A major purpose of the Technical Information Center is to provide the broadest dissemination possible of information contained in DOE's Research and Development Reports to business, industry, the academic community, and federal, state and local governments.

Although a small portion of this report is not reproducible, it is being made available to expedite the availability of information on the research discussed herein.

135
6/9/86 JS (2)

(15) I-26465

DR-1739-6

ornl

ORNL-6236

ORNL--6236

DE86 011350

OAK RIDGE
NATIONAL
LABORATORY

MARTIN MARIETTA

Analytical Chemistry Division Annual Progress Report For Period Ending December 31, 1985

W. D. Shults

MASTER

OPERATED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A05 Microfiche A01

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL-6236
Distribution Category UC-4

Contract No. DE-AC05-84OR21400

ANALYTICAL CHEMISTRY DIVISION ANNUAL PROGRESS REPORT

For Period Ending December 31, 1985

W. D. Shults, Director

Date Published - May 1986

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
operated by
MARTIN MARIETTA ENERGY SYSTEMS, INC.
for the
DEPARTMENT OF ENERGY

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Page

DIVISIONAL MAN-POWER AND FINANCIAL SUMMARY FY 1985 79

ORGANIZATION CHART 80

CONTENTS

	Page
INTRODUCTION	vii
HIGHLIGHTS	ix
1. ANALYTICAL SPECTROSCOPY	1
Analytical Instrumentation R&D	2
Analytical Spectroscopy	2
Laboratory Robotics	4
Special Instrumentation	4
Spectroscopic R&D Programs	5
Organic Mass Spectrometry	6
Resonance Ionization Mass Spectrometry	7
Positron Spectroscopy	7
Heavy-Ion Induced X-Ray Satellite Emission	8
Transuranium Research Laboratory	9
Secondary Ion Mass Spectrometry	10
Organic SIMS	10
Sputter Atomization/Resonance Ionization Mass Spectrometry	11
Actinides and Isotopic Mass Spectrometry	12
2. RADIOACTIVE MATERIALS LABORATORIES	13
Programs and Projects	14
X-Ray Fluorescence Development	14
HTGR Base Technology Program Support	14
Database Software for the Oak Ridge Managed Deer Hunt	15
Radioactive Materials Analytical Laboratory	15
Fuel Recycle Division Support Laboratory	17
Transuranium Analysis Laboratory	17
3. INORGANIC CHEMISTRY	19
Chemical and Physical Analysis	20
Environmental Analysis Laboratory	21
Low-Level Radiochemical Analysis	22
Radiochemical and Activation Analysis	23

Page

4. ORGANIC CHEMISTRY SECTION 25

Organic Analysis 26

Separations and Synthesis 27

Special Projects 29

5. THE ORNL ENVIRONMENTAL RESTORATION AND FACILITIES UPGRADE PROGRAM 33

6. QUALITY ASSURANCE, SAFETY, AND TABULATION OF ANALYSES 35

Quality Assurance 35

Radiation Safety 36

Safety 37

7. SUPPLEMENTARY ACTIVITIES 41

Advisory Committee 41

Consultants 41

Student Assignments 42

Summer Program 42

GLCA Program 42

ORAU Faculty Research Program 42

ORAU Postgraduate Research Training Program 43

Special Awards 43

28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology 43

Analytical Chemistry Division Seminars at ORNL 43

Additional Professional Activities 45

8. PRESENTATION OF RESEARCH RESULTS 51

Publications 51

Contributions to Books, Proceedings, and Reports 51
Articles 56
Reports 62
Oral Presentations 68

Articles Reviewed or Refereed for Periodicals 78

HIGHLIGHTS

We developed a totally new proof-of-principle measurement system capable of providing real-time in situ analysis of absorber concentration within an operating absorption heat pump. The measurement is based on light loss from a stripped optical fiber, when the refractive index of the fluid in contact with the fiber core changes. Initially, experiments were conducted with a single optical fiber model of this "heat pump refractometer." Later, a multiple optical fiber system was developed. The system was used to follow changes in LiBr concentration during operation of an absorption test vessel. This work is continuing with the objective of improving system performance and applying it to other heat exchange fluids.

We have investigated the use of laser optogalvanic detection to observe intermediate molecular species during the chemical vapor deposition (CVD) of amorphous silicon. An optogalvanic signal is generated by illuminating a glow discharge plasma with a pulsed laser beam and then scanning the laser frequency. Silicon hydride was chosen as a test analyte species because it has been well characterized by conventional spectrometric methods, and because it is important in the growth of hydrogenated films. Optogalvanic detection has several advantages over other spectroscopic techniques for CVD interrogation: there is direct electrical signal generation, no optical background noise, and excellent sensitivity. Also, it can be used to analyze non-emitting species present in CVD plasmas.

We have studied the gas-phase ion chemistry and structures of nitroaromatic ions this year. The mechanism for the loss of $OH^{\bullet}$ from o-nitroaromatic compounds by the so-called "ortho" effect has been elucidated. We also studied the energy loss and the mechanism of NO elimination. This work has led to the development of an MS/MS instrument for detecting explosives. It is an extension of the tandem quadrupole/time-of-flight mass spectrometer that we constructed earlier. Much work has gone into designing and testing an atmospheric pressure ionization source for this system.

A Fourier transform mass spectrometer (Nicolet FTMS-2000) was installed in September. It is a new generation mass spectrometer capable of extremely high resolution and mass range. It is the first instrument of its kind to be used within the DOE family of laboratories.

Our research into resonance ionization mass spectrometry (RIMS) has continued, with emphasis on obtaining a better understanding of the optical processes involved. An electron energy analyzer was incorporated into the RIMS system to obtain the electron energy spectra of the photoelectron that is generated in the resonant ionization process. The electron energy spectra we obtained were unexpectedly complex, but once the complexity was understood, various spectra could be calculated for alternate optical processes and compared with experimental spectra. We have done this for about ten transitions.

Our development of sputter atomization/resonance ionization mass spectrometry has continued with emphasis on refinements in the instrumentation and software. Optical and mass spectra of uranium and samarium were studied in some detail, and we established that the RIMS optical spectra observed for sputter atomization agree well with those obtained by thermal atomization. The mass spectra indicated metal ion peaks in the expected isotopic abundancies when the laser was fixed on a resonant wavelength. Metal oxide peaks were also observed at all wavelengths scanned by the laser, which suggests that residual oxygen is interacting with the metal to produce oxide species that are ionized in a nonresonant process.

Studies into the fundamentals of organic secondary ion mass spectrometry (SIMS) have continued. This year we developed a new reservoir system and probe inlet that provides sample to the target surface in a uniform manner by capillary action. This system permits generation of secondary ions of constant intensity and relative abundance for up to 2 h. The reservoir probe system has enabled us to study the relationships between secondary ion intensity characteristics of analytes dissolved in or adsorbed onto a liquid matrix. Secondary ion emission has been found to depend on chemical kinetics. We are attempting to develop a model that describes the behavior of organic secondary ion emission as observed experimentally. A patent is pending on the reservoir probe.

A new GC detector was conceived, designed, and constructed this year. It is an electron capture detector that uses ^{63}Ni as the source and which allows the pressure in the detector to be varied from atmospheric to less than 1 torr. Conventional electron capture response is obtained at atmospheric pressure. At reduced pressure the device gives a uniform response from all analytes, similar to that of a flame ionization detector. At intermediate pressures (about 100 torr) an isomer-selective response is observed. Thus, we have a multimode ionization detector that combines the features of three different detectors. We expect this system to be useful not only for identifying isomers in complex mixtures, but also for detecting classes of compounds. A patent on this device has been filed.

We developed and demonstrated a hybrid instrument of the QEB geometry this year. This was done by interfacing a quadrupole to the front end of an MS50 high-resolution mass spectrometer. This new development enabled a variety of experiments to be done. An EI/CI ion source has been constructed for the new system, which was selected as one of the "Top 100 Innovations" of the year by *Science Digest* magazine.

We are developing a supersonic jet sampling technique for combustion diagnostics. The idea is to rotationally cool combustion gases by supersonic expansion and then study them by high-resolution, laser-induced fluorescence spectroscopy. The apparatus utilizes a 3-hp Briggs and Stratton gasoline engine modified so that combustion gases can be withdrawn while the engine is running; thus dynamic measurements can be made. We have shown that this cooling technique is sufficient for high-resolution spectroscopy under these operating conditions.

We have continued to study the use of passive phase-conjugate reflectors in optical spectroscopy. Our studies this year have been extended to the use of ring dye lasers in conjunction with a $BaTiO_3$ reflector. This system exhibits improved resolution and passive wavelength scanning, as we earlier observed with linear laser systems. Linewidths as narrow as 1.3 GHz are obtained. A scan rate of .0001 nm/s is obtainable, and faster scan rates can be obtained by displacing the reflector by a few centimeters.

Work in developing a ^{68}Ge source for monoenergetic positrons has been completed. Positron scattering studies of W, Mo, Cu, and Si surfaces indicated that the positron spectra at low scattering angles show much higher cross sections than do electron spectra. We are continuing to study positron lifetime spectroscopy, with emphasis on the examination and determination of internal and external surface areas. We have tried to apply this technique to the determination of fumed silicas (cabosils) and composites of carbon fibers and epoxy. These latter materials are widely used in aircraft structures. It is important to know if voids develop or delamination occurs in such structures, since those characteristics can decrease the strength of the aircraft.

A pulsed, helium ionization detector was developed to operate in a constant-current, closed-loop mode. The closed-loop mode was found to decrease noise and background current levels, thus improving operating stability. The dynamic range was extended about two orders of magnitude. This development was awarded an IR-100 award this year by *Industrial Research* magazine.

An important milestone was reached this year when isotopic analyses were completed on a fuel pin that had been irradiated 90 days at full power in the Dounreay prototype fast reactor in Scotland. Isotopic analyses were completed on 21 actinides in this fuel pin. Two other fuel pins will be analyzed as part of this experiment, which is a joint US/UK actinides research program. The program is intended to measure and calculate the burnup and production of various actinides in milligram samples of highly enriched actinide isotopes, as a check on cross sections, measurement techniques, and computational protocols.

There has been public concern recently about the enhanced toxicity of smoke from so-called clove cigarettes imported from Indonesia (kreteks). We were asked by the National Cancer Institute to study the composition of those cigarettes and compare them with normal cigarettes. Both GC and GC/MS were used to survey the vapor and particulate phases of the smoke. No major clove-derived constituents were found in the vapor phase, but five major clove-specific constituents were identified in the particulate phase. Our data have been used to help direct pulmonary toxicity studies being conducted at another laboratory for the National Cancer Institute.

We developed a system this year for probing the chemical composition of deep well waters. A commercially available sample probe was modified extensively for this purpose. The system consists of a sampling probe capable of collecting deep well waters at depths in excess of 1000 ft and a facility designed to measure, collect, and dissolve gases. This system is portable enough to be used in the field. It has performed satisfactorily in preliminary tests in nonradioactive wells. This device makes it possible to make a complete analysis of well waters (including dissolved gases) to obtain a better understanding of the geochemistry of the surrounding formations.

This year for the first time, ORNL, in conjunction with the Tennessee Wildlife Resources Agency, conducted a controlled deer hunt on the Oak Ridge reservation in an attempt to lessen the deer herd population and improve safety in the area. Analytical Chemistry played a major role in this project, because it was our job to monitor the harvested deer individually for radioactivity to ensure public safety. One aspect of that program was the development of a custom-made computer program to handle all the data in a user-friendly manner and in real time. During each hunt, information about the hunter, deer, radioactivity, etc., were entered into the data base. The information could then be formatted in any number of ways to meet the needs of the hunter or ORNL and TWRA personnel. Daily information was merged into a master file so that reports covering the entire hunt could be prepared, or subsets of information could be examined. Some 926 deer were harvested during five weekend hunts in the months of October, November, and December.

During 1985 we initiated separation studies based on the electrokinetic migration of micelles in capillary tubes. In this technique, an open tube is filled with a buffered solution of the surfactant. When a dc voltage is applied to the column, ionic micelles migrate toward the electrode of opposite charge. Analyte molecules diffuse in and out of the migrating micelles and are partitioned there. An efficiency approaching 60,000 theoretical plates was obtained by this approach for a series of derivatized aliphatic amines.

Studies have continued on degenerate four-wave mixing spectroscopy for trace element analysis in flames. This technique offers Doppler free spectra. Theoretical detection limits are 1 ppb for sodium using a pulse laser and 0.1 ppt using a CW laser. Experimentally, we are able to detect sodium at the 200-ppb level. The experimental detection limit is governed by scattered light.

A new research effort in microwave spectroscopy was initiated. Preliminary experiments are aimed at measuring the relative abundancies of ^{16}O and ^{18}O in carbonyl sulfide by microwave absorption spectroscopy. The objective is to develop a simple and reliable technique for measuring stable isotope abundance ratios.

Our collaborative research program with the University of Tennessee at the Transuranium Research Laboratory has continued. A new diamond-anvil cell has been designed and built. It is capable of exerting pressures exceeding 30 GPa. With this cell, we are studying the effect of pressure on the spectra of actinide halides. Several lanthanide compounds have also been studied. In general, our results show that the bromides and iodides transform irreversibly to the most dense structure at less than 5 GPa.

The division was granted approval to operate new laboratories in Building 2026 in August 1985. The facility is being equipped to handle inorganic and organic "priority pollutants" analysis on radioactive materials. This new addition and the existing facilities in Building 2026 will provide the division with unique facilities for handling hazardous materials.

Construction of a new neutron activation analysis laboratory at the High Flux Isotope Reactor is scheduled to begin in March 1986. As part of the project, a second pneumatic tube will be installed, which is expected to provide a well-thermalized neutron flux. This facility will allow us to consolidate all NAA operations into one state-of-the-art facility.

1. ANALYTICAL SPECTROSCOPY

J. A. Carter

The Analytical Spectroscopy Section is the result of the merging of the Analytical Methodology and Mass and Emission Spectrometry Sections and is now composed of four groups: Actinides and Isotopic Mass Spectrometry, Inorganic and Secondary Ion Mass Spectrometry, Analytical Instrumentation R&D, and Spectroscopic R&D Programs. Research and development efforts in each group are directed toward enhancing analytical capabilities through new discoveries and developing a clearer understanding of fundamental physical processes that can be exploited into new instruments or analytical approaches for solving energy problems for DOE. Several projects toward this goal are described in the following technical summaries; however, some of the most outstanding examples of achievements are noteworthy: (a) the QEB (quadrupole/electrostatic/magnetic) high-resolution three-stage mass spectrometer for gas-phase chemistry studies (this project won a "Top 100 Innovation Award" from *Science Digest*); (b) the special design of the mass spectrometry/mass spectrometry (MS/MS) instrument for detecting nitrated compounds; (c) sputter atomization/resonance ionization instrumentation for low level actinide detection; (d) degenerate four wave laser mixing for trace elemental analysis under Doppler-free conditions; (e) real-time in situ analysis of heat pump fluids by fiber optic techniques; and (f) surface area and defect measurements by positron spectroscopy.

About 45% of the section's research and development support is provided by the Division of Chemical Sciences of the Office of Basic Energy Research, U.S. Department of Energy. This effort, broad in nature, provides the Analytical Chemistry Division the technical base from which current and future spectroscopic needs of DOE are addressed. Another 25% of the section's R&D funding is about equally distributed between DOE Offices of Safeguards and Security, International Security Affairs, and Health and Environmental Research. The projects for these funding sources are generally short range and of an applied nature. The balance of our effort is funded by other laboratory programs (seed money), various interagency agreements (FAA, ISPO/State, and IAEA), and other work-for-others contracts.

ANALYTICAL INSTRUMENTATION R&D

H. H. Ross

One of the most satisfying aspects of research in analytical chemistry is seeing one's experimental and theoretical work transformed into the practical solution of a "real-world" measurement problem. ORNL provides an almost perfect environment to realize such an approach. As new analytical techniques are brought from the laboratory, there is almost certainly an on-site opportunity for testing and refinement. In our group, the natural rhythm of the research/implementation cycle has substantially favored new research initiatives during the past few years. This year, in contrast, we have had significant success in bringing our work to the demonstration stage. The result is that some critical analytical measurements can now be done faster, more accurately, or cheaper than before; in other cases, we can make measurements that previously were not even possible!

We have not, however, neglected our commitment to innovative research; many new approaches are described here. Also, we have highlighted interactions between group members and other organizational units at the Laboratory. We feel that such interactions help to maintain the vitality of our overall effort.

Analytical Spectroscopy

We have noted previously that feedback from a $BaTiO_3$ passive phase-conjugate reflector (PPCR) can greatly affect an untuned continuous-wave (CW) dye laser. The salient features of the feedback effect are dramatic line-width reduction (to a few GHz) and repetitive, monotonic self-scanning of the wavelength over tens of nanometers. Earlier experiments made use of a linear standing-wave laser cavity. More recently, we have used a ring laser cavity for the phase conjugate feedback experiments. Ring dye lasers operating in traveling wave mode are known to have narrower bandwidths than comparable linear cavity designs. The reduced bandwidth is the result of a more uniform spatial interaction of the optical fields with the gain medium. We have observed bandwidths as small as 1.3 GHz in experiments where the $BaTiO_3$ PPCR is the sole tuning element for a CW ring dye laser. This bandwidth is a factor of 3 narrower than that observed with the $BaTiO_3$-linear laser.

The $BaTiO_3$-ring laser also exhibits the passive wavelength scanning effect. When the combined length of the external cavity formed by the PPCR is equal to the ring circumference, the frequency is relatively stable with a scan rate of 0.0001 nm/s, and the linewidth is narrow, 1.3 GHz. Displacement of the crystal or retromirror by a few centimeters results in a higher scan rate ($\sim$ 0.02 nm/s), and the output spectrum contains a mode beat pattern with somewhat greater effective linewidth ($\sim$ 3–5 GHz). The additional spectral structure is expected from the interaction of the laser cavity with the additional cavities formed by the PPCR. The output wavelength will scan more than 10 nm to the red of the starting wavelength, then repeat indefinitely, as observed before.

A new research effort has been initiated in the area of microwave spectroscopy. The objective is to develop a simple and reliable technique for the measurement of stable isotope abundance ratios. A preliminary experiment has been designed to measure the relative abundances of ^{16}O and ^{18}O in carbonyl sulfide by microwave absorption spectroscopy. A Fabry-Perot cavity will be used as the absorption cell, thus providing a multipass advantage. The cavity length will be adjusted so that both absorption frequencies are longitudinal modes of the resonator. The $J = 1 \leftarrow 0$ transitions of ^{16}OCS and ^{18}OCS will be monitored. These two transitions differ in frequency by 753 MHz, corresponding to a cavity spacing of 19.9 cm. A super-heterodyne detection scheme will be used to alternately monitor the two transitions.

We have continued our evaluation of degenerate four-wave mixing (dfwm) spectroscopy for trace elemental analysis in analytical flames. The dfwm technique allows the measurement of Doppler-free spectra, thus increasing spectral resolution and potentially enhancing the ability to determine isotopic abundances by optical means.

Theoretical calculations show a fundamental limit of detection for typical atomic transitions of about 10^{-5} absorbance units for 10-ns laser pulses and a 1-s time constant. The use of a CW laser lowers this value by a factor of 10^4. Using typical conversion factors relating solution and flame atom densities, a detection limit of 1 ppb is calculated for sodium using a pulsed laser. This detection limit

compares favorably to that of flame atomic absorption spectrometry. Calculated limits of detection using a CW laser are 0.1 ppt, or better than those achieved with laser-excited fluorescence in a flame or with inductively coupled plasma spectrometry.

Experimental measurements have been made with an Nd-YAG pumped-pulsed dye laser. Spatial filtering and polarization selection have been used in the detection system to reduce background signals, as previously reported. Our current measured detection limit is 200 ppb sodium in water. The detection limit is currently limited by scattered light from the backward pump beam into the detection system. The scattering is from a nebulized solution that has not evaporated before passing into the laser interaction region. This nonresonant scattering can possibly be reduced by using a different polarization scheme. A comparison of measured detection limits with calculated values or those achieved by other techniques is difficult because of the uncertainty associated with transport of species in solution to the flame. A critical evaluation of dfwm for analytical flame spectroscopy can only be made by knowing the atom density in the laser interaction region. We will attempt to determine the atom density by absorption measurements.

A supersonic jet sampling technique for combustion diagnostics is being developed. The technique uses supersonic expansion to rotationally cool combustion gases so that they can be studied with high-resolution laser-induced fluorescence spectroscopy. The apparatus, consisting of a 3-hp Briggs and Stratton gasoline engine, modified cylinder head, optical vacuum manifold, and pumping system, has been completed. Initial experiments were made with the Quanta Ray pulsed dye laser as the excitation source and NO_2 as the analyte. The rotational cooling of NO_2 by combustion gases (with the engine running) to about 16 K compares favorably with the cooling that can be obtained with the same nozzle and pure N_2 (18 K) or Ar (8 K) under stationary conditions. In the latter measurements, the NO_2 and carrier gas were injected through the spark plug hole of the stationary engine. The dynamic measurements were made with NO_2 added to the intake air stream. The experiments showed that cooling by expansion of combustion gases is sufficient for high-resolution spectroscopy.

Chemical vapor deposition (CVD) is widely used to create coatings and thin films for many applications in the microelectronics, wear-resistant coatings, electrooptics, and solar photovoltaic energy conversion industries. However, incomplete understanding of the fundamental processes occurring during glow discharge depositions has caused difficulties in achieving reproducible electrical and optical properties of coatings.

The deposition of hydrogenated amorphous silicon (a-Si:H) films by the glow discharge decomposition of silane is now a common method for solar cell production because economical, large-area depositions can be made on inexpensive substrates at low temperature. We have investigated the use of laser optogalvanic detection to observe intermediate molecular species during the glow discharge deposition of a-Si:H. The optogalvanic signal resulting from the analyte species was generated by illuminating a discharge plasma with a pulsed laser beam and scanning the laser frequency across optical transitions. The two biased electrodes used to sustain the dc discharge served as signal sensors in this detection scheme, and the cathode also served as substrate for deposited films. The intermediate silicon hydride was chosen as a test analyte species because its $A^2\Delta - X^2\pi$ transition has been well characterized by conventional spectrometric methods, and because of its probable role in the growth of hydrogenated films.

A demountable, hollow cathode dc discharge cell was constructed and tested for plasma stability, efficiency, and ease of operation. It was designed so that it could be disassembled, have its electrodes (substrates) replaced, and be reassembled vacuum-tight within seconds without using any tools. Controlled depositions of amorphous silicon films on the cathode substrate were accomplished using silane, silane-He, and silane-H_2 mixtures. The spatial silicon content of the film was examined using energy-dispersive X-ray fluorescence and found to be highest near the hollow cathode cavity at the base of the electrode. Preliminary Raman spectra of the films indicate noncrystallinity. The intermediate species SiH resulting from the decomposition of SiH_4, was monitored by recording its optogalvanic spectrum ($A^2\Delta - X^2\pi$) at 400 to 425 nm. Such gas-phase silicon hydrides are thought to have a bearing on the microscopic structure of the hydrogenated thin film product.

Compared with other spectroscopic techniques, such as fluorescence spectroscopy, optogalvanic

detection generally has many advantages, including direct electrical signal generation, no optical background noise, and excellent sensitivity. Most importantly, it can be used to analyze nonemitting species present in CVD plasmas. Additional studies to demonstrate interesting applications of this technique are currently under way for silane and other discharges.

(J. M. Ramsey, R. W. Shaw, W. G. Tong, W. B. Whitten)

Laboratory Robotics

Our robotics work has largely involved two major activities: programming for method implementation and design of special hardware modules. A second analytical procedure designed for the robot was a fluorometric method for determining uranium. After some preliminary testing, we determined that the conventional laboratory procedure could be used with the robot with only minor changes. The resulting automated method is used to process original samples to the "aliquot-on-pellet" stage; the pellet ignition and fluorescence measurement remain for the technician. During the course of adapting the existing procedure to the robot, we found it necessary to develop a hardware module to handle the necessary solvent extraction step. We designed a simple mixing station to accomplish this task.

A study of the robot procedure was carried out with both uranium control samples and real samples. The results show that the robot system can perform at an acceptable level for the uranium concentrations usually encountered.

We previously reported that a major application of robotics systems is in the automation of procedures that involve very large numbers of identical operations. This type of operation was tested on two occasions. The division needed to prepare more than 1000 sealed glass ampoules containing standards to be used for gas chromatographic calibrations. A variety of materials were to be encapsulated. We were able to develop a procedure in which the robot quantitatively pipetted the desired compound(s) into the ampoule. The procedure was unusual in that it was written to work in concert and in real time with a technician who flame sealed the loaded ampoule. Random samples of the finished standards were analyzed to assess the robot's performance. In all cases, the samples were found to be within the required control limits. Because some of the samples prepared were as small as 0.1 μl, the use of the robot for accurate work seems well established.

During this period, a number of hardware improvements were incorporated into the system. A new ROM operating system was installed in the robot controller that enabled some new system functions and improved others. We also redesigned our shaker controller logic, replaced our disk drive, updated the capping station, and carried out general maintenance.

(C. S. Alley, H. H. Ross)

Special Instrumentation

Funding was obtained through the ORNL Energy Division under the DOE Energy Conservation Program to develop a proof-of-principle measurement system capable of providing real-time in-situ analysis of absorber concentration within an operating absorption heat pump. The measurement is based on light loss from a stripped optical fiber as the refractive index of the fluid in contact with the fiber core changes.

A single optical fiber model of the heat pump refractometer was assembled to determine the response surface for LiBr as the absorber fluid. A multivariant experiment was then conducted to determine the optimum fiber diameter, fiber exposure length, and the effect of solution temperature on the LiBr measurement. The optical response was found to be second order with respect to both LiBr concentration and temperature. An empirical calibration equation was derived to describe this behavior; a theoretical explanation for the observed response was also formulated. A 600-μ optical fiber with at least 2 cm of the fiber core exposed yielded the greatest sensitivity to changes in LiBr concentration and demonstrated the mechanical characteristics required for installation in an absorption heat pump.

Multiple optical fibers were installed in an absorption test vessel to demonstrate real-time in-situ measurement of the LiBr concentration along the heat exchange tubes. A chopper wheel was used to multiplex light from an incandescent source through the optical fibers to a single detector. The temperature of each tube in the heat exchanger, as well as the inlet and outlet cooling water, was monitored with thermocouples.

Data acquisition was based on a HP-85 computer, a HP-3456A digital multimeter, and a 3497A data acquisition control unit. Each signal was integrated over several power line cycles to minimize the noise from this source. The noise on the optical signals (normalized with respect to the source) was approximately 0.14%. Repeatability of the optical signals measured over a 4-d period was less than 0.5%. The system was used to successfully follow changes in LiBr concentration over the 42 to 55 (± 0.5) wt/wt% LiBr range during operation of the absorption test vessel.

Current work is directed toward evaluating alternative light sources and multiplexing concepts to improve the concentration resolution and range of the measurement. The system will also be applied to the measurement of other heat exchange fluids being considered for use in advanced cycle absorption machines.

The development of remote analytical instrumentation has focused on the completion of work on the titrations system. The potentiometric titrator has been in routine use for approximately 2 years in support of operations at our Transuranium Analytical Laboratory. An electronic noise problem was solved by replacing the in-cell transducer preamplifier enclosure system with a unit having revised internal wiring to eliminate a ground loop. Software modifications included the addition of a memory test routine upon power-up and/or a hardware reset, an improved format for the titration plot (with additional features in the replot option), and correction of a problem associated with an occasional failure of the system to automatically terminate a titration. The revised program has functioned without any reported problems.

The assembly of the remote hardware and the electronic system for the amperometric titration system was completed. Initial attempts to use the in-cell amperometric transducer electronics, which employed a grounded load resistor, resulted in this circuit oscillating at the frequency of the computer switching power supply. The circuit was redesigned to use a current-to-voltage converter, thereby eliminating a voltage feedback network required by the former design. The revised circuit performs satisfactorily.

