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.

1

NOTICE

PORTIONS OF THIS REPORT ARE ILLEGIBLE. It has been reproduced from the best available copy to permit the broadest possible availability.

ORNL-6039
Distribution Category UC-4

Contract No. DE-AC05-84OR21400

ORNL--6039

DE84 012044

ANALYTICAL CHEMISTRY DIVISION ANNUAL PROGRESS REPORT

For Period Ending December 31, 1983

W. D. Shults, Director

W. S. Lyon, Editor

Date Published - May 1984

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

DISCLAIMER

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.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

CONTENTS

INTRODUCTION AND SUMMARY

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. The program constituted approximately 23% of the FY 1983 budget.

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. This type of activity accounted for approximately 30% of the division's budget in FY 1983.

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 47% of the budget during FY 1983.

The Analytical Chemistry Division is organized into five major sections, each of which may carry out any type of work falling in the three categories mentioned above. Chapters 1 through 5 of this report highlight progress within the five sections during the period January 1, 1983 to December 31, 1983. A short summary introduces each chapter to indicate work scope. Information about quality assurance and safety programs is presented in Chap. 6, along with a tabulation of analyses rendered. Publications, oral presentations, professional activities, educational programs, and seminars are cited in Chaps. 7 and 8. Approximately 42 articles, 31 proceedings publications and 41 reports have been published, and 115 oral presentations were given during this reporting period.

SOME TECHNICAL HIGHLIGHTS

We have made the surprising discovery that a barium titanate crystal used as a phase conjugate optical feedback element can influence the output characteristics of a dye laser in two ways. First we observe a significant narrowing of the spectral bandwidth of the laser from 1600 GHz to 4 GHz. Also, we observe the laser to spontaneously, repetitively scan in frequency from the center of the dye tuning range to the red edge of the dye tuning curve. Broad wavelength scans at high resolution are thus achieved without any of the mechanical components that are necessary with conventional scanning laser systems.

Gas chromatography-negative chemical ionization mass spectrometry has been found especially promising for the differentiation of isomeric polycyclic aromatic hydrocarbons. Ionization is found to be directly related to the electron affinities of the individual isomers. The selective determination of benzo(a)pyrene in the presence of benzo(e)pyrene is an example of the power of the technique.

The choice of matrix has been shown to have a profound effect on ionization efficiency in organic secondary ion mass spectrometry (SIMS). Matrix enhancement of radical molecular cation emission has been observed, previously observed only rarely. Organic SIMS has been extended to volatile molecules, greatly extending the applicability of this powerful technique.

The effect of the cation in desorption ionization of organic species has been shown to be a function of several properties of the cation, the most important of which is charge transfer from the cation to the organic molecules. Chemical reactions occur in the condensed phase prior to ejection of ion species.

A quadrupole time-of-flight instrument for mass spectrometry-mass spectrometry (MS/MS) studies has been developed. This instrument extends MS/MS to a lower energy regime than could previously be studied and allows investigation of transient species.

A double lutetium spike was evaluated for use in assaying the contents (volumes) of holding tanks, using mass spectrometry. This technique is applicable to any system where irregularly shaped containers of ill-defined volume must be assayed. Precision and accuracy is about 0.1%.

A wavelength dispersive x-ray fluorescence (XRF) instrument utilizing a barrel monochromator and graphite optics was developed for highly radioactive solutions. In a companion project, the fundamental parameters approach was used to provide quantitative XRF results with minimal use of standards.

Studies of heavy-ion induced x-ray satellite emission (HIXSE) as a chemical probe of materials have continued. It was shown, for the first time, that the heavy-ion excited L x-ray satellites can be used to characterize the chemical nature of an element in a solid and that intermediate Z elements are accessible to HIXSE analysis. Alloy studies have shown that HIXSE may yield information about metal valence states and the degree of valence electron delocalization. In collaboration with Metals and Ceramics Division personnel, it was also demonstrated that HIXSE is sensitive to changes in the crystal structure of alloys.

Resonance ionization mass spectrometry has been extended to U/Pu mixtures with good success. Isotope ratios of uranium and plutonium can be measured, without element separation, in 10 ng samples that contain uranium, plutonium, and americium. Precisions comparable to thermal ionization were obtained. Optical spectra of several actinides (Th, U, Np, Pu, Am, and Cm) were obtained in the 580-600 nm region.

Isotopic measurements of einsteinium employing resin bead mass spectrometry methodology were made, in collaboration with Chemistry Division personnel, to redetermine the half-life of ^{253}Es. Inaccuracy of the previous value was causing grief in calculation of reactor characteristics.

In the culmination of several years' work, an assessment of the qualitative and semi-quantitative nature of the chemical and physical consequences of radioactive decay in the solid state was made; a position paper evaluating these results was written.

The division performed many more determinations than usual this year primarily because of environmental activities. Some 319,000 analyses were made; our usual total is ca. 270,000. Much of the extra work was "urgent", hence required considerable special assignments and overtime on the part of the staff.

1. ANALYTICAL METHODOLOGY

W. S. Lyon

Analytical Methodology is composed of two groups: Analytical Instrumentation and Analytical Physics. Major funding for both groups comes from DOE Office of Basic Energy Sciences; major objectives are to develop new instruments and techniques for analytical measurements. In addition the groups perform some development such as remote instrumentation for hot cells or special surface characterization.

Research in Analytical Instrumentation is primarily concerned with lasers and their application. An example of the latter is our cooperative effort with the Mass Spectrometry Section in resonance ionization mass spectrometry (RIMS). Work in Analytical Physics has concentrated on positron spectroscopy and positron source improvement and heavy ion induced satellite x-ray emission. The latter is a cooperative program with a number of other ORNL divisions.

ANALYTICAL INSTRUMENTATION

H. H. Ross

Spectroscopy Research

Our program in analytical spectroscopy remains the most diverse research effort in the Analytical Instrumentation Group. During the past year, we have expanded our work in delayed lasing, pushed ahead in the areas of fluorimetry, Fourier transform microwave spectroscopy, opto-galvanic spectroscopy, and resonance ionization mass spectrometry, and have essentially completed our studies in time-of-flight and opto-acoustic spectrometry. Overall, this has been a most successful year with solid accomplishments in virtually every research project.

One of the most significant developments of the year occurred as a "spin-off" of our main line effort in delayed lasing. In this technique, the absorbance of a sample is determined by its effect on the delay between the excitation of a laser gain medium and the resultant laser emission. We have continued to push our idea of using a laser cavity containing one phase conjugate mirror (PCM) for the delayed lasing phenomena. The nonlinear material used for the phase conjugating process is a single-domain barium titanate crystal. This material is attractive because (1) it can provide gain to the phase-conjugate beam using low power lasers, (2) the non-linear properties are non-resonant and (3) the time response of the gain is relatively slow. The non-resonant properties allow tunability of the absorption measurements while the slow time response essentially eliminates cavity build-up contributions to the delay time. We have performed this experiment and have found the delay time for laser emission to correlate with the intracavity absorbance. Unfortunately the precision of these delay times is rather poor. We have tried experiments which provide a "seed" beam to the PCM cavity in hopes of a more uniform initiation of the PCM gain. These results were also of low precision.

Our PCM studies using $BaTiO_3$ have not been a waste of time however. Specifically, we have made the rather exciting discovery of a way to simultaneously narrow linewidth and also scan a CW dye laser. Such a laser contains no intracavity tuning elements, only an extracavity feedback device. The feedback element is a 5-mm cube, single-domain $BaTiO_3$ crystal. $BaTiO_3$ is a photorefractive material, whose refractive index is a function of the intensity of the light propagating through it. As a result of asymmetric two beam energy coupling, and internal reflections from the corners of the crystal, a nearly-degenerate four wave mixing takes place within the $BaTiO_3$. The result is that the crystal acts as a passive phase conjugate mirror. That is, a device that returns a beam exactly counter propagating on the impingent beam. This feedback results in a narrowing of the spectral bandwidth of the laser from 1600 GHz to 4 GHz, a 400-fold reduction. Additionally, the lasing wavelength sweeps in a quasilinear fashion from the center of the R6G dye tuning curve (618 nm) to either the red (640 nm) or blue (598 nm) wing of the curve. The wavelength range that is actually scanned can be modified by using mirrors of different spectral response and/or using different dyes. The direction and rate of the wavelength scan depend on the distance between the laser output mirror and the phase conjugate feed back device. Thus, very broad wavelength scans are achieved at high resolution and with no mechanical motion.

We have shown that this source can be used for high resolution spectroscopy by measuring sodium transitions via the optogalvanic effect in a hollow cathode lamp. Linewidths of 6-7 GHz were measured for these transitions corresponding to a laser linewidth of 4-6 GHz.

The Fourier transform microwave technique which we developed should exhibit a signal-to-noise advantage over conventional nonmultiplexed methods. Experimentally, however, the sensitivity has not been as good as expected. We are trying to reduce the noise problems by employing Stark effect modulation and a frequency stabilized source. The tests of the prototype spectrometer were made by alternately measuring the sample gas and the evacuated cell. With Stark modulation, the removal of the sample is not required. Also, the detector operates at the modulation frequency rather than at dc for reduced 1/f noise. We are now installing an IBM Instruments Model 9000 computer for data acquisition and rapid calculation of the Fourier transforms and hope to be able to push this work with our enhanced computational ability.

Significant advances have been made in the study of resonance ionization mass spectrometry (RIMS) this year. The process was initially described in the last annual report. Five publications have evolved--either published, in press, or submitted. This work is a cooperative venture of our group and the Mass Spectrometry

Section. RIMS is being evaluated both for its analytical potential and as a research tool. With respect to the first objective, RIMS provides a unique source of inorganic ions. Since the ionization is element-selective, RIMS can minimize isobaric (same mass, different element) interference. These features were demonstrated in the development of a procedure to measure isotope ratios of plutonium and uranium in mixtures of plutonium, uranium, and americium. The procedure requires only 10 ng of sample and can be competitive with existing thermal ionization techniques for the same analysis. It is an improvement over the existing method since it minimizes isobaric interference of the actinides on each other.

Progress has also been made in the use of RIMS as a research tool. RIMS may be considered as a spectroscopic technique that uses a mass analyzer as a detector. Since RIMS is applicable to neutral species, atomic spectral information and information concerning initial states of species evolved from a thermal filament can be obtained. Many more RIMS-active wavelengths were found than originally thought possible; it has been shown that atomic species are present in initial state levels higher than ground state and that these are dependent on the temperature of the sample filament. Initial states are also found that cannot be formed by a Boltzman process. It is postulated that these states are formed by a hybrid-resonance route involving the optical dissociation of neutral dimers or clusters. We have demonstrated that atomic spectral information can be obtained on less than one ng of sample, so the technique could be applied to generating atomic spectral information on very small amounts of man-made elements.

A number of improvements have been made to the phase fluorimeter using the self-modulated argon-ion laser as a source. The primary improvement is the use of a RF vector voltmeter to measure the fluorescence lifetime-induced phase shift rather than a double-balanced mixer. A primary noise source in the phase angle measurement is laser intensity fluctuations. Quadrature measurements allow a large portion of this noise to be removed by numerical division of the two signals. Using a test signal, this system can measure a phase angle to ± 0.001° with less than 1 minute of signal averaging (corresponding to ± 4 ps temporal resolution at 654 MHz modulation). A phase angle uncertainty of only ± 1° was obtained by observing scattered light from polystyrene spheres in the sample cell. This corresponds to a relative lifetime uncertainty of ± 3.5%. A series of lifetimes ranging from 840 to 70 ps were measured and compared favorably with literature values.

