guo, K. and Wunderlich, B. "Single-Molecule Single Crystals of Isotactic Polystyrene," *J. Polym. Sci. B Polym. Phys.* (1994) **32**, 1351.

Chen, W., Fu, Y. and Wunderlich, B. "The Morphology of Gel-Spun Polyethylene Fibers Investigated by Solid State ^{13}C NMR," *J. Polym. Sci. Phys. Ed.* (1994) **32**, 2662.

Cheng, S. Z. D., Chen, J., Wu, X., Yandrasits, M. A., Zhuo, Q., Quirk, R. P., Habenschuss, A. and Zschack, P. R. "Nonintegral and Integral Folding Crystal Growth in Low Molecular Weight Poly(ethylene oxide) Fractions," in *Crystallization of Polymers: Theoretical and Experimental Aspects, NATO ASI-C Series "Mathematical and Physical Sciences"* (1993).

Cheng, S. Z. D., Wu, S. S., Chen, J., Zhuo, Q., Quirk, R. P., von Meerwall, E. D., Hsiao, B. S., Habenschuss, A. and Zschack, P. R. "Isothermal Thickening and Thinning Processes in Low Molecular Weight Poly(ethylene oxide) Fractions Crystallized from the Melt. 4. End Group Dependence," *Macromols.* (1993) **26**, 5105.

Cheng, J., Chen, W., Jin, Y. and Wunderlich, B. "Condis Crystals of Small Molecules VI. The Differences Between Smectic and Condis Phases, Evaluated by a Solid State ^{13}C NMR Study of N,N'-bis(4-n-octyloxybenzyl)-1,4-phenylene-diamine (OOBPD)," *Mol. Cryst. Liq. Cryst.* (1994) **241**, 299.

Cheng, J., Jin, Y., Xenopoulos, A., Chen, W., Wunderlich, B., Diack, M., Compton, R. N. and Guiochon, G. "Motion and Disorder in the Plastic Crystal of the C_{70} Complex with Toluene by Solid State NMR and Thermal Analysis," *Mol. Cryst. Liq. Cryst.* (1994) **250**, 359-371.

Cheng, J., Fone, M., Reddy, V. N., Schwartz, K. B., Fisher, H. P. and Wunderlich, B. "Identification and Quantitative Analysis of the Intermediate Phase in a Linear High Density Polyethylene," *J. Polym. Sci. B Polym. Phys.* (1994) **32**, 2683.

Cheng, J., Jin, Y., Chen, W., Wunderlich, B., Jonsson, H., Hult, A. and Gedde, U. W. "The Chain Conformations of a Polyether Based on Bis(4-hydroxyphenoxy)-p-xylylene and 1,11-Dibromoundecane (HPX-C11) in Its Mesophase States, Derived from ^{13}C NMR," *J. Polym. Sci. B Polym. Phys.* (1994) **32**, 721.

Cheung, Y. W., Stein, R. S., Lin, J. S. and Wignall, G. D. "Small-Angle Scattering Investigations of Poly(ϵ -caprolactone)/Poly (carbonate) Blends," *Mater Res. Symp. Proc.* (1994) **321**, 549.

Curro, J. G., Yethiraj, A., Schweizer, K. S., McCoy, J. D. and Honnell, K. G. "Microscopic Equations-of-State for Hydrocarbon Fluids: Effect of Attractions and Comparison with Polyethylene Experiments," *Macromols.* (1993) **26**, 2655.

- Curro, J. G. "Intermolecular Structure of Vinyl Polymer Liquids: Freely Jointed Chains," *Macromols.* (1994) **27**, 4665.
- Darsey, J. A., Soman, A. G., Noid, D. W. and Sumpter, B. G. "Modeling of Polymeric Systems Using Artificial Neural Network Computing," *Polym. Prepr.* (1993) **34**(1), 622.
- Darsey, J. A., Soman, A. G. and Noid, D. W. "Artificial Neural System Modeling of Monte Carlo Simulation of Polymers," *Makromol. Chem. Theory and Simulat.* (1993) **2**, 711.
- Fu, Y., Annis, B., Boller, A., Jin, Y. and Wunderlich, B. "Analysis of Structure and Properties of Poly(ethylene terephthalate) Fibers," *J. Polym. Sci. B Polym. Phys.* (1994) **32**, 2289.
- Fu, Y., Busing, W. R., Jin, Y., Affholter, K. A. and Wunderlich, B. "Structure Analysis of the Non-crystalline Material in Poly(ethylene terephthalate) Fibers," *Makromol. Chem.* (1994) **195**, 803.
- Fu, Y., Busing, W. R., Jin, Y., Affholter, K. A. and Wunderlich, B. "Poly(ethylene terephthalate) Fibers 1. Crystal Structure and Morphology Studies with Full-pattern X-ray Diffraction Refinement," *Macromols.* (1993) **26**, 2187.
- Gakh, A. A., Sumpter, B. G., Gakh, E. G. and Noid, D. W. "A Neural Network-Graph Theory Approach to the Prediction of the Physical Properties of Organic Compounds," *J. Chem. Inf.* (1994) **34**, 832.
- Gray, S. K., Noid, D. W. and Sumpter, B. G. "Symplectic Integrators for Large Scale Molecular Dynamics Simulations: A Comparison of Several Explicit Methods," *J. Chem. Phys.* (1994) **101**, 4062.
- Grayce, C. J. and Schweizer, K. S. "Solvation Potentials for Macromolecules," *J. Chem. Phys.* (1994) **100**, 6846.
- Grayce, C. J., Yethiraj, A. and Schweizer, K. S. "Liquid-State Theory of the Density-Dependent Conformation of Nonpolar Linear Polymers," *J. Chem. Phys.* (1994) **100**, 6857.
- Hembree, D. M., Pedraza, D. F., Romanski, G. R., Withrow, S. P. and Annis, B. K. "Raman Spectroscopy of C-Irradiated Graphite," *Mater. Res. Symp. Proc.* (1993) **279**, 351.
- Jin, Y., Boller, A., Wunderlich, B. and Lebedev, B. V. "Heat Capacities and Transitions in n-Perfluoroalkanes and Polytetrafluoroethylene," *Thermochim. Acta* (1994) **234**, 103.
- Jin, Y., Xenopoulos, A., Cheng, J., Chen, W., Wunderlich, B., Diack, M., Jin, C., Hettich, R. L., Compton, R. N. and Guiochon, G. "Thermodynamic Characterization of the Plastic Crystal and Non-Plastic Crystal Phases of C₇₀," *Mol. Cryst. Liq. Cryst.* (1994) **257**, 235-250.
- Jin, Y., Cheng, J., Wunderlich, B., Cheng, S. Z. D. and Yandrasits, M. A. "Thermodynamic Functions of Thermotropic Polyethers Based on the Semiflexible Mesogen 1-(4-Hydroxyphenyl)-2-(2-methyl-4-hydroxyphenyl)ethane," *Polym. Adv. Technol.* (1994) **5**, 785-795.