Laboratory evaluation of the amperometric system was completed. Although a few software problems were uncovered, no major difficulties were encountered. The standardization portion of the procedure "Plutonium by Amperometric Titration with Iron(II)," which is defined in ASTM Standard Method C697, was used. Potassium dichromate served as the oxidant in this evaluation. For aliquots of $K_2Cr_2O_7$ ranging from 0.02702 to 0.2161 meq, the standard error of the end point was 0.00022 meq. Expressed in terms of the mass of ^{239}Pu required for an analysis, these aliquots correspond to an approximate sample range of 3.2 to 26 mg, with a standard error of analysis of 0.026 mg.

A trip was made to the United Kingdom Atomic Energy Authority Nuclear Power Development Establishment at Dounreay, Scotland, and to Harwell Laboratory at Oxfordshire, England. The purpose of the trip was to develop the technical portion of a Specific Memorandum of Agreement (SMA) concerning an exchange program on in-line spectrophotometry for breeder fuel reprocessing plants, and to review the process control, process support, and process development activities related to breeder fuel reprocessing. The SMA is being implemented under the Department of Energy and United Kingdom Atomic Energy Authority Liquid-Metal Fast Breeder Reactors Agreement of September 20, 1976.

The Prototype Fast Reactor reprocessing plant at Dounreay has a capacity of 30 kg/d of heavy metal. It has approximately 100 sample points, which yield an average of 200 determinations per day. The chemical support for this plant requires 44% of the plant operating budget. Since 1980, some instrumentation has been added to the plant, and it is estimated that annual savings of $740,000 are being realized. Further details on the analytical chemistry support for the Dounreay reprocessing plant can be obtained from ORNL/FTR-2043.

(D. A. Bostick, L. N. Klatt)

SPECTROSCOPIC R&D PROGRAMS

D. H. Smith

This group is comprised of investigators in a number of disparate disciplines. A single motif informs all the work, however; research is directed at expanding knowledge that will ultimately enhance analytical capabilities. Four examples of this thrust are cited here. The one that seems nearest to fruition is in the area of organic mass spectrometry; fundamental gas-phase ion chemistry studies have led to a

current project to develop an explosives detector based on the principles of mass spectrometry/mass spectrometry. A second effort of this type is in the area of resonance ionization mass spectrometry, where our goal is to develop a sophisticated new instrument for use in isotope ratio measurements. The third example has evolved from our positron research; we have good evidence that positron annihilation can be applied to the measurement of surface areas and to the detection of voids and other internal defects in composite materials. The last such area to be cited is in heavy-ion induced, X-ray satellite emission studies, where important information concerning the chemical state of species in alloys and other solid specimens can be obtained. All of these areas are technically challenging and offer the potential of yielding significant advances in the state of analytical art.

Organic Mass Spectrometry

Much of the effort in organic mass spectrometry has gone into work related to explosive compounds. This work can be divided into two major areas. One is the study of the gas-phase chemistry and ion structures of nitroaromatic ions, and the other is the development of an explosives detector. In the first area, the mechanism behind the loss of OH· from ortho-nitroaromatic compounds by the so-called "ortho" effect has been elucidated. In the radical cation species, transfer of a hydrogen atom to the nitro group occurs from hydrogen containing ortho substituent, with the barrier for reaction being related to the homolytic bond energy of the H bond being ruptured. In the case of the corresponding anions, however, a proton is transferred, with the barrier thus being related to the heterolytic bond energy of the ruptured bond. Although homolytic bond energies show little variation between substituents, heterolytic bond energies can be quite different. This accounts for the fact that the loss of OH· from the cations is universal, whereas this is not true for the anions.

Two other related studies of the gas-phase ion chemistry and structure of nitroaromatic anions are in progress. One involves determination of the energy released during NO loss, with the magnitude of this energy being correlated with properties of substituents. The other study involves elucidating the mechanism of NO loss by determining the structure of the ion that is produced by this reaction.

Work on building an explosives detector has been ongoing since the last report. A tandem quadrupole/time-of-flight (QT) mass spectrometer (similar to the one built previously at ORNL) has been constructed for preliminary experiments. A newer system is planned for the near future that will incorporate an electric sector in the time-of-flight portion of the instrument. This will afford improvement in daughter ion resolution and reduction in background noise. Much work has also gone into designing and testing an atmospheric pressure ionization (API) source. Two different designs have been tried, with both giving similar results to date. Further testing is needed. A novel data acquisition system has been designed for the new QT instrument. Based on CAMAC equipment and an IBM-XT personal computer, it is presently being assembled in conjunction with development.

The other major area of work in organic mass spectrometry this year has been the development and demonstration of a hybrid MS/MS/MS instrument of QEB (quadrupole-electric sectormagnetic sector) geometry. This was done by interfacing a quadrupole to the front end of an MS50 high-resolution mass spectrometer. A variety of experiments have been conducted with the QEB system, including high-resolution daughter analysis, ion/molecule association reactions, improved resolution of high-energy daughter ion spectra, collisional-activation followed by collision-activated or metastable dissociations, and variable-energy, collision-activated decomposition (CAD) mass spectrometry. An EI/CI ion source has been constructed for the new system.

Energy state counting and rate calculation programs have been developed that allow quasi-equilibrium theory (QET) calculations to be performed. Such calculations have been used in conjunction with low-energy CAD results to elucidate the fragmentation mechanism of quaternary ammonium cations.

Work has continued on the ion cyclotron resonance spectrometer in preparation for experiments with positrons. More modifications have been made to the electronics, and tungsten moderator plates have been constructed for two cell walls. Preliminary experiments with unmoderated positrons have been performed to make sure that these would not produce a "background" ion signal that would interfere with the interpretation of results using

moderated positrons. The results were positive in that no signal was observed.

(G. L. Glish, S. A. McLuckey, H. S. McKown, E. H. McBay, D. H. Friar, D. H. Smith)

Resonance Ionization Mass Spectrometry

The study of Resonance Ionization Mass Spectrometry (RIMS) continues; further work has been initiated to obtain a better understanding of the optical processes involved. As described in the 1984 annual report, a limit in precision and sample size has been found that does not permit application of RIMS to the isotopic ratio analysis of lanthanides in samples of 10 ng or less. The problem appears to be inadequate counting statistics caused by the relatively low pulse rate of the ionizing laser (30 Hz). To improve the ion formation rate and counting statistics, we have recently borrowed a copper vapor laser for evaluation and have ordered a dye laser that will be pumped by it. The new system will operate at a considerably higher pulse rate (> 5 kHz) and will be tunable over the 580 to 700-nm range of the spectrum, which is used for exciting lanthanides and actinides of analytical interest. A time-of-flight (TOF) mass analyzer has also been acquired and has been coupled with a nitrogen-pumped dye laser to investigate RIMS processes that occur in the lanthanides. Previous spectral studies using RIMS have revealed that the optical processes leading to ionization are more complex than originally expected. We and others have also seen RIMS transitions that cannot be explained by present knowledge. With the TOF instrument, RIMS studies of all the lanthanides (except promethium) were made over the wavelength range of 430 to 454 nm, and the transitions were cataloged where possible to establish the various optical processes involved. Of the 300 RIMS transitions observed, approximately 65% were identifiable by various routes, including (1) two-photon, single-color through one resonant intermediate; (2) three-photon, single-color through two resonant (or nearly resonant) intermediates; (3) multiphoton excitation to an upper level followed by ionization with another photon; and (4) one case where ionization was caused by a multiphoton nonresonant route. Many of the unidentified transitions were observed with europium and holmium. It is believed that most of these transitions involve a multiphoton transition to an upper level, followed by ionization by absorption of a fin photon. Published energy levels for these two elements do not list these high-lying levels. The location of such levels can be established by RIMS studies. Thus, not only can it be shown that ions can be generated by a number of optical processes, but also that useful spectral information can be obtained by RIMS.

Another approach to understanding the optical processes involved in RIMS is to measure the excess energy of the photoelectron generated in the ionization process. From the maximum excess energy of this photoelectron and a knowledge of the energy of the photons involved, the initial state can be determined, and possible excitation routes of the ionization process can be evaluated. An electron energy analyzer has been incorporated into our RIMS setup to obtain such information about systems of interest. The electron energy spectra obtained were unexpectedly complex because a number of low-lying electronic levels in the ion are available to be populated from the photoelectrons generated. This complexity, however, yields an electron energy spectrum that is usually unique for a given optical process. Once the reason for the complexity was understood, various spectra could be calculated for alternate optical processes and compared with the experimental spectrum. We have done this for about ten lanthanide RIMS transitions and have been able to verify an originally described mechanism or to demonstrate mechanisms which seem to involve excited atomic levels that have not been reported. This work continues.

(D. L. Donohue, J. P. Young, D. H. Smith, L. K. Bertram)

Positron Spectroscopy

Several studies have been made this year of the lifetime spectra of positrons injected into solids. High-energy positrons entering solids penetrate to varying depths, depending on their energies, but they rapidly become thermalized. Before annihilation occurs, some of them may diffuse into regions containing internal or external surfaces, or defects such as atomic vacancies or voids. There they become trapped in an environment of relatively low electron density where lifetimes are measurably longer. Positron lifetime spectroscopy is being used to

study composites of carbon fibers and epoxy. These materials are widely used in aircraft and other structures. Strengths of composites are decreased by voids resulting from inferior carbon fibers or improper curing of the epoxy. Delamination of the epoxy from the carbon fibers also reduces strength. It is expected that these internal surfaces will increase the lifetimes of injected positrons; therefore, the positron lifetime spectroscopy technique might be a viable composite inspection tool. Specimens of carbon fiber-epoxy composites used in aircraft repair were obtained from a Naval Air Rework Facility (NARF). Some of the composites were reported to contain voids, and some were subjected to damage by impact with steel spheres. Spectra of the specimens containing voids and the impacted specimens showed higher probabilities for long positron lifetimes than those of the material free of voids and damage. The NARF specimens were poorly characterized, however, and we cannot be sure of the degree of void content and damage. Collaboration with the University of Tennessee Materials Science Department has begun in an effort to fabricate better characterized samples.

Positron lifetimes are also increased by the presence of external surfaces; therefore, it should be possible to determine specific surface areas of finely divided powders from lifetime spectra. There is need for alternatives to the BET method of gas absorption. The initial work described in the FY 84 report has been continued. Fumed silicas (cabosils) have been used as model materials because their surfaces are all external; specific surface areas are inversely proportional to particle diameters. Measurements for the cabosils have shown that the intensity of the long-lifetime components of the spectra are proportional to surface area. These results have been compared with those for studies of ion exchange resins whose surfaces are mostly internal, which arises from high porosity. It appears that the two correlation curves are approximately parallel but not coincident.

Work with the development of a ^{68}Ge source for monoenergetic positrons has been completed. A rather poor yield of the isotope was achieved, but the activity was high enough to use the source for positron energy loss work. Scattering studies of monoenergetic positrons have been completed for W, Mo, Cu, and Si surfaces. At low angles of scattering, the positron spectra show much higher cross sections for multiple energy losses than electron spectra.

Efforts are continuing to set up a high intensity source of monoenergetic positrons at ORNL. A feasibility study has shown that the Oak Ridge Electron Linear Accelerator (ORELA) can be retrofitted with a tungsten moderator that will convert excess gamma flux into slow positrons. Conceptually, the slow positrons would be conducted through solenoids into a shielded room where the experimenter would be able to work with fluxes as high as 5×10^8 monoenergetic positrons per second in either a pulsed or dc mode. The facility would be used for atomic and molecular physics and solid state and materials science studies. Positron microprobes and microscopes could be developed. Universities, industrial laboratories, and ORNL divisions could make use of the facility.

(L. D. Hulett, J. M. Dale, T. M. Rossseel)

Heavy-Ion Induced X-Ray Satellite Emission

In the diverse field of material science, analytical methods are needed not only to identify the elemental composition of a sample, but also to characterize the chemical state of the constituents and to provide insight into their bonding. Heavy-ion induced, X-ray satellite emission (HIXSE), an X-ray fluorescence technique that uses heavy ions for excitation, is being evaluated for this role.

High-resolution L HIXSE spectra were obtained for a series of Zr, Nb, and Mo alloys and compounds at the EN-tandem accelerator (ENTA). The Mo and Zr spectra were produced with 25-MeV Cl ion bombardment, whereas the Nb results were obtained by 25- and 36-MeV Cl ion excitation. In agreement with previously obtained Zr and Mo data, the Nb spectra obtained with 36 MeV Cl ions exhibited target-specific variations in the intensity profiles of the $L\alpha M^{III}$ and $L\beta M^{III}$ hypersatellites. Also in agreement with Mo and Zr data, the Nb Lα region was more sensitive to compounds, whereas the Lβ region was more sensitive to alloys. In addition, the sensitivity of HIXSE to changes in the Nb-Ti alloy system was found to be independent of projectile energy (0.7–1.0 MeV/u). These results strongly suggest that HIXSE can distinguish between different types of chemical bonding.

Although spectral differences have been qualitatively correlated to the chemical

environment of both alloys and compounds, a mature understanding of the physical nature of these variations is not yet available. To develop the potential of HIXSE as a probe of the bulk chemical environment of an element in a solid and as a complementary technique to electron spectroscopies for the study of chemical bonding in materials, we are participating in the construction of a high-resolution, high-efficiency X-ray spectrometer to identify and measure the satellite transitions that regulate the rate of vacancy transfer and thus the fluorescence yield. The spectrometer is a Van Hamos-type wavelength dispersive device containing a 10- by 10-cm analyzing crystal with a curvature radius of 25.4 cm. The estimated resolution is 0.04%. A commercial position-sensitive proportional counter, having an active length of 10 cm, will detect the X rays. For most experiments, the bandwidth of the counter will be large enough to collect the entire spectrum without moving either the detector or crystal. The major advantage of this spectrometer will be its high efficiency. Preliminary estimates indicate that the efficiency will be greater than ten times that of the Bragg crystal spectrometer currently used for HIXSE experiments. We anticipate a completion date of September 1986.

(T. M. Rosseel, J. P. Young, J. M. Dale, L. D. Hulett, C. R. Vane, P. L. Papmiller,* H. F. Krause,* S. Raman*)*

---

*Physics Division

Transuranium Research Laboratory

Our cooperative research venture with the University of Tennessee continues at the Transuranium Research Laboratory (TRL). This work involves spectral studies of transuranium compounds and is conducted with R. G. Haire of the ORNL Chemistry Division and J. R. Peterson and his students in the Chemistry Department at the University of Tennessee, Knoxville. We have continued spectral studies of actinide compounds at high pressures. A new diamond-anvil cell has been designed to our optical specifications and fabricated by U. Benedict of the European Institut for Transuranium Elements in Karlsruhe, FRG. The new cell is capable of exerting pressures exceeding 30 GPa; we have operated this cell at pressures of about 25 GPa for extended periods of time (days). Preliminary results on AmI_3 and $CfBr_3$ were described in the 1984 report. These results have been further evaluated, and spectral studies of the effect of pressure on PuI_3, $CfCl_3$, and several lanthanide compounds have been conducted. All of the actinide compounds are capable of existing in two or more crystallographic forms of differing unit cell volumes. In general, our results show that the bromides and iodides transform irreversibly to the most dense structure at less than 5 GPa. The expected transformation of hexagonal $CfCl_3$ to orthorhombic $CfCl_3$ was not observed, even at pressures up to 25 GPa. Spectral changes were apparent, but they were reversible and could be ascribed to the hexagonal structure. Several papers have been written concerning these studies, and further work is planned for the $CfCl_3$ system.

An idea for using radioactive transmutation to generate chemical reagents is being developed. A necessary prerequisite of the concept has already been demonstrated in our observation that oxidation states of actinides are preserved in α and β decay. Therefore, we plan to prepare mixtures of $^{91}YBr_3 \cdot CfBr_3$. As the yttrium decays, ($^{91}Y \rightarrow Zr$), Zr(III) should result and may reduce Cf(III) present in the sample. The process can be followed spectrophotometrically. A number of other such transmutation-induced chemical reactions can be envisioned. A patent disclosure has been prepared.

Further studies of progeny species generated by radioactive decay have also been made. We are reexamining the spectra of very old (> 5 years) samples of einsteinium chlorides doped into other host chlorides. Absorption spectra of the actinide chlorides are, in general, weak; therefore, it has taken years for californium granddaughter species to be observable. The study of the $LuCl_3$ host system is of particular interest; $LuCl_3$ exists in a monoclinic structure. $EsCl_3$ and $CfCl_3$ do not normally exist in this structure. The spectrum of einsteinium in the initially prepared $EsCl_3 \cdot LuCl_3$ could be intrepreted as being that of monoclinic $EsCl_3$, possibly forced into that form by the host $LuCl_3$. The result of the current spectral study indicates that the $CfCl_3$ granddaughter is also monoclinic. This represents a new crystalline form of $CfCl_3$ prepared by transmutation. In another study of a $EsCl_2 \cdot GdCl_3$ sample, the spectrum of

Cf(II) was observed. There was also an indication of CfOCl (a trivalent californium compound) in this sample, which was 5 years old or older. The formation of CfOCl was unexpected, but could well have occurred from the long-term reaction of the sample with its container (SiO_2).

(J. P. Young)

SECONDARY ION MASS SPECTROMETRY

W. H. Christie

Rapid growth has occurred in recent years in particle sputtering as a means of producing atoms and ions for mass spectral analysis. More recently, it has been observed that secondary ion mass spectrometry (SIMS) offers a means for studying organic as well as inorganic materials. A significant amount of our research effort has shifted in this direction, and our approach to organic SIMS has been to interface an in-house developed secondary ion source with a tandem three-sector mass spectrometer. This combination is being used to investigate the chemistry and physics of secondary ion emission from both volatile and involatile organic species. In inorganic SIMS, we are investigating laser-induced resonance ionization of sputtered neutrals using a recently acquired micro-beam instrument that has been modified for these studies. The ability to selectively laser ionize nearly every atom emitted during the sputtering process offers the possibility of doing ultra-trace level analysis. Fundamental information concerning the sputtering process is being obtained, because resonance ionization allows one to probe the excited electronic states of neutral atoms ejected during a sputtering event. Experiments have been performed demonstrating the number and type of ions formed along with optical spectral information showing the wave-length at which resonance ionization occurs.

Organic SIMS

Efforts in organic SIMS have been directed toward the goal of obtaining an understanding of organic secondary ion emission. The approach that has been taken is to select chemically well-characterized sample systems and establish relationships between the physical and chemical properties of a sample and its secondary ion emission. Correlations are then either used as a framework in constructing a theoretical model or applied directly toward improving the methodology.

A good example of the practical application of this work is the development of a reservoir probe tip that corrects sample depletion during the course of a SIMS experiment. We observed that the secondary ion spectrum of glycerol/analyte solutions was time dependent. This aspect limits the applicability of any spectral technique; for example, if repeated spectra of a sample show changes during analysis, one is left with the question of which spectrum is correct. We were able to establish that the cause of the changing spectrum was sample depletion. Consequently, a reservoir system that provides capillary action to pump the sample to the target surface during a SIMS experiment was designed, constructed, and tested. A unique feature of this system is that it permits generation of secondary ions of constant intensity and relative abundance for up to 2 h, whereas previous systems limited constant emission to a few minutes. This feature is particularly important for MS/MS work on secondary ions, since MS/MS spectra frequently require time averaging. A patent is pending on the reservoir probe.

Using this reservoir probe system, we have been able to study relationships between the secondary ion intensity characteristics of analytes dissolved in or adsorbed onto a liquid matrix. After measuring the surface activity and Henry's Law constants for a series of amine/glycerol solutions, we can demonstrate that secondary ion intensity does not depend primarily on the thermodynamic properties of the solutions. Rather, the intensity depends on the flux of the analyte reaching the sampling surface and on the primary particle flux; that is, secondary ion emission depends on chemical kinetics. We are in the process of investigating these properties.

Ongoing with these studies is the development of a model which mandates that chemical properties determine the behavior of secondary ion emissions, as observed experimentally. The model developed thus far invokes the existence of a critically heated volume to rationalize the data. Two implicit properties of the model include a mechanism by which the keV energy of the bombarding particle is converted to thermal energy, and a mechanism by which all

intermolecular bonds can be broken without breaking a single intramolecular bond. These two features are important because they are consistent with experimental observation, and they do not require any of the known laws of physical chemistry to be violated when secondary organic ions are generated.

Organic secondary ion emission is important because it extends the range of organic mass spectrometry to involatile compounds. Enhancing organic secondary ion emission has hitherto been empirical. Our studies on this process point to a future when emission enhancement may be effected by design.

(P. J. Todd, C. P. Leibman, W. H. Christie)

Sputter Atomization/Resonance Ionization Mass Spectrometry

Work has continued on the combination of ion beam sputtering and resonance ionization mass spectrometry (RIMS) for ultrasensitive isotope ratio analysis. The use of a micro-focused primary ion beam and knowledge of the energy and angular distribution of the sputtered atoms enables the geometrical overlap of the laser beam with the sputtered plume to be optimized. Additionally, the use of a pulsed primary ion beam enables the temporal overlap between atomization and ionization to be maximized. Saturation of the resonance ionization process gives a predicted sampling efficiency (atomization and ionization) of about 10% (1 ion for each 10 sample atoms removed).

The initial phase of the project involved making a surplus ion microprobe mass analyzer (IMMA) operational and then adapting it for use in SA (sputter atomization)/RIMS experiments; these efforts were described in the 1984 annual report. Our work this year has concentrated on modifying the system to obtain increased sensitivity and ease of use. The IMMA and flashlamp-pumped dye laser were interfaced to an LSI-11/2 microcomputer for data acquisition and control. A stepping motor was attached to the wavelength drive of the dye laser to permit reproducible spectral scans to be made under computer control via a parallel interface board located in the microcomputer. A digital-to-analog converter (DAC) was also installed in the microcomputer to control the magnet for the secondary mass spectrometer and to allow mass scans to be made. The ions formed by resonance ionization produce a signal that is sampled by an analog-to-digital converter (ADC) housed in the LSI-11/2. Software was written to integrate the operation of the analog and digital interfaces and to enable optical spectra at fixed mass or mass spectra at fixed wavelength to be obtained. Programs were also developed to display the spectra in real time on a scope driven by a second DAC in the microcomputer and to store the spectra on disk. This system was used to acquire optical and mass spectra for uranium and samarium samples. The RIMS optical spectra observed for sputter atomization agreed well with those obtained from thermal atomization. The mass spectra showed metal ion (M^+) peaks in the expected isotopic abundances when the laser was fixed on a resonant wavelength; at higher mass the oxide (MO^+) peaks appeared with almost equal intensities. However, the M^+ peaks disappeared, as expected, when the laser was detuned from the resonant wavelengths, whereas the MO^+ peaks occurred at all wavelengths scanned by the laser. These results suggested that residual oxygen (present in the primary ion source) was interacting with the metal to produce metal oxide species that are sputtered and ionized by the laser in a nonresonant process.

A new cryosorption vacuum pump was installed on the IMMA; this enabled us to use pure argon in the primary ion source, thereby eliminating problems associated with residual oxygen in the system. Another experimental benefit resulting from this modification was the decrease in pump-down time compared with the original ion pump found on the system. The new cryosorption pump enables the instrument to be pumped from atmosphere to 10^{-4} torr in less than 3 h compared with 7 to 8 h using the ion pump.

Two additional instrument modifications were made to alleviate problems with the setup of the IMMA for SA/RIMS experiments. A new periscope assembly for lowering the laser beam to the level of the sample was designed and constructed. The new design uses two 1-in. bending prisms rather than the two 1/4 in. mirrors in the previous assembly. This modification simplified the laser alignment procedure. A new "pusher" electrode was also constructed and attached to the primary lens column. The new design permits the assembly to be more easily adjusted and removed without disconnecting any high voltage leads.

Future improvements include the addition of a Nd:YAG-pumped dye laser, a MicroPDP-11 computer system, and electronics for pulsed operation of the primary ion beam. The new laser system is expected to improve overall sampling efficiency by enabling saturation of ionization over a larger volume. The acquisition of the new computer will speed software development and data acquisition, as well as provide improved data display capability. The pulsed primary ion beam will allow us to match the duty cycle for atomization with that of ionization, thereby further improving sample utilization.

(D. E. Goeringer, D. L. Donohue, W. H. Christie, H. S. McKown, L. K. Bertram)

ACTINIDES AND ISOTOPIC MASS SPECTROMETRY

R. L. Walker

A VG-354 isotope ratio mass spectrometer was delivered, installed, and tested. All performance tests with regard to uranium were met; we have obtained external precisions as low as ± 0.005% using an internal standard. The instrument is equipped with an electron impact ionization source to allow analysis of elements that are difficult or impossible to ionize thermally. Performance testing required analyses of mercury and tellurium; the former was successfully analyzed, whereas the latter failed. (This issue still awaits resolution.) The instrument is presently in routine operation, primarily for uranium and mercury analyses.

We continued to participate in various projects funded by the International Safeguards Projects Office (ISPO) to assist the International Atomic Energy Agency (IAEA). Analyses were performed on the samples taken for ISPO Task A-126, a joint experiment to evaluate internal standards as applied to reprocessing facilities; the participants are ORNL, IAEA, the French nuclear laboratory at Saclay, and the French reprocessing plant at LaHague. All four laboratories have analyzed all samples, and a meeting will be held in Paris to evaluate the results.

A second ISPO project involved evaluating quadrupole mass spectrometers for on-site safeguards analyses. A custom-assembled ORNL instrument was installed at the IAEA laboratory in Seibersdorf, Austria. Also installed at Seibersdorf was a Finnigan-MAT THQ quadrupole mass spectrometer designed expressly to measure isotope ratios. H. S. McKown visited the laboratory to evaluate both instruments. He concluded that neither spectrometer (in its present form) is suitable for its intended purpose; however, with proper modification, either would be acceptable.

We continued to provide analytical support for the transuranium production and stable isotopes sales programs. In addition, many low-level actinide analyses have been conducted in support of environmental control programs at ORNL and Y-12. Several research programs have required high-precision isotopic composition and isotope dilution analyses for plutonium, uranium, and neodymium in highly radioactive spent reactor fuels, e.g., for ORIGEN code verification of burnup.

Isotopic analyses were completed on 21 actinides taken from a fuel pin irradiated 90 days at full power (600 MW) in the Dounreay Prototype Fast Breeder Reactor in Scotland. This work was in support of the joint US/UK actinides research program to study the behavior of these nuclides in this type of reactor. This was the first of three pins prepared for this experiment. One of the primary purposes of the experiment was to measure and calculate the burnup and production of various actinides in milligram samples of highly enriched actinide isotopes as a check on measurement techniques, nuclear cross sections, and calculational methods.

Another unique support activity of the group was the acquisition and standardization of a beryllium solution containing $^{9}Be/^{10}Be$ (~75:1) as the starting material for two projects. A portion of the solution will be used by the National Bureau of Standards as the starting material for preparing a tandem accelerator mass spectrometry standard; the expected $^{9}Be/^{10}Be$ ratio is 10^{10} to 10^{11}. Another portion will be used jointly by S. Raman and others at ORNL and by Professor Wolfli of the Institut fur Mittelenergiephysik, ETH-Honggerberg, Zurich, Switzerland, to redetermine the half-life of ^{10}Be.

(L. K. Bertram, M. P. May, E. H. McBay, C. A. Pritchard, G. I. Gault, L. Quinn, M. M. Honaker, H. S. McKown, E. G. Miller, H. C. Smith, D. H. Smith)

2. RADIOACTIVE MATERIALS LABORATORIES

W. R. Laing

The Radioactive Materials Laboratories Section is composed of three groups: Radioactive Material Analytical Laboratories, Transuranium Analytical Laboratory, and Programs and Projects. A satellite laboratory is also operated within the Consolidated Fuel Reprocessing Facility. These groups provide support for many Laboratory programs, primarily those in the Chemical Technology, Fuel Recycle, Metals and Ceramics, and Operations divisions. They also perform work for other federal and nonfederal agencies.