The matrix-isolation/optoacoustic spectroscopy project is now complete. The goal of this study has been to develop a companion technique for high-resolution, matrix-isolation fluorescence spectroscopy, hopefully exhibiting comparable sensitivity, but useful for non-fluorescent compounds. Ultraviolet optoacoustic (OA) spectra were recorded for several PAH and heterocyclic compounds isolated in argon, xenon, and nitrogen matrices. Among the heterocycles were representatives of O-, N- and S-substituted PAHs. Detection limits of 50 to 500 ng were measured for several of these compounds, depending on the molar absorbtivity of the particular molecule. The minimum detectable absorbance measured was 0.01 a.u., limited primarily by the acoustically-unconstrained nature of these thin film samples. Resolution enhancements of two-to four-fold over room temperature solution spectra were observed. In only one case did this rather modest improvement affect our ability to spectrally quantify mixture of isomers: the benzoquinolines. A synthetic mixture of equal parts of 3,4-; 5,6-; and 7,8-benzoquinoline was prepared and examined using matrix-isolation OA spectroscopy. In room temperature solution, the individual (0,0) bands of the three isomers were not resolved; however, in solid argon at 5K, where the bandwidth had been reduced to approximately 100 cm^{-1}, the (0,0) bands were sufficiently separated to allow quantification of the mixture components.

The sensitivity of matrix-isolation OA spectroscopy is comparable to that of matrix-isolation Fourier transform infrared spectroscopy but the observed spectral resolution is poorer. This work was reported at the 26th ORNL-DOE Conference on Analytical Chemistry in Energy Technology and a manuscript describing these results has been submitted to *Analytical Chemistry*.

Optogalvanic spectroscopy (OGS) experiments have been continued on a limited basis. The majority of this effort has been aimed at the improvement of our instrumentation for the determination of cesium in sodium/potassium/magnesium brines. Different electrode configurations and the use of an RF pulse transformer for signal pick-up (rather than a load resistor) have been examined. Neither resulted in significantly improved performance. The laser spectral output was narrowed with an intracavity etalon so as to more closely match the atomic linewidth of the analyte in the flame. Greater sensitivity resulted, but this improvement was offset by increased wavelength instability. Because of that difficulty, laser linewidth narrowing has not been routinely used for sample analysis. Our sensitivity for cesium determination in concentrated brine samples from nuclear waste isolation leaching studies remains at seven ppm.

This optogalvanic research has recently been extended to low pressure plasmas such as those found in chemical vapor deposition (CVD) processes. A joint study with staff members from the Metals & Ceramics Division is being developed to identify the active species in CVD plasmas optimized for the deposition of boron nitride films on substrates.

As noted previously, we have completed our work in time-of-flight optical spectroscopy. We have made some theoretical calculations of the spectral resolution which could be obtained with this method using a single-mode optical fiber. Such fibers have no modal dispersion; thus the spectral resolution is a tradeoff between the material dispersion of the fiber and the transform-limited spectral width of the short pulses. It is found that the ultimate resolving power which can be obtained varies as the square root of the fiber length. The dispersion is such that at 600 nm, a 1-km single mode could resolve 0.7 cm^{-1} if a time resolution of 8 ps were attainable. All of the work on time domain spectrometry with fiber optic waveguides has been summarized in a review article which was recently published.

(J. M. Ramsey, R. W. Shaw, W. B. Whitten, J. P. Young)

Advanced Instrumentation

Changing objectives in the Fuel Recycle Program mandate that our development effort for new process instrumentation for fuel reprocessing be stopped. However, we are particularly proud of the fact that many of the devices we developed are now installed in process streams at the Y-12 plant and have proven to be superior to any previously used measurement system.

Another major effort, remote analytical instrumentation, continues to make excellent progress. This past year the project focused upon conversion of the prototype remote titration system into a unit suitable for installation into an operating hot-cell. A testing and evaluation protocol of the system was conducted in a mock-up facility. This protocol involved carrying out titrations with all operations performed via the master-slave manipulators, demonstration of remote maintenance, and training sessions with personnel who will operate the final system. This testing protocol resulted in thirteen mechanical modifications. These modifications significantly improved the ease of remote maintenance and solved an unexpected problem involving remote changing of the buret. Software modifications were directed toward making the system more tolerant of operator errors. An algorithm was also developed which allows the operator to locate end-points when the automatic end-point calculation feature fails. This capability is required when dealing with very small breaks or two very closely positioned end-points.

The revised system has three interchangeable burets of 5,10, and 25 ml capacity. The accuracy and precision of volume delivery are 1.6 and 1.3 μl, respectively, and are independent of the buret capacity and the volume delivered. Experiments designed to ascertain what factors limit the accuracy and precision of results obtained from the system indicate that the variance associated with the preparation of standard samples can dominate and, in many applications, will limit the accuracy of the final result. Testing of the revised system was completed and the unit delivered to building 7920 for installation in cell No. 8.

The program funded by the Consolidated Fuel Recycle Program (CFRP) concerning the detection of low levels of uranium in aqueous waste streams was completed in April.

An ORNL/TM summarizes the problems associated with the direct photometric determination of low level uranium as the uranyl ion using the multiwavelength photometer developed under the CFRP program. An alternative procedure was recommended in which the uranyl ion was initially reduced to U(IV) prior to photometric analysis. Such a scheme has the advantages that (1) the optical background can be determined before uranyl reduction, (2) the absorption coefficients of U(IV) at 647 and 1075 nm are 3 to 5 times greater than uranyl absorption, and (3) the major fission and corrosion product contaminants in Purex streams do not optically absorb at wavelengths greater than 600 nm. The multiwavelength photometer can be used to correct the absorbance data for sample nitrate concentration, as well as predict the final sample absorbance from initial reduction data. This predictive ability can decrease the time required for complete uranium analysis to less than two minutes.

The multiwavelength photometer was also applied to the analysis of uranium in an aqueous raffinate stream at the Y-12 Uranium Recovery facility. The installation, calibration, and evaluation of the in-line spectrometer proved so successful for process control that two additional in-line cells were multiplexed to the photometer to enhance operator control of the unit. The concentrations of uranium in the raffinate (0-15 g/L uranium), an aqueous feed (170-220 g/L) and an organic extraction (70-130 g/L uranium) stream are now measured at half minute intervals and displayed on a CRT screen and at remote repeaters in the process control areas. Control samples from each stream are collected weekly and the instruments completely recalibrated quarterly. Over a six month period, the standard deviation between photometer analysis and Davies-Gray determination of uranium were 1, 8, and 4 g/L uranium for the raffinate, aqueous feed, and organic extraction streams, respectively. Four more triply-multiplexed photometer systems are planned for installation over the next two years. We are presently studying specific monitoring locations to identify modifications that may be required to adapt the photometer algorithms and optics to expected sample parameters.

A new effort has begun in cooperation with personnel from the Materials and Chemical Technology Department, ORGDP, to study the thermal decomposition of UF_6 and related compounds. As atomic fluorine is one of the reaction products, it can be used as a diagnostic to determine the extent and rate of UF_6 degradation under a variety of reaction conditions. ORGDP personnel currently monitor atomic fluorine concentration by introducing Cl_2 into the gas stream to form ClF; the concentration of which is followed by infra-red absorption, using a diode laser light source. An alternate procedure is now being investigated to improve the detection limit of atomic fluorine and also provide a calibration technique for the infrared determination. Here, atomic fluorine is titrated with Cl_2; the intensity of chlorine atom recombination emission is used as the end-point indicator. The detection limit of the chemiluminescent procedure is at least comparable to the infra-red absorption method and can ultimately be reduced by a factor of 20. Currently the chemiluminescent reaction chamber is being modified to achieve this additional sensitivity and also to allow laser interrogation of the chemiluminescent reaction products.

In a cooperative program with the Department of Chemistry, University of Tennessee, we have continued the development of an optical spectroelectrochemical technique and the study of iridium carbonyl, $Ir_4(CO)_{12}$, as a catalysis precursor for the hydrogenation of carbon monoxide in molten $AlCl_3$-NaCl. The previous optical multipass spectroelectrochemical arrangement which involved positioning the optically transparent thin-layer electrode, OTTLE, cell between two mirrors could not be extended to the molten salt system due to the physical restrictions imposed by the presence of the furnace. A system involving the use of right angle prisms attached to the outside of the molten salt OTTLE cell is being pursued.

The study of the iridium carbonyl system has focused on the UV-visible spectral region. In $AlCl_3$-NaCl (63:37 mole percent) at 150°C, absorption bands at 278, 326, and 498 nm associated with the catalytic reaction of $Ir_4(CO)_{12}$ are observed. The identical bands are observed when chlorotricarbonyliridium, $IrCl(CO)_3$, is the starting material, suggesting that the monomer may be the reactive species. The rate of appearance of these bands depends upon the CO partial pressure. Experiments are underway to determine this CO partial pressure dependence.

(D. A. Bostick, B. Harward, H. E. Howell, L. N. Klatt, G. Mamantov, J. E. Strain)

Special Projects

Work on the analytical applications of heavy-ion induced x-ray satellite emission (HIXSE) is a combined effort between our group and the Analytical Physics group of ACD along with personnel of the Physics Division. Heavy-ion beam time was at a premium this year, but some experimental progress was made. Also, a more refined interpretation of previous results was carried out. Although HIXSE can easily be used to determine compound identity (and we have demonstrated this use), there are more readily available and cheaper techniques for performing this function. The value of HIXSE lies in the area of materials characterization and study, such as the determination of the valence state of pure metals and their alloys. It will be in the future, however, before direct valence state measurements can be made in pure metals, but suitable samples have been obtained and such experiments are planned. It has been shown that practical use can be made of the valence state capability in alloys; HIXSE has been used to identify different members of a Mo-Ti binary alloy system and differentiate between crystal structures of the same alloy. Several publications are in press or in preparation.

We requested and received seed money support this year for a project to initiate a study to determine active biomass in immobilized biological systems. While methods are available for the measurement of active biomass of freely suspended cells in cultures and natural waters, reliable methods for the measurement of active biomass of attached cells are unavailable.

Microorganisms are the basic process units in both biotechnological waste water treatment and in natural ecological systems. They control the degradation of organic substrates and the remineralization of essential nutrients from organic matter. As such, the estimation of active cellular biomass is a fundamental parameter of a given biological system, relating the concentration and activity of the microorganisms in the process. The measurement of active biomass in a bioreactor can be used to extrapolate such control parameters as column efficiency, chemical poisoning and microbial contamination. Biomass measurements in ecological samples are used to study and predict environmental responses to nutrients, toxic substances, anaerobic conditions, etc. We are considering two different approaches to achieve the desired measurement. In the first, the gelatinous polymer surrounding and attaching the microorganisms to the solid matrix could be dissolved, forming a free suspension of cells. Once the cells are freed, active biomass could be determined directly and rapidly by equipping a Coulter cell counter with a fiber optic system oriented perpendicular to cellular flow. Such a system would automatically provide a count of total cell population electronically, as well as the live cell count based on the measurement of either the absorbance of tetrazolium-stained cells or the native fluorescence of such labile cellular biochemicals as NADH. If cellular detachment cannot be demonstrated, active biomass will be determined indirectly by quantitatively extracting a biochemical indicator of cellular activity. Several new techniques are being considered for the analytical measurement. If we are able to successfully demonstrate that immobilized biomass measurements are possible, a major proposal will be prepared to expand and refine the methods.