- Lebedev, B. V., Bycova, T. A., Vasil'yev, V. G. and Wunderlich, B. "Thermodynamics of Normal Perfluorododecane, Perfluorotetradecane and Perfluorohexadecane in the Range of 0-320 K at Standard Pressure," *Z. Fiz. Khim.* (1994) **68**, 15.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Dynamics of a Paraffin Crystal," *Makromol. Chem. Theory Simulat.* (1993) **2**, 245.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Gauche Defects, Positional Disorder, Dislocations, and Slip Planes in Crystals of Long Methylene Sequences," *J. Phys. Chem* (1994) **98**, 11739.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Atomistic Details of Disordering Processes in Superheated Polymethylene Crystals," *Acta Polym.* (1993) **44**, 214.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Dynamics and Structure Simulation of Polymethylene Crystals with Explicit Hydrogen Atoms," *J. Comput. Polym. Sci.* (1993) **3**, 101.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Molecular Dynamics Simulations of the Hexagonal Structure of Crystals With Long Methylene Sequences," *J. Polym. Sci. B Polym. Phys.*, (1993) **31**, 1909.
- Londono, J. D., Narten, A. H., Wignall, G. D., Honnell, K. G., Hsieh, E. T., Johnson, T. W. and Bates, F. S. "The Composition Dependence of the Interaction Parameter in Isotopic Polymer Blends," *J. Chem. Phys.* (1994) **27**, 2864.
- Londono, J. D., Annis, B. K., Turner, J. Z. and Soper, A. K. "The Intermolecular Hydrogen-Hydrogen Structure of Chain-molecule Liquids from Neutron Diffraction," *J. Chem. Phys.* (1994) **101**, 7868.
- Melenkevitz, J. M., Curro, J. G. and Schweizer, K. S. "Variational Approach to the Conformation of Flexible Polymers in Solution," *J. Chem. Phys.* (1993) **99**, 5571.
- Melenkevitz, J. M., Schweizer, K. S. and Curro, J. G. "Self-Consistent Integral Equation Theory for the Equilibrium Properties of Polymer Solutions," *Macromols.* (1993) **26**, 8190.
- Roles, K. and Wunderlich, B. "Heat Capacities of Solid Copoly(amino acid)s," *J. Polym. Sci. Polym. Phys.* (1993) **31**, 279-285.
- Roles, K., Xenopoulos, A. and Wunderlich, B. "Heat Capacities of Solid Poly(amino acid)s. II. The Remaining Polymers," *Biopolym.* (1993) **33**, 753-768.
- Schweizer, K. S. "Analytical RISM Theory of Polymer Alloys: Molecular Closure Predictions for Structurally Symmetric Blends," *Macromols.* (1993) **26**, 6033.
- Schweizer, K. S. "Analytic PRISM Theory of Structurally Asymmetric Polymer Blends and Copolymers," *Macromols.* (1993) **26**, 6050.

- Schweizer, K. S. and Yethiraj, A. "Polymer RISM Theory: New Molecular Closures for Phase Separating Fluids and Alloys," *J. Chem. Phys.* (1993) **98**, 9053.
- Schweizer, K. S. and Curro, J. G. "Polymer RISM Theory of the Structure, Thermodynamics and Phase Transitions of Polymer Liquids and Alloys," *Adv. Polym. Sci.* (1994) **116**, 319.
- Sen, C. S., Cohen, J. M., McCoy, J. D. and Curro, J. G. "The Structure of a Rotational Isomeric State Alkane Melt Near a Hard Wall," *J. Chem. Phys.* (1994) **101**, 9010.
- Spining, M. T., Darsey, J. A., Sumpter, B. G. and Noid, D. W. "An Introduction to Artificial Neural Networks," *J. Chem. Ed.* (1994) **71**, 406.
- Sumpter, B. G., Getino, C., Noid, D. W. and Wunderlich, B. "Computer Simulations of Atomic Force Microscopy: Crystalline Polymers and the Effects of Surface Contaminants," *Makromol. Chem. Theory Simulat.* (1993) **2**, 55.
- Sumpter, B. G., Noid, D. W. and Wunderlich, B. "Computer Simulation and Modeling of Polymeric Crystals," *Trends Polym. Sci.* (1993) **1**, 160.
- Sumpter, B. G., Noid, D. W. and Wunderlich, B. "Computational Experiments on the Motion and Generation of Defects in Polymer Crystals," *Macromols.* (1993) **25**, 7247.
- Sumpter, B. G., Noid, D. W., Liang, G. L. and Wunderlich, B. "Atomistic Dynamics of Macromolecular Crystals," *Adv. Polym. Sci.* (1994) **116**, 27.
- Sumpter, B. G. and Noid, D. W. "Computational Experiments on the Migrations of Internal Energy in Macromolecular Systems," *Chem. Phys.* (1994) **186**, 323.
- Sumpter, B. G., Getino, C. and Noid, D. W. "Theory and Applications of Neural Computing in Chemical Science," *Ann. Rev. Phys. Chem.* (1994) **45**, 439.
- Sumpter, B. G. and Noid, D. W. "Neural Networks and Graph Theory as Computational Tools for Predicting Polymer Properties," *Makromol. Chem. Theory Simulat.* (1994) **3**, 363.
- Wang, Q., Annis, B. and Wunderlich, B. "Surface Studies of Tetraalkylammonium Bromides and Iodides Using Atomic Force Microscopy," *J. Polym. Sci. B Polym. Phys.* (1994) **32**, 2653.
- Wozny, C. E., Sumpter, B. G. and Noid, D. W. "Calculating the Vibrational Spectra of Linear Polymers from Molecular Dynamics Trajectories," *Trends Polym. Sci.* (1994) **2**, 375.
- Wozny, C. E., Sumpter, B. G. and Noid, D. W. "Semiclassical Theory of Group Vibrations for Linear Polymer Chains," *Makromol. Chem. Theory Simulat.* (1994) **3**, 347.
- Wozny, C. E., Sumpter, B. G. and Noid, D. W. "The Existence of Nonlinear Resonances in Collective Modes of Linear Macromolecules," *J. Chem. Phys.* (1994) **100**, 8540.

Wozny, C. E., Sumpter, B. G. and Noid, D. W. "A Molecular Dynamics Method for Obtaining the Vibrational Spectra of Macromolecules," *J. Chem. Phys.* (1994) **100**, 3520.

Wozny, C. E., Sumpter, B. G. and Noid, D. W. "A Dynamical Analysis of Linear Polymers Using Mode Specific Trajectories," *Mol. Phys.* (1994) **82**, 597.

Wunderlich, B. "Glass Transitions of Partially Ordered Macromolecules," *Colloid Polym. Sci.* (1994) **96**, 22.

Wunderlich, B., Jin, Y. and Boller, A. "Mathematical Description of Differential Scanning Calorimetry Based on Periodic Temperature Modulation," *Thermochim. Acta* (1994) **238**, 277.

Xenopoulos, A., Wunderlich, B. and Narten, A. H. "Proton Motion in Aliphatic Nylons from Neutron Scattering," *Macromols.* (1993) **26**(7), 1576.