Development is an inherent activity and includes work on X-ray fluorescence, gas-cooled reactor fuels, reprocessing, mercury purification, testing of coatings for the nuclear industry, and the division's computer-based Data Management and Sample Transaction System.

PROGRAMS AND PROJECTS

D. A. Costanzo

X-Ray Fluorescence Development

Quantitative X-ray fluorescence (XRF) analysis for uranium and plutonium in highly radioactive solutions presents several unique problems. These problems include excitation of the uranium and plutonium by passive radiation in the sample (gamma, X-ray, alpha, and beta activity), the spontaneous emission of X rays resulting from internal conversion following the decay of radioactive isotopes (e.g., uranium L X rays following the alpha decay of americium and plutonium isotopes), and coping with the high degree of scattered radiation from the sample. Passive excitation and interference from internal conversion can be managed by appropriate analytical techniques; however, conventional XRF spectrometer designs cannot tolerate a very high degree of passive radiation from the sample. Therefore, the goal of this project is to circumvent these problems and provide an XRF system to monitor uranium and plutonium in highly radioactive feed solutions to a nuclear fuel reprocessing plant.

Investigations by C. J. Sparks, Jr., of the ORNL Metals and Ceramics Division, led to the design of a wavelength dispersive XRF system that can be used to determine concentrations of uranium and plutonium (and many other elements) in highly gamma-active backgrounds. Mechanical simplicity, a basic feature incorporated into the design of the XRF spectrometer, makes the system unique for use in remote and inaccessible environments. Pyrolytic graphite, which is used for X-ray optics in the system, offers excellent radiation resistance and high diffraction efficiency (40% of incident power). The graphite diffraction crystal also provides simultaneous diffraction of the entire energy region, from PuL_α to UL_α, with sufficient resolution (30 eV FWHM at 14 keV) to permit the use of a fixed single-crystal spectrometer. Therefore, an operational system would have no moving parts after initial alignment, thus simplifying instrument maintenance and enhancing reliability. The constant optical geometry should also result in improved accuracy and precision.

Capital funds ($\sim$ \$115,000) have been obtained during the last two years to purchase equipment for fabricating a prototype XRF system. New equipment includes an LSI-11/23 Plus-based computer system, a Tracor TN-7200 multichannel analyzer, a TEC high-resolution position-sensitive proportional counter with all control electronics, and a Philips constant-potential 3-kW X-ray generator. All new equipment, except the X-ray generator, has been incorporated into the prototype XRF system. The X-ray generator was installed in November, 1985 and is currently being tested.

Most software development for the acquisition, peak processing, and quantitation of XRF data has been completed. A special device handler has been written to provide a communication link with the TN-7200 MCA on a serial line at speeds up to 4800 baud. The device handler, along with an application program, supports bidirectional transfer of spectral data and transfer of control commands under either RT-11 or TSX-Plus operating systems. Integration of the software into a single menu driven application package remains to be completed.

Remaining work includes the setup, testing, and integration of new equipment and material into the prototype XRF system. Following final testing of the new X-ray generator, system performance will be reevaluated and optics will be optimized.

(J. M. Keller)

HTGR Base Technology Program Support

This project involves the upgrading and replacement of equipment and instrumentation for the HTGR Coated-Particle Fuel-Performance Assessment. An ORNL-designed Irradiated-Microsphere Gamma Analyzer (IMGA) was upgraded from control by an obsolete TP-5000 gamma analysis system to a Nuclear Data ND-6700 system. A complete new software package was developed for the ND-6700 to control and acquire data with the IMGA system.

A new automated fuel particle handler for the IMGA system was successfully tested with new control software and then installed in the hot cell during July. The status of the IMGA upgrade at that time was sufficient to satisfy an ORO milestone, which did not include the installation of a new particle handler. The new automated fuel particle handler has continued to undergo testing with the new control software. The handler has successfully been used for

numerous runs (with 2000 particles), which consisted of continuous operation for several days per run. The particle handler has been installed in the hot cell and has successfully undergone additional testing. All additional equipment required for operation of the IMGA system has also been installed and the hot cell was closed at the end of November. Remaining work on the IMGA upgrade includes development of data processing software and documentation of the new system.

The upgrade of a shielded electron microprobe (SEMP) is in progress. An initial evaluation of the SEMP indicated a need to upgrade or replace most of the current electronic components. The SEMP is based on out-of-date technology, and the vendor for the probe is no longer in business. The existing vacuum tube technology used on the SEMP is questionable regarding reliability and performance characteristics relative to present standards. The lack of vendor support has created maintenance problems because of the inability to obtain replacement parts.

The electronic components scheduled for replacement include both the high- and low-voltage power supply modules, the beam-scanning electronics, and the wavelength dispersive spectrometers. The present SEMP single-channel analyzer should be replaced with a computer-based multichannel analyzer that also provides advanced image processing capabilities. To meet projected requirements for the SEMP, a shielded-energy dispersive spectrometer will be added to the system.

A consultant has been contacted to evaluate the SEMP and provide information and advice about the required electronics. When discussions are complete, procurement of the necessary equipment required for a functional SEMP will be initiated; approximately $90,000 has been approved for the upgrade.

(J. M. Keller)

Database Software for the Oak Ridge Managed Deer Hunt

To handle all of the information generated during the 1985 ORNL/Tennessee Wildlife Resources Agency (TWRA) managed deer hunts on the Oak Ridge Reservation, a custom package was developed using dBASE III for an IBM PC. The package was compiled (with Wordtech Systems, Inc.) to permit legal distribution of information and to simplify user interaction with the computer.

The program is completely menu driven and uses formated input screens to provide a "user friendly" environment. The customized package consists of three primary functions selected from a master menu. The first function is used each hunt day to handle input of hunter information (name, address, etc.), deer statistics (sex, age, number of points, weight, and kill location), and counting data (gross counts for total ^{40}K and ^{137}Cs). Based on counting data and sample weight, the program then calculates ^{137}Cs activity (pCi/g) and alerts the user if the activity has exceeded a preset limit. At the end of a hunt day the user can generate a report on all information obtained, for internal use and a special report form (for TWRA officials) that provides additional blank fields for other statistics of interest to the TWRA.

The second function of the program is to merge daily data into a master database for all hunts. The third function provides the user with the means to manipulate the master summary database. From the master summary, the user can select numerous formats of information sorted by various criteria (by hunter, deer weight, kill location, ^{137}Cs activity, etc.). The user can also select subsets of information based on relational combinations (such as, sex = male and weight $\geq$ 100 lb) and generate reports of these subsets.

(J. M. Keller)

RADIOACTIVE MATERIALS ANALYTICAL LABORATORY

D. A. Costanzo

The Radioactive Materials Analytical Laboratory (RMAL) provides support to various nuclear-related ORNL programs. Support for the Consolidated Edison Uranium Solidification Program, Consolidated Fuel Reprocessing Program, hydrofracture waste disposal, isotopes production, Environmental Restoration and Facilities Upgrade Program, and environmental monitoring are representative activities. Many ORNL divisions are supported, including Chemical Technology, Fuel Recycle, Physics, Environmental Sciences, Environmental and Occupational Safety, Operations, Quality Assurance and Inspection,

Health, and Plant and Equipment. Analysis of intermediate- and high-level radioactive samples that require glove-box and/or hot-cell operations are the primary services provided; in addition, X-ray fluorescence, testing of coatings for application in nuclear facilities, and referee analysis of uranium ore concentrates are also performed.

During this report period, 1574 samples were processed, and 4967 determinations were performed. A large number of highly radioactive samples were prepared for analysis by other sections within the division for isotopic compositions, mass spectrometry, gamma spectrometry, neutron activation, and gas and ion chromatography. A variety of analytical techniques were used in RMAL, including potentiometric titrimetry, coulometry, X-ray fluorescence, alpha pulse-height analysis, liquid scintillation counting, spectrophotometry, BET surface area, particle size distribution, free acid, and infrared analysis for carbon.

Radiation tolerance, decontamination, and design basis accident (DBA) testing of coatings for application within nuclear facilities is provided to coating manufacturers, utilities, architect-engineering firms, and testing agencies. Testing has been performed for ten clients this year. Radiation tolerance testing is performed at the High Flux Isotope Reactor using the intense radiation emitted by the spent fuel elements. Samples are examined visually for physical damage to the coating. In the decontamination test, a mixture of gamma-emitting nuclides is applied to the surface of stainless steel panels or coated cement blocks and then removed with various decontamination solutions. This test is performed by the Transuranium Analytical Laboratory. In the DBA test, coated specimens are exposed to an emergency coolant spray solution at an elevated temperature and then examined for physical damage, chalking, and change in film thickness. These tests conform to ASTM specifications.

We have continued to upgrade the DBA autoclave equipment; pneumatic temperature controllers have been replaced with solid state proportional temperature controllers. Also, a computer program, written by C. K. Bayne of Computing and Telecommunications Division, is being used to calculate the irradiation time necessary to obtain a desired dose as a function of the elapsed time after the spent fuel element is removed from the reactor. During this report period, the quality assurance program for testing coatings was audited and approved by three different clients.

For a number of years, the New Brunswick Laboratory provided analytical chemistry services to the uranium mining and processing industry in the form of measurements of the uranium content of ore concentrates. Current contracts between shipper and receiver require that a certain percentage of samples be analyzed independently, including those samples where shipper and receiver differ by more than 0.1 wt %. In mid-1984, the Department of Energy determined that the New Brunswick Laboratory should not do this work since it is not safeguards related. Thus, the Radioactive Materials Analytical Laboratory was selected by commercial uranium suppliers to provide referee analyses. Since the program was initiated in late 1985, 310 ore concentrate samples have been analyzed. This service has also been provided to the Y-12 Product Certification Group to assist in resolving shipper/receiver differences between the Y-12 facility and the Savannah River Plant on the uranium assay of process waste. A weightbased version of the Davies-Gray potentiometric titration is being used. The relative standard deviation at the 95% confidence interval has been demonstrated to be 0.05% for samples containing 65 to 80 wt % uranium.

Construction of an addition to the west end of Building 2026 was started in mid-May 1983 and terminated in August 1984, at which time the facility was accepted by the Engineering Division. Certain deficiencies have been corrected, and the facilities were reviewed and approved by the Radiation Operation Committee in August 1985. The addition contains a radiochemistry counting room ($\sim$600 ft^2) on the first floor and three chemistry laboratories and an office on the second floor ($\sim$2000 ft^2). The counting room was occupied in April 1985 when the intermediate-level radiochemical operations in Building 3019B were moved and consolidated with the operations in Building 2026. The second floor laboratories are being equipped to screen, handle, and prepare radioactive samples for priority inorganic and organic pollutant analysis by other groups within the division. The new addition and existing facilities in Building 2026 will provide the division with a unique complex for the analysis of radioactive, chemically hazardous materials.

Fuel Recycle Division Support Laboratory

The service laboratory located in Building 7603 performed 3430 analyses in support of process and engineering studies conducted by the Fuel Recycle Division (FRD). This was a 15% increase over the previous year (1984). The types of analyses performed were uranium by volumetry and spectrophotometry, free acid, silver, chloride, iodine, oxides of nitrogen, density, viscosity and conductivity, gadolinium, foam break time, and disengaging time.

During the year, additional work was done on uranium and nitric acid distribution coefficients in the Integrated Equipment Test (IET) solvent extraction system. Extractions were performed using various organic-to-aqueous ratios, and both phases were analyzed for uranium and acid before and after extractions.

Solutions of zinc bromide having densities of 1.491 and 1.495 g/mL, respectively, were prepared for use in calibrating in-line density meters for the IET. Also, solutions of nitric acid were prepared for use as conductivity standards to calibrate in-line IET instrumentation.

Special studies were conducted on a cerrobase alloy (Pb/Bi), on dissolution at various temperatures and nitric acid concentrations, and on the oxides of nitrogen produced by the dissolution.

A leaching study of a vespel-21 bushing was conducted during January, February, and March. Using a nitric acid and uranyl nitrate solution, we determined that this mixture is suitable for use in the United Kingdom centrifuge. The UK machine is to be used as a polishing clarifier for the Breeder Reactor Engineering Test (BRET). The bushing is made of a polyimide resin containing 15% graphite.

(P. W. Pair)

TRANSURANIUM ANALYSIS LABORATORY

J. L. Botts, Group Leader

The Transuranium Analytical Laboratory (TAL) continued to provide support to two main Laboratory programs: (1) the Transuranium Production Program and Solvent Extraction Test Facility (SETF) within the Chemical Technology Division and (2) the monitoring of radioactive waste effluents for the Operations Division. More than 45,000 analytical determinations were made during the past year.

The TAL provided analytical support to the SETF in the processing of a high burnup, short-cooled Fast Flux Test Facility reactor fuel. Because of the radiation levels of the samples from this process, most of the analysis required the use of a hot-cell facility. The analyses included in-cell plutonium and uranium extractions, with subsequent alpha counting and spectrophotometry, to determine concentrations. Free-acid determinations were made using the in-cell ORNL model Q5895 automatic titrator. All in-cell dilutions were made using the computer-controlled remote pipettor.

The Transuranium Production Program was involved in two campaigns processing a total of 25 HFIR targets; the transuranium isotopes ^{244}Cm, ^{252}Cf, ^{249}Bk, ^{253}Es, and ^{255}Fm were recovered. In support of these campaigns, we performed some 12,000 determinations. Measurements included alpha and gamma spectrometry, in-cell free acid, and the separation of the transcurium actinides of Bk, Cf, Es, and Fm from dissolver solutions using a high-pressure ion exchange column. Actinides Es and Fm were subsequently determined by alpha counting, Bk by beta counting, and Cf by neutron counting.

As a result of the interest generated by an article in the May 1984 issue of *Nuclear News* on the problems of shift work, personnel rotation at TAL has been changed. The rotation was changed, as suggested in the article, to a days, afternoon, and midnight sequence. The new sequence replaced the old schedule of days, midnight, and afternoon, and has been very beneficial to shift workers in eliminating some of the inherent shift-work problems. The new schedule has been used at the ORGDP facility for some time with great success.

An ACS course on radiochemistry was made available to shift technicians working at TAL. A cassette recorder, tapes, and manuals were made available to be used at work as time permitted. The course has been beneficial in familiarizing the technicians with basic radiochemistry.

Pocket meter readings for the first three quarters of this year show a significant decrease (68%) in the radiation exposure received by TAL personnel. The total exposure decreased from 1760 mR for the first quarter to

560 mR for the third quarter. This decrease in personnel exposure can be attributed to better waste handling, better sample storage facilities, and improved techniques for handling dilutions and samples taken from the hot cells.

Methods and techniques have been developed and improved to characterize candidate materials by the hydrofracture injection technique. To satisfy the requirement that all materials be completely characterized, the TAL has analyzed a number of samples. The required analyses included gross alpha, beta, and gamma measurements, gamma spectral analysis, plus the determination of the actinides (U, Pu, Am, and, Cm).

(R. A. Jones, C. C. Foust, J. M. Peele, M. E. Peters, R. T. Pack, R. Peralez, M. E. Garcia, S. C. Wells, J. D. Mayton)

3. INORGANIC CHEMISTRY

J. R. Stokely

The Inorganic Chemistry Section performs inorganic and low-level radiochemical analyses for a large number of Laboratory programs. The section also does development work to upgrade capabilities and to solve applied problems requiring inorganic analytical chemistry or radiochemical expertise. Approximately 200,000 analyses are performed by the section each year.

During this year, the section has become heavily involved with new Laboratory environmental monitoring and waste management programs and environmental acid rain projects. New staff, equipment, and procedures are being acquired to handle expanding sample loads from these programs. In addition, the section continues to provide general inorganic analytical support for numerous basic research projects within the Laboratory and to assist outside private corporations and other government agencies with special analytical expertise.

CHEMICAL AND PHYSICAL ANALYSIS

J. H. Stewart, Jr.

Analytical support of the ORNL hydrofracture waste encapsulation programs required development of a series of new techniques for measuring trace and ultratrace levels of both cations and anions. A unique vapor transport separation and subsequent measurement of sub-part-per-million levels of fluoride in saturated NaCl brine was developed. A Dionex anion analyzer was modified to provide bromide measurements at low part-per-million levels in the brine. Crystallization of NaCl from the brine, using HCl gas saturation, permitted simultaneous inductively coupled plasma (ICP) detection of approximately 25 elements at the 50-ppb concentration level. Cadmium and lead were measured polarographically. Further improvements to achieve even lower detection limits are under way.

Methods development for the removal of both toxic metals and radionuclides from the 4 million gallon Bechtel Niagara Falls liquid waste site was completed. The methods were successful and permitted the release of water that met all New York State discharge specifications. This technology should be applicable to other mixed waste liquids. As part of this work, we developed a practical method for the reduction of hexavalent selenium and the subsequent removal of all selenium (to less than 20 ppb) in very large volumes of water. With additional development, we believe the method could be extended to selenium contaminated irrigation water.

Characterization of uranium mill tailing ponds in Wyoming and Colorado was completed for the Nuclear Regulatory Commission (NRC). In a continuing survey program, several additional sites were sampled and analyzed for toxic metals, anions, and radionuclides.

Environmental monitoring of ORNL surface and well waters continued to increase in both total samples and in the number of parameters being monitored. We have added coliform, ammonia, biochemical oxygen demand, cyanide, total phenols, thallium, and sulfide to the measurements performed. We discovered that the four-plant environmental method for determining the presence of polychlorinated biphenyls (PCB) in fish was not adequate; consequently, an improved methodology is being investigated. The new SOXTEC rapid (1.5 h) extraction system is being evaluated as a potential replacement for the conventional Soxhlet (16 h) method; initial results of the evaluation are very encouraging. The SOXTEC system can be used for sediment specimens.

Zymark robotic methods development has continued with the completion and successful testing of the fluorimetric uranium extraction procedure. All hardware and software is now available for colorimetric analysis; only the interfacing of the Zymark to the Hach spectrophotometer remains to be completed.

The PGT System 4 analyzer, interfaced to the scanning electron microscope, has been widely used in such diverse applications as measuring ratios of solid-solution crystals of gadolinium-terbium phosphates and tantalum niobates to determine the cause of failure of a bioreactor for nitrate destruction, identifying TVA slag from other types of slag in cinder blocks used in construction, and assisting in the location of the source of ductwork failure in an ORNL air conditioning fan room. A forensic-type examination of work gloves enabled us to identify the work area in which the gloves were used and the type of work done by the wearer of the gloves. We also examined a section of plaster wall removed from the Hiroshima area in 1945 to determine the iron content of the "black rain droplets."

The X-ray diffraction area has been heavily involved in the support of new compound syntheses (bismuth and samarium titanates, boron nitrides, and phosphates) and the identification of Al_2O_3 in the iota, -O, -K, and corundum forms. We determined diffraction index data for 29 new rare earth titanate compounds and submitted the data to the International Centre for Diffraction Data for publication.

Inductively coupled plasma spectrometry (ICP) was used to map the location of metals in 13 specific areas of the human brain. This work, which supports the University of Tennessee's research on possible causes of Alzheimer's disease, has contributed new information on concentrations of elements in both normal and Alzheimer's patients. A paper on this work was presented at the combined Southeast-Southwest Regional ACS Meeting in Memphis.

By using mannitol to control the loss of volatile metals, during a ten-fold concentration step, we were able to attain low parts-per-billion detection limits for trace elements in very pure process water via ICP. Our support for Savannah River, Bechtel, and NRC continued to increase.

Unusual analytical requests also included high-accuracy measurements of nickel aluminide crystals. This required the painstaking development of separation procedures prior to analysis. A method was also developed for the detection of parts-per-million levels of fluoride in tungsten metal.

We were asked to provide very rapid uranium analyses to the North Dakota Public Health Department, following a truck-train collision that involved some release of uranium. Our results indicated that the uranium exposure to those on site was negligible which immediately reduced public concern. This is an example of good interplant collaboration between Martin Marietta Energy Systems analytical laboratories. The work resulted in a commendation from the Governor of North Dakota.

(C. S. Alley, S. J. Bobrowski, C. Feldman, B. C. Grant, J. H. Hackney, R. L. Holmes, C. S. MacDougall, B. Philpot, J. C. Price, W. P. Rogers, K. I. Webb)

ENVIRONMENTAL ANALYSIS LABORATORY

N. M. Ferguson

The Environmental Analysis Laboratory (EAL) provides analytical support primarily for the Environmental Sciences Division (ESD) but does a significant amount of work for other ORNL divisions. Support for other divisions increased this year and required analysis of a wide variety of materials.

A very large portion of our work during this report period derived from the acid rain program in ESD. Oak Ridge National Laboratory is the prime contractor for this work. This program, funded by the Electric Power Research Institute (EPRI), produced throughfall, rain, dry deposition, and soil samples. Three groups generated samples for this program - the University of Pennsylvania from Whiteface Mountain in New York; the Coweta Hydrological Laboratory in Coweta, North Carolina; and ESD from the Smoky Mountains. Since there was a delay in EPRI funding for 1985, the sampling program was also delayed. There was a tremendous influx of water and soil samples during the last 4 months of this report period. All water samples were analyzed for Al, Ca, Mg, Na, K, NH_3-N, Cl, NO_3-N, PO_4-P, SO_4, and Kjeldahl nitrogen. The soil samples were analyzed for Na, Ca, K, Mg, P, and Kjeldahl nitrogen.

We also provided analytical support for many new ESD programs during the year. One group was involved with a program to characterize soils from Pearl Harbor for the U. S. Navy. Numerous samples generated for the project were analyzed for Cd, Pb, Hg, Zn, and organic carbon. Another project dealt with a round-robin evaluation of The soil samples were analyzed for Na, Ca, K, Mg, P, and Kjeldahl nitrogen.

We also provided analytical support for many new ESD programs during the year. One group was involved with a program to characterize soils from Pearl Harbor for the U. S. Navy. Numerous samples generated for the project were analyzed for Cd, Pb, Hg, Zn, and organic carbon. Another project dealt with a round-robin evaluation of the new Toxicity Characteristic Leaching Procedure (TCLP) proposed by EPA for utility waste samples. This study evaluated TCLP performance in comparison with the existing extraction procedure. The three laboratories involved with the evaluation were Battelle, Richland, Washington; Radian Corporation, Austin, Texas; and ORNL. This program produced approximately 200 acetic acid and sodium acetate leachates of fly ash. The extracts were analyzed for As, Ba, Cd, Cr, Mn, Pb, Hg, Ag, Se, V, Zn, and SO_4. The analyses were time consuming and very difficult to perform. Quality assurance requirements were very strict.

We provided much technical support for programs of the Department of Environmental Management. A project involving a Non-Radiological Process Waste Water Abatement Facility generated the largest number of samples. Samples were also generated to obtain information for a National Pollution Discharge and Elimination System permit application that would allow ORNL to discharge liquid waste into state waterways. Another ongoing project that monitors surface waters and groundwaters for compliance with the Resource Conservation and Recovery Act (RCRA) produced large numbers of samples, which were subsequently analyzed for Sb, As, Be, Ba, Cd, Cr, Cu, Fe, Hg, Pb, Ni, Se, Ag, Tl, and Zn. Total and dissolved metals were determined in many samples. Organic carbon, Kjeldahl nitrogen, ammonia, and total phosphorus were determined in most samples. Extreme care and attention was required to obtain the desired low concentration levels (ppt and ppb). Numerous fish were analyzed for mercury.

During this report period, there was a considerable increase in the volume of work done for the Chemical Technology Division. One group

studying various methods to remove mercury from liquid wastes at ORNL generated hundreds of water samples for mercury analysis. This work required fast turnaround time and very low limits of detection (ppt). Another project dealt with the hydrofracture waste disposal technique. One group performed many experiments in an attempt to understand and predict what might be leached from the hydrofracture waste site by various solutions. Grout samples containing several concentrations of metals were prepared and leached with deionized water and brine for various periods of time and at various temperatures. The leachates were analyzed for Hg, Cd, Cr, Cu, Ni, Pb, Co, Ba, As, and Sb. All metal concentrations were at the low parts-per-billion level.

We have been heavily involved with mercury analyses for the Y-12 Plant. Several hundred soil samples from various locations at the plant were analyzed. Concentrations ranged from 1 μg/g to 10 mg/g. Several techniques to remove mercury from various waste solutions were investigated. This project produced hundreds of samples for analysis.

The EAL obtained a new, very versatile carbon analyzer this year. The instrument determines organic carbon and inorganic carbon in aqueous samples, and organic carbon in solid samples. The cost of an analysis is approximately half that of the old system. A new atomic absorption instrument (acquired this year) has been put into operation; it has Zeeman-based background correction capability. This instrument is used for both flame and flameless atomic absorption analyses. All of our graphite furnace procedures were modified for use with the new system.

Several projects required the development of new procedures or the modification of existing ones. A procedure was developed to determine methylmercury in water. The method involves concentrating methylmercury on a resin column (Amberlite XAD-2), eluting the mercury with an HCl-methanol solution, and extracting the mercury with benzene. Gas chromatography was then used to determine the methyl mercury.

(L. S. Barringer, S. A. MacIntyre, M. L. Moore, S. J. Morton, W. R. Musick, J. W. Wade, C. L. Watson)

LOW-LEVEL RADIOCHEMICAL ANALYSIS

T. G. Scott

During the past year, our Low-Level Radiochemical Analysis Laboratory performed more than 20,000 determinations for both man-made and natural radionuclides in a multitude of materials. Support was provided for all of Martin Marietta Energy Systems facilities, as well as a number of outside organizations such as USGS, NRC, and DOE. Although our laboratory's primary function is to provide services for environmental radiochemical analyses, a sizable portion of work involved analysis of unusual matrices and elevated levels of radioactivity.

Early this year, a release of radioactivity into the sewage system created an emergency situation that required rapid identification and quantification of several radionuclides in sludge, sediments, core samples, and sewage water. Procedures were modified to provide a quick turnaround of data that led to locating the source of release and subsequent corrective measures. A major portion of the analyses was for the determination of gross alpha, gross beta, and ^{90}Sr; the gamma emitters were measured to a lesser extent. A screening process was established in which only materials exceeding 10^4 Bq/kg in gross beta were analyzed for ^{90}Sr which was the major radionuclide found.

Brine solutions taken from deep wells at the shale hydrofracture site and wells around waste ponds at Y-12 contained stable elements such as barium, calcium, magnesium, sodium, and strontium in concentrations (several mg/mL) high enough to cause serious problems with normal analysis procedures for ^{90}Sr, ^{99}Tc, and ^{129}I. Procedures were developed in our laboratory to determine the concentrations of these radionuclides in brine solutions (see ORNL/CF-85/251). The problem with strontium was resolved by the development of a procedure for separating and purifying ^{90}Y (daughter of ^{90}Sr). Both the technetium and iodine problems were alleviated by the development and/or modification of anion exchange separations.

We also participated in the study of Niagara Falls waste water mentioned earlier in this chapter. Our part in the effort was to perform gross alpha, gross beta, and ^{226}Ra analyses. Our radioanalysis data were used in conjunction

with other data to develop procedures for treating millions of gallons of wastewater to reduce chemical and radiological contaminants to permissible levels for discharge into public streams. This work was performed for the Bechtel Corporation under the sponsorship of DOE..

Under an agreement between ORNL (Energy Division) and NRC, samples from uranium waste mill ponds in Wyoming were sent to the Analytical Chemistry Division for the measurement of anionic species, toxic metals, organics, and radionuclides of the natural uranium chain. Gross alpha and gross beta measurements were made without much difficulty; however, determinations of ^{230}Th, ^{226}Ra, and ^{210}Pb were complicated by the high salt content of many samples. As a general rule, aqueous samples were analyzed for both dissolved and total radionuclides. Some modifications to normal procedures were required to circumvent the problems. Levels of activity ranged from detection limits to a few hundred becquerels per liter.