We have been working very closely with technical support groups in the division to handle a number of special, complex analytical tasks. These studies include:

(1) The clean-up of wastewater from uranium ore processing.

(2) Use of lithium metaborate to solubilize traces of refractory minerals,

(3) Collection and determination of traces of cerium, lanthanum, and zirconium in turbid wastewater, and

(4) Determination of iridium in heterogeneous Ir/Si/Fe/Cu/Zn residues.

In each case, a satisfactory (if not excellent) solution to the problem was achieved. Some of these studies have been written up for publication and one (lithium metaborate) has been accepted by *Analytical Chemistry*.

A minor effort continues in spectral studies related to the transuranium research interests of the laboratory. This work is carried out in cooperation with personnel of the Chemistry Division of ORNL and the Chemistry Department of the University of Tennessee. Three publications have evolved, either published or in press. The work involves developing absorption spectral techniques required in the research effort and applying these techniques to the characterization of solid state materials that are prepared or develop because of radioactive decay. The research will branch out to a study of the effect of high pressure on 4f and 5f transitions in lanthanide and actinide compounds. Preliminary design studies have been completed, and a prototype high-pressure cell is being constructed for use with μg-sized samples in our microscope-spectrophotometer. The use of spectral information to establish the structure of transplutonium compounds and to follow the ingrowth of, and identify the nature of, progeny species continues. This study has expanded, from the studies of halides, to include oxides, phosphates, and other oxyanions.

Finally, the group has just received and installed a Zymark Laboratory robot system. Our initial plans for the system are 1) to study its characteristics and potential applications *vis-a-vis* the technical service work carried out in the division and 2) to develop new concepts in analytical methods and instrumentation to maximize the benefits that might be obtained by the marriage of a laboratory robot to an analytical system. A preliminary study in the division indicates that several radiochemical procedures might be excellent candidates for "robotization". One such procedure has been selected for the first demonstration test and evaluation.

(D. A. Bostick, C. Feldman, H. H. Ross, J. P. Young)

ANALYTICAL PHYSICS

L. D. Hulett, Jr.

Positron Spectroscopy

The development of monoenergetic positron spectroscopy techniques for surface and bulk analysis of solids is going on at ORNL, at three other national laboratories (BNL, ANL, LLNL), at commercial laboratories (e.g., Bell Labs), and at several universities. The common impediment to all of this work is the limited intensities of monoenergetic positrons that can be produced. This past year our group has taken several approaches to the achievement of more intense fluxes. Our work has involved interactions with other groups at ORNL, LLNL, the State University of New York, and the Hochschule der Bundeswehr, Munich.

At ORNL we have worked with the Physics Division to generate ^{11}C from ^{11}B by bombardment with 10 MeV protons. The ^{11}C isotope emits fast positrons, having a maximum energy of 1.8 MeV, with a half-life of about 20 minutes. These fast particles were impinged on a tungsten moderator. Intensities of moderated positrons produced with the EN Tandem facility were very low. A possible reason for this is that the ^{11}C that was generated in the ^{11}B target was buried so deep that the positrons could not escape. The Physics Division has plans to try to improve yields by using lower energy protons and orienting the target at grazing angles such that they do not penetrate so deeply. At the present time, however, the EN Tandem is undergoing extensive renovations and this work has been halted. The Analytical Chemistry Division has shifted its efforts to the preparation of another positron isotope, ^{68}Ge. It will be electroplated from cupric cyanide solutions onto a platinum substrate as the Cu_3Ge alloy. Commercial vendors offer this isotope but only in limited activities of 10 mCi or less. The reason for this is probably due to difficulties with the electroplating process. When one attempts to use the commonly prescribed techniques for plating large quantities of this alloy, the result is a spongy non-adherent deposit. We have determined that part of this problem is due to the dissipation of cyanide by the anodic reaction of the electrolysis. By continuously replenishing the cyanide during the course of the electrolysis we have suppressed the onset of non-adherent deposit formation. It appears that we will be able to produce safe, adherent sources with activities in excess of 100 mCi.

Concurrent with the above work, we have done collaborative studies with R. H. Howell and R. A. Alvarez of Lawrence Livermore National Laboratory in the use of an electron linear accelerator (LINAC) for generating monoenergetic positrons. The high energy (60 MeV) electron beam is directed onto tantalum bremsstrahlung targets. Positrons produced by pair production are thermalized and re-emitted by tungsten moderators. An overall yield of about 2×10^{6} slow positrons per LINAC electron was obtained. This means that a LINAC beam current of one microamp could produce a slow positron flux of about 12 million particles per second. LLNL is presently constructing shielding facilities that will allow beams of this intensity to be generated. ORNL and LLNL have discussed development of a positron emission microscopy device.

In addition to increasing the intensity of the fast positron source, we are also trying to improve moderation efficiency. There is a general concensus that this can be accomplished with thin film transmission moderators but techniques for fabricating free standing films of tungsten and other moderator materials are not very well worked out. We have succeeded in growing polycrystalline films of tungsten on copper substrates and in removing them in a free-standing form. Thicknesses are about 500 nm. The as-grown films were very fine grained, and it was necessary to anneal them to produce suitable moderators. After annealing at temperatures greater than 1800°C the grain sizes were 2-3 μm. In the as-grown state the films had face-centered cubic crystal structures. After annealing the structure reverted to the normal body-centered cubic type. Moderation efficiencies of these films have not yet been tested.

A low-pass/high-pass differential retarding field spectrometer has been used to measure spectra of scattered positrons. The device has a very large solid angle and it can accept broad diffuse beams. The spectrometer has an electrostatic lens at its entrance. The potential of the lens is adjusted so that its focal point coincides approximately with the point from which the particles are scattered. This causes the positrons to be focused into a beam in which the particles have parallel trajectories; collimated beams of this type can be energy analyzed with flat plate retarding grids which are very inexpensive to construct. Energy resolution of the spectrometer varied from 1/2–1%. It appears to be unsuitable, however, for studying positron scattering. Energy loss spectra were smeared and did not show the detail of those measured with a spherical spectrometer. Presumably, the reason for this is that energy loss cross sections are functions of scattering directions as well as energy. The spectrometer integrated spectra for a large range of scattering angles, giving convoluted data.

(J. M. Dale, L. D. Hulett, T. M. Rosseel, W. Triftshauser)

Heavy-Ion Induced X-Ray Satellite Emission

Heavy-ion induced x-ray satellite emission (HIXSE) is being evaluated as a tool for the chemical analysis of solids and as a method to provide new insight into the bonding characteristics of complex materials. The development of HIXSE as a chemical probe has focused on the expansion of the range of elements which can be analyzed and the concomitant materials applications. For example, we have expanded the element range to the second row transition metal elements (intermediate Z elements) by demonstrating that variations in the intensity profiles of the heavy-ion induced L x-ray satellite difference spectra of molybdenum alloys and compounds can be correlated with the valence electron density of the material. Analysis of the data revealed that the refilling mechanism for the compounds is dominated by inter-atomic relaxation (ligand effects). Although the alloy and molybdenum metal spectra exhibit a linear correlation between the relative yield of Lβ satellites and the valence electron density, no conclusions could be reached about the nonradiative relaxation mechanism. The difference between the observed correlations may indicate that HIXSE is sensitive to the degree of delocalization of the valence electrons and thus the type of chemical bonding. The alloy data are also significant because they indicate that HIXSE may provide an avenue for the identification of metal valence states. Just as a valence state can be used to describe inorganic compound formation, metal valence states may help codify and predict alloy bonding and crystal structure formation.

In another region of the periodic table high resolution V Kβ HIXSE spectra were obtained for a series of $V(Fe_xCo_yNi_z)_3$ long-range ordered (LRO) alloys. Variations in the relative intensity distribution of their satellite lines were observed and are attributed to differences in the vanadium valence electron density of the various alloys. These alloys are of interest because in the cubic form they possess unusual strength and ductility at high temperatures. HIXSE was also used to differentiate between different crystal structures of the same alloy. For example, by generating V Kβ difference spectra, we were able to distinguish between an LRO alloy in a disordered cubic (fcc) form and an ordered hexagonal ($BaPb_3$-type) form. Although it won't replace diffraction methods, the ability to detect changes in the crystal structure provides additional evidence that HIXSE is a sensitive probe of the valence electron distribution. These preliminary results also suggest that HIXSE may be more sensitive to chemical bonding effects than the various electron spectroscopies. In addition, surface anomolies are eliminated because the soft x-rays probe the bulk phase (0.5 mg/cm is the mean depth of x-ray production).

In order to investigate the ability of HIXSE to yield information about metal bonding, a new analyzing crystal (LiF(220)) was installed and aligned in the Applied Research Laboratory x-ray scanning monochromater. The new crystal will allow us to probe the Lα and Lβ heavy-ion induced x-ray satellites of the lanthanide elements (through gadolinium) for variations caused by differences in their metal valence states. In addition, higher resolution vanadium Kβ spectra can be obtained with this crystal. The improved resolution should enhance our capacity to correlate variations in the satellite spectra of LRO alloys with changes in their electronic structure.

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

---

*Metals and Ceramics Division

**Physics Division

Solids/Surface Characterization Team

A Solids/Surface Characterization Team, consisting of a coordinator and a matrix organization of members from many separate groups, has been established to develop and apply materials analysis techniques. Many problems require more than one method for complete analysis, and the integration of chemistry (separations, specimen preparation) with spectroscopy is often needed. Materials analysis methods are frequently applied to other problems such as environmental research and monitoring. The job of the Solids/Surface Characterization Team is to take a broad-based approach to situations such as these. Another function is to keep the division and its management updated on methodology. This past year the team made a survey of surface analysis capabilities in the Oak Ridge 3-plant area and in the industry at large.

Two examples of materials characterization are the analysis of a single crystal stainless steel specimen and the diagnosis of a nickel cathode contamination problem. The stainless steel crystal was a 2 cm boole, 8 mm diameter, grown by zone refining. Using x-ray fluorescence for non-destructive analysis it was determined that the chromium, iron, and nickel concentrations did not differ by more than 2% between the two ends, implying that little or no gradients existed in the crystal. Wet chemical methods were used to analyze a small chip for carbon and silicon. The contamination on the nickel cathode was found to be from brass. The film on the surface was leached and concentrated with ammonium hydroxide. X-ray fluorescence indicated copper, zinc, and lead of concentration ratios typical for brass.

ORNL, and also the Technology for Energy Corporation, has developed a position sensitive detector for use on x-ray diffractometers. Initial applications were mainly in materials problems such as the determination of strain in cast steel parts. We are now experimenting with the use of this detector on a diffractometer designed for asbestos analysis. Preliminary tests indicate that sample turnaround time can be decreased by factors of 5-10. We presently have a high background problem, but we think that this can be overcome and that the instrument will provide both speed and high sensitivity. This is another example of how materials analysis techniques can be applied to other problems.

(L. D. Hulett, J. H. Stewart)

2. MASS AND EMISSION SPECTROMETRY

J. A. Carter

The Mass and Emission Spectrometry Section is engaged in research and development in three broad areas: inorganic mass spectrometry, organic mass spectrometry, and secondary ion mass spectrometry. Each area provides effective support for various laboratory programs, both by developing new analytical procedures and by providing support analyses. The long range goal of the section in general is to develop new techniques to allow extension of mass spectrometric analysis to new areas; this requires research aimed at understanding the fundamental physical processes involved and using the information thus obtained in development of new analytical procedures and instrumentation. Some of the areas receiving attention are: organic secondary ion mass spectrometry, surface characterization, isotopic abundance measurements (particularly as applied to safeguards and the nuclear fuel cycle), multi-element trace analysis, the technique of mass spectrometry-mass spectrometry in organic analysis, and isotopic characterization of enriched stable isotopes.