Xenopoulos, A., Subirana, J. A. and Wunderlich, B. "Thermal Properties of Nylons Related to Polyglycine," *Eur. Polym. J.* (1993) **29**, 927.

Xenopoulos, A., Cheng, J. and Wunderlich, B. "Mesophases of Alkylammonium Salts. V. Heat Capacities of Symmetric Halides with Alkyl Chains Longer than Ethyl," *Mol. Cryst. Liq. Cryst.* (1993) **226**, 87-102.

Xenopoulos, A., Londono, J. D., Wignall, G. D. and Wunderlich, B. "Phase Separation in Blends of Polystyrene and Poly(p-methylstyrene) Using Thermal Analysis and Small-Angle Neutron Scattering," *Mater. Res. Symp. Proc.* (1994) **321**, 107.

Yethiraj, A. and Schweizer, K. S. "Integral Equation Theory of Polymer Blends: Numerical Investigation of Molecular Closures for Symmetric Mixtures," *J. Chem. Phys.* (1993) **98**, 9080.

Yethiraj, A., Curro, J. G., Schweizer, K. S. and McCoy, J. D. "Microscopic Equations-of-State of Polyethylene: Hard Chain Contributions to the Pressure," *J. Chem. Phys.* (1993) **98**, 1635.

Yethiraj, A., Kumar, S., Hariharan, A., and Schweizer, K. S. "Surface Segregation in Polymer Blends Due to Stiffness Disparity," *J. Chem. Phys.* (1994) **100**, 4691.

Presentations/Conference Proceedings

Alamo, R. G., Mandelkern, L., Stehling, F. C., Wignall, G. D. and Londono, J. D. "The Phase Behavior of Blends of Linear and Branched Polyethylenes in the Molten and Solid States by SANS," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.

Boller, A. and Wunderlich, B. "Temperature-modulated DSC," Colloquium at the Sektion fuer Kalorimetrie, Department of Physics, University of Ulm, Ulm, Germany, June 20, 1994.

Boller, A., Annis, B. and Wunderlich, B. "Three-Phase Structure-Property Analysis of PET Fibers," Poster, American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Boller, A. and Wunderlich, B. "Temperature-modulated DSC," Department of Physics, University of Rostock, Rostock, Germany, June 10, 1994.

Chen, W. and Wunderlich, B. "Investigation of Polyethylene Fibers by Solid State NMR," Poster, American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Cheng, J., Jin, Y., Chen, W. and Wunderlich, B. "The Chain Conformation of a Polyester Based on Bis(4-hydroxyphenoxy)-p-xylylene and 1,11-Dibromoundecane (HPX-C11) and Its Mesophase States," Poster, American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Cheng, S. Z. D., Wu, S. S., Chen, J., Zhuo, Q., Quirk, R. P., von Meerwall, E., Habenschuss, A., Zschack, P. R. and Hsiao, B. S. "End Group and Molecular Weight Effects on Thickening and Thinning Processes in Low Molecular Weight Poly(ethylene oxide) Fractions, Nonintegral and Integral Folding Crystal Growth in Low Molecular Weight Poly(ethylene oxide) Fractions," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.

Cheng, J., Fone, M. and Wunderlich, B. "Solid State ^{13}C NMR Study on the Intermediate Phase and Domain Sizes of Polyethylene," American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Curro, J. G. "Molecular Modeling of Polymer Melts and Alloys," in *Proc., ANTEC '94, Society of Plastics Engineers Meeting*, May 1-5, 1994.

Curro, J. G. "Intermolecular Structure of Vinyl Polymer Liquids," American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Curro, J. G. "Molecular Modeling of Polymer Melts and Alloys," Department of Chemical Engineering, Michigan State University, September 22, 1994.

Curro, J. G. "Molecular Modeling of Polymer Melts and Alloys," Department of Chemistry, Stanford University, Stanford, CA, May 3, 1994.

Curro, J. G., Donley, J. P. and Yethiraj, A. "Equation-of-State of Polymer Melts for Integral Equation Theory: Thermodynamic Consistency," American Physical Society Meeting, Seattle, WA, March 22-25, 1993.

Darsey, J. A., Sumpter, B. G. and Noid, D. W. "Neural Network Prediction of Properties of Polymers and Other Organic Molecules and Prediction and Deconvolution of Mathematical Functions," American Physical Society National Meeting, Pittsburgh, PA, March 1994.

Darsey, J. A., Soman, A. G., Noid, D. W. and Sumpter, B. G. "Modeling of Polymeric Systems Using Artificial Neural Network Computing," American Chemical Society National Meeting, Denver, CO, March 1993.

Darsey, J. A., Sumpter, B. G. and Noid, D. W. "Prediction and Deconvolution of Mathematical Functions," 1st DOE Workshop on Applications of Neural Networks in Materials Science, February 28-March 2, Knoxville, TN, March 1994.

Darsey, J. A., Sumpter, B. G. and Noid, D. W. "Neural Network Prediction of Properties of Polymers and Other Organic Molecules," 1st DOE Workshop on Applications of Neural Networks in Materials Science, February 28-March 2, Knoxville, TN, 1994.

Darsey, J. A., Sumpter, B. G. and Noid, D. W. "Correlating Physical Properties of Polymeric Materials and Organic Precursors of Polymers Using Artificial Neural Networks," Artificial Neural Networks in Engineering Meeting, St. Louis, MO, November 1994.

Donley, J., Curro, J. G. and McCoy, J. D. "A New Integral Equation for Pair Correlations in Molecular Liquids," American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Fu, Y., Boller, A., Jin, Y. and Wunderlich, B. "X-ray Diffraction of Super-drawn Polyethylene Fibers," Poster, Fibers Gordon Conference, New London, NH, July 11-16, 1993.

Fu, Y., Annis, B. and Wunderlich, B. "Two-dimensional Rietveld Refinement Studies of Fibers," 43rd Annual Denver Conference on Applications of X-Ray Analysis, Steamboat Springs, CO, August 1-5, 1994.

Fu, Y., Annis, B., Boller, A. and Wunderlich, B. "Structure Analysis of High-Modulus Polyethylene Fibers Using a Three-Phase Model," Poster, American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Fu, Y., Busing, W. R., Affholter, K. A. and Wunderlich, B. "Full-pattern Refinement of Poly(ethylene terephthalate) Fibers," Poster, American Crystallographic Association '93 Meeting, Albuquerque, NM, May 23-27, 1993.

Gakh, A., Gakh, B., Sumpter, B. G. and Noid, D. W. "Neural Network Prediction of Properties of Fluorocarbons," American Chemical Society National Meeting, San Diego, CA, March 1994.

Gakh, A. A., Sumpter, B. G. and Noid, D. W. "Estimation of Properties of Fluororganic Compounds Using a Computer Neural Network: A Technique Intelligible to Everyone," American Chemical Society Meeting, San Diego, CA, March 13-18, 1994.