In addition to a routine suite of annual samples submitted to us by National Lead of Ohio (NLO), we received several special samples to estimate possible doses related to a release of contamination by NLO. Routine aqueous samples were analyzed for ^{90}Sr, ^{137}Cs, ^{237}Np, ^{99}Tc, and the isotopes of plutonium, thorium and uranium. The special samples were composed primarily of stack dust materials that included UF_4, U_3O_8, UO_2, UO_3, and MgF_2 and required ^{90}Sr and ^{106}Ru determinations.

We received more than 300 samples from projects involved in the Environmental Restoration and Facilities Upgrade Program. A major portion of these samples (~200) was composed of gravel, surface water, and groundwater. Pieces of gravel of selected size and composition were fashioned into "bugs" and placed in several of the streams at ORNL. We leached portions of the gravel used in the bugs with a prescribed leach solution (2% hydroxylamine hydrochloride in 3% ammonium citrate) and determined the ^{90}Sr concentration of the leach solutions. Gamma-emitting radionuclides were determined by nondestructive Ge(Li) gamma-ray spectrometry. Activities ranged from a few to 10^5 becquerels per kilogram.

To comply with the Resource Conservation and Recovery Act, the Department of Environmental Management collected groundwater samples at several locations at ORNL and submitted portions of these samples to our laboratory for determination of gross alpha, gross beta and ^{226}Ra. To be in compliance with the EPA safe drinking water regulations, the gross alpha and ^{226}Ra activity levels must be no greater than 0.55 Bq/L, and the gross beta (indicator for ^{90}Sr) must be no greater than 0.12 Bq/L. We were able to measure ^{226}Ra in these materials by two orders of magnitude lower than the requirements; however, we were barely able to meet the requirements for gross activities because of the limitation on dissolved solids which should produce a weight no greater than 5 mg/cm^2 on the counting planchet for gross alpha and gross beta.

(L. D. Bible, W. M. Caldwell, P. S. Gouge, C. C. Granger, R. D. Johnson, L. L. Kohring, W. C. Massey, S. H. Prestwood, and T. L. Rucker)

RADIOCHEMICAL AND ACTIVATION ANALYSIS

J. F. Emery

The Radiochemistry and Activation Analysis Group provides general neutron activation analysis (NAA) services for a number of Laboratory divisions and programs, as well as radioisotope assay and gamma-ray spectrometry services and technical assistance.

This year we determined Al, Br, Ce, Cl, Hf, I, ^{129}I, Na, O, Ta, Te, and U in alloys, ceramics, metals and soils for the Chemistry, Chemical Technology, Environmental and Occupational Safety, Health and Safety Research, Operations, Physics and Solid State divisions. Multielement analysis was also performed on alloys, glasses, niobium, plastic, and soils. Isotope products (^{13}C–^{244}Cm γ source), ^{24}Na, ^{54}Mn, ^{59}Fe, ^{60}Co, ^{68}Ge, ^{75}Se, ^{85}Sr, ^{93m}Nb, ^{119m}Sn, ^{144}Ce, ^{153}Gd, ^{169}Yb, and ^{231}Pa were assayed by gamma-ray spectrometry.

Our addition to the High Flux Isotope Reactor (HFIR) NAA laboratory was approved and funded. Architectural design is near completion and construction is scheduled to begin in March 1986. This addition will consolidate our ORR NAA facility with the NAA research facility at the HFIR. The radiochemistry laboratory at the HFIR will be enlarged, an office area will replace the present counting room, and a new counting room will be constructed as an addition to the HFIR building. As part of the project, a

second pneumatic tube will be installed in the slant engineering facility No. 3. This location is adjacent to, but part of, the beryllium reflector and is expected to provide a well thermalized neutron flux.

Our work-for-others activities consisted of determining uranium and thorium in semiconductors and semiconductor materials. We have added Alcoa, International Minerals and Chemical Corporation (IMC), Jet Propulsion Laboratory, and Norton Company to our present customers, Cominco Electronic Materials, DuPont, Harbison-Walker, and Varian. We have analyzed more than 100 samples. Some of the semiconductor materials were refractory, thus required a method that involved less exposure to extremely radioactive samples. A method was developed to determine uranium in refractory metals, including tungsten, tantalum, and others. In this method a high-purity polished quartz disk was contacted by the sample and irradiated in a graphite rabbit in the HFIR pneumatic tube. The disk was remotely removed from the sample in the hot cell and etched in concentrated HF to cause fission tracks formed in the silica to be visible when magnified 100X. A series of standards containing a range of uranium concentrations was treated in the same manner, and photographs of the track patterns formed on the disks from the standards and unknown were made. The images of the track patterns were then visually compared, and when the track density for the unknown was judged to be similar to a particular standard, the uranium concentration in the unknown could be estimated from that of the standard and the relative neutron fluences to which the samples were exposed.

One project this year was the result of NRC's decision to convert all reactors using highly enriched fuel to low enriched fuel. A safeguards program based at Argonne National Laboratory has the objective of developing methods to determine fuel inventory in low enriched uranium (LEU) fuel elements that will soon be used in the Oak Ridge Research Reactor. Reactor Operations with our assistance and that of the Instrumentation and Controls Division, is designing and building a gamma scanning system that will be used to determine the fission product distribution in the elements at intervals in their power history. Fuel burnup will be deduced from the fission product inventory. The gamma scanning system will make use of the ND 6620 computer-based gamma spectroscopy system in the Analytical Chemistry Division's NAA laboratory at the ORR. Our responsibility is to assist in the design of the system, to ensure that valid gamma spectroscopy results are obtained, and to ascertain if the gamma spectroscopy system meets the experiment's needs.

Other projects and programs include the design and operation of the radiological monitoring program for the Oak Ridge Reservation. We have provided radioactive monitoring of deer taken on managed hunts from the Oak Ridge reservation. During the first two hunts of two days duration each, 281 animals were surveyed for ^{137}Cs and ^{90}Sr contamination. One animal was found to contain Sr concentrations in its bones at levels exceeding our release limit. Subsequent radiochemical analysis showed 140 pCi/g in the bone sample. The maximum ^{137}Cs concentration was found to be less than 4 pCi/g. A special database was established to provide both radioactivity and animal characteristic information for future hunts in which these same hunters might participate. A collection of liver and bone samples from each animal was kept for archival purposes.

Biological studies have also included the measurement of ^{137}Cs and ^{60}Co contamination in Canada geese residing near one of the ORNL settling basins. Whole-body counts on a live female, as well as measurements on the sacrificed male, were performed. Several whole eggs were measured, followed by subsequent determinations on the hatched goslings. It was found that most of the ^{137}Cs and ^{60}Co from the whole eggs was transferred to the goslings or embryos. Significant concentrations of ^{90}Sr were found in the emptied shells following the incubation period.

Radioactivity concentrations were determined in honey, hive bees, flowers, and source-water supplies from or in the vicinity of the five stations in the honeybee sampling network. Cesium-137 continued to be the nuclide of greatest consequence in these materials; however, ^{7}Be, ^{60}Co, and ^{75}Se concentrations were also measured. The general levels of radioactivity in the 1985 collection are lower than those of 1984.

(L. D. Bible, F. F. Dyer, J. S. Eldridge, L. Robinson, N. A. Teasley)

4. ORGANIC CHEMISTRY SECTION

M. R. Guerin

Each of the three groups in this section, Organic Analysis, Separations and Synthesis, and Special Projects, carries out applied analytical research and provides specialty services to Laboratory programs. The Organic Analysis group is also establishing a general organic analytical services operation. Applied research deals with the chemistry and toxicology of complex mixtures, with particular attention to fossil fuels, hazardous wastes, cigarette smoke, and military formulations. Analytical research currently emphasizes gas-phase ion chemistry in the form of chemical ionization techniques and Fourier Transform Mass Spectrometry for the identification and quantification of organic chemicals. A major effort was initiated this year to establish an analytical services operation responsive to new Laboratory needs in environmental monitoring and characterization. Literature and data studies in support of environmental and health assessments and as input to research initiatives for others have continued. Support for this section is provided primarily by the Department of Energy, Department of Defense, the Department of Health and Human Services, and increasingly by other ORNL programs.

ORGANIC ANALYSIS

J. E. Caton

The Organic Analysis group combines various areas of analytical spectroscopy and chromatography to achieve its research and support goals. Analytical research emphasizes studies designed to develop methods for unambiguously identifying organic compounds found at trace levels in complex organic mixtures. Studies are also directed toward the development of advanced techniques in liquid chromatography, with special emphasis on narrow-bore or open-tube liquid chromatography (OTLC). In addition to research, there is a growing effort in analytical services to support internal programs; much of this effort is directed toward environmental analysis. The primary sources of funding are provided by the Department of Energy and by the support of other Laboratory programs.

Negative ion processes in the gas phase have continued to receive primary attention in analytical research designed to elucidate concepts and methods for the unambiguous isomeric identification of organics in complex mixtures. Previously, it was demonstrated that negative ion chemical ionization (NICI) processes could be used to distinguish various isomeric polycyclic aromatic hydrocarbons (PAHs) based on differences in electron affinity (EA) values. PAHs with EA values greater then 0.5 eV undergo ionization to produce molecular anions, whereas compounds with lower EA values do not ionize. Based on this observation, a number of isomeric PAHs are readily differentiated. More recently, the NICI technique has been extended to the characterization of nitrogen-substituted PAHs. As predicted, the addition of a nitrogen into an aromatic ring system raised the EA value of the azaarene slightly over that of the corresponding PAH. In addition to differentiation of the structural isomers of azaarenes, it was observed that the position of the nitrogen in the ring system can affect the relative ionization response of positional isomers, allowing them to be distinguished by careful NICI studies.

Although the basis for the differences in ionization of various isomers appears to be related to a threshold EA of 0.5 eV, the mechanism responsible for such ionization behavior is not understood. Thus, work has been initiated to elucidate this mechanism. To this end, the observation of an M+14 anion for PAH, with a saturated five-membered ring, prompted studies which revealed that trace levels of oxygen present in the source can participate in gas-phase reactions. The participation of oxygen in these NICI reactions, along with the fact that oxygen has an EA value of 0.5 eV, has raised the possibility that oxygen could compete with compounds with lower EA values, thus preventing them from ionizing via electron capture.

During these NICI mechanism studies, we observed that the pressure of the reagent gas in the ion source had a pronounced effect on the gas-phase reactions. This suggested that isomeric discrimination similar to the NICI technique could be achieved in conventional gas chromatography by operating an electron capture detector at reduced pressure. Consequently, a new detector was designed and constructed by enclosing an electron capture cell with a ^{63}Ni source in a vacuum chamber. The pressure in this detector can be varied from atmospheric to less than 1 torr. A capillary GC column was connected directly to the detector, and the reagent gas was mixed with the GC carrier gas prior to introduction to the detector. Studies with the detector, using a reagent gas of 10% methane in argon at atmospheric pressure, yielded conventional electron capture response. When the pressure in the detector was reduced to about 5 torr, inverted peaks were observed. The peaks resulted from direct ionization of the analytes by the argon metastables because of the increase in the electron population at low pressure. This reduced pressure ionization mode yielded a uniform response from all analytes, similar to that of a flame ionization detector. However, when the pressure in the detector was raised to about 100 torr, an isomer selective response was observed. At intermediate pressures, electron emission competes with electron capture, and the extent of the competing reactions can be controlled by the pressure in the detector. Thus, a multimode ionization detector, combining the features of three different detectors (a conventional electron capture response, a universal emission response, and a selective response), can be attained by simply changing the pressure within the detector. This detector will be useful not only for identifying isomers in complex mixtures but also for detecting classes of compounds. A patent on the device is being filed.

A Fourier Transform Mass Spectrometer (Nicolet FTMS-2000) was installed in September. This instrument is based on the principles of

ion cyclotron resonance (ICR) and represents a radical departure from the design of conventional mass spectrometers. The design of the instrument is unique in that it can be operated in a number of modes simply by changing a few operating parameters through the computer keyboard. This versatility allows the instrument to emulate a variety of different conventional configurations, such as double focusing, quadrupole, and tandem mass spectrometry. In the FTMS technique, the frequency of an ion's circular path in the analyzer cell is measured and related to its mass. Because this frequency can be so accurately measured, ultra-high mass resolution can be obtained. We have obtained a mass resolution exceeding 1 million at mass 131. In addition to high resolution, the mass range of the instrument exceeds 3000 amu. Thus, accurate mass measurement can be obtained on high molecular weight species such as polymers and biological molecules.

Separation studies based on the electrokinetic migration of micelles in capillary tubes are in progress. In this technique, an open tube (25–60 μm ID) is filled with a buffered solution of surfactant. When a voltage (0–30 kV) is applied to the column, the ionic micelles migrate toward the electrode of opposite charge. Analyte molecules diffuse in and out of the migrating micelles, with the amount of time spent in the micelles being a function of the partition coefficient of the analyte between the buffer and the micelle. Those analytes that spend a greater proportion of time in the micelle migrate through the column at a faster rate. Cetyltrimethylammonium chloride (CTAC) and sodium dodecylsulfate (SDS) have been used as micelles, with CTAC being preferred for molecules containing aromatic rings and SDS being the surfactant of choice for molecules that were mainly alkyl in nature. Using this technique, an efficiency approaching 60,000 theoretical plates was obtained for a series of derivatized aliphatic amines. Another success using this technique was the separation of metabolites of Vitamin B6.

A general organic analysis capability is being established to support various Laboratory functions and programmatic efforts. The total scope of this capability is being designed to include sample receiving (tracking, storage, and custody) and sample preparation and analysis, including quality assurance and quality control procedures. This was a development year for this effort; therefore, much time has been devoted to assembling adequate staff and equipment to fulfill this support function. Essential equipment needs include duplicate GC/MS facilities for both volatile organics and semivolatile organics, sample preparation facilities capable of processing at least ten samples daily, a data management and archival system, facilities to process hazardous samples, and miscellaneous analytical facilities, including gas chromatography, liquid chromatography, and routine spectrometry (fluorescence, infrared, and ultraviolet-visible). At the close of FY-1985 50% to 60% of the needed facilities were in place.

Analytical procedures used in this activity will generally be established and documented methods, such as those prescribed by the EPA. To this end, several methods have been adapted, and personnel have been trained to carry them out. Sample preparation methods, such as EPA methods 3510 (separatory funnel liquid-liquid extraction) and 3540 (soxhlet extraction), are now being used by trained personnel. In addition, the following analysis methods have been adapted:

1. Method 8010 — Halogenated volatile organics
2. Method 8015 — Nonhalogenated volatile organics
3. Method 8020 — Aromatic volatile organics
4. Method 8080/608 — Organochlorine pesticides and PCB's
5. Method 8240/1624 — GC/MS method for volatile organics
6. Method 8250/1625 — GC/MS method for volatile organics using capillary column
7. Method 8310/610 — Polynuclear aromatic hydrocarbons by HPLC

(M. V. Buchanan, S. H. Harmon, R. W. Harvey, G. M. Henderson, S. K. Holladay, D. L. Manning, M. P. Maskarinec, G. Olerich, S. K. Parks, M. B. Wise)*

---

*Summer employee, 1985.

SEPARATIONS AND SYNTHESIS

W. H. Griest

The chemistry of complex mixtures, especially in regard to toxicology, was the major focus of this group during 1985. Health effects issues

involving synthetic and petroleum-derived fuels and means of mitigating the toxicity of crude coal liquids were studied for the U.S. Departments of Energy and Defense. Separations research and chromatographic methods development projects have recently been combined under this group to consolidate analytical and applied research, depending on separation technologies. Progress will be reported next year.

The comparative chemistry of crude and upgraded coal liquids and of finished fuels refined from synthetic and natural crude oils continues as a main activity contributing to the understanding of the toxicology of complex mixtures. Lifetime mouse dermal tumorigenicity studies recently completed by collaborators in the Biology Division have demonstrated that catalytic hydrogenation is a very effective means of reducing the toxicity of crude coal liquids. However, a small residual level of tumorigenicity remains in finished products refined from coal liquids. An important observation is that a coal-derived reformed naphtha and a coal-derived home heating oil contain similar concentrations of certain polycyclic aromatic hydrocarbon (PAH) dermal tumorigens. The coal-derived naphtha is devoid of detectable tumorigenicity, whereas the heating oil is a weak tumorigen. In contrast, a small level of tumorigenicity was found in a petroleum-derived light, catalytically cracked naphtha that does not contain detectable PAH dermal tumorigens. A detailed high resolution gas chromatographic and mass spectroscopic comparison of the fuel matrices revealed major differences that may influence the expression of tumorigenicity according to PAH content. The nontumorigenic coal-derived naphtha consists of normal and branched-chain C_5 through C_7 alkanes, benzene and its C_1 through C_4 alkylated homologs, naphthalene, and indane. The slightly tumorigenic petroleum naphtha also contains more numerous branched-chain C_6 and C_7 alkanes and C_5 through C_7 alkenes. The coal-derived home heating oil is composed largely of cycloparaffins, such as alkylated decalins, cyclohexanes, and cyclopropanes. Radiolabeled PAH tracers synthesized in our laboratory are being used to study the influences of these sample matrices on the uptake, transport, and metabolism of tumorigens.

The chemical characterization of complex diesel fuel-related mixtures is a part of overall studies to determine the amounts and kinds of personnel exposure to fuel and lubricant fumes and engine exhaust in the military workplace. Differences in the toxicology of shale- and petroleum-derived fuels also are being studied. Dermal tumorigenicity and inhalation toxicity are the main biological end points of concern. A comparison of the major organic compounds in shale- and petroleum-derived diesel fuels revealed group-specific compositional differences. Although both groups of fuels are very similar in their content of C_8 through C_{25} n-alkanes, alkyl benzenes, and benzo(a)pyrene, the shale oil-derived diesel fuels are distinguished by their lower levels of parent and alkylated two- and three-ring aromatic hydrocarbons. The volatile organic compound content of the inhalable fuel vapors also shows group-specific differences. The shale oil-derived fuel vapors appear to contain fewer branched-chain and partially unsaturated hydrocarbons.

Another significant observation is that diesel engine exhaust is not an entirely suitable material for toxicological studies of fuel-related personnel exposure in the military workplace. A comparison between air particulate matter collected in motor-pool garages and diesel exhaust particulates from military vehicles showed that the latter is compositionally different from the former, although diesel exhaust particulates probably contribute significantly to air particulate matter in garages. The concentration of the dermal tumorigen benzo(a)pyrene found in workplace air was similar to that found in diesel exhaust (16 μg/g vs 11 to 17 μg/g). However, the concentration of the highly mutagenic 1-nitropyrene was somewhat higher in workplace air than in diesel exhaust (4.5 μg/g vs 0.32 to 2.1 μg/g); and the concentration of a bulk organic matrix indicator species, eicosane, was considerably lower in workplace air than in diesel exhaust (74 μg/g vs 2500 to 7400 μg/g). A more detailed sampling and analysis study of workplace air and emission sources in military garages is planned to better characterize fuel-related personnel exposure.

The chemistry of complex synfuel mixtures is being examined for DOE Oak Ridge Operations to aid in interpreting bioassay results being generated by other contractors. In an inhalation bioassay using rats, a coal-derived solid has been characterized for properties relevant to lung tumor inducement. Particle structure and morphology, trace elemental composition, and the concentrations of selected PAH dermal

tumorigens have been determined. A study of the bioavailability of PAHs in particles demonstrated that parts-per-billion concentrations (each PAH) can be leached by phospholipid vesicles, detergents, and serum solutions. Two coal-derived middle distillates from mouse dermal toxicity studies were compared for phenols content. One sample caused much more severe dermal irritation than did the other; the phenols were suspected as the cause of the differential response. Surprisingly, the sample that caused the more severe dermal irritation contained much lower concentrations of phenol, cresols, and dimethyl phenols. This finding suggests that other compounds are responsible for the irritation.

An evaluation of the chemical and toxicological characteristics of coal liquids refining technologies has been a major research activity. The focus of the evaluation is now on identifying optimum catalytic hydrogenation conditions and supplemental treatments that will improve the efficiency of hydrotreatment for eliminating tumorigens and tumorigenicity in crude coal liquids. The sulfide form of alumina-based catalysts has been found much more efficient than the oxide form for reducing the content of benzo(a)pyrene in a vacuum gas oil fraction (>343°C/650°F) of a heavy coal oil. Multiple hydrogenations with fresh catalyst [or prolonged (about 2 h) hydrogenation at 8370 kPa (1200 psig) and 320°C (608°F)] are required to reduce the benzo(a)pyrene content to about 15% of the original (322 ppm). Catalyst poisoning by high-boiling components appears to be the major factor limiting the effectiveness of tumorigen hydrogenation in heavy coal liquids. Some improvement in efficiency is achieved by pretreating the sample with 10 N sodium hydroxide solution. Higher temperature and pressure hydrogenation conditions and other pretreatments are being evaluated.

Toxicological studies of crude coal liquids have often been conducted using petroleum crude oils as "benchmarks" for comparison. Interpretation of the results of these studies has been hindered by differences in the boiling range or the degree of processing between the two groups. To solve this problem, a set of high-boiling petroleum crude oils and crude oil distillates (equivalent in boiling range to commonly studied coal liquids) has been prepared and compared chemically and physically with coal liquids in terms of relevance to dermal tumorigenicity. A major finding is that concentrations of selected four-ring to six-ring PAH dermal tumorigens are one or two orders of magnitude lower (even in the highest-boiling distillates) than in crude coal liquids. The distribution of PAH isomers also is different in the petroleum samples, with the less tumorigenic isomers generally being present in higher concentrations than those with greater tumorigenicity. The concentrations and isomer distributions in the petroleum samples are more similar to those in hydrogenated coal liquids.

Synthesis and measurement of radiolabeled compounds to support fundamental studies of the toxicology of complex mixtures is a new activity initiated this year. Tritiated 10-azabenzo(a)-pyrene and ^{14}C-labeled 4,5-dihydrobenzo(a)-pyrene samples have been prepared and are being purified. Samples of these model compound radiotracers and of synthetic fuels will be supplied to investigators in the Biology Division by the DOE Synfuels Repository. A sample matrix oxidizer has been rebuilt, and optimum conditions have been established for the combustion, collection, and measurement of radioactivity in physiological tissue specimens. Separation and near-quantitative recovery of both ^{14}C and tritium activity from as much as 200 mg of tissue homogenate can be readily achieved.

Our work this year represents the completion or near completion of standing commitments to the DOE and DOD Program offices. Work in the coming year will be to increasingly emphasize separations methods and research while continuing to address the chemistry of complex mixtures.

(A. R. Jones, C. E. Higgins, C.-h. Ho, C. Y. Ma, R. R. Reagan, I. B. Rubin, B. A. Tomkins, J. W. Russell[a]*)*

---

*Summer student, 1985.

SPECIAL PROJECTS

R. W. Holmberg

Although programmatic work for the National Institutes of Health (NIH) and the Department of Defense (DOD) on the chemical properties of concentrated smokes has continued as the main thrust in funding and efforts, work with other

ORNL divisions and groups has broadened. Substantive collaborative projects with the Information Resources Organization, Instrumentation and Controls Division, Environmental Sciences Division, and Solid State Division have been undertaken this year. Particularly noteworthy is the collaborative work of R. S. Ramsey with R. A. Todd of the Instrumentation and Controls Division on a pulsed Helium Ionization Detector that received an IR-100 award. We also note that the collaborative work with Solid State Division on the composition of lead phosphate glasses used to contain nuclear wastes is a direct spin-off of our DOD-sponsored phosphorus obscurants work. Department of Defense work related to the toxicology of military smokes has been essentially concluded with the publication of results on the analysis of RPN03 smokes and the completion of aerosol support activities relating to the study of phosphorus smoke toxicology at the Illinois Institute of Technology Research. New initiatives for continued work with this branch of the military are being discussed.

Projects supported by the NIH comprise two components: (1) the chemical characterization of tobacco and marijuana smoke and (2) the development of specialty instrumentation to determine both exposure to smoke and the magnitude of that exposure. At the request of the National Cancer Institute, we substantially redirected our research efforts on cigarette smoke to include studies of "kreteks", Indonesian cigarettes containing both tobacco and cloves. There has been public concern recently about the enhanced toxicity of smoke from these cigarettes. Our work was directed toward the analysis of major smoke constituents contributed by the cloves. Cigarettes, including a specially prepared cigarette containing only clove, were smoked under standard conditions. Both GC and GC/MS were used to survey the vapor and particulate phases of the smoke. No major clove-derived constituents were found in the vapor phase. Five major clove-specific constituents were identified in the particulate phase. They were eugenol, acetyl-eugenol, beta-caryophylene (BC), alpha-humulene (AH), and caryophylene epoxide. Deliveries of these constituents in the smokes of six brands of kreteks were determined using gas/liquid chromatography. Eugenol deliveries ranged from 9 to 17 mg per cigarette, whereas acetyl-eugenol levels were a few percent of those of the eugenol. Beta-caryophylene deliveries were in the range of 1 mg per cigarette, and AH levels were 13% of those of BC. Caryophylene epoxide deliveries were less than 100 µg per cigarette. These data have since been used to help direct pulmonary toxicity studies being conducted at another laboratory.

The emission rates of sidestream tobacco smoke constituents from smoldering cigarettes are related to their contribution to indoor air pollution. For this reason, we have initiated a project to determine those emission rates. An especially critical aspect of this project is the development of standardized generation and sampling conditions for sidestream smoke, because much of the methodology currently used radically alters the immediate combustion environment of the cigarette, which can change the composition of the material that is ultimately collected and analyzed. For example, measurements of temperature, humidity, and localized air velocity conducted in our laboratory on one popular chamber indicated these parameters could affect the particle/vapor phase distribution of nicotine. A new chamber under development in our group promises to address many of these concerns. Air flow into the chamber and around the smoldering cigarette is essentially laminar, and temperature mapping in and around the smoke plume suggests that laboratory-tested cigarettes smoulder under conditions which closely mimic those encountered in the real world. The effect of air sampling rates on smoke particulate collection efficiencies is currently under investigation.

We have previously described an ORNL cigarette smoke dosimeter that uses analog electronics to process and manipulate signals from both a light-emitting diode/phototransistor-based particle sensor and an orifice flow meter built into a small cigarette holder to measure the mass of particles moving through the holder and into the smoker's mouth. Software and hardware have been developed around an IBM-PC to replace the analog signal processing. The new system uses a Data Translation DT2805 digitizer board to acquire data from both the flow and the particulate signals. A program, written in C, controls data acquisition and analyzes the information. Flow rate and particle concentration are displayed graphically in real time, along with the derived integrated smoke delivery. The program also tabulates and stores (for later statistical analysis) various aspects of smoking topography that may be of interest to behavioralists. The program operates completely

passive mode after startup; in particular, the smoker is not required to signal that he is about to puff. A working prototype program is currently being evaluated for reproducibility and accuracy.

Cooperative work with the National Center for Toxicological Research on the subject of marijuana smoke has continued. Samples have been collected and analyzed to better understand the factors that influence the amount of smoke generated by primate smoke exposure systems. Work has also been done to determine the amount of constituents retained by animals as a result of exposure to the smoke of full strength [2.8% delta-9 tetrahydrocannabinol (THC)] marijuana cigarettes. Exhaled breath samples analyzed for delta-9 THC at ORNL confirmed the findings of previous experiments performed with half-strength material; the animals retain half of the smoke particulates to which they are exposed.

As a joint project with the Information Resources Organization, we are conducting a literature study to characterize and evaluate emissions from rifles and large caliber guns. This work is funded by the Department of Defense, which is interested in understanding the potential health effects of occupational exposure to gunsmoke, particularly as it occurs in armored vehicles and other confined areas. Most of the analytical literature deals with the primary gaseous combustion products of the propellant and primer: oxygen, nitrogen, carbon dioxide, carbon monoxide, and water vapor. With the exception of carbon monoxide, little is known about compounds of potential toxicity. There is a particular lack of information about trace constituents from partially oxidized propellant. It is known that in the explosion process, combustion is not complete, and organic compounds and particulate matter from the partially consumed charge exits the gun barrel. Metallic erosion products from gun barrels also find their way into the exposure atmosphere. From this perspective, there is an obvious need for analytical studies of gunsmoke. Sampling and analytical techniques used to characterize combustion products from other sources, such as cigarette smoke, diesel, and gasoline exhaust, have been reviewed for their applicability to this problem. A second phase of the study will be concerned with the development of plans for a laboratory in which to perform inhalation toxicology experiments and conduct analytical investigations of the exhausts from weapons systems.