About 30% of our research and development support is provided by the Division of Chemical Sciences of the Office of Basic Energy Sciences, Department of Energy. This effort, which is very broad in scope, provides the technical base from which current and future mass spectrometric needs of DOE are addressed. Special safeguard projects of diverse origin provide substantial support; the rest of our funding comes through several laboratory programs and various Work-for-Others contracts. Examples of these are the waste isolation projects at Hanford and Sandia and the Three-Mile Island reactor clean-up.

RESEARCH IN INORGANIC MASS SPECTROMETRY

R. L. Walker and D. H. Smith

Resonance ionization mass spectrometry (RIMS) has emerged as a powerful new analytical tool for isotope ratio measurements. The technique relies on the high elemental selectivity inherent in the laser-induced resonance ionization process, which can eliminate isobaric interferences encountered by conventional thermal ionization. Optimum RIMS parameters have been established for analysis of uranium and plutonium. Small samples of each element (10 ng) loaded on anion resin beads yielded isotopic measurements with good precision (0.3–0.7% RSD) with acceptable selectivity and accuracy. The selectivity ratio for plutonium relative to americium at mass 241 also was found to be adequate (1.5×10^3). In other studies, RIMS has been used to investigate the physical processes associated with atom formation at the surface of a heated metal filament. These studies, involving the element europium, indicated that molecular species may provide a route for non-resonant photo-excitation of atoms into highly excited states. RIMS has also been used to study the optical spectroscopy of the actinide elements: Th, U, Np, Pu, Am, and Cm in the wavelength range of 580–610 nm, thus paving the way for measurements of the higher actinides Bk, Fm, and Cf.

An ion optical bench was assembled and put into service. Initial experiments were preliminary evaluations of a position-sensitive detector and a quadrupole/time-of-flight system for mass spectrometry/mass spectrometry (MS/MS) experiments. An internal standard for use in isotopic dilution analyses of plutonium was synthesized, characterized, and put into use. This standard improved precision to about ±0.1%. Both uranium and plutonium internal standards were evaluated for use in our quadrupole mass spectrometer. An improvement in precision of about a factor of two (to about ±0.7%) was realized. A new approach to statistical treatment of isotope ratio data was developed by C. K. Bayne of the Math Panel. This approach uses a model to predict values for the ratios; we hope to develop it to the point where more information can be obtained than is available from conventional treatment.

Recently, we have developed a resin-bead technique for burnup measurement. It involves a very simple separation scheme similar to that developed here for plutonium and uranium analysis. Anion resin beads are contacted with a methanolic nitric acid mixture (90% MeOH.10% 8M HNO_3) containing 100–200 ng or more of neodymium. Good separation from samarium, the main interference in neodymium method, is achieved.

(D. L. Donohue, H. S. McKown, L. K. Bertram, C. A. Pritchard, G. I. Gault, D. I. Whaley, J. P. Young, E. G. Miller, H. C. Smith).

ELEMENTAL AND SECONDARY ION MASS SPECTROMETRY

W. H. Christie

Secondary Ion Mass Spectrometry (SIMS) has been used to study the effect of pulse duration time of XeCl lasers on the annealing of ion-implanted silicon. Boron implanted samples were XeCl laser annealed using energies of 0.5–3.0 J cm^{-2} and pulse duration times of 25 and 70 ns. SIMS depth profiles demonstrated that the shorter laser pulse provided deeper dopant spreading, as expected. The sample that was annealed with 70-ns pulses yielded a very "abrupt" profile when an energy just above threshold for complete annealing (i.e., 2.5 J cm^{-2} in this case) was used. The "abrupt" (sharp fall off) change in B concentration at 400 nm depth has not been observed with ruby or short pulse (25 ns) XeCl laser annealed samples. Clearly, the shorter pulse time is more energy efficient for annealing but longer pulses have the advantage of providing shallow-surface melting and a more "abrupt" dopant profile which appears to have significant implications for high switching speed devices.

In another study, a comparison of laser-induced surface melting and dopant diffusion in ruby and XeCl laser-annealed samples of B-implanted silicon was made by SIMS profiling. Both lasers had a pulse duration time of 25 ns. The SIMS results indicated that at the same energy density, the resulting profiles arising from the two lasers were almost identical. These results suggest that, regardless of the large differences in the optical properties of silicon at UV and visible wavelengths, the efficiency of usage of the incident energy for melting silicon surface regions to comparable depths is approximately the same for the two lasers at similar pulse duration times.

A surplused ion microprobe, essentially identical to our previously existing instrument, has been obtained. This instrument is currently being repaired and reassembled for use in our research program. The instrument is being modified to allow resonance ionization of sputtered atoms to be studied. One potential advantage of this instrument is the availability of a micro focused (~2 μm) primary ion beam. This should allow resonance ionization techniques to be applied to small inclusions and micro particles.

Pu-238 oxide is used as a general purpose heat source (GPHS) to power radioisotopic thermoelectric generators for NASA deep space probes, such as the upcoming Galileo mission to Jupiter (launch 1985). After being fabricated into ceramic pellets approximately 2.5 cm long by 2.5 cm in diameter, the PuO_2 is encapsulated in a 700 μm thick iridium shell. The major purpose of the iridium shell is to provide containment of the PuO_2 in the event of a mission failure involving a high velocity impact of the GPHS capsules with the ground. An iridium alloy (DOP 26) consisting of 0.3% tungsten, and nominally 50 wt ppm aluminum and 60 wt ppm thorium was chosen as the cladding material because of its high temperature strength and ductility and chemical inertness, especially to PuO_2. The alloying elements enhance the impact strength and ductility by increasing the coherent strength of the grain boundaries. Perhaps even more importantly these elements, in particular thorium, help maintain ductility during high temperature aging of the iridium by preventing grain growth. Thorium is effective as grain growth inhibitor because it exists primarily as discreet particles on the grain boundaries.

Although the microstructure and grain boundary chemistry of the iridium have been well characterized for the case where the iridium has been heat treated alone, the effects of high temperature aging in the presence of PuO_2 are unknown. We were asked by scientists at the Savannah River Laboratory to provide analytical assistance in an ongoing iridium/$^{238}PuO_2$ $^{238}PuO_2$ compatibility test. These workers observed that the iridium cladding alloy showed greatly enhanced near-surface grain growth when exposed to PuO_2 for six months at 1440°C. It was felt that SIMS would provide a means for investigating the grain boundary chemistry under different conditions of aging in the presence of PuO_2. SIMS studies demonstrated that chromium and nickel impurities in the PuO_2 tended to diffuse into the cladding alloy along grain boundaries. No plutonium was found in any of the samples studied. Aluminum was observed to diffuse out of the cladding in areas where chromium, iron, and nickel had intruded. Thorium was also observed to diffuse out of the alloy along grain boundaries. The most striking and also unexpected finding of the study was that oxygen diffused inward along grain boundaries and formed ThO_2 *in situ* in one sample. This sample was also observed to have exhibited the least near surface grain growth.

The current state of this investigation is summarized as follows. Chromium, iron, and nickel migrate from the PuO_2 fuel to the iridium cladding and alter the chemistry of the near-surface grains and grain boundaries. Although the effect of these impurities is not now known, they should probably be excluded from the iridium until their effect is understood. The observation that *in situ* oxidation of thorium on grain boundaries seems to reduce grain growth should be investigated further. Currently, no information is available concerning the effect of grain boundary ThO_2 on high temperature impact ductility. This study does suggest that this oxidation phenomena may be a way to stabilize the alloy against exaggerated grain growth and thereby improve its impact resistance.

(R. E. Eby, L. Landau, G. I. Gault)

ORGANIC MASS SPECTROMETRY

G. L. Glish and P. J. Todd

The research in organic mass spectrometry has focused on fundamental aspects of MS/MS and on novel ionization processes. In the area of MS/MS, research has been initiated into the effects that various cationizing species have on MS/MS spectra. Preliminary results using glycerol as a model compound have shown two effects. The first one is the degree of structurally significant fragmentation observed in the MS/MS spectra. This effect correlates well with the cation affinity of the cationizing species: the higher the affinity of the cation the less ion current it takes away in the fragmentation of the ion and thus more structurally significant fragmentation is observed. The other effect observed is the amount of odd-electron ion current produced in the fragmentation processes. This effect correlates well with the amount of charge delocalization from the cationizing species to the glycerol molecule. Further studies are planned to examine the generality of these observations.

Another area of endeavor in MS/MS has been the design and construction of a new type of instrument. This instrument consists of a tandem quadrupole mass analyzer (Q) and time-of-flight (T) mass spectrometer. Such an instrument has several attractive features. First, it is relatively simple and inexpensive. This could allow untold numbers of labs access to MS/MS which presently only have quadrupole mass spectrometers. Second and more important, it should allow rapid acquisition of MS/MS spectra and be especially good for transient type experiments such as pulsed laser desorption. Initial results on the crude prototype QT confirm these expectations. MS/MS spectra of very low intensity signals can be readily obtained as well as MS/MS spectra on transient ion pulses. This instrument was designed with thermal desorption experiments in mind due to the often transient nature of the signal obtained and looks to be very promising for studies in this area.

A collaborative project with researchers from Purdue University used MS/MS to investigate some of the processes involved in desorption ionization of involatile organic molecules by ion bombardment. Several interesting results were observed. Unusual adduct ions were found from sample/sample and sample/matrix interactions and also analyte ions that had undergone chemical transformations. This demonstrated that complex chemistry can occur in the energized condensed phase. It was also shown that the matrix from which the ions are sampled can influence substantially the fragmentations observed. These results show the need for extreme care when using desorption ionization methods for quantification and qualitative identification of organic molecules.

<u>Organic SIMS</u>. Enhancement of organic secondary ion emission by various matrices has been studied in an attempt to better describe and understand the process. Intact, thermally labile, high molecular weight species can be ionized and pass from a condensed phase into the gas phase. Our efforts have been divided into two parts: study of the physical properties of glycerol--the most common matrix employed--and attempts to generate secondary organic species from other matrices, chemically different from glycerol.

For example, consideration of the vapor pressure of glycerol shows that glycerol molecules depart the target surface (i.e., evaporate) at a rate greater than the rate of primary ion bombardment. Involatile species dissolved in the glycerol matrix, cannot, of course, evaporate, so their surface concentration is increased as the glycerol evaporates. While in contrast to the widely-accepted model proposed by McGee, this explanation is consistent with observed variation of secondary emission with time, apparent absence of surface damage, and secondary emission of elemental ions such as Na^+, K^+, etc. which should not be present in significant concentrations at the glycerol surface.

Secondary ion emission from analytes dissolved in matrices chemically similar to glycerol is essentially identical to the emission observed from glycerol. However, secondary ion emission for some analytes dissolved in matrices chemically different from glycerol can be substantially enhanced. For example, polyphosphoric acid (PPA) enhances secondary ion emission from dissolved organic phosphonates by a factor of 400. At the same time, it appears to somewhat suppress the secondary ion signals from other organic species such as amines, which normally produce copious secondary ion signals from a glycerol matrix.