Getino, C., Meyer, S., Sumpter, B. G. and Noid, D. W. "Conformational Studies of Polymer Chains," American Physical Society National Meeting, Pittsburgh, PA, March 1994.

Getino, C., Sumpter, B. G. and Noid, D. W. "A Neural Network Approach to the Study of Dynamics and Structure of Molecular Systems," Artificial Neural Networks in Engineering Meeting, Rollo, MO, November 13-16, 1994.

Gray, S. K., Noid, D. W. and Sumpter, B. G. "Simple, Accurate Time Integration Method for Polymer Dynamics," American Physical Society National Meeting, Pittsburgh, PA, March 21-25, 1994.

- Grayce, C. J., Yethiraj, A. and Schweizer, K. S. "Liquid State Theory of Polymer Dimensions in Solutions and Melts," Poster, Gordon Research Conference on Chemistry and Physics of Liquids, Holderness, NH, August 1993.
- Grayce, C. J., Schweizer, K. S. and Yethiraj, A. "Solvation Potentials for Macromolecules," Poster, American Physical Society Meeting, Pittsburgh, PA, March 1994.
- Guenther, R. A., Noid, D. W. and Sumpter, B. G. "Implications of Quantum Chaology for Heat Capacities and Thermal Conductivities of Solids," American Physical Society National Meeting, Seattle, WA, March 1993.
- Habenschuss, A., Xenopoulos, A., Narten, A. H. and Wunderlich, B. "Structural Changes During Mesophase Transitions of Tetra-n-alkylammonium Halides," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.
- Habenschuss, A., Varma-Nair, M., Wunderlich, B. "The Phase Diagram of Copolymers of 4-Hydroxybenzoic Acid and 2,6-Hydroxynaphthoic Acid from X-Ray Diffraction and Thermal Analysis," Poster, American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.
- Jin, Y. and Wunderlich, B. "Single Run Heat Capacity Measurement by DSC: Principle, Experimental Detail and Data Analysis," in *Proc., 21st NATAS Conference*, Atlanta GA, Sept. 13-16, pgs. 151-156 (1992), *Thermochim. Acta*, (1993) **226**, 155.
- Jin, Y., Boller, A. and Wunderlich, B. "Heat Capacity Measurement by Modulated DSC at Constant Temperature," in *Proc., 22nd Annual North American Thermal Analysis Society Meeting*, Denver, CO, September 19-22, 1993, K. R. Williams, ed., pg. 59. Full paper: A. Boller, Y. Jin and B. Wunderlich, *J. Thermal Anal.* (1994) **42**, 307.
- Jin, Y., Xenopoulos, A., Wunderlich, B., Diack, M., Guiochon, G. A. and Compton, R. N. "Thermodynamic Properties of C_{70} ," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.
- Jin, Y., Boller, A. and Wunderlich, B. "Heat Capacities and Transitions in Perfluorinated Paraffins and Poly(tetrafluoroethylene)," Pitcon '93, Atlanta, GA, March 8-11, 1993.
- Lee, S. W., Cheng, S. Z. D., Lee, S. K., von Meerwall, E. D., Habenschuss, A. and Zschack, P. R. "Molecular Shape Effects on the Crystallization and Melting Behavior of Poly(ethylene oxide) Fractions," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.
- Lee, S. W., Cheng, S. Z. D., Lee, S. K., von Meerwall, E. D., Habenschuss, A. and Zschack, P. R. "Molecular Shape Effects on the Crystallization and Melting Behavior of Poly(ethylene oxide) Fractions," MACROAKRON '94, 35th International Union of Pure and Applied Chemistry International Symposium on Macromolecules, Akron, Ohio, July 11-15, 1994.
- Liang, G. L., Noid, D. W., Sumpter, B. G. and Wunderlich, B. "Molecular Dynamics: Effects of Surface-Constraints on the Crystal Structure. Phase Transition, Defect Distribution, Mass Transport

and Surface Melting in Polymethylene Crystals," American Physical Society National Meeting, Pittsburgh, PA, March 21-25, 1994.

Liang, G. L., Noid, D. W., Wozny, C. E., Sumpter, B. G., and Wunderlich, B. "Large Scale Molecular Dynamics Simulation on Polymer Systems," North Carolina Symposium on Molecular Modeling: Integration of Theory and Experiments, Research Triangle Park, NC, October 1993.

Londono, J. D. and Wignall, G. D. "Toward an Understanding of Polyethylene Blends: Miscibility and Morphology," Materials Science Department, The University of Tennessee, Knoxville, TN, August 1994.

Londono, J. D., Annis, B. K., Turner, J. Z. and Soper, A. K. "The Intermolecular Structure of Chain Liquids from Neutron Diffraction," American Institute of Chemical Engineers Meeting, San Francisco, CA, November 13-18, 1994.

Londono, J. D., Wignall, G. D., Narten, A. H., Honnell, K. G., Yethiraj, A. and Schweizer, K. S. "Asymmetries in the Flory-Huggins Interaction Parameter in Isotopic Polymer Blends," American Chemical Society General Meeting, Chicago, IL, August 22-27, 1993.

Londono, J. D. and Wignall, G. D. "The Flory-Huggins Interaction Parameter in Blends of Polystyrene and Polyparamethylstyrene from SANS," American Chemical Society Meeting on SANS and X-ray Scattering from Amphiphilic Block Copolymers in Solution, Washington, D. C., August 22-26, 1994.

Londono, J. D. and Wignall, G. D. "The Composition Dependence of the Interaction Parameter in Isotopic Polymer Mixtures," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.

McCoy, J. D., Honnell, K. G., Honeycutt, J. D., Curro, J. G. and Schweizer, K. S. "Single-Chain Structure in Model Polyethylene Melts," Centre European de Cacul Atomique et Moleculaire, University of Paris, Workshop on Generating Starting Structures for Polymer Simulation, April 13-15, 1993.

McCoy, J. D., Honnell, K. G., Curro, J. G., Schweizer, K. S. and Honeycutt, J. D. "Single-Chain Structure in Model Polyethylene Melts," American Physical Society Meeting, Seattle, WA, March 22-25, 1993.

Melenkevitz, J. G. and Curro, J. D. "Theory of Phase Behavior in Polymer Blends," American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Melenkevitz, J. and Curro, J. G. "Optimized Cluster Theory of Condensed Polymer Systems," American Physical Society Meeting, Seattle, WA, March 22-25, 1993.

Noid, D. W. "Use and Development of Massively Parallel Processing at Oak Ridge National Laboratory," University of Arkansas, Little Rock, AR, July 1993.

Noid, D. W. and King, W. L. "Research on Nanotechnology," Farragut Middle School, Farragut, TN, October 1993.

Noid, D. W., Darsey, J. A. and Sumpter, B. G. "Applications of Neural Networks in Polymer Simulations," in *Proc., Society of Plastics Engineers, ANTEC '93*, New Orleans, LA, March 22-26, 1993, 750 (1993).