A pulsed helium ionization detector has been configured to operate in a constant-current closed-loop mode. Electronic circuitry includes a stable, low-noise current source; a high-speed electrometer; intermediate low-noise gain stages; and a voltage-to-frequency (V/F) converter circuit. A high voltage pulser capable of operating from 0 to 500 V from dc to 300 kHz at the highest voltage was also designed and incorporated. Operation of the detector in a closed-loop mode has been found to decrease noise and background current levels, which improves operating stability, especially at conditions necessary for high sensitivity measurements (i.e., high voltages). The dynamic range, in comparison to dc operation, has been extended approximately two orders of magnitude (from 10^5 to 10^7), thus permitting the analysis of both very high and low concentrations (% to ppb) of the permanent gases. Catastrophic breakdown of the detector under overload conditions is also prevented. Applications for this device include the analysis of high-purity gases for semiconductor processing, environmental pollutants, workplace air for industrial hygiene monitoring, and (because of its universal response mechanism) volatile compounds that are difficult to measure with other detector systems. Presently, efforts are being directed toward transferring this technology to the industrial sector.

As part of a joint project with Environmental Sciences, we have developed a system for probing the chemical composition of deep well waters. While the prime purpose of this investigation is to characterize radioactive and chemical ground water contaminants to very deep levels, it is planned to make a complete analysis of the waters, including dissolved gases, to obtain a better understanding of the geochemistry of the surrounding formations. The system consists of a sampling probe capable of collecting deep well waters to depths in excess of 1000 ft and a facility designed to measure and collect the dissolved gases. The gases will be isolated from the liquid so that both can be analyzed by procedures we have developed. The transfer system was designed and fabricated at ORNL and is sufficiently portable to be used in the field. No commercial probe was available for sampling deep wells that retained the dissolved gases; accordingly, a commercial probe was extensively modified for this purposes. The system has performed satisfactorily in preliminary tests in non-radioactive wells to a depth of 950 ft. Brine solutions (principally NaCl

and $CaCl_2$) containing about 180 mL of dissolved gases per liter of solution were obtained. Mass spectral analyses of the gases indicate that they are predominantly nitrogen (90%) with small, but significant, amounts of methane, helium, argon, carbon dioxide, and oxygen. The quantity of gas found indicates that the solution is essentially saturated at the ambient pressure.

We have collaborated with investigators from Solid State to investigate the structure of mixed lead and iron phosphate glasses that are being considered as a medium for the long-term storage of nuclear wastes. The lead and iron form solid state polymeric phosphates that can be detected using ion exchange HPLC techniques developed for the elucidation of polymeric phosphoric acids in phosphorus combustion aerosols. The solid materials are crushed and then leached with water or salt solutions containing EDTA. The solution is passed through the HPLC column to develop the polyphosphate chromatogram. It has been determined that the average phosphate chain length decreases as the iron content of the phosphate glass increases. More than 50% of the total phosphate in pure lead phosphate glass is composed of unresolved long-chain polymers (greater than P_{13}) whereas the glass with 9% added Fe_2O_3 contains only P_1 to P_8. The solubility of all glasses studied is greater in NaCl/EDTA solution than in pure water.

(T. M. Gayle, G. M. Henderson, S. K. Holladay, R. A. Jenkins, J. H. Moneyhun, D. D. Parr, R. S. Ramsey)*

---

*Instrumentation and Controls Division

5. THE ORNL ENVIRONMENTAL RESTORATION AND FACILITIES UPGRADE PROGRAM

B. R. Clark

An effort was initiated in 1985 to remedy the accumulated environmental problems of the ORNL portion of the Oak Ridge reservation. Past waste disposal and control practices are inadequate by today's standards. The Laboratory is required to identify and remedy the present and potential problems of release of hazardous substances into the environment. Actions needed to remedy and abate environmental pollution are being defined and executed by the Environmental Restoration and Facilities Upgrade Program (ERFU). The ERFU Program is funded by DOE through "taxation" of the R&D programs that the DOE sponsors.

Three major components make up the Program: (1) remedial action, (2) restoration, and (3) monitoring. Remedial actions include identifying and rectifying pollutant releases from solid waste storage areas, surface holding basins, storage tanks, low-level waste lines, and others. Also, unused facilities are being decommissioned as part of the remedial action activities. Restoration projects are the capital intensive actions needed to modernize the waste systems to minimize further releases. A major example is the construction of a new low-level waste drainage, handling and storage system. Monitoring activities are broad; both remedial action sites and routine waste handling operations will require extensive monitoring.

With this brief description of the ERFU Program, the importance of chemical analyses should be evident. The Analytical Chemistry Division (ACD) has a huge responsibility to the Program; and because the Program is large, complex, and continuously evolving, an ACD Program Manager was named to establish and maintain the best possible interface between ACD sections and the numerous projects comprising the ERFU Program. The interface is much more than the usual processing of samples through the division. The program manager helps plan sampling and analysis campaigns "up front" with the ERFU project manager; schedules, sampling protocols, designation of analytes, and quality control procedures can then be established early and orderly. This mode of operation gives ACD the opportunity to plan work loads, acquire special or additional equipment and arrange subcontracts as necessary. Furthermore, ACD people in specialized areas of analysis can be enlisted in the planning stages and contribute to making a better program.

In terms of facilities, the ACD is developing new, expanded capabilities to accommodate the ERFU and other related programs. In particular, a hazardous materials laboratory (HML) was established to receive and prepare samples for analyses of potentially toxic chemical, radiochemical, or mixed substances. A soil testing laboratory is to be included in the HML to measure mechanical and other parameters needed for the Remedial Action Program. Additional radioanalytical and organic analytical equipment is being acquired to handle the rapidly expanding workloads in these areas.

The ACD/ERFU interface through a program manager helps the ACD in its relationship with the ERFU Program. Program activities are better coordinated because the ACD program manager interacts with many people at all levels.

INTRODUCTION

W. D. Shults, Director

The Analytical Chemistry Division of Oak Ridge National Laboratory (ORNL) is a large and diversified analytical chemistry organization. As such, it serves a multitude of functions for a clientele that exists both in and outside ORNL. These functions fall into the following general categories.

1. **Analytical Research, Development, and Implementation.** The division maintains a program to conceptualize, investigate, develop, assess, improve, and implement advanced technology for chemical and physicochemical measurements. Emphasis is on problems and needs identified with ORNL and Department of Energy (DOE) programs, but attention is also given to needs in the analytical sciences themselves. This program is composed of medium- to long-term projects and is supported primarily by the DOE. Fundamental R&D constitutes approximately 20% of our effort.

2. **Programmatic Research, Development, and Utilization.** The division carries out a wide variety of chemical work that typically involves analytical research and/or development plus the utilization of analytical results or special analytical capabilities to expedite programmatic interests. The effort in this category comes from ORNL and DOE programs and from "Work-for-Others" agreements. Emphasis here is on "applied" chemistry. Programmatic R&D constitutes ca. 11% of our work.

3. **Technical Support.** The division performs chemical and physicochemical analyses of virtually all types. Development of methodology is an inherent part of this activity because of the variety of analytical problems that arise in a multiprogram institution like ORNL. Consultation, collaboration, and special projects are involved. Much of this work is short-term in nature and comes from other divisions and programs within ORNL, but a significant fraction originates outside of ORNL and involves the use of talent and/or facilities in which the division is particularly strong or unique. This type of work accounted for approximately 69% of the effort this year.

The Analytical Chemistry Division is organized into four major sections, each of which may carry out any type of work falling in the three categories mentioned above. Chapters 1 through 4 of this report highlight progress within the five sections during the period January 1, 1985 to December 31, 1985. A brief discussion of the division's role in the Laboratory's Environmental Restoration and Facilities Upgrade is given in Chapter 5. Information about quality assurance and safety programs is presented in Chapter 6, along with a tabulation of analyses rendered. Publications, oral presentations, professional activities, educational programs, and seminars are cited in Chapters 7 and 8. Approximately 35 articles, 22 proceedings publications, and 34 reports have been published; 113 oral presentations were given during this reporting period. Some 310,000 determinations were performed with an overall quality factor of 96%.

6. QUALITY ASSURANCE, SAFETY, AND TABULATION OF ANALYSES

W. R. Laing
P. L. Howell
H. G. Davis
A. L. Harrod
R. E. Jones

QUALITY ASSURANCE

The quality control program increased by 68% to over 9000 results this year (Table 6.1). The overall quality level was 96%, the same as 1984. There was an increase of 10% in the number of control elements and/or compounds covered by controls (Tables 6.2 and 6.3). In cooperation with the Department of Environmental Management and the Energy Division, samples from seven programs were spiked, and blind controls were prepared for submission to ACD laboratories. Quality problems were addressed in several areas, including inductively coupled plasma spectrometry; alpha, beta, and gamma counting; spectrophotometry; and ion chromatography.

In other work, monthly and quarterly reports were prepared, and a customer satisfaction survey was conducted. Three programs were audited internally, and ACD was reviewed eight times by external audits.

RADIATION SAFETY

The division supports the ALARA principle (as low as reasonably achievable) and has demonstrated this by continually reducing exposure to personnel over the past 5 years. New audible personnel radiation monitors, known as Bristol Beepers, are being worn by Transuranium Laboratory and Radioactive Materials Analytical Laboratory personnel. The use of daily pencil meter monitors has been discontinued, and visual dosimeters have been assigned to appropriate personnel; individual readings are recorded daily.

During the year, a new analytical chemistry facility, the Hazardous Materials Analytical Laboratory in Building 2026, has been reviewed and approved by the Radioactive Operations Committee. The necessary signs, radiation monitors and safety equipment have been installed in rooms 212 and 213 in the new facility.

SAFETY

The safety policy of the Analytical Chemistry Division is described in the following statements:

1. Conduct all activities with the lowest reasonable risk of personal injury or property loss due to preventable accidents.
2. Perform all work and maintain the working environment in accordance with Laboratory safety regulations and designated national codes and standards.
3. Investigate all significant accidents, determine their causes, and take steps to prevent recurrence of similar accidents.
4. To improve employee awareness of safety while off the job as well as on the job.

The Analytical Chemistry Division had only four first aid cases this year, no recordable injuries/illnesses, no lost workday cases, and only one off-the-job injury. The employees have accumulated 2,843,221 workday hours since the last lost time accident in June 1972. This record is possible because of an excellent safety awareness program within the division and the high priority given to safety. All division employees are expected to attend a safety meeting each quarter. During this period, 95% of the employees attended such a meeting.

The division conducted the following safety training and orientation workshops this year:

1. ACD Local Emergency Organization, Fire and CPR.
2. QA Orientation, New Employees.
3. ACD General Orientation Workshop. This included hazardous materials, radiation control, affirmative action, and the division's open door program.

Quarterly safety audits were made by the division's safety committee and the division safety officer.

Division Appearance Inspection Program. This program was initiated this year to review facilities and equipment and to help ensure an orderly, safe working environment and good employee attitudes about their place of work. This program includes the following features:

1. Semiannual inspections.
2. Division-wide walk-throughs.
3. Division-level management visibility and participation.

Table 6.1 Distribution of control tests by group

Group	Total	No. Outside fixed limits	Quality level (%)[a]
Chemical and Physical Analysis	3333	166	95
Environmental Analysis	738	45	94
Low Level Radio-chemical Analysis	273	14	95
Radioactive Materials Analysis	851	27	97
TRU	4022	127	97
TOTAL	9217	379	96[b]

[a]Quality level, % = $\frac{\text{No. results in control}}{\text{total No. of results}} \times 100$

[b]Average

Table 6.2 Control samples prepared for October 1984 through September 1985

Method	No. of control elements	No. of control solutions	Concentration range (mg/mL)
Atomic absorption/flame emission/flameless AA spectrometry	15	27	0.002-0.250
Coulometry	1	3	8-12
Counting methods			
alpha	1	11	0.03-0.05
Beta and liquid scintillation	7	26	10^1 to 10^6 Bq/mL
Fluorimetry	1	4	0.001-0.01
Gamma spectrometry	13	52	10^1 to 10^7 Bq/mL
Gas chromatography	1	5	0.001 to 1000 mg/L
Gravimetry	3	11	2-75%
Gravimetry (Leco)	2	4	100-800 μg/g
Ion chromatography	7	4	0.001-0.06
Ion selective electrode	3	9	0.001-0.1
Inductively coupled plasma (ICP)	30	20	0.001-0.15
Infrared absorption spectrophotometry	1	6	0.004-0.1
Solution measurements (pH and conductivity)	2	5	
Spectrophotometry	10	20	0.0001-5
Volumetric titrimetry			(acid)
In the laboratory	14	40	0.1-7 normal
In hot cells	?	12	2-120
X-ray fluorescence spectrometry	4	6	0.50-150
TOTAL	117	265	

Table 6.3 Distribution of control results by method for October 1984 through September 1985

Method of analysis	No. of control elements	No. of control results
Atomic absorption/flame emission/ flameless AA spectrometry	15	458
Coulometry	1	17
Counting methods		
alpha	1	488
beta and liquid scintillation	7	231
Fluorimetry	1	132
Gamma spectrometry	13	3314
Gas chromatography	1	11
Gravimetry	3	95
Gravimetry (Leco)	2	68
Ion chromatography	7	1014
Ion selective electrode	3	86
Inductively coupled plasma (ICP)	30	1820
Infrared absorption spectrophotometry	1	35
Solution measurements (pH and conductity)	2	32
Spectrophotometry	10	269
Volumetric titrimetry		
In the laboratory	14	947
In the hot cells	2	103
X-ray fluorescence	4	97
TOTAL	117	9217

7. SUPPLEMENTARY ACTIVITIES

The division continues to maintain liaison with the academic community through its Advisory Committee, consultants, and various ORNL and ORAU programs. We also make facilities available for student and faculty research and training programs.

ADVISORY COMMITTEE

The Information Meeting was held July 22-24, 1985. The interval between meetings has been extended to 18 months. The next meeting will be held in January 1987. The 1985 Advisory Committee was composed of:

J. W. Frazer, 6767 Alisal Street, Pleasanton, CA.
J. G. Grasselli, Standard Oil Company, 4440 Warrensville Center Road, Cleveland, OH.
E. D. Pellizzari, Director for Analytical Sciences, Research Triangle Institute, P. O. Box 12194, Research Triangle Park, NC.
J. W. Taylor, Chemistry Department, University of Wisconsin, Madison, WI.
R. C. Wymer, Chemical Technology Division, Oak Ridge National Laboratory, P. O. Box X, Oak Ridge, TN.

CONSULTANTS

The following specialists were brought to ORNL on a short-term consulting basis this past year as part of our Seminar Program. Details of the seminars are listed below.

K. D. Cook, University of Tennessee, Knoxville, TN
C. S. Alley, Analytical Chemistry Division, ORNL, Oak Ridge, TN
P. R. Griffiths, University of California, Riverside, CA
D. C. Hoffman, Lawrence Berkeley Laboratory, Berkeley, CA
K. A. Rahn, University of Rhode Island, Narragansett, RI
A. G. Marshall, Ohio State University, Columbus, OH
J. W. Russell, Humboldt State University, Arcata, CA
J. E. Riley, Jr., AT&T Bell Laboratories, Murray Hill, NJ
M. Martini, EG&G ORTEC, Oak Ridge, TN
D. L. Illman, Infometrix, Inc., Seattle, WA
D. M. Lubman, University of Michigan, Ann Arbor, MI
F. Brech, Jarrell-Ash (Retired), Dover, MA
B. Wilson and R. Boyd, ARL Division of Bausch & Lomb, Sunland, CA

Michael L. Gross, University of Nebraska, presented the plenary lecture at the 28th Conference on Analytical Chemistry in Energy Technology.

Willard Harrison, University of Virginia, and Larry Hrubesh, Lawrence Livermore Laboratory, were consultants for the Office of Basic Energy Sciences Site Review.

G. Mamantov and M. J. Sepaniak, of the University of Tennessee, continued working in the division as adjunct research participants.

STUDENT ASSIGNMENTS

B. A. Tomkins served as "Dean" for the division's student guests during 1985. Brisco Harward, a predoctoral student from the University of Tennessee, completed his work in the Analytical Methodology Section as an ORAU graduate research participant.

The division maintains a subcontract with the University of Tennessee to enable advanced graduate students to participate in environmental analysis programs. Chris P. Leibman continued his work with P. J. Todd on organic SIMS studies. Also under this contract, C. N. Kettler completed his work with Mike Maskarinec in developing an electron capture detector for open tubular liquid chromatography. D. E. Burton also worked with Mike Maskarinec to develop micellar electrokinetic separations.

The division also hosted another ORAU graduate research participant this year. J. R. Parrish worked with Juel Emery in performing neutron activation analysis at the HFIR.

SUMMER PROGRAM

During the summer the division was host to two representatives of the ORAU Undergraduate Research Program, which offers laboratory experience to exceptional college students. Sharon K. Parks, Wake Forest University, worked with Michelle Buchanan and Mark Wise in the Organic Analysis Section in developing a new type of chromatographic detector. Jay W. Russell, Humboldt State University, worked with C.-h. Ho and Wayne Griest on synthesizing selective stationary phases for gas chromatography.

GLCA PROGRAM

During the fall semester, Jennifer L. Dyke, DePauw University, was assigned to the Organic Analysis Section and worked with Michelle Buchanan and Mark Wise in the development and evaluation of a new chromatographic detector.

ORAU FACULTY RESEARCH PROGRAM

S. Ballou Skinner worked in the Radiochemical and Activation Analysis Group with Frank Dyer in evaluating fission track counting methodology for determining uranium in human urine.

ORAU POSTGRADUATE RESEARCH TRAINING PROGRAM

W. G. Tong continued his postdoctoral research in laser analytical chemistry in the Analytical Methodology Section.

SPECIAL AWARDS

W. B. Whitten and J. M. Ramsey received a Publications Award from Martin Marietta Energy Systems, Inc., for "Self-scanning of a Dye Laser Due to Feedback from a $BaTiO_3$ Phase-Conjugate Reflector."

M. V. Buchanan and G. Olerich also received a Publications Award from Martin Marietta Energy Systems, Inc., for "Differentiation of Polycyclic Aromatic Hydrocarbons Using Electron Capture Negative Chemical Ionization."

D. A. Bostick received the DOE Weapons Complex Award of Excellence for the In-Line Photometric Uranium Concentration Monitor being applied in the Enriched Uranium Recovery Improvement Program at Y-12.

R. S. Ramsey received an I-R 100 Award for development of a Helium-Ionization Detector for GC ("PHIDELS").

G. L. Glish received a "Top 100 Innovator" award from *Science Digest*.

28th ORNL/DOE CONFERENCE ON ANALYTICAL CHEMISTRY IN ENERGY TECHNOLOGY

This year's conference was held at the Knoxville Hilton, October 1-3, 1985. The theme of the conference was "Analytical Chemistry in Energy Technology." Attendance was 225, with representatives from foreign countries, academia, industrial institutions, and other government agencies. There were 19 exhibits (31 representatives) and 17 booths. Topics emphasized during the meeting included lasers, mass spectrometry, and nuclear and plasma spectroscopy.

A. L. Harrod was Arrangements Chairman, W. R. Laing was Technical Program Chairman, and Z. H. Benson was Treasurer. Terrye Danner and Doris Smith were Conference Secretaries. Other conference committee members included D. A. Costanzo, J. S. Eldridge, M. P. Maskarinec, S. A. McLuckey, M. L. Parsons (LANL), W. D. Shults, and J. P. Young.

ANALYTICAL CHEMISTRY DIVISION SEMINARS AT ORNL

Speaker	Title	Date
Cook, K. D. Univ. of Tennessee, Knoxville, TN	"Solution Mass Spectrometry: Better Results Through Chemistry"	April 3, 1985
Alley, C. S. Anal. Chem. Div., ORNL	"The Evaluation of a Zymark Robotics System for Multitasking Applications in a Complex Process Laboratory"	May 30, 1985

Griffiths, P. R. Univ. of California, Riverside, CA	"Hyphenated Techniques with FTIR"	June 14, 1985
Hoffman, D. C. Lawrence Berkeley Laboratory, Berkeley, CA	"Production and Identification of New Heavy and Superheavy Element Isotopes"	June 18, 1985
Rahn, K. A. Univ. of Rhode Island, Narragansett, RI	"Sources and Transport of Pollution Aerosol in the Northeast as Deduced from Regional Elemental Tracers"	June 25, 1985
Marshall, A. G. Ohio State Univ., Columbus, OH	"Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy"	Aug. 9, 1985
Russell, J. W. Humboldt State Univ., Arcata, CA	"Qualitative and Quantitative Determination of Dermal Tumorigen Polycyclic Aromatic Hydrocarbons in Coal Conversion Products"	Aug. 21, 1985
Riley, Jr., J. E. AT&T Bell Laboratories, Murray Hill, NJ	"Monitoring Trace Levels of Radioactive Contaminants in Semiconductor Materials"	Sept. 18, 1985
Martini, M. EG&G ORTEC, Oak Ridge, TN	"Cooling Gamma-Ray Spectrometers to Liquid Nitrogen Temperature without Liquid Nitrogen"	Sept. 24, 1985
Illman, D. L. Infometrix, Inc., Seattle, WA	"Exploratory Data Analysis Using the ARTHUR and Ein*Sight Computer Program Packages"	Oct. 4, 1985
Lubman, D. M. Univ. of Michigan, Ann Arbor, MI	"Analytical Applications of Laser Ionization in Mass Spectrometry"	Oct. 15, 1985
Brech, F. Jarrell-Ash (Retired), Dover, MA	"Application of Science in Examination of Works of Art"	Nov. 5, 1985
Wilson, B., and Boyd, R. ARL Division of Bausch & Lomb, Sunland, CA	"Glove Box Application of a Sequential Inductively Coupled Plasma Spectrometer Laboratory"	Nov. 21, 1985

ADDITIONAL PROFESSIONAL ACTIVITIES

ATTRILL, J. E.

Advisory Committee:	Subcommittee E-38.01 on Energy, ASTM
Member:	ASTM Committee E-38 on Resource Recovery
	ORNL Emergency Oil Spill Response Team
Sample Coordinator:	ACD/Department of Environmental Management

BROOKSBANK, R. D.

Member:	ASTM Committee D-33, Protective Coating and Lining Work for Power Generation Facilities
Division Assistant Representative:	Material Balance Area Representative for Nuclear Materials Management

BUCHANAN, M. V.

Member:	ORAU Traveling Lecture Program

CARTER, J. A.

Advisory Board:	*Analytical Chemistry*
Advisory Panel Member:	DOE/ISA Laboratory Advisory Group for Effluent Research (LAGER)
Laboratory Coordinator:	ISPO Programs
Secretary:	Subcommittee C-5:05, Analytical Task Group (Reactor Grade Graphite), Committee C-5, Manufacturer of Carbon and Graphite Products, ASTM

CATON, J. E.

Member:	ACD Long Range Planning Committee

CHRISTIE, W. H.

Member:	ACD Long Range Planning Committee
	ACD Solids/Surface Characterization Team
	Program Committee, SIMS V, Fifth International Conference on Secondary Ion Mass Spectrometry, Washington, DC, Sept. 29-Oct. 4, 1985

COSTANZO, D. A.

Member:	ASTM Committee C-26, Nuclear Fuel Cycle, and Subcommittee C-26:05, Test Methods
	ACD Long-Range Planning Committee
	Planning Committee, 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Chairman and Organizer:	Poster Session: "Interactive Analytical Seminars," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology

DALE, J. M.

Member:	Ad Hoc Committee for Physics Division Staff Member Appointment

ELDRIDGE, J. S.

Member:	Lab Committee 8 of the International Society Committee for the Methods of Air Sampling and Analysis
	Planning Committee, 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology

Organizer:	Session on "Radioanalytical Methods: Environmental," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
President-Elect:	Environmental Radiation Section of the Health Physics Society

BERRY, J. F.

Division Representative:	Laboratory Emergency Sample Coordinator Division Computer Systems Security Officer

FELDMAN, C.

Fellow:	American Society for Testing and Materials
Member:	Committee E-2 on Emission Spectroscopy, ASTM, Subcommittees on Fundamental Methods, Editorial Practices, and Nomenclature
Scientific Editor:	*Optics and Spectroscopy* (English translation of Russian journal, *Optika i Spektroskopita*)

FERGUSON, N. M.

Division Representative:	Energy Systems Environmental Analysis Committee

GLISH, G. L.

Chairman:	American Society for Mass Spectrometry History Committee
Lecturer:	ORAU Traveling Lecture Program

GOERINGER, D. E.

Chairman:	ACD Seminar Committee

GRIEST, W. H.

Consultant:	Department of Energy - BES Electric Power Research Institute Environmental Protection Agency - IERL/TSO

GUERIN, M. R.

Consultant:	Department of Energy (OHER) Complex Mixtures Program Committee National Institutes of Health NCI Passive Smoking Grant Review

HIGGINS, C. E.

	ACD Ombudsman

HOLMBERG, R. W.

Coordinator:	ACD Metric Coordinator

HOWELL, F. L.

Coordinator:	ACD Quality Control Program

HULETT, L. D.

Coordinator:	ACD Solids/Surfaces Characterization Team

JENKINS, R. A.

Consultant:	National Cancer Institute: Program/Project Review of American Health Foundation
Member:	ORNL Speaker's Bureau

JONES, R. E.

Chairman:	Task Group on Methods of Coatings Analysis, D-33
Division Representative:	ACD Radiation Control Officer
	Respirator Trainer
Member:	ASTM Committee D-33, Protective Coating and Lining Work for Generation Facilities

KELLER, J. M.

Member:	ACD Seminar Committee
	Digital Equipment Company Users Society (DECUS)

KLATT, L. N.

Member:	Energy Systems, PhD Recruiting Team
	ACD Long-Range Planning Committee
	ACD Safety Committee
Secretary:	ACS Division of Analytical Chemistry

LAING, W. R.

Chairman:	Subcommittee C-26:05, Test Methods, Nuclear Fuel Cycle, ASTM
	ASTM Long-Range Planning Committee
Coordinator:	ACD Quality Assurance Program
Fellow:	American Society for Testing and Materials
Member:	ASTM Committee D-33, Protective Coatings
	ASTM Committee on Technical Committee Operations
	ISO Technical Committee 85, Subcommittee 5
	ORNL Pregrievance Committee
	INMM Group 5.1, Analytical Chemistry Laboratory Measurement Control
	Energy Systems-GAT Analytical Committee
Technical Program Chairman:	28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Vice-Chairman:	ASTM Committee C-26, Nuclear Fuel Cycle

LYON, W. S.

Advisory Board:	*Analyst*
Chairman:	Honors & Awards Committee, Isotopes & Radiation Division, ANS
	Session on "Analytical Chemistry and the Environment," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Fellow:	American Nuclear Society
Honorary Member:	Committee E-10, Nuclear Technology and Applications, ASTM
Member:	Organizing Committee, 7th International Conference on Modern Trends in Activation Analysis
	Scientific Committee 25 on Radiation Protection in the Use of Small Neutron Generators, NCRP
Regional Editor:	*Journal of Radioanalytical and Nuclear Chemistry*

MASKARINEC, M. P.

Member:	ASTM E-19 Committee on Chromatography
	ASTM D-34 Committee on Waste Disposal
	Planning Committee, 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Organizer:	Session on "Analytical Chemistry and the Environment," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology

McKOWN, H. S.

Division Representative:	Interplant Computer Communications Committee

McLUCKEY, S. A.