(E. H. McBay, L. K. Bertram, H. S. McKown, D. E. Goeringer, G. S. Groenewold, W. H. Christie, D. H. Smith)

3. RADIOACTIVE MATERIALS ANALYSIS

W. R. Laing

The Radioactive Materials Analysis Section is composed of three groups: Radioactive Material Analytical Laboratories, Transuranium Analytical Laboratory and Special 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, porosity and surface area measurements, 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

Porosimetry of High-Temperature Gas-Cooled Reactor Graphite

A continuing program on the particle technology analysis of HTGR core graphite has been pursued. Oxidation studies of H-451 and Stackpole 2020 graphite have produced many samples for examination. Recently Stackpole 2020 samples have been analyzed by mercury porosimetry and nitrogen adsorption-desorption to determine pore surface area and pore volume distributions as well as surface areas. These analyses have been completed.

During this period it was found that graphite samples smaller than 5 g. could not be analyzed reliably for micropore surface area and pore volume distributions by nitrogen adsorption-desorption with the present apparatus. However, excellent reproducibility was found for pore volume and surface area distribution plot profiles with samples larger than 5 g. Helium densities and BET surface area analyses were also performed on graphite and fly ash.

(D. A. Lee)

X-Ray Fluorescence Development

Quantitative x-ray fluorescence (XRF) analysis for uranium and plutonium in highly radioactive solutions depends on a number of factors, many of which are common to all XRF applications and include background radiation (scatter and detector noise), overlapping peaks, mass adsorption of both the exciting and fluorescent radiation, and enhancement by secondary (and higher order) excitation. In addition, highly radioactive samples introduce two other factors that must be considered. These radiation related factors include excitation of the uranium and plutonium by passive radiation in the sample (gamma, x-ray, alpha, and beta activity) and the spontaneous emission of x-rays which result from internal conversion following the decay of radioactive isotopes (e.g. uranium L x-rays following the alpha decay of plutonium isotopes). Unfortunately, conventional XRF spectrometer designs cannot tolerate a high degree of passive radiation associated with the sample. We are studying designs for an XRF system that may be used to monitor uranium and plutonium in highly radioactive feed solutions to a nuclear fuel reprocessing plant.

Investigations by C. J. Sparks, Jr. (ORNL Metals and Ceramics Division) led to the design of a wavelength dispersive XRF system which can be applied to the determination of uranium and plutonium (or most other elements) in highly gamma-active backgrounds. Because of the requirement that the system operate in a remote and inaccessible environment, a basic feature incorporated into the ORNL XRF spectrometer design is mechanical simplicity. The XRF system employs pyrolytic graphite for the x-ray optics which has the advantage of excellent radiation resistance, high diffraction efficiency (40% of incident power), and 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, a final operational system would have no moving parts after initial alignment, which simplifies instrument maintenance and enhances reliability. The constant optical geometry should also result in improved accuracy and precision.

To achieve the energy resolution and analytical sensitivity to meet process control and accountability requirements for the Westinghouse-Hanford reprocessing demonstration facility (BRET), an intense point source is required for sample excitation. The excitation source for the ORNL XRF system employs a barrel monochromator to select and focus AgK_α radiation from a standard 2KW silver target diffraction x-ray tube (side-window). Quantitative detection limits of < 0.4 mg/ml for uranium have been obtained with a barrel fabricated from singly-bent graphite. However, the graphite barrel monochromator did not provide a sufficiently small focal area to meet both sensitivity and resolution requirements.

The performance of the high-gamma XRF system is strongly dependent upon the focal spot dimensions (primarily the vertical dimension) obtained with the barrel monochromator. The original barrel design with singly-bent graphite (Johann optics) is limited to a minimum vertical dimension of approximately 2.5 mm. This can be improved significantly by using doubly-bent graphite. The expense of doubly-bent graphite would result in the barrel monochromator cost in excess of $50 K, therefore, lithium fluoride is being considered as an alternative for barrel fabrication. With doubly-bent and ground

(Johansson optics) lithium fluoride, LiF(200), we should be able to approach a vertical dimension of 0.4 mm. This reduction in the focal area would yield at least a 10-20 fold increase in sensitivity with a 30 eV FWHM resolution and a cost of less than $10 K. Therefore, current work is directed toward the fabrication of a lithium fluoride barrel monochromator.

Background discrimination against high passive radiation from the sample was empirically evaluated at low energy (10-30 keV) and high energy (greater than 100 keV). In both cases the wavelength selection performance of the graphite crystal spectrometer was more than adequate to yield good analytical results. An empirical evaluation of contributions to measured uranium and plutonium fluorescence from radiation resulting from internal conversion of radioactive isotopes indicated that this interference could be corrected by subtracting spectra taken with and without the exciting silver radiation. Although this correction requires two measurements on the sample and doubles the analysis time, it cannot be avoided.

(J. M. Keller)

Software Development for Quantitative XRF Spectra

We are developing computer programs for peak processing of XRF spectra and for quantitative interpretation of spectral data. This effort is necessary because commercially available software often fails to meet our needs. Additionally, vendors often fail to supply source codes. This omission makes adequate evaluation of the commercial program impossible as well as prevents us from customizing the software for a particular application.

The first phase of software development for the quantitative interpretation of XRF spectral data has been completed. This phase of the software permits the computation of XRF spectra from known sample composition, and provides a means of testing program algorithms and the accuracy of parameters in the x-ray data base. Included in the x-ray data base for most elements are regression coefficients for photoionization and scattering (coherent and incoherent) cross sections, jump ratios, atomic weight and atomic densities. The fluorescent yields, fractional radiative rates and energies for the 15 most intense x-ray emissions are also included. In addition, the L-shell Coster-Kronig yields have been added to the data base for Z=12 (Mg) through Z=94 (Pu).

The next phase of software development for quantitation is the complement of the first phase: computation of sample composition from XRF spectral data. This calculation is based on a nonlinear combination of functions which account for the presence of each element in the sample. However, these functions cannot be solved in closed form but require an iterative solution by successive approximations. The functions for computing sample composition also account for both matrix absorption effects and secondary (and higher order) fluorescence enhancements.

(J. M. Keller)

RADIOACTIVE MATERIALS ANALYTICAL LABORATORY

D. A. Costanzo

The Radioactive Materials Analytical Laboratories provide support to various nuclear related Laboratory programs. The Consolidated Edison Uranium Solidification Program (CEUSP), Consolidated Fuel Reprocessing Program (CFRP), and work related to gunite tank sludge recovery, isotopes production, Three Mile Island (TMI), the Nuclear Regulatory Commission (NRC), radioluminescent lights and enviromental surveillance are representative of these programs. Analysis of intermediate and high level radioactive samples that require glove box or hot cell operations are the main services provided by the group; in addition, x-ray fluorescence analysis and testing of coatings for application in nuclear facilities are also provided.

During this reporting period, approximately 3000 samples were processed and 10,000 determinations were performed. A large number of highly radioactive samples were prepared for analyses by other sections within the division for isotopic analysis, mass spectrometry, gamma spectrometry, neutron activation and gas and ion chromatography.

The majority of analyses were performed in support of nuclear fuel reprocessing and uranium and plutonium gel microsphere development activities within the Chemical Technology and Fuel Recycle Divisions, and radioactive waste disposal and isotopes production activities within the Operations Divison. A variety of analytical techniques have been employed for the determination of uranium and plutonium. Potentiometric titrimetry, coulometry, x-ray fluorescence, alpha pulse height analysis, spectrophotometry and fluorometry are representative of the methods. Other analyses routinely performed included free acid, neutron poisons (gadolinium and cadmium), fission product and corrosion product elements, tritium, C-14, Sr-90, I-129 and -130, and gross alpha, beta, and gamma activity.

The energy dispersive x-ray fluorescence technique has been applied to a wide variety of sample types and matrices. The number of determinations performed by this technique has increased 50% above the last reporting period to approximately 3000.

Sample types included stainless steels and other alloys, uranium ores, soil, deposits on filter disks and aqueous and organic process solutions containing uranium, plutonium or fission product elements. Two commercial computer programs from Tracor Northern Company have been used for quantitative analysis of XRF spectra. One program, SORT, compares an unknown spectrum to a library of standard spectra, and the other, EXACT, employs the fundamental parameter technique for matrix corrections.

Special analyses and material preparations are also provided by the group. In the hydrofracture program large crystals (octahedron in shape and 90 mm in the maximum dimension) obtained from a gunite radioactive waste storage tank were characterized by neutron activation, ion chromatography, spark-source mass spectrometry, gamma spectrometry, Karl Fischer water and pycnometric density measurements. The composition of the crystals corresponded to $[NaFPO_4 \cdot 7H_2O]_{0.7}[NaF]_{0.3}$. Thermal analyses (TGA and DSC) have been made on $UO_2(NO_3)_2$ process samples. Dissolution of SiC and B_4C was accomplished by chlorination of these compounds with Cl_2 and S_2Cl_2. Methods were developed for the preparation of anhydrous $ZrCl_4$ and zirconium 1,1,1-trifluoro-2,-4-pentanedione. Preparations of these materials were used by the Metals and Ceramics Division for chemical vapor deposition studies of ZrO_2 on silicon. Isotopically pure U-234 was separated from daughter activities by ion exchange chromatography and converted to the oxide for Operations Division. A combustion-gravimetric method was developed for the determination of total hydrogen in highly concentrated uranium-plutonium solutions in support of Consolidated Fuel Reprocessing Program criticality studies being conducted at Battelle Northwest Laboratories.

A facility for reprocessing mercury has been installed. Used mercury is purified by a counter current liquid-liquid extraction technique. The impurities content of the reprocessed mercury is typically less than 5 ppm and meets ACS reagent specifications. Approximately 2500 pounds o mercury have been purified for reuse within UCCND and for companies under contract to DOE.

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. The number of requests and funding support for these services has increased to the highest level since the Nuclear Coating Testing program was established in 1977. Testing has been performed for eleven different clients and has involved a 1.5 man year effort. Radiation tolerance testing is performed in the High Flux Isotope Reactor using the intense radiation emitted by the spent fuel elements. In the decontamination test, a mixture of gamma-emitting nuclides are applied to the surface of coated stainless steel panels or coated cement blocks and removed with various decontaminating solutions. In the DBA test, the coated specimens are exposed to an emergency coolant spray solution at elevated temperature. These tests conform to ASTM specifications.

A number of modifications have been made to the DBA apparatus to improve operation of the equipment and reliability of the measurements. Temperature and pressure recorders are now used for continuous monitoring and a super heated steam line was installed to obtain temperatures up to 196°C.

Construction of an addition to the west end of building 2026 was started in mid-May 1983, and is scheduled for completion in February 1984. Occupancy of the addition should occur in mid-1984. The addition contains approximately 600 sq. ft. of floor space on the ground floor and 2000 sq. ft. on the second floor. A counting room will be on the ground level and a glove box laboratory, two cold laboratories and an office will be located on the second floor. The addition will be used to relieve the crowded conditions that have existed for the past several years in the low-level chemistry and glove box laboratories in building 2026. In addition, the intermediate-level radiochemical operations being performed in building 3019-B will be moved into the new facilities.