Noid, D. W. and Sumpter, B. G. "Computational Studies of Polymeric Materials," Department of Materials Research, The University of Tennessee, Knoxville, TN, January 1993.

Noid, D. W., Wozny, C. E. and Sumpter, B. G. "The Spectral Analysis of Linear Polymers Using Classical Trajectories," American Physical Society National Meeting, Pittsburgh, PA, March 21-25, 1994.

Noid, D. W. and Sumpter, B. G. "Computational Simulations of Polymeric Materials," First Joint Meeting of Northeastern Ohio Modeling Interest Group and Pittsburgh Academic and Industrial Modeling Group, Youngstown, OH, May 1994.

Noid, D. W. "Applications of Neural Networks in Material Science," Master Builders, Inc., Cleveland, OH, August 1994.

Noid, D. W. "Applications of Neural Networks in Material Science," Argonne National Laboratory, Argonne, IL, August 1994.

Noid, D. W., Sumpter, B. G. and Tuzun, R. E. "Computational Nanotechnology," Third Annual Workshop of the Consortium For Nanostructured Materials, Oak Ridge, TN, October 1994.

Noid, D. W., Tuzun, R. E. and Sumpter, B. G. "Molecular Dynamics Simulation of a Graphite Molecular Bearing," 1994 Summer Computer Simulation Conference, La Jolla, CA, July 1994.

Schweizer, K. S. "Microscopic Theory of Polymer Liquids: A Unified Approach to Conformation, Structure and Phase Transitions," Chemistry Colloquium, University of Nebraska, Lincoln, NE, January 1993.

Schweizer, K. S. "Integral Equation Theories of Polymer Alloys," Physics Department, University of Mainz, Germany, March 1993.

Schweizer, K. S. "A Liquid State Theory Approach to the Statistical Mechanics of Polymers," Theoretical Physics Seminar, Department of Physics, University of Illinois, December 1993.

Schweizer, K. S. "Statistical Mechanics of Chain Molecule Liquids," Gordon Research Conference on Chemistry and Physics of Liquids, Holderness, NH, August 1993.

Schweizer, K. S. and Yethiraj, A. "Bulk Phase Transitions and Surface Segregation of Structurally Asymmetric Polymer Blends," American Physical Society Meeting, Seattle, WA, March 1993.

Schweizer, K. S. "Microscopic Theory of Polymer Liquids: A Unified Approach to Conformation, Structure and Phase Transitions," Department of Chemistry, Tulane University, April 1994.

Schweizer, K. S. "Integral Equation Theories of Polymer Alloys," Gordon Research Conference on Polymer Physics, Newport, RI, August 1994.

Singh, C. and Schweizer, K. S. "Correlation Effects and Phase Stability of Structurally Asymmetric Polymer Blends," Poster, Polymer Physics Gordon Conference, Newport, RI, August 1994.

Singh, C., Schweizer, K. S. and Yethiraj, A. "Fluctuation Phenomena in Polymer Blends," Poster, American Physical Society Meeting, Pittsburgh, PA, March 1994.

Sumpter, B. G. "Applications of Computational Neural Networks in Materials Science: An Introduction," Artificial Neural Networks in Engineering, St. Louis, MO, November 1994.

Sumpter, B. G. and Noid, D. W. "Neural Networks and Graph Theory as Tools for Predicting Polymer Properties," 1st DOE Workshop on Applications of Neural Networks in Materials Science, Knoxville, TN, February 28-March 2, 1994.

Sumpter, B. G., Noid, D. W. and Gakh, A. "Neural Network Prediction of Polymer Properties," American Chemical Society National Meeting, Washington DC, August 21-25, 1994.

Sumpter, B. G. "Computational Neural Networks as Tools for Predicting Materials Properties," Pittsburgh Paint and Glass Co., Pittsburgh, PA, August 1994.

Sumpter, B. G. and Noid, D. W. "Potential Energy Surfaces for Macromolecules: A Neural Network Approach," 1st DOE Workshop on Applications of Neural Networks in Materials Science, Knoxville, TN, February 28-March 2, 1994.

Sumpter, B. G. "Computational Simulations of Polymeric Materials," Chemistry Division, Cornell University, October 1993.

Sumpter, B. G. and Noid, D. W. "New Tools for Molecular Dynamics Simulation of Polymers," Scientific Computing and Automation Conference: Accessing New Resources--The Solutions for Science and Technology in the '90s, Washington, DC, October 11-13, 1993.

Sumpter, B. G., Getino, C. and Noid, D. W. "Computational Experiments on the Migration of Internal Energy in Macromolecular Crystals," 2nd International Discussion Meeting on Relaxations in Complex Systems, Alicante, Spain, June 28-July 8, 1993.

Sumpter, B. G., Noid, D. W. and Gakh, A. "A Computational Paradigm for Predicting Materials Properties," First Joint Meeting of Northeastern Ohio Modeling Interest Group and Pittsburgh Academic and Industrial Modeling Group, Youngstown, Ohio, May 1994.

Sumpter, B. G., Getino, C. and Noid, D. W. "A Neural Networks Approach to the Study of Internal Energy Flow in Macromolecular Systems," 1st DOE Workshop on Applications of Neural Networks in Materials Science, Knoxville, TN, February 28-March 2, 1994.

Sumpter, B. G., Noid, D. W., Gakh, A. and Darsey, J. A. "The Correlation of Properties for Polymers and Organic Compounds Using Neural Networks," American Physical Society National Meeting, Pittsburgh, PA, March 1994.

Sumpter, B. G., Noid, D. W. and Gray, S. K. "Computational Studies of the Mechanisms for Hydrogen Abstraction," 1994 Summer Computer Simulation Conference, La Jolla, CA, July 1994.

Sumpter, B. G., Gakh, A. A. and Noid, D. W. "Predicting Materials Properties Using Neural Networks," Artificial Neural Networks in Engineering Meeting, St. Louis, MO, November 1994.

Varma-Nair, M., Wunderlich, B., Grebowicz, J. and Bauer, R. "Thermal Analysis of Epoxy Resins," in *Proc., 21st NATAS Conference*, Atlanta GA, Sept. 13-16, pgs. 54-59 (1992). *Thermochim. Acta* (1993) 226 99.

Varma-Nair, M., Habenschuss, A. and Wunderlich, B. "The Phase Diagram of Copolymers of 4-hydroxybenzoic Acid and 2,6-hydroxynaphthoic Acid from X-ray Diffraction and Thermal Analysis," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.

Wang, Q., Annis, B. K., Habenschuss, A. and Wunderlich, B. "Investigation of the Surface Structure in Tetra-n-alkylammonium Halides by Atomic Force Microscopy," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.

Wang, Q., Annis, B. K., Habenschuss, A. and Wunderlich, B. "Investigation of the Surface Structure in Tetraalkyl Ammonium Halides by Atomic Force Microscopy," Polymer Division, American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1993.

Weeks, T., Zorlu, M., McCoy, J. D. and Curro, J. G. "Analysis of Polyolefin Blends by Differential Scanning Calorimetry: Detectability of Polypropylene in High Density Polyethylene/Polypropylene Blends," in *Proc., ANTEC '94, Society of Plastics Engineers Meeting*, May 1-5, 1994.