Member:	Planning Committee, 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Organizer:	Session on "Advances in Analytical Mass Spectrometry," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology

RAMSEY, J. M.

Member:	Advanced Gas Centrifuge Review Team

RAMSEY, R. S.

Member:	ACD Seminar Committee
	Steering Committee, Separation Science and Technology

ROSS, H. H.

Chairman:	ORNL Graduate Student Selection Panel
	ORNL Postdoctorate Selection Panel
Faculty Member:	Dept. of Chemistry, University of Tennessee, Knoxville (Science Alliance Professor, Part-time)
Member:	Editorial Advisory Board, *Journal of Radioanalytical and Nuclear Chemistry*
	Fellowship Committee, ACS, Division of Analytical Chemistry
	ORNL Technology Utilization Committee
Organizer:	Symposium on "Nuclear Methods in Analytical Chemistry," ACS SE-SW Regional Meeting, Memphis, TN, Nov. 3-5, 1985

ROSSKEL, T. M.

Chairman:	Awards Committee, Tennessee Valley Chapter, American Vacuum Society
	Scholarship Committee, Tennessee Valley Chapter, American Vacuum Society
Chairman and Organizer:	Session on "First Student Paper Competition," 5th Annual Tennessee Valley Chapter, AVS Symposium and Equipment Exhibition, Knoxville, TN, April 30-May 2, 1985

SCOTT, T. G.

Member:	Committee D-19, Water, ASTM, and Subcommittee 4, Methods of Radiochemical Analysis
	Health Physics Society

SHULTS, W. D.

Consultant:	Energy Systems Career Planning Program
Member:	Advisory Committee, "Analytical Approach," *Analytical Chemistry*
	Canvassing Committee for the ACS Award for Creative Advances in Environmental and Technology
	Editorial Board, *Analytica Chimica Acta*
	ORNL In-House Continuing Education Committee
	Technical Services Committee, Energy Systems

SMITH, D. H.

Chairman	American Society of Mass Spectrometry Isotopes Ratio Committee
Member:	ACD Long-Range Planning Committee
Organizer:	Symposium on Frontiers in Isotope Ratio Measurements, 33rd Annual Conference on Mass Spectrometry and Applied Topics, San Diego, CA, May 1985

STEWART, J. H., Jr.

Division Representative:	ACD Environmental Protection Officer
Member:	ACD Solids/Surfaces Characterization Team, Fluorescence Methods
	International Working Group, "Analytical Standards of Minerals, Ores, and Rocks"
	Manuscript Review Board for *Analytical Chemistry*
Task Leader:	ASTM C-26 Nuclear Fuel Cycle Task: C-26.05 X-Ray Task Group

STOKELY, J. R.

Coordinator:	ACD MS/BS Recruiting

TODD, P. J.

Coordinator:	ACD Awards

TOMKINS, B. A.

Coordinator:	ACD University Relations

WALKER, R. L.

Advisory Panel Member:	DOE/ISA Laboratory Advisory Group for Effluent Research (LAGER)

WISE, M. B.

Member:	ACD Seminar Committee

WHITTEN, W. B.

Lecturer:	ORAU Traveling Lecture Program

YOUNG, J. P.

Fellow:	American Association for the Advancement of Science
Member:	Planning Committee, 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology
Chairman and Organizer:	Session on "Broadened Horizons in Fourier Transform Spectroscopy," 28th ORNL/DOE Conference on Analytical Chemistry in Energy Technology

Table 6.4 Summary of analytical work

Organization	Number of results reported by					
	Mass and Emission Spectrometry	Transuranium Laboratory	Radioactive Materials Analytical Laboratory	Bio/Organic Analysis	General and Environmental Analysis	Total
ORNL Unit						
Analytical Chemistry	125		58	23	3,546	3,752
Biology	210				4,224	4,434
Central Management					19,356	19,356
Chemical Technology	3,757	27,808	2,709	2,277	38,719	75,270
Chemistry	150		5	213	692	1,060
Energy			8		6,590	6,598
Engineering Physics	25					25
Engineering Technology	1,053				1,200	2,253
Environmental and Occupational Safety	122		68	3,887	19,699	23,776
Environmental Sciences			421	6,916	83,799	91,136
Finance and Materials				24		24
Fuel Recycle	175		4,179		219	4,573
Fusion Energy	207				140	347
Health			8	61	916	985
Health and Safety Research	131			783	3,795	4,709
Laboratory Protection				12	119	131
Metals and Ceramics	3,745		28	50	2,184	6,007
Operations	10,780	23,338	1,948	9,478	7,471	53,015
Physics	76		6		102	184
Plant and Equipment				156	869	1,025
Solid State	1,053			141	1,249	2,443
Others						
Protective Coating Testing			801			801
K-25 and Y-12			261	538	3,958	4,757
Miscellaneous	688	732	12	43	793	2,268
Nuclear Regulatory Commission				1,017		1,017
Savannah River Laboratory	378					378
Work for Others			211			211
TOTAL	22,675	51,878	10,723	25,619	199,640	310,535

8. PRESENTATION OF RESEARCH RESULTS

As in past years, the division has actively responded to the changing priorities of the ORNL research effort by changing the emphasis of some of its own programs or instituting new studies. The increasing concern with energy - nuclear as well as non-nuclear - is reflected in the research results listed below. The multidisciplinary approach required in many such problems is indicated by the number of papers and talks coauthored by members of other ORNL divisions. Such persons are designated by an asterisk.

PUBLICATIONS

Contributions to Books, Proceedings, and Reports

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Bertram, L. K.	Glish, G. L.; McBay, E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 709
Buchanan, M. V.	Buchanan, M. V.; Hamming, M. C.* *TRC Spectral Data-Mass*	Supplement No. 2, July 1, 1985, Thermodynamics Res. Ctr.
Christie, W. H.	Christie, W. H.; Donohue, D. L.; Goeringer, D. E.; McKown, H. S. "Sputter Atomization/ Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 59
	James, R. B.;* Narayan, J.;* Christie, W. H.; Eby, R. E.; Holland, O. W.;* Wood, R. F.* Pulsed CO_2-Laser Annealing of Ion-Implanted Silicon"	Proc., *Mater. Res. Soc. Symp.*, Vol. 35, Boston, MA, Nov. 26-30, 1984, p. 413 (1985)
	Taylor, D. H.;* Christie, W. H.; Pavone, D.* "Ir/PuO_2 Compatibility: Transfer of Impurities from Plutonium Dioxide to Iridium Metal during High Temperature Aging"	*Optimizing Materials for Nuclear Applications*, Los Angeles, CA, F. A. Garner, D. S. Gelles, F. W. Wiffen, eds., The Metallurgical Soc., Warrendale, PA, 1985, p. 201
	Aziz, M. J.;* Nygren, E.;* Christie, W. H. White, C. W.;* Turnbull, D.* "Effect of Pressure on Self Diffusion in Crystalline Silicon"	Proc., *Mater. Res. Soc. Symp.*, Vol. 36, Boston, MA, Nov. 26-30, 1984, p. 101 (1985)

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Christie, W. H.	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ultra-Sensitive Isotopic Analysis by Resonance Ionization Mass Spectrometry"	Proc., *Int. Conf. on Lasers*, San Francisco, CA, Nov. 26-30, 1984, p. 295 (1985)
	Tsao, J. Y.;* Thompson, M. O.;* Percy, P. S.;* White, C. W.;* Christie, W. H. "Test of Two Solute Trapping Molds"	Proc., *Mater. Res. Soc. Symp.*, Vol. 35, Boston, MA, Nov. 26-30, 1984 p. 153 (1985)
	James, R. B.;* Christie, W. H.; Eby, R. E. Darken;* Mills, B. E.* "Intervalence-Band Absorption Saturation and Optically Induced Damage of Ga As by Pulsed CO_2 Laser Radiation	*SPIE*, Vol. 540, SW Conf. on Optics, Albuquerque, NM, Mar. 4-8, 1985, p. 453
Donohue, D. L.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Spectral Studies Using Resonance Ionization Mass Spectrometry Combined with Photoelectron Spectroscopy"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 52
	Christie, W. H.; Donohue, D. L.; Goeringer, D. E.; McKown, H. S. "Sputter Atomization/ Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 59
	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ultra-Sensitive Isotopic Analysis by Resonance Ionization Mass Spectrometry"	Proc., *Int. Conf. on Lasers*, San Francisco, CA, Nov. 26-30, 1984, p. 295 (1985)
Dyer, F. F.	Roseberry, L. M.; Dyer, F. F. "Instrumental Neutron Activation Analysis in the Measurements of Trace Element Distribution at Two Coal Conversion Plants"	Proc., *Fifth Int. Conf. on Nucl. Methods in Environ. and Energy Res.*, Puerto Rico, Apr. 2, 1984, p. 1334, (1985)
Eby, R. E.	James, R. B.;* Narayan, J.;* Christie, W. H.; Eby, R. E.; Holland, O. W.;* Wood, R. F.* Pulsed CO_2-Laser Annealing of Ion-Implanted Silicon"	Proc., *Mater. Res. Soc. Symp.*, Vol. 35, Boston, MA, Nov. 26-30, 1984, p. 413 (1985)
	James, R. B.;* Christie, W. H.; Eby, R. E. Darken;* Mills, B. E.* "Intervalence-Band Absorption Saturation and Optically Induced Damage of Ga As by Pulsed CO_2 Laser Radiation"	*SPIE*, Vol. 540, SW Conf. on Optics, Albuquerque, NM, Mar. 4-8, 1985, p. 453
Glish, G. L.	Glish, G. L.; McBay, E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 709

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Glish, G. L.	Glish, G. L.; McLuckey, S. A.; Goeringer, D. E. "Low Energy Collisional Activation: Internal Energy Considerations"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics,* San Diego, CA, May 26-31, 1985, p. 128
	McLuckey, S. A.; Glish, G. L. "Substituent Effects in the Collisionally Activated Decompositions of Nitroaromatic Anions"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics,* San Diego, CA, May 26-31, 1985, p. 591
	McLuckey, S. A.; Glish, G. L. "Kinetic Energies Released in the Loss of Nitrogen Oxide from Substituted Nitroaromatic Anions"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics,* San Diego, CA, May 26-31, 1985, p. 148
Goeringer, D. E.	Glish, G. L.; McLuckey, S. A.; Goeringer, D. E. "Low Energy Collisional Activation: Internal Energy Considerations"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics,* San Diego, CA, May 26-31, 1985, p. 128
	Christie, W. H.; Donohue, D. L.; Goeringer, D. E.; McKown, H. S. "Sputter Atomization/ Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics,* San Diego, CA, May 26-31, 1985, p. 59
	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ultra-Sensitive Isotopic Analysis by Resonance Ionization Mass Spectrometry"	Proc., *Int. Conf. on Lasers,* San Francisco, CA, Nov. 26-30, 1984, p. 295 (1985)
Griest, W. H.	Griest, W. H.; Guerin, M. R.; Ho, C.-h. "Dermal Tumorigen PAH and Complex Mixtures for Biological Research"	*Proc., 1st Annual DOE Contractor's Meeting on the Health and Environmental Effects of Complex Chemical Mixtures* Chicago, IL, June 17-18, 1985, p. 115
Guerin, M. R.	Griest, W. H.; Guerin, M. R.; Ho, C.-h. "Dermal Tumorigen PAH and Complex Mixtures for Biological Research"	*Proc., 1st Annual DOE Contractor's Meeting on the Health and Environmental Effects of Complex Chemical Mixtures,* Chicago, IL, June 17-18, 1985, p. 115

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Ho, C.-h.	Griest, W. H.; Guerin, M. R.; Ho, C.-h. "Dermal Tumorigen PAH and Complex Mixtures for Biological Research"	*Proc., 1st Annual DOE Contractor's Meeting on the Health and Environmental Effects of Complex Chemical Mixtures*, Chicago, IL, June 17-18, 1985, p. 115
Lee, D. A.	Lee, D. A. "Separation of Lithium Ions by Chromatography"	*Lithium: Current Applications in Science, Medicine, and Technology*, John Wiley & Sons, Inc., 1985, p. 25
Maskarinec, M. P.	Maskarinec, M. P.; Francis, C. W.*; and Goyert, J. C.* "Mobility of Organic and Inorganic Constituents from Energy and Combustion-Related Wastes Under Codisposal Conditions"	Proc., *Mater. Res. Soc. Symp.*, Boston, MA, Nov. 26-30, 1984, p. 227 (1985)
McBay, E. H.	Glish, G. L.; McBay, E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 709
McKown, H. S.	Christie, W. H.; Donohue, D. L.; Goeringer, D. E.; McKown, H. S. "Sputter Atomization/Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 59
	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ultra-Sensitive Isotopic Analysis by Resonance Ionization Mass Spectrometry"	Proc., *Int. Conf. on Lasers*, San Francisco, CA, Nov. 26-30, 1984, p. 295 (1985)
McLuckey, S. A.	McLuckey, S. A.; Glish, G. L. "Kinetic Energies Released in the Loss of Nitrogen Oxide from Substituted Nitroaromatic Anions"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 148
	McLuckey, S. A.; Glish, G. L. "Substituent Effects in the Collisionally Activated Decompositions of Nitroaromatic Anions"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 591
	Glish, G. L.; McBay, E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 709

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
McLuckey, S. A.	Glish, G. L.; McLuckey, S. A.; Goeringer, D. E. "Low Energy Collisional Activation: Internal Energy Considerations"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 128
Roseberry, L. M.	Roseberry, L. M.; Dyer, F. F. "Instrumental Neutron Activation Analysis in the Measurements of Trace Element Distribution at Two Coal Conversion Plants"	Proc., *Fifth Int. Conf. on Nucl. Methods in Environ. and Energy Res.*, Puerto Rico, Apr. 2, 1984, p. 1334, (1985)
Smith, D. H.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Spectral Studies Using Resonance Ionization Mass Spectrometry Combined with Photoelectron Spectroscopy"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 52
	Smith, D. H. "Isotope Ratio Committee Report"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 1008
Todd, P. J.	Todd, P. J.; Leibman, C. P.;* Mamantov, G.* "Lewis Acid Enhanced Emission of Organic Secondary Molecular Ions"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 970
	Leibman, C. P.;* Todd, P. J. "Secondary Ion Mass Spectrometry of Lewis Acids"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 170
	Todd, P. J.; Groenewold, G. S.* "Evaporation and Ion Damage in Molecular SIMS"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 571
Tomkins, B. A.	Tomkins, B. A. "Chromatographic Detectors Used for the Determination of Nitrated Polycyclic Aromatic Hydrocarbons"	*Nitrated Polycyclic Aromatic Hydrocarbons* C. White, ed., Huethig Publ., p. 87, 1985
Young, J. P.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Spectral Studies Using Resonance Ionization Mass Spectrometry Combined with Photoelectron Spectroscopy"	Proc., *33rd Annu. Conf. on Mass Spectrom. and Allied Topics*, San Diego, CA, May 26-31, 1985, p. 52

Articles

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Buchanan, M. V.	Rubin, I. B.; Buchanan, M. V. "Carbon-13 NMR Spectra of Anthraquinone-Derived Dyes"	*Magn. Reson. in Chem.* 23(3), 161, 1985
Carter, J. A.	McLuckey, S. A.; Glish, G. L.; Carter, J. A. "The Analysis of Explosives by Tandem Mass Spectrometry"	*J. of Forensic Sci.* 30, 773, 1985
Christie, W. H.	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ion Microprobe Mass Spectrometry Using Sputtering Atomization and Resonance Ionization	*Anal. Chem.* 57, 1193, 1985
	Narayan, J.;* Holland, O. W.;* Christie, W. H.; Wortman, J. J.* "Rapid Thermal and Pulsed Laser Annealing of Boron Fluoride-implanted Silicon"	*J. Appl. Phys.* 57(8), 2709, 1985
	Christie, W. H. "Sleuthing with Secondary Ion Mass Spectrometry"	*ORNL Review* 18(1), 10, 1985
Costanzo, D. A.	Ryan, J. L.;* Bryan, G. H.;* Burt, M. C.;* Costanzo, D. A. "Preparation of Standards and the Determination of Free Acid in Concentrated Plutonium-Uranium Solutions"	*Anal. Chem.* 57, 1423, 1985
Dale, J. M.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.;* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission (HIXSE) Spectra"	*Nucl. Instr. Meth. B* 10,11, 195, 1985
Donohue, D. L.	Smith, D. H.; Donohue, D. L.; Young, J. P "Determination of Isotopic Ratios of Neodymium by Resonance Ionization Mass Spectrometry"	*Int. J. Mass Spectrom. Ion Processes* 65, 287, 1985
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Spectral Studies of Actinide Elements by Resonance Ionization Mass Spectrometry"	*Appl. Spectrosc.* 39, 93, 1985
	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ion Microprobe Mass Spectrometry Using Sputtering Atomization and Resonance Ionization	*Anal. Chem.* 57, 1193, 1985
Dunn, H. W.	Bamberger, C. E.;* Begun, G. M.;* Brynestad, J.;* Dunn, H. W. "Lanthanide Titanates and $Ln_xBi_{4-x}Ti_3O_{12}$ Solid Solutions; their Raman Spectra"	*Inorg. Chim. Acta* 109, 14, 1985
Eldridge, J. S.	Voshell, J. R.;* Eldridge, J. S.; Oakes, T. W.* "Transfer of ^{137}Cs and ^{60}Co in a Waste Retention Pond with Emphasis on Aquatic Insects"	*Health Phys.*, 49, 777, 1985

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Glish, G. L.	McLuckey, S. A.; Glish, G. L.; Carter, J. A. "The Analysis of Explosives by Tandem Mass Spectrometry"	*J. of Forensic Sci.* 30, 773, 1985
	Brown, A. J.;* Glish, G. L.; McBay, E. H.; Snyder, F.* "Alkyldihydroxyacetonephosphate Synthase Mechanism: ^{18}O Studies of Fatty Acid Release from Acyldihydroxyacetone Phosphate"	*Biochemistry* 24, 8012, 1985
Goeringer, D. E.	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ion Microprobe Mass Spectrometry Using Sputtering Atomization and Resonance Ionization"	*Anal. Chem.* 57, 1193, 1985
Griest, W. H.	Tomkins, B. A.; Manning, D. L.; Griest, W. H.; Jones, A. R. "Selective Detection of 1,2-Propylene Glycol Dinitrate, 1-Propylene Glycol Mononitrate, and 2-Propylene Glycol Mononitrate Using Gas Chromatography/Thermal Energy Analyzer Detection and Liquid Chromatography/Electrochemical Detection"	*Anal. Chim. Acta* 169, 69, 1985
	Griest, W. H.; Harris, L. A.* "Microscopic Identification of Carbonaceous Particles in Stack Ash from Pulverized-Coal Combustion"	*Fuel* 64, 821, 1985
	Tomkins, B. A.; Jenkins, R. A.; Griest, W. H.; Reagan, R. R.; Holladay, S. K. "Liquid Chromatographic Determination of Benzo(a)-Pyrene in the Total Particular Matter of Cigarette Smoke"	*J. of Assoc. Off. Anal. Chem.* 68(5), 935, 1985
Guerin, M. R.	Henry, C. J.;* Dansie, D. R.;* Kanagalingam, K. K.;* Kouri, R. E.;* Gayle, T. M.;* Guerin, M. R.; Florant, L.;* Greenspan, J.* "Chronic Inhalation Studies in Mice: I. Facilities and Equipment for 'Nose-Only' Exposure to Cigarette Smoke"	*Beitrag. zur Tabakforsch* 13(1), 37, 1985
Ho, C.-h.	Vo-Dinh, T.;* Miller, G. H.;* Abbott, D. W.;* Moody, R. L.;* Ma, C. Y.; Ho, C.-h. "Luminescence Determination of Benzoquinoline Isomers in Complex Samples	*Anal. Chim. Acta* 175, 181, 1985
Holladay, S. K.	Tomkins, B. A.; Jenkins, R. A.; Griest, W. H.; Reagan, R. R.; Holladay, S. K. "Liquid Chromatographic Determination of Benzo(a)-Pyrene in the Total Particular Matter of Cigarette Smoke"	*J. of Assoc. Off. Anal. Chem.* 68(5), 935, 1985
Hulett, L. D.	Rossael, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.;* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission (HIXSE) Spectra"	*Nucl. Instr. Meth. B* 10,11, 195, 1985

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Jenkins, R. A.	Nolan, J.;* Jenkins, R. A.; Kurihara, K.;* Schultz, R. C.* "The Acute Effects of Cigarette Smoke Exposure on Experimental Skin Flaps"	*Plastic and Reconstr. Surgery* 75(4), 544, 1985
	Tomkins, B. A.; Jenkins, R. A.; Griest, W. H.; Reagan, R. R.; Holladay, S. K. "Liquid Chromatographic Determination of Benzo(a)-Pyrene in the Total Particular Matter of Cigarette Smoke"	*J. of Assoc. Off. Anal. Chem.* 68(5), 935, 1985
Jones, A. R.	Tomkins, B. A.; Manning, D. L.; Griest, W. H.; Jones, A. R. "Selective Detection of 1,2-Propylene Glycol Dinitrate, 1-Propylene Glycol Mononitrate, and 2-Propylene Glycol Mononitrate Using Gas Chromatography/Thermal Energy Analyzer Detection and Liquid Chromatography/Electrochemical Detection"	*Anal. Chim. Acta* 169, 69, 1985
Klatt, L. N.	Harward, B. L.;* Klatt, L. N.; Mamantov, G.* "Multipass Apparatus for Molten Salt Spectroelectrochemical Experiments"	*Anal. Chem.* 57, 1773, 1985
Lyon, W. S.	Lyon, W. S. "Technostress - Technodisease?"	*J. Radioanal. Nucl. Chem., Ltrs.* 94(5), 287, 1985
	Braun, T.;* Bujdoso, E.;* Lyon, W. S. "The Impact of Some Research Published in the *Journal of Radioanalytical Chemistry*, 1968-1981"	*J. Radioanal. Nucl. Chem., Articles*, 91(2), 419, 1985
	Lyon, W. S. *Technostress: The Human Cost of the Computer Revolution* (Book Review)	*ORNL Review* 18, 8, 1985
Ma, C. Y.	Vo-Dinh, T.;* Miller, G. H.;* Abbott, D. W.;* Moody, R. L.;* Ma, C. Y.; Ho, C.-h. "Luminescence Determination of Benzoquinoline Isomers in Complex Samples"	*Anal. Chim. Acta* 175, 181, 1985
Manning, D. L.	Tomkins, B. A.; Manning, D. L.; Griest, W. H.; Jones, A. R. "Selective Detection of 1,2-Propylene Glycol Dinitrate, 1-Propylene Glycol Mononitrate, and 2-Propylene Glycol Mononitrate Using Gas Chromatography/Thermal Energy Analyzer Detection and Liquid Chromatography/Electrochemical Detection"	*J. Of Chromatogr. Sci.* 169, 69, 1985
Maskarinec, M. P.	Balchunas, A. T.;* Capacci, M. J.;* Sepaniak, M. J.;* Maskarinec, M. P. "Dynamically Modified Capillary Columns for Liquid Chromatographic Separations of Biological Compounds"	*Anal. Chim. Acta* 23, 381, 1985
McKown, H. S.	Donohue, D. L.; Christie, W. H.; Goeringer, D. E.; McKown, H. S. "Ion Microprobe Mass Spectrometry Using Sputtering Atomization and Resonance Ionization"	*Anal. Chem.* 57, 1193, 1985

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
McLuckey, S. A	McLuckey, S. A; Glish, G. L.; Carter, J. A. "The Analysis of Explosives by Tandem Mass Spectrometry"	*J. of Forensic Sci.* **30**, 773, 1985
	van der Zande, W. J.;* de Bruijn, D. P.;* Los, J.;* Kistemaker, P. G.;* McLuckey, S. A. "Angular Scattering in Dissociative Collisions of Ionized Acetone with Helium"	*Int. J. Mass Spectrom. Ion Proc.* **67**, 161, 1985
Ramsey, J. M.	Ramsey, J. M.; Whitten, W. B. "Phase-Conjugate Feedback into a CW Ring Dye Laser"	*Optics Letters* **10**, 362, 1985
	Whitten, W. B.; Ramsey, J. M. "Molecular Spectrometry with a Holographically-Scanned CW Dye Laser and Supersonic Cooling"	*Appl. Spectrosc.* **39**, 582, 1985
Reagan, R. R.	Tomkins, B. A.; Jenkins, R. A.; Griest, W. H.; Reagan, R. R.; Holladay, S. K. "Liquid Chromatographic Determination of Benzo(a)-Pyrene in the Total Particular Matter of Cigarette Smoke"	*J. of Assoc. Off. Anal. Chem.* **68**(5), 935, 1985
Robinson, L.	Robinson, L.; Wahl, A. C.;* Semkow, T. M.;* Norris, A. E.* "Nuclear-Charge Distribution for A = 121 from Thermal-Neutron-Induced Fission of ^{235}U"	*Phys. Rev. C*, **31**, 1334, 1985
Rosseel, T. M.	Rosseel, T. M.; Taylor, J. W.;* Negri, R. E.* "Energy Dependence of the Titanium, Chromium, and Manganese 3p Photoionization Cross Sections Using Synchrotron Radiation"	*Anal. Chem.* **57**, 2685, 1985
	Rosseel, T. M.; Dale, J. M.; Hulett, L. D. Krause, H. F.;* Pepmiller, P. L.;* Raman, S.;* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission (HIXSE) Spectra"	*Nucl. Instr. Meth. B* **10,11**, 195, 1985
	Andrews, M. C.;* McDaniel, F. D.;* Duggan, J. L.;* Mehta, R.;* Lapicki, G.;* Miller, P. D.;* Pepmiller, P. L.;* Krause, H. F.;* Rosseel, T. M.; Rayburn, L. A.* "L-Shell X-ray Production Cross Sections in Nb, Gd, Ho, Yb, Au, and Pb for 25-MeV Carbon and 32-MeV Oxygen Ions"	*Nucl. Instr. Meth. B* **10,11**, 181, 1985
	Andrews, M. C.;* McDaniel, F. D.;* Duggan, J. L.;* Miller, P. D.;* Pepmiller, P. L.;* Krause, H. F.;* Rosseel, T. M.; Rayburn, L. A.;* Mehta, R.;* and Lapicka, G.* "M-Shell Electron Capture and Direct Ionization of Gold by 25-MeV Carbon and 32-MeV Oxygen Ions"	*Nucl. Instrum. Meth. B* **10,11**, 186, 1985

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Rubin, I. B.	Rubin, I. B.; Buchanan, M. V. "Carbon-13 NMR Spectra of Anthraquinone-Derived Dyes"	*Magn. Reson. in Chem.* 23(3), 161, 1985
Smith, D. H.	Smith, D. H.; Donohue, D. L; Young, J. P. "Determination of Isotopic Ratios of Neodymium by Resonance Ionization Mass Spectrometry"	*Int. J. Mass Spectrom. Ion Processes* 65, 287, 1985
	Smith, D. H.; Walker, R. L. "Internal Standards Applied to Isotopic Ratio Measurements of Uranium and Plutonium"	*J. Inst. Nucl. Mater. Manage.* 13(2), 44, 1985
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Spectral Studies of Actinide Elements by Resonance Ionization Mass Spectrometry"	*Appl. Spectrosc.* 39, 93, 1985
Todd, P. J.	Groenewold, G. S.;* Todd, P. J. "Detection of Gaseous Organophosphorous Compounds Using Secondary Ion Mass Spectrometry"	*Anal. Chem.* 57, 888, 1985
Tomkins, B. A.	Tomkins, B. A.; Manning, D. L.; Griest, W. H.; Jones, A. R. "Selective Detection of 1,2-Propylene Glycol Dinitrate, 1-Propylene Glycol Mononitrate, and 2-Propylene Glycol Mononitrate Using Gas Chromatography/Thermal Energy Analyzer Detection and Liquid Chromatography/Electrochemical Detection"	*Anal. Chim. Acta* 169, 69, 1985
	Tomkins, B. A.; Jenkins, R. A.; Griest, W. H.; Reagan, R. R.; Holladay, S. K. "Liquid Chromatographic Determination of Benzo(a)-Pyrene in the Total Particular Matter of Cigarette Smoke"	*J. of Assoc. Off. Anal. Chem.* 68(5), 935, 1985
Walker, R. L.	Smith, D. H.; Walker, R. L. "Internal Standards Applied to Isotopic Ratio Measurements of Uranium and Plutonium"	*J. Inst. Nucl. Mater. Manage.* 13(2), 44, 1985
Whitten, W. B.	Ramsey, J. M.; Whitten, W. B. "Phase-Conjugate Feedback into a CW Ring Dye Laser"	*Optics Letters* 10, 362, 1985
	Whitten, W. B.; Ramsey, J. M. "Molecular Spectrometry with a Holographically-Scanned CW Dye Laser and Supersonic Cooling"	*Appl. Spectrosc.* 39, 582, 1985
Young, J. P.	Smith, D. H.; Donohue, D. L.; Young, J. P. "Determination of Isotopic Ratios of Neodymium by Resonance Ionization Mass Spectrometry"	*Int. J. Mass Spectrom. and Ion Processes* 65, 287, 1985