(J. L. Botts, R. D. Brooksbank, R. E. Jones)

Fuel Recycle Division
Support Laboratory

Approximately 2000 analyses were performed by the satellite service laboratory in building 7603 in support of process and engineering studies carried out by the Fuel Recycle Division. The samples were generated in fuel dissolver, iodine trapping, nitric acid recycle, NO off-gas and concentration profile studies. Analyses included free acid by volumetry and thermometric titrimetry, iodine by volumetry and spectrophotometry, oxides of nitrogen by acidimetry and spectrophotometry, hydrogen by combustion, silver by volumetry and solids by gravimetry.

Procedures for the determinations of uranium, gadolinium, viscosity, density, tributyl phosphate and disengaging time are presently under investigation in anticipation of the start-up of the integrated equipment test during the first quarter of 1984.

(F. L. Layton)

TRANSURANIUM ANALYSIS LABORATORY

J. H. Cooper

The Transuranium Analysis Laboratory continued to provide support to the Transuranium production program and to the Operations Division in monitoring radioactive waste effluents. The sample load was slightly less than last year.

Normally Am-243 has been determined in the presence of curium by alpha pulse height analysis or isotope dilution mass spectrometry. In cases where the radioactivity of curium is excessively higher (100 times) than the activity of the americium, alpha pulse height analysis is not practical because the americium alpha peak is lost in the tail from the curium activity. One solution to this problem has been to determine Am-243 by isotope dilution mass spectrometry. However, this method is expensive and time consuming. We have attempted to determine Am-243 by direct gamma spectrometry. The gamma lines of Am-243 are often obscured by all the curium gammas. The daughter of Am-243, Np-239, has gamma energies sufficiently intense and separated from curium gammas. This phenomenon was used to determine Am-243. After initial separation of americium from its daughter Np-239, time was allowed for fresh neptunium to grow in. Standard Am-243 samples were analyzed simultaneously with the unknowns to eliminate the need for the calculation of recovery and ingrowth of Np-239.

An exercise to evaluate decontamination methods for simulated nuclear accidents was carried out using shortlived ($T_{1/2}$ = 11.4 days) Ra-223 as an alpha emitting contaminant. The Ra-223 was produced by irradiating Ra-226 in the High Flux Isotope Reactor and allowing the products to decay to Th-227. This nuclide was separated from the other radioactive contaminants and allowed to decay to Ra-223. The production and separation processes provided many samples for radiochemical analyses. Gamma-spectrometry and alpha pulse height analyses were used to determine the purity of the final product.

Free acid in solutions of plutonium and uranium was determined after separation of the plutonium from the other constituents by iodate precipitation. Since no standards of acid in plutonium were available, standard addition techniques were used to assure the correct value of acid concentration.

Reducing normality of hydroxylamine nitrate was measured by titrating the ferrous ion produced by ferric ion reduction. Normally, reducing normality is determined by direct titration with potassium dichromate. This method produced erratic results. An excess of Fe(III) was added to the hydroxylamine in an acid medium and the resulting Fe(II) was titrated with standard permanganate.

Some of the instrumentation in the Transuranium Analysis Laboratory is being updated. A pipettor and a titrator for use in the shielding cells have been fabricated and tested. A new analyzer system for alpha spectrometry has been ordered. This system will allow the simultaneous analysis of four different samples.

4. BIO/ORGANIC ANALYSIS SECTION

M. R. Guerin

This section is composed of three groups, Analytical Chromatography, Separations and Spectroscopy, and Special Projects. Each group carries out analytical research, applied studies, and analytical services to varying degrees. Analytical research currently emphasizes chemical ionization mass spectrometry, analytical separations, and chromatographic detection. Applied studies continue to focus on toxicology-related issues associated wtih cigarette smoke, other dense aerosols, and synthetic fuels technologies. Increased attention is being given to providing quantitative and qualitative organic analytical services in general support of Laboratory programs. Principal support for Section activities is provided by the Department of Energy, the Department of the Army, and Health and Human Services.

ANALYTICAL CHROMATOGRAPHY

W. H. Griest

The main activities of the Analytical Chromatography group are chromatographic methods development and applications associated with health and environmental effects studies. Projects are funded by the Department of Energy, the Environmental Protection Agency, the Electric Power Research Institute, the National Cancer Institute, and in a new area, the Department of Defense. A small effort in fundamental chromatographic separations research is funded by the Department of Energy. In-house organic analytical services have been an increasingly important activity.

Basic chromatography research continues to focus upon separations employing open tubular liquid chromatography (OTLC) and also capillary electrophoresis. The technology has been developed for the preparation of high resolution 7.5 μm I.D. reverse phase columns from either borosilicate or soda-lime glass. Collaboration with researchers at the University of Tennessee and in the ACD Analytical Methodology section has resulted in the development of a laser-fluorescence OTLC detector sensitive to 2 pg of 7-chloro-4-nitrobenzooxadiazole-derivatized alkyl amines, and a thermal lens absorbance detector sensitive to 30 pg of nitroanilines. Capillary zone electrophoresis utilizing a 25 kV constant current power supply and 100 cm x 75 μm I.D. fused silica column with phosphate buffer supporting media has produced more than 10^5 theoretical plates for 9-aminoacridine.

Methods development has relied heavily upon the use of selective detectors coupled with sequential chromatographic separations. A sensitive, specific, and reliable method for the determination of nitro-derivatives of polycyclic aromatic hydrocarbons (NO_2PAH) in particulate matter has been developed. It features semi-preparative scale normal phase HPLC to provide a polar fraction enriched in the nitroaromatics class, and GC with the thermal energy analyzer to achieve extreme selectivity with good sensitivity for compounds substituted with the nitro group. Several NO_2PAH were measured in diesel exhaust particulates, including 1-nitropyrene at 10 ppm. This same NO_2PAH was measured at 0.2 ppm in coal combustion stack ash, with a limit of detection of 0.05 ppm. The GC procedure, without the HPLC isolation, has been used also for determining nitroglycols in solvent extracts of XAD-2 resin used to collect air chamber samples.

The sequential HPLC/HPLC procedure for determination of benzo(a)pyrene in synthetic fuels was found applicable to cigarette smoke total particulate matter (TPM). A preseparation of the TPM extract on a silica Sep-Pack cartridge prior to the HPLC was the only procedural modification required. Sensitivity is at least 10 ng of benzo(a)pyrene per cigarette when 100 mg of TPM are used, and is limited only by the number of cigarettes which can be conveniently smoked to generate the TPM. Two TPM samples can be analyzed per man-day.

Procedures requiring minimal isolation and relying mainly upon selective detection have allowed very rapid and facile analyses. Phenol and cresols in cigarette smoke TPM are determined by basic extraction and and reverse phase HPLC fluorescence. The limit of detection is approximately 0.1 μg phenol per cigarette. As many as 20 samples can be analyzed per man-day.

A new applied research area initiated this year also relies upon selective chromatographic detection. Sorbent resins are being evaluated for their efficiency and practicality in the collection of munitions components in ground and surface waters. Solvent extracts of the resin eluates are directly analyzed using reverse phase HPLC with electrochemical detection. Very sensitive determinations of nitrated compounds such as nitroglycerin, nitrotoluenes, and nitramines are achieved down to the 0.5-2 ppb level in water. In the field, eight to ten water samples per pump can be collected on resin cartridges in an 8-hour shift. The same electrochemical-LC procedure also can detect nitroglycols in solvent extracts of air chamber samples collected on XAD-2 resin.

Developmental activities in GC include the refinement of the thermal-desorption GC method for analyzing volatile and semivolatile particulate organics. Particulate samples are heated in an inert gas stream and the volatilized components are collected on Tenax resin for analysis by thermal-desorption GC. A wide range of one- through three-ring aromatics and their alkyl-substituted homologs, aliphatic hydrocarbons, and oxygenated PAHs were determined in a coal combustion stack ash sample at levels from 6 ppb to 3 ppm. A chemical subtractor column for selectively removing acidic species from the volatilized components was developed to simplify the chromatograms and to allow additional chemical information to be obtained on the components present.

A multielement GC analysis capability is being established to allow simultaneous detection of C, S, and N-compounds in complex mixtures. A capillary column GC has been fitted with flame ionization (general detector for carbon-compounds), flame photometric (sulfur or phosphorus), and thermionic bead (nitrogen or phosphorus) detectors with separate electrometers. Each detector has been optimized individually. Three-way splitting of the capillary column effluent to allow simultaneous analysis with all detectors is being perfected.

Research has continued on the nature of carbonaceous particulate matter emitted into the atmosphere. For the first time, solvent-extractable matter from air particulates has been separated into molecular weight fractions by size-exclusion chromatography, and characterized using FT-IR and FT-NMR. The results were complicated by coextracted inorganic matter, but suggested that the higher molecular weight, "chromatographic intractables" have molecular weights of at least 800 AMU, aliphatic protons and C=O and OH functional groups. Identification and quantitation will require advances in chromatogrpahic technology for moderate- molecular weight polar organics. Carbonaceous particles have been isolated from coal combustion stack ash. Light and scanning electron microscopy indicate that they consist of uncombusted coal macerals, partially combusted coal, semicoke, and cokes. They contribute significantly to the surface area and organic-compound sorptivity of fly ash. They appear to act as the vehicle for release and transport of organic matter from coal combustion into the environment.

The in-house demand for organic analytical services increased considerably this year, leading to the establishment of a services lab and subgroup. HPLC and GC instrumentation and procedures for the preparation of aqueous, particulate, filter, or adsorbent samples for quantitative determination of organic compounds have been established. The primary demand has been for measurements of priority pollutant PAHs, phenols, and volatile organic compounds in aqueous matrices.

Research sample management has been a continuing special responsibility of the group. This year, additional coal liquefaction product samples have been obtained from the H-Coal and EDS pilot plants. These samples have received baseline chemical and physical characterization and are being archived to support current and future studies of synthetic fuels. A sample handling laboratory is being prepared in building 3001 to allow the homogenization and aliquotting of 200 L drum quantities of synthetic fuels as well as the preparation and storage (in freezers) of smaller quantities (<1 L) of samples for near-term distribution and study.

(P. A. David, S. H. Harmon, R. W. Harvey, C. E. Higgins, D. L. Manning, M. P. Maskarinec, P. J. Pellechia,** R. R. Reagan, M. J. Sepaniak,† B. A. Tomkins, J. D. Vargo††)*

---

*GLCA Student

**ORAU Summer Fellow

†Assistant Professor, University of Tennessee

††Oak Ridge Associated Universities Research Fellow now employed at General Motors

SEPARATIONS AND SPECTROSCOPY

J. E. Caton

Research, technical support, and/or applied chemistry are carried out in several areas of spectroscopy, in separations science, in fossil fuel chemistry, and in the compilation of fossil fuel information. Research in spectroscopy is mainly centered around chemical ionization techniques associated with gas chromatography/mass spectrometry. Basic studies in separation science have been initiated to evaluate and understand the effects of selected chemical and physical perturbations on conventional separation techniques. For fossil fuels a minor research effort is devoted to the interrelationship among the chemical, physical, and biological characteristics of synfuel products. Applied studies are carried out in two principal areas: (1) to elucidate certain chemical processes which effect the reduction of toxicity in synfuels and (2) to develop separation methods which can reproducibly isolate groups of compounds for further analytical studies. Technical support is provided in several spectroscopy areas including nuclear magnetic resonance spectrometry, infrared spectrometry and gas chromatography/mass spectrometry. Samples are prepared for biological or environmental testing. Chemical and biological data associated with fossil fuels are assembled, interpretated, reduced and evaluated. When required, organic compounds are synthesized to produce standards and model compounds for biological, environmental, or chemical studies.