Wignall, G. D., Londono, J. D., Alamo, R. G., Mandelkern, L. and Stehling, F. C. "The Morphology of Blends of Linear and Branched Polyethylenes in the Solid State by SANS," American Physical Society Meeting, Pittsburgh, PA, March 21-25, 1994.

Wignall, G. D. "SANS from Synthetic Polymers," Exxon Chemical Company Research Center, Baytown, TX, April 29, 1994.

Wignall, G. D. "SANS Analysis of Compatibility and Demixing in Polymer Blends," Dow Chemical Company Research Laboratories, Freeport, TX, April 28, 1994.

Wignall, G. D., Londono, J. D., Alamo, R. G., Mandelkern, L. and Stehling, F. C. "The Morphology of Blends of Linear and Branched Polyethylenes in the Solid State by SANS," American Chemical Society Meeting, Washington, DC, August 22-26, 1994.

Wignall, G. D., Londono, J. D., Lin, J. S., Alamo, R. G. and Mandelkern, L. "The Morphology of Blends of Linear and Long Chain Branched Polyethylenes by Small Angle Neutron and X-ray Scattering," in *Proc., Materials Research Society Meeting*, Boston, MA, November 28-December 2, 1994 (in press).

Wozny, C. E., Sumpter, B. G., Noid, D. W. "Novel Methods for Spectral Analysis of Polymers," First Joint Meeting of Northeastern Ohio Modeling Interest Group and Pittsburgh Academic and Industrial Modeling Group, Youngstown, OH, May 1994.

Wozny, C. E., Noid, D. W. and Sumpter, B. G. "Mode-Specific Classical Trajectories and the Vibrational Analysis of Linear Polymer Chains," American Physical Society National Meeting, Pittsburgh, PA, March 21-25, 1994.

Wozny, C. E., Sumpter, B. G. and Noid, D. W. "Calculating the Vibration Spectra of Linear Polymers from Molecular Dynamics Trajectories," North Carolina Symposium on Molecular Modeling: Integration of Theory and Experiments, Research Triangle Park, NC, October 1993.

Wozny, C. E., Sumpter, B. G., Noid, D. W. and Wunderlich, B. "Vibrational Analysis of Random Coil Polyethylene," American Physical Society National Meeting, Seattle, WA, March 1993.

Wunderlich, B. "Molecular Dynamics Simulation and Thermal Analysis of Macromolecular Crystals," 13th Nordic Symposium on Thermal Analysis, *Thermochim. Acta* (1993) **214**, 103.

Wunderlich, B. and Jin, Y. "Thermal Properties of the Three Allotropes of Carbon," in *Proc., 21st NATAS Conference*, Atlanta GA, Sept. 13-16, 1992, pgs. 278-383 (1992). Updated and published as "Thermal Properties of the Four Allotropes of Carbon," *Thermochim. Acta* (1993) **226**, 169.

Wunderlich, B. "Unsolved Problems of Crystallization of Flexible Macromolecules. - Attempts at the Understanding of the Molecular Process by Experiments and Computer Simulation," *Proc., NATO Advanced Research Workshop on Crystallization of Polymers*, Mons, Sept. 7-11, 1992. Published in M. Dosire, ed., "Crystallization of Polymers," NATO ASI Series, C, Volume 405, Kluwer Academic Publishers, Dordrecht, The Netherlands, pgs. 237 (1993).

Wunderlich, B. "Remarks on Gradual Change of Conformational Disorder," American Physical Society Meeting, Pittsburgh, PA, March 21-24, 1994.

Wunderlich, B., Liang, G. L., Sumpter, B. G. and Noid, D. W. "Atomistic Details of Disordering Processes in Superheated Polymethylene Crystals II. Effects of Surface Constraints" Materials Research Society Meeting, Boston, MA, November 1993.

Wunderlich, B., Liang, G., Sumpter, B. G. and Noid, D. W. "Analysis of the Hexagonal Phases of Polymers and Oligomers," American Physical Society National Meeting, Seattle, WA, March 1993.

Wunderlich, B., Liang, L., Noid, D. W. and Sumpter, B. G. "Atomic Details of the Disordering Process in Superheated Polymethylene Crystals II. Effect of Surface Constraints," Materials Research Society Meeting, Boston, MA, November 29-December 3, 1993; published in *Crystallization and Related Phenomena in Amorphous Materials*, M. Libera, T. E. Haynes, P. Cebe, and J. E. Dickinson, Jr., eds. *MRS Proceedings*, Pittsburgh, PA, (1994) 321, 93.

Wunderlich, B. "Thermodynamische Charakterisierung von Mesophasen," Awards Lecture, Joint German Society for Thermal Analysis (GEFTA) and the Swiss Society for Thermoanalytic and Calorimetry (STK), Munich, Germany, September 13-15, 1993.

Wunderlich, B. "Thermal Properties of Fullerenes," Material Research Society Fall Meeting, Boston, MA, November 28-December 3, 1993.

Wunderlich, B. "Thermal Properties and Motion in C₆₀, C₇₀, and C₇₀ C₆H₅CH₃- Complex as Analyzed by DSC and NMR," Poster, Material Research Society Fall Meeting, Boston, MA, November 28-December 3, 1993.

Wunderlich, B. "Thermal Analysis of Mesophases," University of Osaka, Osaka, Japan, June 10, 1993.

Wunderlich, B. "The Three Phases in PET Fibers, Analyzed by Thermal Analysis and X-ray Diffraction," Materials Engineering Department, The University of Tennessee, Knoxville, TN, October 14, 1993.

Wunderlich, B. "The Three Phases in PET Fibers, Analyzed by Thermal Analysis and X-ray Diffraction," Fibers Gordon Conference, New London, NH, July 11-16, 1993.

Wunderlich, B. "The Rigid Amorphous Fraction of Crystalline Polymers," Two Lecture Series and Discussion at the Research Laboratory of the Toray Research Center, Otsu, Japan, June 7, 1993.

Wunderlich, B. "The Nature of the Glass Transition and Its Determination by Thermal Analysis," American Society for Testing and Materials Symposium on the Assignment of Glass Transition Temperatures Using Thermomechanical Analysis, Atlanta GA, March 3-5, 1993, in *ASTM STP 1249*, R. J. Seyler, Ed., American Society for Testing and Materials, Philadelphia, (1994) pg. 75.

Wunderlich, B. "The Basis of Thermal Analysis," 17th Symposium on Thermal Analysis, New York Polytechnic University, Park Ridge, NJ, April 19-21, 1993.

Wunderlich, B. "Solid State Physics of Polymers," Rensselaer Polytechnic Institute, Troy, NY, May 10, 1993.

Wunderlich, B. "Production of Single-Molecule Phases in Microgravity," Workshop on Organic and Polymeric Materials, NASA, Huntsville AL, April 27-28, 1993.