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Young, J. P.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.;* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission (HIXSE) Spectra"	*Nucl. Instr. Meth. B* **10,11**, 195, 1985
	Ensor, D. D.; Young, J. P.; Haire, H. G.;* Peterson, J. R.* "Characterization of Anhydrous Transcurium Halides by Absorption Spectrophotometry"	*Rev. in Inorg. Chem.* **4**, 383, 1983
	Haire, R. G.;* Benedict, U.;* Young, J. P. Peterson, J. R.;* Begun, G. M.* "The Effect of Pressure on the Absorption Spectrum and the Crystal Structure of Anhydrous AmI_3"	*J. Phys. C: Solid State Phys.* **18**, 4595, 1985
	Peterson, J. R.;* Young, J. P.; Haire, R. G.;* Benedict, U.;* Begun, G. M.* "Transformation of Monoclinic $CfBr_3$ to Orthorhombic $CfBr_3$ by the Application of Pressure"	*Inorg. Chem.* **24**, 2466, 1985
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Spectral Studies of Actinide Elements by Resonance Ionization Mass Spectrometry"	*Appl. Spectrosc.* **39**, 93, 1985

Reports

AUTHOR	AUTHOR(S) AND TITLES	REPORT NO. AND DATE
Buchanan, M. V.	McCarthy, J. F.;* Caton, J. E.; Whitmore, D. K.;* Jones, A. R.; Singley, P. T.;* Buchanan, M. V.; Rubin, I. B.; Ho, C.-h.; Hurst, G. B.* *Support for Establishing Structure-Activity Relationships Between a Series of Phthalate Esters and Toxicity to Aquatic Organisms*	ORNL/TM-9254 (Feb. 1985)
Carter, J. A.	Carter, J. A. *Analytical Chemistry Division Research and Development Summary: Mass and Emission Spectrometry Section*	ORNL/CF-85/31 (Feb. 6, 1985)
	Christie, W. H.; Shults, W. D.; Carter, J. A. *A New Mass Spectrometry Laboratory at ORNL*	ORNL/CF-85/32 (April 1985)
	Carter, J. A. *Analytical Chemistry Division Research and Development Summary: Mass and Emission Spectrometry Section*	ORNL/CF-85-283 (June 1, 1985)
	Carter, J. A. *Analytical Chemistry Division Research and Development Summary: Analytical Spectroscopy Section*	ORNL/CF-85/431 (Oct. 1, 1985)
	Smith, D. H.; Walker, R. L.; Carter, J. A. *ISPO Task A-126: Application of Mixed Internal Standards to the Mass Spectrometric Analysis of Plutonium and Uranium in Spent Fuel Dissolver Solutions: ORNL Results*	ORNL/TM-9820 (ISPO-230) (Nov. 1985)
	Walker, R. L.; Smith, D. H.; McKown, H. S.; Smith, H. C.; Carter, J. A. *Resin Beads as a Sample Acquisition and Loading Medium Mass Spectrometric Analysis*	ORNL/TM-5505/R1 (Sept. 1985)
	Smith, D. H.; Walker, R. L.; Carter, J. A. *Evaluation of Uranium and Plutonium Internal Standards*	ORNL/TM-9779 (Sept. 1985)
	McLuckey, S. A.; Glish, G. L.; Carter, J. A. *Mass Spectrometry/Mass Spectrometry Applied to the Detection of Explosives; Background, Progress Report for FY 1984 and Future Plans*	ORNL/TM-9447 (Jan. 1985)
Caton, J. E.	McCarthy, J. F.;* Caton, J. E.; Whitmore, D. K.;* Jones, A. R.; Singley, P. T.;* Buchanan, M. V.; Rubin, I. B.; Ho C.-h.; Hurst, G. B.* *Support for Establishing Structure-Activity Relationships Between a Series of Phthalate Esters and Toxicity to Aquatic Organisms*	ORNL/TM-9254 (Feb. 1985)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Caton, J. E.	Ho, C.-h.; Jones, A. R.; Caton, J. E.; Griest, W. H.; Smith, L. H.;* Guerin, M. R. *Upgrading Coal-Derived Liquids by Means Other Than Hydrotreatment: II. Tumorigenicity and Tumorigens*	ORNL/TM-9324 (May 1985)
Christie, W. H.	Christie, W. H.; Shults, W. D.; Carter, J. A. *A New Mass Spectrometry Laboratory at ORNL*	ORNL/CF-85/32 (April 1985)
Clark, B. R.	Clark, B. R.; Roseberry, L. M.; Rubin, I. B. *Environmental Health and Safety Assessments for Direct Coal Liquefaction: Vol. 5. Physico-chemical Measurements of Process Streams Products and Emissions*	ORNL/FETEP-5 (Feb. 1985)
Dale, J. M.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission Spectra" in *Physics Division Progress Report*	ORNL-6120 (Jan. 1985) p. 195
Donohue, D. L.	Donohue, D. L. *Report of Foreign Travel*	ORNL/FTR-2037 (June 18, 1985)
Glish, G. L.	McLuckey, S. A.; Glish, G. L.; Carter, J. A. *Mass Spectrometry/Mass Spectrometry Applied to the Detection of Explosives; Background, Progress Report for FY 1984 and Future Plans*	ORNL/TM-9447 (Jan. 1985)
	Glish, G. L. *Report of Foreign Travel*	ORNL/FTR-2108 (Oct. 4, 1985)
Griest, W. H.	Maskarinec, M. P.; Manning, D. L.; Griest, W. H. *Characterization of Potential Wastes from Human Manufacture and Processing*	ORNL/TM-6167 (Apr. 1985)
	Ho, C.-h.; Jones, A. R.; Caton, J. E.; Griest, W. H.; Smith, L. H.;* Guerin, M. R. *Upgrading Coal-Derived Liquids by Means Other Than Hydrotreatment: II. Tumorigenicity and Tumorigens*	ORNL/TM-9324 (May 1985)
Guerin, M. R.	Ho, C.-h.; Jones, A. R.; Caton, J. E.; Griest, W. H.; Smith, L. H.;* Guerin, M. R. *Upgrading Coal-Derived Liquids by Means Other Than Hydrotreatment: II. Tumorigenicity and Tumorigens*	ORNL/TM-9324 (May 1985)
	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; February, 1985, Bio/Organic Analysis Section*	ORNL/CF-85/79 (March 1985)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Guerin, M. R.	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; June, 1985, Organic Chemistry Section*	ORNL/CF-85/315 (July 1985)
	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; October, 1985, Organic Chemistry Section*	ORNL/CF-85/467 (Nov. 1985)
Ho, C.-h.	McCarthy, J. F.;* Caton, J. E.; Whitmore, D. K.;* Jones, A. R.; Singley, P. T.;* Buchanan, M. V.; Rubin, I. B.; Ho, C.-h.; Hurst, G. B.* *Support for Establishing Structure-Activity Relationships Between a Series of Phthalate Esters and Toxicity to Aquatic Organisms*	ORNL/TM-9254 (Feb. 1985)
	Ho, C.-h.; Jones, A. R.; Caton, J. E.; Griest, W. H.; Smith, L. H. Guerin, M. R. *Upgrading Coal-Derived Liquids by Means Other Than Hydrotreatment: II. Tumorigenicity and Tumorigens*	ORNL/TM-9324 (May 1985)
Holmberg, R. W.	Ramsey, R. S.; Moneyhun, J. H.; Holmberg, R. W. *The Chemical and Physical Characterization of Phosphorus Smokes for Inhalation Exposure and Toxicology Studies*	ORNL/TM-9571 (Apr. 1985)
	Holmberg, R. W.; Moneyhun, J. H.; Gayle, T. M.* *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: A System for the Continuous Generation of Phosphorous Aerosols from Red Phosphorus-Butyl Rubber*	ORNL/TM-9649 (June 1985)
Hulett, L. D.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission Spectra" in *Physics Division Progress Report*	ORNL-6120 (Jan. 1985) p. 195
Jones, A. R.	McCarthy, J. F.;* Caton, J. E.; Whitmore, D. K.;* Jones, A. R.; Singley, P. T.;* Buchanan, M. V.; Rubin, I. B.; Ho, C.-h.; Hurst, G. B.* *Support for Establishing Structure-Activity Relationships Between a Series of Phthalate Esters and Toxicity to Aquatic Organisms*	ORNL/TM-9254 (Feb. 1985)
	Ho, C.-h.; Jones, A. R.; Caton, J. E.; Griest, W. H.; Smith, L. H.;* Guerin, M. R. *Upgrading Coal-Derived Liquids by Means Other Than Hydrotreatment: II. Tumorigenicity and Tumorigens*	ORNL/TM-9324 (May 1985)
Klatt, L. N.	Klatt, L. N.; McCue, D. D. *Report of Foreign Travel*	ORNL/FTR-2043 (June 26, 1985)

AUTHOR	AUTHORS(S) AND TITLE	REPORT NO. AND DATE
Laing, W. R.	Laing, W. R. *Status Report: Radioactive Material Laboratories Section*	ORNL/CF-85/201 April 1, 1985
	Laing, W. R. *Status Report: Radioactive Material Laboratories Section*	ORNL/CF-85/370 Aug. 1, 1985
Lyon, W. S.	Lyon, W. S. *Analytical Chemistry Division Research and Development Summary for December 1984; Analytical Methodology Section*	ORNL/CF-94/449 (Jan. 2, 1985)
Manning, D. L.	Maskarinec, M. P.; Manning, D. L.; Griest, W. H. *Characterization of Potential Wastes from Human Manufacture and Processing*	ORNL/TM-6167 (Apr. 1985)
Maskarinec, M. P.	Maskarinec, M. P.; Manning, D. L.; Griest, W. H. *Characterization of Potential Wastes from Human Manufacture and Processing*	ORNL/TM-6167 (Apr. 1985)
McKown, H. S.	McKown, H. S. *Report of Foreign Travel of H. S. McKown*	ORNL/FTR-1986 (Apr. 4, 1985)
	McKown, H. S. *Report of Foreign Travel*	ORNL/FTR-2092 (Sept. 9, 1985)
	Wa''er, R. L.; Smith, D. H.; McKown, H. S.; Smith, H. C.; Carter, J. A. *Resin Beads as a Sample Acquisition and Loading Medium Mass Spectrometric Analysis*	ORNL/TM-5505/R1 (Aug. 1985)
McLuckey, S. A.	McLuckey, S. A.; Glish, G. L.; Carter, J. A. *Mass Spectrometry/Mass Spectrometry Applied to the Detection of Explosives; Background, Progress Report for FY 1984 and Future Plans*	ORNL/TM-9447 (Jan. 1985)
Moneyhun, J. H.	Ramsey, R. S.; Moneyhun, J. H.; Holmberg, R. W. *The Chemical and Physical Characterization of Phosphorus Smokes for Inhalation Exposure and Toxicology Studies*	ORNL/TM-9571 (Apr. 1985)
	Holmberg, R. W.; Moneyhun, J. H.; Gayle, T. M.* *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: A System for the Continuous Generation of Phosphorous Aerosols from Red Phosphorus-Butyl Rubber*	ORNL/TM-9649 (June 1985)
Ramsey, R. S.	Ramsey, R. S.; Moneyhun, J. H.; Holmberg, R. W. *The Chemical and Physical Characterization of Phosphorus Smokes for Inhalation Exposure and Toxicology Studies*	ORNL/TM-9571 (Apr. 1985)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Rosseel, T. M.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission Spectra" in *Physics Division Progress Report*	ORNL-6120 (Jan. 1985) p. 195
Rubin, I. B.	McCarthy, J. F.;* Caton, J. E.; Whitmore, D. K.;* Jones, A. R.; Singley, P. T.;* Buchanan, M. V.; Rubin, I. B.; Ho, C.-h.; Hurst, G. B.* *Support for Establishing Structure-Activity Relationships Between a Series of Phthalate Esters and Toxicity to Aquatic Organisms*	ORNL/TM-9254 (Feb. 1985)
	Clark, B. R.; Roseberry, L. M.; Rubin, I. B. *Environmental Health and Safety Assessments for Direct Coal Liquefaction: Vol. 5. Physicochemical Measurements of Process Streams, Products and Emissions*	ORNL/FETEP-5 (Feb. 1985)
Shults, W. D.	Christie, W. H.; Shults, W. D.; Carter, J. A. *A New Mass Spectrometry Laboratory at ORNL*	ORNL/CF-85/32 (April 1985)
	Shults, W. D. *Analytical Chemistry Division Annual Progress Report for Period Ending December 31, 1984*	ORNL-6139 (April 1985)
Smith, D. H.	Smith, D. H.; Walker, R. L.; Carter, J. A. *ISPO Task A-126: Application of Mixed Internal Standards to the Mass Spectrometric Analysis of Plutonium and Uranium in Spent Fuel Dissolver Solutions: ORNL Results*	ORNL/TM-9820 (ISPO-230) (Nov. 1985)
	Smith, D. H.; McKown, H. S.; Carter, J. A. *ISPO Task A-109: Evaluation of Quadrupole Mass Spectrometers as On-Site Inspection Devices*	ORNL/TM-9839 (ISPO-230) (Nov. 1985)
	Walker, R. L.; Smith, D. H.; McKown, H. S.; Smith, H. C.; Carter, J. A. *Resin Beads as a Sample Acquisition and Loading Medium for Mass Spectrometric Analysis*	ORNL/TM-5505/R1 (Aug. 1985)
	Smith, D. H.; Walker, R. L.; Carter, J. A. *Evaluation of Uranium and Plutonium Internal Standards*	ORNL/TM-9779 (Sept. 1985)
	Smith, D. H. *INSTD: A Computer Program to Perform Internal Standard Calculations for Isotopic Ratio Mass Spectrometric Data Using General Solutions to the Equations*	ORNL/TM-9842 (Nov. 1985)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Smith, H. C.	Walker, R. L.; Smith, D. H.; McKown, H. S.; Smith, H. C.; Carter, J. A. *Resin Beads as a Sample Acquisition and Loading Medium Mass Spectrometric Analysis*	ORNL/TM-5505/R1 (Aug. 1985)
Stokely, J. R.	Stokely, J. R. *Analytical Chemistry Division Summary Report: General and Environmental Analysis Section*	ORNL/CF-85/19 Jan. 11, 1985
	Stokely, J. R. *Analytical Chemistry Division Summary Report: Inorganic Chemistry Division*	ORNL/CF-85/251 May 1, 1985
	Stokely, J. R. *Analytical Chemistry Division Summary Report Inorganics Chemistry Division*	ORNL/CF-85/377 Sept. 1, 1985
Todd, P. J.	Todd, P. J. *Report of Foreign Travel*	ORNL/FTR-1107 (Sept. 27, 1985)
Walker, R. L.	Smith, D. H.; Walker, R. L.; Carter, J. A. *ISPO Task A-126: Application of Mixed Internal Standards to the Mass Spectrometric Analysis of Plutonium and Uranium in Spent Fuel Dissolver Solutions: ORNL Results*	ORNL/TM-9820 (ISPO-230) (Nov. 1985)
	Walker, R. L.; Smith, D. H.; McKown, H. S.; Smith, H. C.; Carter, J. A. *Resin Beads as a Sample Acquisition and Loading Medium Mass Spectrometric Analysis*	ORNL/TM-5505/R1 (Aug. 1985)
	Smith, D. H.; Walker, R. L.; Carter, J. A. *Evaluation of Uranium and Plutonium Internal Standards*	ORNL/TM-9779 (Sept. 1985)
Young, J. P.	Young, J. P. *Report of Foreign Travel of J. P. Young, Senior Staff, Analytical Chemistry Division*	ORNL/FTR-2101 (Sept. 23, 1985)
	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.;* Pepmiller, P. L.;* Raman, S.* Vane, C. R.;* Young, J. P. "Effect of the Chemical Environment on the L and M Heavy-Ion-Induced X-ray Satellite Emission Spectra" in *Physics Division Progress Report*	ORNL-6120 (Jan. 1985) p. 195

ORAL PRESENTATIONS

As in previous years, staff members have made presentations at local, national, and, in a few instances, international meetings. The papers covered a wide variety of subjects, reflecting the division's broad spectrum of activities.

At Meetings of Professional Societies, Conferences, and the Like

SPEAKER	AUTHORS(S) AND TITLE	PRESENTED AT
Alley, C. S.	Alley, C. S.; Ross, H. H.; Stewart, J. H. "The Evaluation of a Zymark Robotics System for Multitasking Applications in a Complex Process Laboratory"	Nat. Am. Chem. Soc. Mtg., Miami, FL, Apr. 28-May 1, 1985
Bobrowski, S. J.	Bobrowski, S. J.; Stewart, J. H. "Evaluation Inductively Coupled Plasma (ICP) Spectrometry for Multielement Analysis of Blood and Brain Tissue"	SE/SW Reg. Am. Chem. Soc., Mtg., Memphis, TN, Oct. 9-11, 1985
Buchanan, M. V.	Buchanan, M. V. "New Analytical Techniques for the Characterization of Bioactive Constituents in Fossil-Derived Fuels"	Univ. of Alabama, Tuscaloosa, AL, Oct. 31, 1985
	Buchanan, M. V. "Chemical Ionization Processes for Isomer Differentiation"	FACSS Mtg., Philadelphia, PA, Oct. 2-5, 1985
	Buchanan, M. V. "Case History of a Communication Problem"	IRI Manage. Study Group, Charleston, SC, Jan. 9-11, 1985
	Buchanan, M. V. "Probing Molecular Structure with Chemical Ionization Processes"	33rd Annu. Conf. in Mass Spectrom. and Allied Topics, San Diego, CA, May 26-31, 1985
	Buchanan, M. V.; Rubin, I. R. "Isomeric Differentiation of Nitrogen-Containing Aromatics with Negative Chemical Ionization Mass Spectrometry"	36th Pittsburgh Conf., New Orleans, LA, Feb. 25-March 1, 1985
	Buchanan, M. V. "Characterization of Bioactive Constituents in Fossil-Derived Fuels"	Univ. of Ala., Huntsville, AL, Apr. 26, 1985
	Buchanan, M. V. "Chemical Ionization Processes Isomeric Differentiation by Mass Spectrometry"	Univ. of Tenn., for Chem. Dept., Anal. Chem. Div. Sem., Knoxville, TN, May 7, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Buchanan, M. V.	Buchanan, M. V. "Chemical Ionization Processes: Obtaining Isomeric Information Using GC/MS"	ACS Central Regional Mtg., Akron, OH, June 6, 1985
Carter, J. A.	Carter, J. A.; Walker, R. L.; Smith, D. H.; Christie, W. H. "Mass Spectrometry in Nuclear Science and Industry"	Nat. Am. Chem. Soc. Mtg., Miami, Fl., Apr. 28-May 3, 1985
Christie, W. H.	Christie, W. H.; Donohue, D. L.; Goeringer, D. E.; McKown, H. S. "Sputter Atomization/ Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	Christie, W. H. "New Directions in Secondary Ion Mass Spectrometry"	ACD Inf. Mtg., Exec. Sess., ORNL, Oak Ridge, TN, July 22, 1985
	Christie, W. H. "Mass Spectrometry Laboratory Status Report"	ACD Inf. Mtg., Exec. Sess., ORNL, Oak Ridge, TN, July 22, 1985
Clark, B. R.	Clark, B. R. "Voltammetry Applied to Effluent Monitoring at Oak Ridge National Laboratory"	1985 ORO Contractors Environ. Workshop, Knoxville, TN, Apr. 23-24, 1985
	Clark, B. R. "ACD Radiochemical Hazardous Waste Program"	24th Martin Marietta-Goodyear Anal. Forum, Nov. 19, 1985
Dale, J. M.	Dale, J. M.; Rosseel, T. M.; Hulett, L. D. "Positron Studies"	DOE-BES Chem. Sci. Site Rev., ORNL , April 17, 1985
	Dale, J. M.; Rosseel, T. M.; Hulett, L. D. "Positron Spectroscopy"	ACD Inf. Mtg., ORNL, July 23, 1985
	Dale, J. M. "Positron Spectroscopy"	Special ACD Inf. Mtg., ORNL, July 29, 1985
	Dale, J. M.; Rosseel, T. M.; Hulett, L. D. "Surface Areas by Positron Annihilation Spectroscopy"	28th ORNL-DOE Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Sept. 30-Oct. 3, 1985
Donohue, D. L.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Resonance Ionization Mass Spectrometry for Isotopic Analysis of Uranium and Plutonium"	Karlsruhe Int. Conf. on Anal. Chem. in Nucl. Techn., Karlsruhe, FRG, June 3-6, 1985
	Donohue, D. L.; Smith, D. H.; Young, J. P. "Spectral Studies Using Resonance Ionization Mass Spectrometry Combined with Photoelectron Spectroscopy"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Donohue, D. L.	Donohue, D. L. "Recent Advances in Resonance Ionization Mass Spectrometry"	Univ. of Alabama, Tuscaloosa, AL, Mar. 21, 1985
	Donohue, D. L.; Smith, D. H.; Young, J. P. "Advances in Resonance Ionization Mass Spectrometry"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985
Dyer, F. F.	Dyer, F. F.; Emery, J. F.; Bate, L. C. "Determination of Thorium and Uranium at the Nanogram per Gram Level in Semiconductor Potting Plastics by Neutron Activation Analysis"	Int. Symp. for Nucl. Anal. Chem., Dalhousi, Univ., Halifax, Canada, June 5-7, 1985
	Dyer, F. F. "A Review of Isotope Dilution Mass Spectrometry for Bioassay of Uranium in Urine"	Public Meeting of the Off. of NRC, Washington, DC, Dec. 3, 1985
Eldridge, J. S.	Eldridge, J. S.; Teasley, N. A.; Oakes, T. W.;* Stegnar, P.* "Applications of a Unique Lyophilization Apparatus for Sample Preparation in Environmental Surveillance Programs"	13th Symp. of the Yugoslavia Protect. Assoc., Pula, YU, June 10-15, 1985
	Eldridge, J. S.; Oakes, T. W.;* Stegnar, P.* "Radiological Emergency Response: Laboratory Measurements Under Field Conditions"	13th Symp. of the Yugoslavia Protect. Assoc. Assoc., Pula, YU, June 10-15, 1985
	Eldridge, J. S.; Oakes, T. W.* "A 'State-of-the-Art' Air Monitoring Network for Environmental Radioactivity"	Conf. on Anal. Chem. in Nucl. Techn., FRG, Karlsruhe, June 3-6, 1985
	Eldridge, J. S. "Special Analytical Techniques for Analysis of Radioactivity in Water"	Toxins and Pathogens: Impact on Drinking Water, course presented by Univ. of Missouri-Columbia, St. Louis, MO, May 22-23, 1985
	Eldridge, J. S. "A System for Precious Metals and Special Nuclear Material Inventories"	IAEA Consultant's Mtg. on Advances in Nucl. Anal. Tech. and Their Appli. for Use in Dev. Countries, Karlsruhe, FRG, June 7, 1985
	Eldridge, J. S.; Teasley, N. A.; Oakes, T. W.* Stegnar, P.* "The Use of Bio-Indicator Organisms in Environmental Surveillance--Vehicle-Killed Deer Thyroids for Radioiodine Releases"	ACD Inf., Mtg., ORNL, Oak Ridge, TN, July 23, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Eldridge, J. S.	Rhea, T. A.; Eldridge, J. S. "Consideration for Selection and Installation of Radiological Emergency Response Instrumentation"	28th ORNL-DOE Conf. on Anal. Chem. in Energy Techn., Knoxville, TN, Oct. 2-3, 1985
	Eldridge, J. S.; Oakes, T. W.* "New Air Monitoring Methods for Environmental Radioactivity"	SE/SW Reg. Am. Chem. Soc. Mtg., Memphis, TN, Oct. 9-11, 1985
Glish, G. L.	Glish, G. L.; McLuckey, S. A.; Goeringer, D. E.; McBay, E. H. "Low Energy Collisional Activation: International Energy Considerations"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	Glish, G. L.; McBay E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	Glish, G. L.; McLuckey, S. A.; McBay, E. H. "MS/MS Applications of a New Hybrid Instrument"	36th Pittsburgh Conf. & Expo. on Appl. Spectrosc., New Orleans, LA, Feb. 25-Mar. 1, 1985
	Glish, G. L.; McLuckey, S. A.; McKown, H. S. "A Tandem Mass Spectrometer for the Detection of Nitroaromatic Compounds and Other Electronegative Species in Ambient Air"	28th ORNL-DOE Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Sept. 30-Oct. 3, 1985
	Glish, G. L.; McLuckey, S. A.; Bertram, L. K.; McBay, E. H. "Multi-Stage Mass Spectrometry with a Quadrupole Mass Filter Interfaced to a High Resolution Sector Mass Spectrometer"	28th ORNL-DOE Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Sept. 30-Oct. 3, 1985
	Glish, G. L.; McLuckey, S. A. "The Effect of Para Substituents on the 'Ortho' Effect in Anions of Substituted Nitrosromatics"	10th Int. Mass Spectrom. Conf., Swansea, UK, Sept. 9-13, 1985
	Glish, G. L.; McBay, E. H.; McLuckey, S. A.; Bertram, L. K. "A 'Reverse' Geometry Hybrid Instrument for MS/MS"	10th Int. Mass Spectrom. Conf., Swansea, UK, Sept. 9-13, 1985
Goeringer, D. E.	Goeringer, D. E.; Donohue, D. L.; Christie, W. H.; McKown, H. S. "Sputter Atomization/ Resonance Ionization Mass Spectrometry for High Sensitivity Isotopic Analysis"	36th Pittsburgh Conf. & Expo. on Appl. Spectrosc., New Orleans, LA, Feb. 25-Mar. 1, 1985
	Donohue, D. L.; Christie, W. H.; Goeringer, D. E. "Ion Microprobe Mass Spectrometry Using Sputtering Atomization and Resonance Ionization"	Fifth Int. Conf. on Secondary Ion Mass Spectrom., Washington, DC, Sept. 29-Oct. 4, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Goeringer, D. E.	Goeringer, D. E.; Christie, W. H.; Carter, J. A.; Walker, R. L. "Ultrasensitive Particulate Analysis via Sputter Atomization/Resonance Ionization Mass Spectrometry"	LAGER Program Review, Washington, DC, Nov. 13, 1985
Griest, W. H.	Griest, W. H.; Higgins, C. E.; Guerin, M. R. "Comparative Chemical Characterization of Shale Oil- and Petroleum-Derived Diesel Fuels"	24th Hanford Life Sci. Symp., Richland, WA, Oct. 21-24, 1985
	Griest, W. H.; Ho, C.-h.; Witschi, H. R.:* Smith, L. H.;* Guerin, M. R. "Toxicological Beneficiation of Coal Liquids and Comparison with Petroleum Products"	Contractors Conf., Pittsburgh, PA, Nov. 19-21, 1985
	Griest, W. H.; Guerin, M. R.; Ho, C.-h. "Dermal Tumorigen PAH and Complex Mixtures for Biological Research"	DOE/OHER Complex Mixtures Res. Program, Argonne Nat. Lab., Chicago, IL, June 17-18, 1985
Guerin, M. R.	Guerin, M. R.; Ho, C.-h.; Buchanan, M. V. "Identification and Quantification of Mutagens in Complex Mixtures"	Am. Chem. Soc. Metrochem '85, Pocono Manor, PA, Oct. 13, 1985
	Guerin, M. R.; Higgins, C. E.; Holladay, S. K.; Jenkins, R. A. "Measuring Environmental Emissions from Tobacco Combustion"	Charac. of Contaminant Emissions from Indoor Sources Conf., Research Triangle Park, NC, May 13-15, 1985
Ho, C.-h.	Ho, C.-h.; Jones, A. R.; Smith, L. H.;* Epler, J. L.;* Griest, W. H.; Guerin, M. R. "Upgrading Coal-Derived Liquids for Toxicity Mitigation. I. Evaluation of Non-Hydrotreatment Processes as Alternates or Supplements to Hydrotreatment"	24th Hanford Life Sci. Symp., Richland, WA, Oct. 21-24, 1985
James, R. B.*	James, R. B.;* Christie, W. H.; Eby, R. E.; Darken, L. S.* "Nonlinear Adsorption and Optically Induced Melting of GaAs:Zn by Pulsed CO_2 Laser Radiation"	Int. Mtg. on Optics, Albuquerque, NM, Mar. 4-8, 1985
Klatt, L. N.	Klatt, L. N. "Hot-Cell Instrumentation"	UKAEA Nuclear Power Development Estab., Dounreay, Scotland, May 21, 1985
	Klatt, L. N. "Hot-Cell Instrumentation"	UKAEA, Harwell Lab., Oxfordshire, England, May 30, 1985
	Klatt, L. N. "Analytical Chemistry Development for Breeder Fuel Processing in the United Kingdom"	Consolidated Fuel Reprocessing Program, ORNL, August 1, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Laing, W. R.	Laing, W. R. "QA for Environmental Samples - Difficult Task"	Energy Systems-Goodyear Atomic 5-Plant Anal. Chem. Forum, July 16, 1985
Leibman, C. P.*	Leibman, C. P.;* Mamantov, G.;* Todd, P. J. "Use of Lewis Acids in Secondary Ionization Mass Spectrometry of Arenes"	SE Reg. Am. Chem. Soc. Mtg., Memphis, TN, Oct. 7-9, 1985
Lyon, W. S.	Lyon, W. S. "Scientometrics with Some Emphasis on Communication at Scientific Meetings and Through the 'Invisible' College"	Nat. Am. Chem. Soc. Mtg., Miami, FL, Apr. 28-May 3, 1985
	Lyon, W. S. "Radioanalytical Chemistry: Past Imperfect, Future Tense"	SE-SW Reg. Am. Chem. Soc. Mtg., Memphis, TN, Oct. 9-11, 1985
Maskarinec, M. P.	Maskarinec, M. P.; Burton, D. E.* "Using Electrokinetic Migration of Micelles for Liquid Chromatographic Separations"	10th Annu. Spring Training Workshop, Assoc. Off. Anal. Chem., Dallas, TX, Apr. 9, 1985
	Maskarinec, M. P.; Kimmell, T. A.* "Presentation of the Draft TCLP"	10th Annu. Spring Training Workshop, Assoc. Off. Anal. Chem., Dallas, TX, Apr. 9, 1985
	Maskarinec, M. P. "Use of the TCLP Zero Headspace Extractor for Determining the Liquid Content of Wastes"	10th Annu. Spring Training Workshop, Assoc. Off. Anal. Chem., Dallas, TX April 9, 1985
	Maskarinec, M. P.; Harmon, S. H. "Analysis of Volatile Priority Pollutants in Water"	DOE/ORO Contractors' Environ. Workshop, Knoxville, TN Apr. 22-23, 1985
	Maskarinec, M. P.; Francis, C. W.* "Mobility of Toxic Compounds in Hazardous Waste: Comparison of Three Test Methods to a Lysimeter Model"	Symp. on Solid Waste Testing and Quality Assurance, Washington, DC, July 23-26, 1985
McLuckey, S. A.	McLuckey, S. A.; Glish, G. L. "MS/MS Studies of Explosives and Related Compounds"	36th Pittsburgh Conf. & Expo. on Appl. Spectrosc., New Orleans, LA, Feb. 25-Mar. 1, 1985
	McLuckey, S. A.; Glish, G. L. "Substituent Effects in the Collisionally Activated Decompositions of Nitroaromatic Anions"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
McLuckey, S. A.	McLuckey, S. A.; Glish, G. L. "Kinetic Energies Released in the Loss of Nitrogen Oxide from Substituted Nitroaromatic Anions"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	McLuckey, S. A.; Glish, G. L. "Studies of Gas Phase Ion Chemistry Using MS/MS"	DOE-BES Chem. Sci. Site Rev., ORNL, Oak Ridge, TN, Apr. 16-17, 1985
	McLuckey, S. A.; Glish, G. L. "MS/MS with an Instrument of QEB Geometry"	DOE-BES Chem. Sci. Site Rev., ORNL, Oak Ridge, TN, Apr. 16-17, 1985
	McLuckey, S. A.; Glish, G. L. "Applications of a New Tandem Mass Spectrometer to the Study of Fundamental Factors Underlying MS/MS"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985
	McLuckey, S. A.; Glish, G. L.; Carter, J. A. "Explosives Detection with MS/MS"	FBI Conf. on Explosive Detection, Quantico, VA, Oct. 1-2, 1985
Peterson, J. R. *	Peterson, J. R.;* Young, J. P.; Haire, R. G.;* Begun, G. M.;* Benedict, U.* Using Pressure for Synthesis: Preparation of Orthorhombic Californium Tibromide, $CfBr_3$"	190th Nat. Mtg. Am. Chem. Soc., Chicago, IL, Sept. 9, 1985
	Haire, R. G.;* Young, J. P.; Peterson, J. R.* "Structural and Chemical Studies of Californium and Einsteinium Oxides"	Nat. Am. Chem. Soc. Mtg., Miami FL, Apr. 28-May 3, 1985
Ramsey, J. M.	Ramsey, J. M.; Whitten, W. B. "Degenerate Four Wave Mixing: A New Approach to Spectrochemical Analysis"	190th Nat. Mtg. Am. Chem. Soc., Chicago, IL, Sept. 9, 1985
	Ramsey, J. M.; Whitten, W. B. "Atomic Spectroscopy by Degenerate Four Wave Mixing"	36th Pittsburgh Conf. & Expo. on Appl. Spectrosc., New Orleans, LA, Feb. 25-Mar. 1, 1985
	Ramsey, J. M.; Whitten, W. B. "High Resolution Laser Spectroscopy"	DOE-BES Chem. Sci. Site Rev., ORNL, Oak Ridge, TN, Apr. 16-17, 1985
	Ramsey, J. M.; Whitten, W. B. "Fourier Transform Microwave Spectroscopy"	28th ORNL-DOE Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Sept. 30-Oct. 3, 1985
Ramsey, R. S.	Ramsey, R. S.; Todd, R. A.* "Constant-Current, Pulse-Modulated Helium Ionization Detection"	36th Pittsburgh Conf., New Orleans, LA, Feb. 25-Mar. 1, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Ramsey, R. S.	Ramsey, R. S. "Chemical Characterization of Selected Military Obscurants"	Wayne State Univ., Detroit, MI, Sept. 20, 1985
	Ramsey, R. S.; Todd, R. A.* "Pulse Modulated Helium Ionization Detection"	ACD Inf. Mtg., ORNL July 25, 1985
Ross, H. H.	Ross, H. H.: Alley C. S. "Evaluation of a Laboratory Robotics System"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985
	Ross, H. H. "Radiochemical Measurements in Environmental Analysis"	Univ. of Tennessee, Knoxville, TN, Aug. 1, 1985
Rosseel, T. M.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D. Krause, H. F.;* Pepmiller, P. L.;* Raman, S.;* Vane, C. R.;* Young, J. P. "Chemical Effects in the Heavy-Ion-Induced X-ray Satellite Emission (HIXSE) Spectra of Niobium Alloys and Compounds"	6th Symp. on X- and Gamma-Ray Sources and Applications, Univ. of Michigan, Ann Arbor, MI, May 21-23, 1985
Rucker, T. L.	Rucker, T. L. "A Multi-Column Step-Gradient Chromatography System for Automated Ion Exchange Separations"	28th ORNL/DOE Conf. on Anal. Chem. in Energy Techn., Knoxville, TN, Oct. 1-3, 1985
Sales, B. C.*	Sales, B. C.;* Ramsey, R. S.; Bates, J. B.;* Boatner, L. A.* "Liquid Chromatography and Raman Spectroscopy Studies of Lead-Iron Phosphate Glasses"	Amer. Phys. Soc., Baltimore, MD, March 25-29, 1985
Smith, D. H.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Challenges in Isotope Ratio Mass Spectrometry"	DOE-RES Chem. Sci. Site Rev., ORNL, Oak Ridge, TN, Apr. 16-17, 1985
	Smith, D. H.; Walker, R. L.; McBay, E. H.; Carter, J. A. "Development of Internal Standards for Plutonium and Uranium"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985
Stewart, J. H.	Stewart, J. H.; Dunn, H. W. "Quantitative Determination of Amosite, Anthophilite, Crocidolite and Chrysotile Asbestos in Solid Materials by X-Ray Diffractometry"	1985 ORO Contractors Environ. Workshop, Knoxville, TN, Apr. 23-24, 1985
	Stewart, J. H. "Rapid Combined Method for Quantitative Determination of Amosite Anthophyllice, Crocidolite and Chrysotile Asbestos in Solid Materials by X-ray Diffractometry"	SE-SW Reg. Am. Chem. Soc. Mtg., Memphis, TN, Oct. 9-11, 1985
Teasley, N. A.	Teasley, N. A.; Eldridge, J. S. "A System for Precious Metals-and Special Nuclear Materials Inventories"	Nat. Am. Chem. Soc. Mtg., Miami, FL, Apr. 28-May 1, 1985