The ongoing research on chemical ionization techniques in mass spectrometry has resulted in new and promising observations. These include the use of metals as chemical ionization reagents and the differentiation of isomeric polycyclic aromatic hydrocarbons (PAH) by negative chemical ionization. Using methane as an ionization reagent for negative chemical ionization, electrons with essentially thermal energy are generated. These thermal electrons can ionize those PAH compounds with electron affinities above some threshhold level which has been experimentally estimated by initial studies on standard compounds. From this threshold level it should be possible to predict the formation of the negative molecular ion for a given PAH either from electron affinity values in the literature or from Huckel molecular orbital calculations. Such selective ionization should provide a useful tool for differentiating a number of isomeric PAH and in some cases could eliminate the need for comparison to standard compounds. For example, PAH compounds which contain an unsaturated five-membered ring such as fluoranthene generally have a high electron affinity and can be ionized. On the other hand, pyrene with the same molecular weight as fluoranthene contains only six-membered rings and is not ionized by the thermal electrons. Thus, these two isomeric PAH compounds which are common in environmental samples can be readily distinguished.

The use of metal ions as chemical ionization reagents for the differentiation of isomeric compounds is also being studied. Iron pentacarbonyl has been used to generate various iron-containing ions including Fe^+, $Fe(CO)^+$, and $Fe(CO)_2^+$. Upon the introduction of standard alkenes into this atmosphere, complexes corresponding to the addition of an iron ion to each alkene bond are observed. Following this demonstration of the utility of chemical ionization by metal ions at relatively high pressures, future studies will be directed toward the formation of metal-arene complexes.

Preliminary studies have been initiated to investigate the effects of fields such as microwave radiation and radio-frequency energy on chromatographic separations. The first experiments in this area utilized the broad band microwave field generated by a domestic microwave oven. Although most of the effects induced by this microwave field are likely to be related to thermal excitation of either the sample or the chromatographic phases, some special selectivity might be expected because such a field tends to heat substances with permanent dipoles. Thus, polar phases, polar samples, polar solvent molecules, and even glass containers would tend to be heated before non-polar substances such as hexane, carbon tetrachloride, or benzene. Naturally, when any part of a system is heated, heat will flow to the cooler parts of the system; but, one can imagine a polar stationary phase being eluted with a slightly cooler non-polar solvent. This overall differential thermal effect on eluent, stationary phase, and sample could lead to significant changes in separation characteristics, and preliminary results indicate this to be true. Ongoing work will further evaluate both the broad band microwave field and radio-frequency energy fields.

Several processes other than hydrotreatment are being evaluated for their utility in eliminating the toxic characteristics of crude coal-derived liquids. It appears that the most efficient first step in any non-hydrotreating process for removing toxicity should be a simple distillation, because essentially all mutagenicity as measured by the Ames bioassay is concentrated in that fraction boiling above 240°C. After the portion of material requiring further upgrading has been reduced by distillation, four procedures which are related to processes already carried out in petroleum refining have shown much promise in reducing the mutagenic activity. These treatments are equilibration with concentrated sulfuric acid, pentane deasphalting, partitioning between pentane and furfural, and percolation through clay. Although each of these processes has been quite successful in removing mutagens, further evaluations are in progress. The toxicity is being determined by other bioassays. More quantitative chemical treatments are being completed in order to estimate relative amounts of chemical reagents needed to upgrade the high boiling fraction. Subsequently, a laboratory-scale investigation of the relative efficiency and effectiveness of these four processes will be compared to hydrogenation.

The eight isomers of acridine (benzoquinolines) were used as model compounds in several different separation and spectroscopic studies. The infrared spectrum of each isomer was determined by the diffuse reflectance technique with each isomer showing a unique spectrum. This set of isomers also offered a unique set of compounds for nuclear magnetic resonance spectrometry studies where spectra were recorded and simulated spectra were calculated in order to determine precise coupling constants and chemical shift values for each isomer. These acridine isomers also offered a challenging set of compounds to test separation methods. Liquid chromatography on normal phase columns allowed the isocratic separation of six isomers with the final two isomers eluting together. Similar results were obtained for capillary gas chromatography where only six distinct peaks were observed.

Because the eight acridine isomers have similar chromatographic and mass spectral characteristics, the question concerning which of these compounds might be present in a synfuel was studied in detail. Accordingly, a careful isolation of the benzoquinoline compounds from a crude coal-derived liquid by multiple liquid chromatography steps indicated that for at least one coal oil two or three of the benzoquinoline isomers were present in greater quantities than acridine. In this study, both phenanthridine and 5,6-benzoquinoline were isolated from a coal-derived oil, and their structures were definitely confirmed by essentially perfect matches of the mid-infrared spectra. This isolation work served to emphasize that most routine gas chromatography/mass spectral identifications on samples derived from complex mixtures must be considered tentative. Absolute structure assignments require further confirmation such as that provided by careful comparisons of infrared spectra, nuclear magnetic resonance spectra, or in some cases, ultraviolet-visible spectra and fluorescence spectra. Such spectral matches require the generation of spectra of pure compounds and the labor-intensive and time-consuming isolation of an essentially pure compound which ultimately limits the number of compounds which can be unequivocally identified.

An evaluation of Fourier Transform Mass Spectrometry has been made and indicates that this technique might substantially reduce the effort required for absolute isomeric discrimination. This evaluation, carried out at the instrument manufacturer's site, indicated that a spectral resolution of greater than 350,000 was easily achieved. In addition, ions of a single mass could be trapped and several successive generations of daughters of that ion could be studied thereby revealing much structural information about isomers in a mixture.

A number of special projects were completed this year. A conventional spectrofluorometer was interfaced with an Apple II+ computer which was also interfaced to an ultraviolet-visible spectrophotometer thereby allowing digitized electronic spectral data to be collected, stored, manipulated, and plotted. Another project involved assembling a multiple column semipreparative HPLC system which should provide for the efficient preparation of analytical samples from much larger initial samples. For example, preliminary experiments have resulted in the isolation and subsequent analysis of a sample containing parts-per-million quantities of several nitrogen-containing compounds from five grams of a coal-derived oil in a one-day period. A third special project was carried out in conjunction with workers at the University of Mississippi where it was shown that the potent cricket teratogen, benzo(g)quinoline-5,10-dione, exhibited microbial toxicity similar to that produced by strong antibiotics.

Technical support efforts increased significantly during this year with much of this increase being provided to the Fossil Energy Technology Environmental Program in the form of contributions to program development, preparing review documents, contributing to information data bases, and reviewing environmental monitoring plans. Two documents were prepared: (1) A document detailing the "lessons learned" concerning health effects from the direct coal liquefaction work which has been carried out in the United States and outlining the additional studies needed in order to assess the health and environmental effects associated with coal liquefaction; and (2) A document enumerating selected sampling and analysis guidelines needed to monitor direct coal liquefaction processes. In addition to these documents, several computer data bases containing health and environmental assessment data for coal liquefaction processes were prepared; and more than twenty outlines for environmental monitoring submitted to the Synthetic Fuels Corporation were critically reviewed.

Spectroscopic services in support of Laboratory-wide programs continued at essentially a constant level. Both raw data and interpretation were provided to personnel in several divisions, including Biology, Instrumentation and Controls, Chemical Technology, Health and Safety Research, Industrial Safety and

Applied Health Physics, Chemistry, Environmental Sciences, and Metals and Ceramics.

(M. V. Buchanan, R. R. Clark, C.-h. Ho, G. B. Hurst, A. R. Jones, C. Y. Ma, G. Olerich, R. B. Quincy, L. M. Roseberry, and I. B. Rubin).*

SPECIAL PROJECTS

R. W. Holmberg

Studies of the chemical and physical properties of concentrated aerosols continue as the primary emphasis of the Special Projects group. Primary project support is provided by the National Cancer Institute for cigarette smoke studies and by the Department of Defense for toxicology related studies on military smokes and obscurants. Additionally, work is in progress on the characterization of marijuana smoke and on the development of animal delivery devices for its neurological testing. The development of a modified helium ionization detector for chromatographic detection is being pursued.

Work on Army smokes and obscurants has reached a mature phase with on-going toxicological studies being performed by the Environmental Protection Agency at Research Triangle Park, NC and by the Illinois Institute Of Technology Research Institute (IITRI) at Chicago. Both projects use generation and monitoring equipment developed and built here. We continue to provide technological support to these projects and prepare, store, and supply some of the specialized materials used by them.

The smoke being investigated by IITRI is a phosphorous aerosol produced by the burning of a red phosphorus-butyl rubber formulation. We have undertaken a chemical and physical comparison of this smoke with a similar one produced from white phosphorus impregnated into a wool felt matrix. It is hoped that the chemical and physical comparison will indicate sufficient similarity of the smokes so that a complete toxicological investigation of the white phosphorus obscurant will not be necessary.

The two formulations were burned under conditions which simulates smoke production in the field. The smoke was delivered to chambers where it was sampled and analyzed. Chemically, the aerosols were found to be composed primarily of a complex mixture of phosphoric acids. The HPLC anion exchange profiles for phosphate speciation were very similar with regard to the number of compounds detected and their concentration levels. The highest polymeric phosphoric acid species resolved was $H_{13}P_{11}O_{34}$. No resolved cyclic compounds were seen in either the red or white phosphorus smokes. Despite the appreciable organic content of the raw materials (i.e., 5% butyl rubber and 20% felt) the concentration of the organic compounds in the gas phase and particulate phase was found to be very low. Other gaseous constituents such as P_4, PH_3, and CO were detected, but at sufficiently low levels that they should not contribute to the toxicity of the smokes. The mass median particle diameter for each aerosol was generally below 1.0 μm. The aerosols produced from these static burns were also compared to those produced with the ORNL extrusion generator. The major difference seen was in the phosphate speciation. Cyclic phosphates, and long straight chain and branched polymers were detected in the generator produced aerosols.

In our tobacco smoke studies, there has been an increasing shift in emphasis toward the characterization of cigarette smokes generated under conditions of human exposure. Fifteen of the most popular commercial products and several products representing the ultra-low tar delivery class are being studied for their deliveries of nitrogen oxides and of selected particulate and vapor phase organic constituents. Smoke is being generated under both traditional analytical conditions and under conditions reported to better mimic current human smoking practices. Selected products purchased up to five years ago are being compared with their newly purchased equivalents to determine whether detectable changes might have occurred due to processing or crop year. Development of a micro-computer controlled variable puff smoking machine has proceeded to the point where the operator can control the shape, size, duration, and frequency of the puff. Actual testing of the system using human puffing characteristics should begin soon.

We have recently initiated a new study for the National Institute for Drug Abuse involving marijuana smoke exposure of primates and rodents. We have been asked to develop inhalation exposure systems and methodology which will maximize exposure to active cannabinoids while limiting exposure to carbon monoxide, a major toxin in the smoke complicating the bioassay. Our first task is to determine the cannabinoid

---

*Co-op Student, University of Tennessee

deliveries of the marijuana cigarettes under a wide range of puffing conditions.

Both field sampling activities and the development of instrumentation continue to play an important role in our Group's activities. An early analog version of an instrumental cigarette smoke monitor designed by ORNL to measure the amount of smoke that humans generate has been sent to another laboratory for evaluation of its use with human subjects. A more advanced, micro-computer controlled version of the monitor is now under development. Instrumental smoke concentration monitors were field tested as part of a project to assist the Department of Plastic Surgery, University of Illinois Medical Center with tobacco smoke inhalation exposure of rodents. This study sought to determine whether smoking impeded the healing process following large scale skin grafts. The Navy's Inactive Ships Facility at Bremerton, WA was visited by members of the Group. Air and internal surface samples were obtained from the battleship Missouri and other vessels to scope the existence and magnitude of organics contamination.