Wunderlich, B. "Polymer Films and Their Analysis" Research Facility of Medtronics Co., San Diego, CA, January 29, 1993.

Wunderlich, B. "Heat Capacities of C₆₀, C₇₀, and C₇₀ C₆H₅CH₃ and Their Transitions," Calorimetry Conference, Durham, NC, July 19-22, 1993.

Wunderlich, B. "Glass Transitions of Partially Ordered Macromolecules," Extended abstract in *Proc., 28th European Conference on Macromolecular Physics*, Sept. 27-Oct. 1, 1993, Ulm, Germany, Volume 17H, Paper G-8, pg. 1 (1993), *Colloid Polym. Sci.* (1994) 96, 22.

Wunderlich, B. "Defects in Polyethylene," EXXON Research Company, Linden, NJ, November 19, 1993.

Wunderlich, B. "Computer Simulation of Macromolecular Crystals and Their Defects," Osaka University International Macromolecular Symposium on Ordering in Macromolecular Systems (to recognize the 30 Year Anniversary of the Department of Macromolecular Science of the University of Osaka), Osaka, Japan, June 3-6, 1993.

Wunderlich, B. "Atomistic Details of the Disordering Process in Superheated Polymethylene Crystals," Material Research Society Fall Meeting, Boston, MA, November 28-December 3, 1993.

Wunderlich, B. "Analysis of the Hexagonal Phases of Polymers and Oligomers," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.

Wunderlich, B. "Thermal Analysis Instrumentation for the Measurement of Transitions in Polymers," Tutorial, 23rd NATAS Conference, Toronto, Canada, September 24-28, 1994.

Wunderlich, B. "The Measurement of the Glass Transition with Modulated DSC and Its Relation to Dynamic Mechanical and Electrical Analyses," 23rd North American Thermal Analysis Society Conference, Toronto, Canada, Sept. 24-28, 1994.

Wunderlich, B. "The Glass Transitions and Disordering Transitions in Polymers," Tutorial, 23rd North American Thermal Analysis Society Conference, Toronto, Canada, September 24-28, 1994.

Wunderlich, B. "The Defect State of Polymers Analyzed by Calorimetry, Solid State NMR and Molecular Dynamics Simulation," RayChem Research Laboratory, Menlo Park, CA, April 29, 1994.

Wunderlich, B. "The Defect State of Polymers, Analyzed by Calorimetry, Solid State NMR, and Molecular Dynamics Simulation," ICI Research Laboratory, Wilton, England, May 24, 1994.

Wunderlich, B. "The Crystal Morphology, Macroconformations and Defects of Polyethylene," Tutorial, RayChem Research Laboratory, Menlo Park, CA, April 29, 1994.

Wunderlich, B. "The Basis of Thermal Analysis," 18th Symposium on Thermal Analysis, Polytechnic University of New York, Park Ridge, NJ, April 18-20, 1994.

Wunderlich, B. "The ATHAS Data Bank of Heat Capacities of Linear Macromolecules," Plenary Lecture, International Union of Pure and Applied Chemistry International Symposium on Thermochemistry, Clermont-Ferrand, France, July 17-22, 1994.

Wunderlich, B. "The Advanced Thermal Analysis System (ATHAS)," Keynote Lecture on The Application of Differential Scanning Calorimetry to Physical Characterization of Polymers of the Royal Society of Chemistry, Society of Chemistry Industry and Analytical Division (Thermal Methods Group), London, England, May 26, 1994.

Wunderlich, B. "Single Chain Single Crystals," 35th International Union of Pure and Applied Chemistry Symposium on Macromolecules, MacroAkron '94, Akron, OH, July 11-15, 1994.

Wunderlich, B. "Bestimmung von Umwandlungsenthalpien ausserhalb des Umwandlungsbereiches," invited Introductory Lecture at the III Laehnwitz Seminar on Calorimetry about "Bestimmung von Umwandlungsenthalpien," Serrahn, Germany, June 2-4, 1994.

Wunderlich, B. "Crystallization During Polymerization," Shell Development Laboratories, Amsterdam, The Netherlands, May 31, 1994.

Wunderlich, B. "Gradual Change of Conformational Disorder," International Polymer Physics Symposium Honoring Professor Torhu Kawai's 70th Birthday, Tokyo, Japan, October 25, 1994.

Wunderlich, B. "Large-Amplitude Motion in Polymer Crystals and Mesophases," in *Proc., 35th International Union of Pure and Applied Chemistry International Symposium on Macromolecules, MacroAkron '94*, Akron, OH, July 11-15, 1994.

Wunderlich, B. "Large-Amplitude Motion in Polymer Crystals and Mesophases," University of Hiroshima, Higashi-Hiroshima, Japan, October 26, 1994.

Wunderlich, B. "Large-Amplitude Motion in Polymer Crystals and Mesophases," in *Proc., International Symposium on Polymer Crystallization*, Gakunan, Okayama, Japan, October 28-29, 1994.

Wunderlich, B. "Modulated Differential Scanning Calorimetry," ICI Paints Research Laboratory, Slough, Berkshire, England, May 23, 1994.

Wunderlich, B. "Modulated DSC - Capabilities and Limits," III Laehnwitz Seminar on Calorimetry (Bestimmung von Umwandlungsenthalpien), Serrahn, Germany, June 2-4, 1994.

Wunderlich, B. "Molecular Motion in Polymers Simulated by Supercomputer and Measured by Calorimetry," ICI Paints Research Laboratory, Slough, Berkshire, England, May 23, 1994.

Wunderlich, B. "New Observations about Phase Transitions," Department of Chemistry, December 8, 1994.

Xenopoulos, A., Mucha, M. and Wunderlich, B. "Nonequilibrium States of Symmetric Tetraalkylammonium Halides," 1993 MRS Meeting, Boston, MA, November 29- December 3, 1993; published in *Crystallization and Related Phenomena in Amorphous Materials*, M. Libera, T. E. Haynes, P. Cebe, and J. E. Dickinson, Jr., eds., *MRS, Proceedings*, Pittsburgh, PA., (1994) **321**, 53.

Xenopoulos, A., Cheng, J., Habenschuss, A. and Wunderlich, B. "Relaxations in Biopolymers: Studies of Main-Chain and Side-Chain Mobility in Three Poly(amino acids)," 2nd International Discussion Meeting on Relaxation in Complex Systems, Alicante, Spain, June 28-July 8, 1993.

Xenopoulos, A., Habenschuss, A., Narten, A. H. and Wunderlich, B. "X-ray Studies of Symmetric Tetra-n-alkylammonium Halides," Poster, American Physical Society Meeting, Seattle, WA, March 22-26, 1993.

Xenopoulos, A., Habenschuss, A. and Wunderlich, B. "X-Ray Diffraction Studies of Mesophase Transitions in Homologous Series of Symmetric Tetra-n-alkylammonium Halides," American Crystallographic Association '93 Meeting, Albuquerque, NM, May 23-27, 1993.

Xenopoulos, A., Jin, Y., Diak, M., Guichon, G., Compton, R. N. and Wunderlich, B. "Thermodynamic Properties of C70," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.