SPEAKER	AUTHOR(S) AND TITLE	TITLE
Todd, P. J.	Todd, P. J.; Leibman, C. P.* "Secondary Ion Mass Spectrometry of Lewis Acids"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	Todd, P. J.; Leibman, C. P.* "Lewis Acid Enhanced Emission of Organic Secondary Molecular Ions"	33rd Annu. Conf. on Mass Spectrom. Allied Topics, San Diego, CA, May 26-31, 1985
	Todd, P. J.; Leibman, C. P.* "Organic Secondary Ion Intensity and Analyte Concentration"	Fifth Int. Conf. on Ion Mass Spectrom., Washington, DC, Sept. 29-Oct. 4, 1985
	Todd, P. J. "Local Thermal Equilibrium Model of Molecular Secondary Ion Emission"	Fifth Int. Conf. on Ion Mass Spectrom., Washington, DC, Sept. 29-Oct. 4, 1985
	Todd, P. J.; Christie, W. H. "Secondary Ion Mass Spectrometry"	DOE-BES Chem. Sci. Site Rev., ORNL, Oak Ridge, TN, Apr. 16-17, 1985
	Todd, P. J.; Groenewold, G. S. "Evaporation and Ion Damage in Molecular SIMS"	33rd Annu. Conf. on Mass Spectrom. and Allied Topics, San Diego, CA, May 26-31, 1985
	Todd, P. J. "Secondary Ion Mass Spectrometry of Volatile Amines"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985
	Todd, P. J.; Leibman, C. P.;* Mamantov, G.* "Lewis Acid Enhanced Emission of Secondary Molecular Ions"	10th Int. Mass Spectrom. Conf., Swansea, UK, Sept. 9-13, 1985
	Todd, P. J. "Secondary Ion Mass Spectrometry of Volatile Amines"	AT&T Bell Labs, Murray Hill, NJ, July 17, 1985
Tomkins, B. A.	Tomkins, B. A.; Jenkins, R. A.; Reagan, R. R.; Griest, W. H.; Holladay, S. K. "Liquid Chromatographic Determination of Trace Levels of Benzo(a)pyrene in the Total Particulate Matter of Cigarette Smoke"	36th Pittsburgh Conf., New Orleans, LA, Feb. 25-Mar. 1, 1985
	Tomkins, B. A. "Chromatographic Detectors Used for the Determination of Nitrated Polycyclic Aromatic Hydrocarbons"	Nat. Am. Chem. Soc. Mtg., Miami Beach, FL, Apr. 28-May 3, 1985
Whitten, W. B.	Ramsey, J. M.; Whitten, W. B. "High Resolution Laser Spectroscopy"	ACD Inf. Mtg., ORNL, Oak Ridge, TN, July 23, 1985

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Wise, M. B.	Wise, M. B.; Holladay, S. K.; Higgins, C. E.; Jenkins, R. A.; Guerin, M. R. "The Chemical Characteristics of Smoke Delivered by Clove-Containing Cigarettes"	39th Tobacco Chemists' Res. Conf., Montreal, Quebec, Canada, Oct. 2-5, 1985
	Wise, M. B. "Fourier Transform Mass Spectrometry: Advanced Instrumentation for Research and Chemical Analysis"	Five Plant Anal.Conf., Oak Ridge Nat. Lab., Oak Ridge, TN, July 16, 1985
	Wise, M. B.; Guerin, M. R. "Chemical Analysis of Clove-Cigarette Smoke"	Banbury Center Conf. on New Aspects of Tobacco Carcinogenesis, Cold Spring Harbor, New York, Sept. 8-11, 1985
Young, J. P.	Donohue, D. L.; Smith, D. H.; Young, J. P. "Resonance Ionization Mass Spectrometry at Oak Ridge National Laboratory"	Central Reg. Mtg. Am. Chem. Soc., Akron, OH, June 5-7, 1985
	Young, J. P. "Counting Atoms and Isotopes by Resonance Ionization Techniques"	Chemical Inst. of Beijing, Beijing, People's Republic of China, Aug. 19, 1985
	Young, J. P. "Counting Atoms and Isotopes by Resonance Ionization Techniques"	Inst. of Atomic Energy, Beijing, People's Republic of China Aug. 29, 1985
	Young, J. P. "Counting Atoms and Isotopes Resonance Ionization Techniques"	Modern Inst. of by Chemistry, Xian, People's Republic of China, Aug. 24, 1985
	Young, J. P. "Counting Atoms and Isotopes Resonance Ionization Techniques"	Fuijian Inst. of by Research on the Structure of Matter, Fuzhou, People's Republic of China, Aug. 28, 1985
	Young, J. P.; Rosseel, T. M.; Hulett, L. D.; Dale, J. M. "Heavy-Ion Induced X-ray Satellite Emission, HIXSE, A New Analytical Technique"	36th Pittsburgh Conf. & Expo. on Appl. Spectrosc., New Orleans, LA, Feb. 25-Mar. 1, 1985
	Wilmarth, W. R.;* Peterson, J. R.;* Young, J. P. "Spectrophotometric Studies of Californium in Selected Lanthanide Trihalide Hosts"	SE-SW Reg. Am. Chem. Soc. Mtg., Memphis, TN, Oct. 9-11, 1985
	Young, J. P.; Donohue, D. L.; Smith, D. H. "Application of Resonance Ionization Mass Spectrometry: Survey of the Lanthanide Elements in the Region of 430-455 nm"	Annu. Mtg. Opt. Soc. of Am., Washington, DC, Oct. 14-18, 1985
	Young, J. P. "Counting Atoms and Isotopes by Resonance Ionization Techniques"	Soc. Appl. Spectrosc., Cincinnati, OH, Oct. 29, 1985

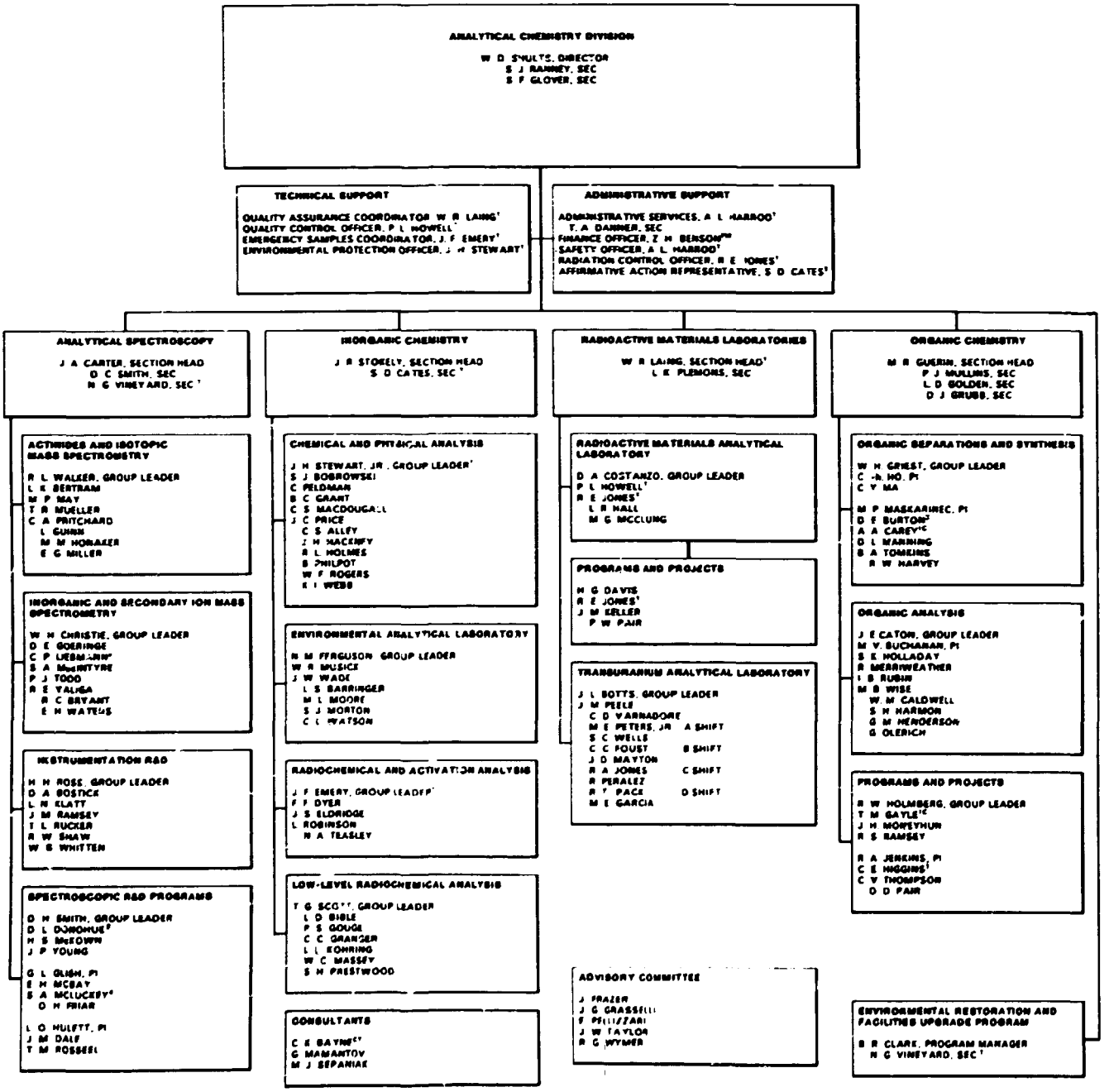
ARTICLES REVIEWED OR REFERRED FOR PERIODICALS

	Anal. Chem.	Anal. Chim. Acta	Fuel	Health Physics	J. Radioanal. Nucl. Chem. Lett.	ORNL Reports	Optics Letters	Proposals	Others	Total
Buchanan, M. V.	5	1								6
Carter, J. A.	2							2		4
Christie, W. H.								1		1
Clark, B. R.				2				2		4
Costanzo, D. A.						2				2
Dale, J. M.								1		1
Eldridge, J. S.			2							2
Feldman, C.	5									5
Glish, G. L.	2								1	3
Griest, W. H.	4								3	7
Guerin, M. R.									10	10
Hulett, L. D.								4	2	6
Jenkins, R. A.									1	1
Lyon, W. S.					3			2	3	8
Maskarinec, M. P.	3								4	7
Ramsey, J. M.	2						1			3
Ramsey, R. S.	5							1		6
Ross, H. H.	1							4	2	7
Rosseel, T. M.								2		2
Shaw, R. W.								1		1
Shults, W. D.	2							2	6	10
Todd, P. J.		1						6	2	9
Tomkins, B. A.	12							2	7	21
Whitten, W. B.							1	2		3
Wise, M. B.								1		1
Young, J. P.	4							2		6
Total	47	2	2	2	3	2	2	35	41	136

DIVISIONAL MAN-POWER AND FINANCIAL SUMMARY
FY 1985

Source	$K	PY
DOE programs		
Health and Environmental Research	658	4.9
Basic Energy Sciences	1,382	10.0
Nuclear Energy	340	2.5
Fossil Energy	321	2.6
Safeguards and Security	497	3.5
DOE - Miscellaneous	89	0.7
Total DOE programs	3,287	24.2
Work for others - federal agencies		
Department of Defense (U.S. Army)	444	3.8
National Cancer Institute	388	3.1
Department of State	124	1.1
National Institute on Drug Abuse	163	1.4
Miscellaneous	44	0.4
Total work for others - federal agencies	1,163	9.8
Work for others - nonfederal agencies		
Protective coating companies	108	0.9
Uranium ore testing companies	46	0.4
International Research and Development Corporation	128	1.1
Miscellaneous	176	1.5
Total work for others - nonfederal agencies	458	3.9
Support/Services		
ORNL divisions	4,479*	69.1
Other clients	1,145*	16.0
	5,624*	85.1
Total financial plans	10,532	123.0

*Does not reflect Laboratory general and administration expense or general plant services.



CT COMPUTING AND TELECOMMUNICATIONS DIVISION
FM FINANCE AND MATERIALS DIVISION
I INSTRUMENTATION AND CONTROLS DIVISION

MULTIPLE ASSIGNMENT
PREDOCTORAL STUDENT UT-K
LEAVE OF ABSENCE IAEA
WIGNER FELLOW

ORNL-6236
Distribution Category UC-4

INTERNAL DISTRIBUTION

1. ". Adair
2. 1. D. Anderson
3. B. R. Appleton
4-28. J. T. Atherton
29. S. I. Auerbach
30. J. B. Ball
31-32. V. B. Baylor
33. Z. H. Benson
34. D. A. Bostick
35. J. L. Botts
36. M. V. Buchanan
37. W. D. Burch
38-39. J. A. Carter
40. J. E. Caton, Jr.
41. W. H. Christie
42. B. R. Clark
43. D. A. Costanzo
44. J. M. Dale
45. R. M. Davis
46. J. G. Dorsey
47. F. F. Dyer
48. B. G. Eads
49. J. S. Eldridge
50. J. F. Emery
51. L. D. Eyman
52. C. Feldman
53. N. M. Ferguson
54. J. C. Franklin
55. W. Fulkerson
56. T. M. Gayle
57. G. L. Glish
58. D. E. Goeringer
59. R. A. Griesemer
60. W. H. Griest
61. M. R. Guerin
62. R. L. Hahn
63. C.-h. Ho
64. L. L. Horton
65. L. D. Hulett
66. R. A. Jenkins
67. J. M. Keller
68. L. N. Klatt
69. E. H. Krieg
70. W. R. Laing
71. C. E. Lamb
72. A. P. Malinauskas
73. D. L. Manning
74. M. P. Maskarinec
75. S. A. McLuckey
76. L. E. McNeese
77. O. B. Morgan
78. R. W. Morrow
79. W. R. Musick
80. D. C. Parzyck
81. J. M. Peele
82. H. Postma
83. M. L. Poutsma
84-85. R. H. Powell
86. J. M. Ramsey
87. R. S. Ramsey
88. C. R. Richmond
89. D. E. Reichle
90. L. Robinson
91. P. S. Rohwer
92. H. H. Ross
93. T. M. Rosseel
94. T. H. Row
95. I. B. Rubin
96. T. L. Rucker
97. T. G. Scott
98. R. W. Shaw
99-123. W. D. Shults
124. D. H. Smith
125. J. H. Stewart
126. J. O. Stiegler
127. J. R. Stokely
128. P. J. Todd
129. C. S. Travaglini
130. B. A. Tomkins
131. H. E. Trammell
132. R. L. Walker
133. C. W. Weber
134. R. S. Wiltshire
135. M. B. Wise
136. J. C. White
137. W. B. Whitten
138. M. K. Wilkinson
139. P. Wooldridge-Paducah
140. R. G. Wymer
141. J. P. Young
142. A. Zucker
143. Biology Library
144. Laboratory Shift Supv.
145. ORNL Y-12 Library, Document Reference
146. Laboratory Records, ORNL-RC
147. ORAU Technical Library (MERT)
148. ORAU/UPD Beth Jinkerson
149. Patent Section
150. PGDP Library (B. Barbre)
151-152. Central Research Library
153-156. Laboratory Records
157-158. Technical Publications

EXTERNAL DISTRIBUTION

158. D. A. Coffin, Health Effects Research Laboratory, MD-52, EPA, Research Triangle Park, NC 27711
159. Paul Cunningham, Analytical Chemistry Division, Los Alamos National Laboratory, CMB-1, MS G740, Los Alamos, NM 87545
160. P. Duhamel, Pollutant Characterization & Safety Research, Office of Health & Environmental Research, USDOE, GTN, Washington, DC 20545
161. J. W. Frazer, 6767 Alisal Street, Pleasanton, CA 94566
162. J. E. Garneir, Sohio Engineered Materials Company, P.O. Box 832, Niagara Falls, NY 14302
163. C. Giddings, 3978 Emigration Canyon, Salt Lake City, UT 84108
164. G. Goldstein, Pollutant Characterization & Safety Research, Office of Health & Environmental Research, USDOE, GTN, Washington, DC 20545
165. J. A. Goleb, Division of Safeguards and Security, USDOE, GTN, Washington, DC 20545
166. David W. Green, Chemical Technology Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439
167. Institute for Energy Analysis, P.O. Box 117, Oak Ridge, TN 37830
168. G. Hieftje, Chemistry Department, Indiana University, Bloomington, IN 47401
169. R. Hirsch, Division of Chemical Sciences, Office of Energy Research, USDOE, ER-162, GTN, Washington, DC 20545
170. G. Mamantov, Dept. of Chemistry, University of Tennessee, Knoxville, TN 37916
171. R. S. Marianelli, Division of Chemical Sciences, Office of Energy Research, USDOE, ER-14, GTN, Washington, DC 20545
172. R. B. Neel, US Nuclear Regulatory Commission, MS-130SS, Willste Bldg., 7915 Eastern Avenue, Silver Springs, MD 20210
173. T. B. Owen, National Cancer Institute, Bethesda, MD 20014
174. E. Pellizzari, Director for Analytical Sciences, Research Triangle Park, NC 27709
175. D. Stevenson, Division of Chemical Sciences, Office of Basic Energy Sciences, USDOE, ER-142, GTN, Washington, DC 20545
176. USDA SEA-TIS National Agricultural Bldg., Current Serial Records, Beltsville, MD 20705
177. R. W. Wood, Deputy Director, Office of Health & Environmental Research, USDOE, ER-74, GTN, Washington, DC 20545
178. D. J. Wynn, USATHAMA, DRX TH-TE-A, Bldg. E4585, Aberdeen Proving Ground, MD 21010
179. Office of Assistant Manager, Energy Research and Development, DOE, Oak Ridge Operations Office, Oak Ridge, TN 37830

180-324. Distribution as shown in DOE/TIC-4500 under category UC-4 (Chemistry) (25 copies—NTIS)

☆U.S. GOVERNMENT PRINTING OFFICE: 1986-631-056/20290