Xenopoulos, A., Londono, J. D., Wignall, G. D. and Wunderlich, B. "Phase Separation in Polystyrene-Poly(p-methylstyrene) Blends Using Thermal Analysis and Small Angle Neutron Scattering," Poster, Material Research Society Fall Meeting, Boston, MA, November 28-December 3, 1993.

Xenopoulos, A., Mucha, M. and Wunderlich, B. "Nonequilibrium States of Symmetric Tetraalkylammonium Halides," 2nd International Discussion Meeting on Relaxation in Complex Systems, Alicante, Spain, June 28-July 8, 1993.

Xenopoulos, A., Mucha, M. and Wunderlich, B. "Nonequilibrium States of Symmetric Tetraalkylammonium Halides," Materials Research Society Fall Meeting, Boston, MA, November 28-December 3, 1993.

Xenopoulos, A., Roles, K. and Wunderlich, B. "A Possible Glass Transition for Poly(L-methionine) and Poly(L-serine)," American Physical Society Meeting, Seattle, WA, March 22-26, 1993.

Yethiraj, A. and Schweizer, K. S. "Integral Equation Theory of Polymer Alloys: New Molecular Closure Approximations," American Physical Society Meeting, Seattle, WA, March 1993.

Other

Sumpter, B. G., Guenther, R. E., Halloy, C., Getino, C. and Noid, D. W. "Neural Network Simulations on Massively Parallel Computers: Applications in Chemical Physics," *Lecture Notes in Computation No. 686*, Springer Verlag (1994).

APPENDIX D: HONORS, AWARDS, AND PROFESSIONAL ACTIVITIES

M. D. Barnes

Martin Marietta Energy Systems Publication Award (with J. M. Ramsey and W. B. Whitten), 1994

C. M. Barshick

Co-Chairman, North American Glow Discharge Users Group, 1994-1995

P. V. Bonnesen

Martin Marietta Energy Systems Technology Transfer Award (with B. A. Moyer and R. A. Sachleben), 1994

A. C. Buchanan

DOE/BES Program Review on Coal Chemistry at Pacific Northwest Laboratory, 1994

R. A. Glenn Award (with P. F. Britt), Division of Fuel Chemistry, American Chemical Society, 1994

A. L. Compere

R&D-100 Award for development of the Cl_2 *LEANOUT* process (with W. L. Griffith, W. P. Huxtable, J. M. Googin, B. G. Davis, and R&D Solutions), 1993

D. C. Duckworth

Chairman-elect, American Society for Mass Spectrometry Elemental Interest Group, 1995-1996

Chairman-elect, North American Glow Discharge User Group, 1995-1996

W. H. Griest

Technical Communication Award, East Tennessee Chapter of the Society for Technical Communication, 1994

W. L. Griffith

R&D-100 Award for development of the Cl_2 *LEANOUT* process (with A. L. Compere, W. P. Huxtable, J. M. Googin, B. G. Davis, and R&D Solutions), 1993

G. A. Guiochon

Alexander von Humboldt Foundation Research Award for Senior American Scientists, 1994

R. L. Hettich

Martin Marietta Energy Systems R&D Accomplishment Award, 1994

B. A. Moyer

Secretary/Treasurer of the Separation Science and Technology Subdivision, Industrial and Engineering Division, American Chemical Society, 1991-1993

Associate Editor, *Solvent Extraction and Ion Exchange*, 1993-present

Vice Chairman elect, Separation Science and Technology Subdivision, Industrial and Engineering Division, American Chemical Society, 1994

Lind Lecture Committee, East Tennessee Section, American Chemical Society, 1994

Martin Marietta Energy Systems Technology Transfer Award (with P. V. Bonnesen and R. A. Sachleben), 1994

Editorial Board, *Hydrometallurgy*, 1994-present

D. R. Mullins

Newsletter Editor, Tennessee Valley Chapter, American Vacuum Society, 1994

J. R. Peterson

Member, Program Advisory Council, The Glenn T. Seaborg Institute for Transactinium Science, Lawrence Livermore National Laboratory, 1992-present

Councilor, Division of Nuclear Chemistry and Technology, American Chemical Society, 1993-1995

International Advisory Board, 2nd International Conference on f Elements, Helsinki, Finland, 1993-1994

Vice Chairman, Committee on Nuclear and Radiochemistry, Board on Chemical Sciences and Technology, National Academy of Sciences - National Research Council, 1992-1993

Alternate Councilor, East Tennessee Section, American Chemical Society, 1991-1993

M. L. Poutsma

Elected Fellow, American Association for the Advancement of Science, 1994

Editorial Advisory Board, *Energy and Fuels*, 1993-present

Board of Visitors, Chemistry Department, The University of Tennessee/Knoxville, 1994-present

J. M. Ramsey

Editorial Advisory Board, *Analytical Chemistry*, 1995-present

Instrumentation Advisory Panel, *Analytical Chemistry*, 1993-1995

Martin Marietta Energy Systems Publication Award (with M. D. Barnes and W. B. Whitten), 1994

L. Robinson

Chairman-elect, Board of Directors, Oak Ridge Housing Development Corporation, 1995

Member, Martin Marietta Energy Systems Honors and Awards Committee, 1993-present

Martin Marietta Energy Systems Outstanding Community Service Award, 1994

R. A. Sachleben

Martin Marietta Energy Systems Technology Transfer Award (with P. V. Bonnesen and B. A. Moyer), 1994

R. L. Schenley

Technical Publications and Art Competition Award for Mechanical Illustration and Tone Distinction, Local East Tennessee Chapter of the Society for Technical Communication (with D. G. Cottrell), 1994

R. W. Shaw

Chairman, Chemical and Analytical Sciences Division Improvement Council, 1994-1995

J. M. Simonson

Sunner Memorial Award of The Calorimetry Conference, 1993

Chairman, The Calorimetry Conference, 1993-1994

Pluperfect Chairman, The Calorimetry Conference, 1993-1994

ORNL Exploratory Studies Review Committee Chairman, 1992-1993

D. H. Smith

Martin Marietta Energy Systems R&D Accomplishment Award, 1994

F. J. Smith

ORNL Operations Support Award, 1994

Staff of Bldg. 2026

ORNL ALARA Award for dose reduction efforts during electrical upgrade of hot cells, 1994

P. J. Todd

Chairman-elect, East Tennessee Mass Spectrometry Discussion Group, 1994

D. J. Wesolowski

Associate Editor, *Geochimica et Cosmochimica Acta*, 1992-present

Adjunct Associate Professor, Department of Geological Sciences, The University of Tennessee at Knoxville, 1990-present

W. B. Whitten

Martin Marietta Energy Systems Publication Award (with M. D. Barnes and J. M. Ramsey), 1994

M. C. Woody

ORNL Most Valuable Player Award, 1993

J. P. Young

American Chemical Society representative to WATTEC Sponsors Committee, 1993-1995

Chairman, East Tennessee Section, American Chemical Society, 1993

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