An additional instrumentation project involving design modifications for a helium ionization detector (HID) has been funded by the Exploratory Studies Program at ORNL. The design changes are expected to improve the overall performance and extend the applications of this sensitive, universal chromatographic detector. Modifications include changes in cell geometry from the parallel plate configuration to a symmetrical design, changes in the radioactive source, and changes in the method of sampling the detector current from the application of a constant DC voltage to a pulsed frequency voltage. A pulse generator with variable width and interval adjust has been assembled and allows up to 500 V to be pulsed in a minimum of 100 nsec. The pulse width, interval, and voltage supplied to the detector cell all influence electron collection. The effect of these variables on the background current, noise level, sensitivity, and linear range will be investigated.

(R. W. Holmberg, R. A. Jenkins, R. S. Brazell, J. H. Moneyhun, S. K. Holladay, D. D. Pair, G. M. Henderson, and T. M. Gayle)*

---

*Instrumentation and Controls Division

5. GENERAL AND ENVIRONMENTAL ANALYSIS

J. R. Stokely

The General and Environmental Analysis Section provides a diversity of analytical chemical services in support of Laboratory and Nuclear Division programs. Activities within the section are organized into five groups: Chemical and Physical Analysis, Environmental Analysis, Low-Level Radiochemical Analysis, Activation Analysis, and Special Projects. The section performs routine analyses using established procedures and is involved in developmental activities to upgrade capabilities, to devise new methods of analysis, or to solve applied problems requiring analytical expertise. Over 200,000 analyses are performed annually for a large number of programs and projects.

For several years, the section has supported Laboratory programs to monitor possible releases of toxic metals, organics, and radioactive elements into the environment of the Oak Ridge-DOE reservation and the East Tennessee area. This year, there has been an intensification and diversification of this monitoring effort that has put heavy demands on the section. Continuation of this intense monitoring effort is expected in the foreseeable future.

Analysis capabilities have been improved significantly this year by acquisition of new equipment. A new transmission electron microscope with x-ray analysis capability was put into routine service. A new ion chromatographic system was acquired for environmental analysis of anions and organic acids. A low-level beta counter is being put into service for monitoring of radionuclides in Laboratory effluents. Plans have been made for expansion of neutron activation analysis facilities at the High Flux Isotope Reactor, and funding for construction is expected within the next 1-2 years.

CHEMICAL AND PHYSICAL METHODS GROUP

J. H. Stewart, Jr.

Applications of laboratory analytical chemistry to a large scale industrial environmental problem were made to support the Bechtel Corporation. Special DOE funding for our group allowed characterization of the waste liquid storage areas within the formerly-used Niagara Falls Site and supported our development of a practical method for removing toxic metals and radiochemical contamination from a one-million-gallon concrete storage basin. The solution contained radium and daughter products, carbonate-complexed uranium and numerous environmentally harmful metals. Two additional 300,000 gallon outside storage basins were also included in our study of the Niagara Site. An ad hoc ACD group analyzed the liquids, formulated a method for removal of contaminants, and developed the procedures needed for analytical measurements. A very practical flowsheet was developed and successfully tested in the laboratory. The gross alpha beta counts were reduced from 2×10^5 Bq/L to less than 50 Bq/L which more than met the release criteria of 600 Bq/L. The treated effluent also met the State of New York discharge guidelines for uranium, fluoride, and toxic metals. The Bechtel staff is purchasing tank car lots of the chemicals required for treating the first basin in early FY-84, using the ORNL procedure.

The determination of metals and organics at trace levels in local surface waters assumed new significance this year. The intensive survey of effluents from ORNL facilities at the Y-12 area resulted in approximately 8000 additional analyses during a six week sampling program. Improved methodology was required to meet stringent regulations for PCB, methoxychlor, aldrin, lindane, heptachlor, and heptachlor epoxide at the nanogram level in water. A revision of the EPA florisil column was needed to obtain suitable specimens for the PCB analysis.

Other nonroutine development activities were a demonstration that a DOD procedure for determining phosphorus in butylrubber was not adequate, measurement of 2-ethyl hexanol in LiBr reactor coolant, determination of six-separate organic tracers in groundwater measurements, determination of carbonate-bicarbonate ratios in clay to be used as natural barriers in landfills, and measurement of organic acids in surface water. A lithium metaborate microfusion method was developed to prepare solid materials for ICP analysis while still retaining the silicon for quantitative analysis. A gas chromatographic technique for measuring the free silicon content of minerals was re-established. Accountability measurements of iridium in scrap material were provided by three separate methods with excellent agreement between the methods and with the vendor.

The inductively coupled plasma (ICP) spectrometer continued to be a vital support technique to major Laboratory programs. The spectrometer was used for measurement of trace impurities in high purity graphite (used for a new reactor core) and analysis of a larger number of surface and ground water samples and lysimeter extract solutions.

Two new instruments now provide major improvements in analytical capabilities. The JEOL 120 CX transmission electron microscope (TEM) is fully operational and has TEM, x-ray elemental analysis, and electron diffraction capabilities. A PGT System 4 x-ray fluorescence analyzer was purchased with design specification to permit easy interconnection for use with our ISI and AMR scanning electron microscope or to the JEOL transmission instrument. The console is on wheels to ensure mobility, and it is also capable of expansion to provide quantitative tube excited x-ray fluorescence analysis.

The Analytical Chemistry Division emergency response team again provided rapid identifications of spilled oils and organic materials within the required 4-hour response time. The team responded to an August 3-4 fish kill in White Oak Creek and, with cooperative analyses by the ORGDP GC-MS facility, the complex organic waste was identified as acetaldehyde, freon 11, freon 113, and butyl cellusolve. The ORNL Department of Environmental Management staff then determined by stores issue records that no UCC-ND facility used acetaldehyde, and that the fish kill was probably due to dumping by an outside source. The same emergency response team performed measurements to assure no contamination of the local surface water by aldrin, endrin, lindane, heptachlor or heptachlor epoxide.

Our data management and sample transactions system was significantly improved. Rapid retrieval of specific customer charges, together with specific types and number of each type of analysis provided for each customer charge, greatly reduced the efforts required to produce monthly time charge summaries.

(C. S. Alley, J. E. Attrill, L. D. Bible, H. G. Davis, H. W. Dunn, C. Feldman, J. H. Hackney, D. R. Heine, B. Philpot, J. C. Price, W. F. Rogers, K. I. Webb)*.

*Analytical Methodology Section

ENVIRONMENTAL ANALYSIS LABORATORY

N. M. Ferguson

The Environmental Analysis Laboratory (EAL) provides technical support for the Environmental Sciences Division (ESD), other ORNL divisions, and outside organizations. Approximately 50,000 analytical results were reported during this year with fewer staff members than the previous year.

Because the ESD was involved with several environmental mercury projects for one UCC-ND facility, the mercury lab has been extremely busy. These projects required the analysis of a wide variety of environmental materials (soils, water, hair, air filters, and aquatic animals). A major effort was required to measure the mercury in the discharge from some ORNL facilities for the ORNL Department of Environmental Management. These programs generated numerous samples for mercury analyses. Fast turnover time and a heavy quality assurance burden were required for this work. To meet these program commitments, it was necessary that personnel work overtime and reschedule vacation. The acquisition of an ion chromatography instrument provided a much needed new analytical capability for the group. The instrument has been in constant use since October. Although it will be used to support all programs, an acid rain project was the primary user. The instrument was used to determine fluoride, chloride, nitrate, phosphate, and sulfate in soil leachates, solid waste leachates, stream and throughfall samples. The determination of sulfate is one of the major concerns of the acid rain program. Previously, many problems were encountered with the spectrophotometric method (methylthymol blue) for sulfate analysis. Organic rich samples, phosphate, and pH all presented problems. This technique determines sulfate in the ppb concentration range and overcomes all of these problems. Ion chromatography will also be used in the future to analyze samples for organic acids.

A method to determine fluoride in soils for a National Park Service project was investigated, completed, and placed in operation. The procedure determines fluoride with a fluoride ion-selective electrode by the method of standard addition, following fusion with lithium metaborate.

Graphite furnace analyses were improved by the use of a platform and matrix modification. Increased sensitivities and fewer interferences were observed for many elements. These techniques were used extensively for continued support of the ORNL Industrial Hygiene Department. Lead was determined in blood and urine. Air filters were analyzed for cesium in the ppb concentration range for the Solid State Division.

After overcoming many instrumental and chemical problems, we placed a gaseous hydride method for the determination of total arsenic and total selenium in operation. Less than one nanogram per mL of arsenic and selenium can be determined by this method. Several hundred samples were analyzed for the Chemical Technology Division. Also, numerous samples were analyzed for an ORNL program monitoring liquid effluents.

A very large portion of the group's work for this year continued to come from the Terrestrial Ecology Section of the ESD. Programs producing large numbers of samples were the acid rain harvest studies, the Walker Branch Watershed mineral cycling studies, and a project to establish the effect of acid rain on forest nutrients. These programs were funded by the Environmental Protection Agency, the Department of Energy, and the Electric Power Research Institute. Aqueous (throughfall, soil leachates, dry deposition), soil, and plant tissue samples were received from these projects. Aqueous samples were routinely analyzed for calcium, sodium, magnesium, potassium, aluminum, phosphorus, nitrate, chloride, sulfate, and Kjeldahl nitrogen.

(L. S. Barringer, S. J. Morton, W. R. Musick, J. W. Wade)

LOW-LEVEL RADIOCHEMICAL ANALYSIS

T. G. Scott

The Low-Level Radiochemical Analysis Group continues to provide support to ORNL and Nuclear Division programs needing radioanalyses of natural and man-made radionuclides in environmental and other types of materials at very low concentrations. This year, we have been required to analyze a significant number of samples that were quite different and that required modified procedures and/or techniques.

Three radiation incidents at ORNL (an iodine-131 release into the waste treatment system, a sodium-24 release from the HFIR, and a technetium-99m release into the sewage treatment system) created emergency situations that required special attention. The iodine-131 incident involved the analysis of drinking water samples at a required sensitivity of 1 pCi/L on approximately 10 samples per day for over a month. Radiochemical separations on one-liter samples followed by low-background beta counting were performed to acquire both the turn-around time (24 hours) and sensitivity (1 pCi/L). The normal Ge(Li) gamma-ray spectrometry method for iodine-131 was not used because of the limited number of detectors (three) and the counting time necessary for 1 pCi/L sensitivity is 24 hours. Since the sensitivities for sodium-24 and technetium-99m were much higher, Ge(Li) gamma-ray spectrometry was used for these determinations.

Biota samples (fish, frogs, and turtles) were analyzed for uranium isotopes in a program to determine the environmental effects of the operations of one Nuclear Division facility. Special arrangements in laboratory operations and modification of ashing and radiochemical procedures were made to provide the requested data and to meet the rigid schedule. Concentrations of the uranium isotopes ranged from 0.02 to 3 Bq/kg in these samples. Sediment samples taken for the same purpose as the above biota also required rigid scheduling in order to determine the concentrations of stronium-90, neptunium-237, technetium-99, and the isotopes of uranium, thorium, and plutonium so as to meet deadlines for reports going to DOE and an inter-agency committee. Radioactivities in the sediments were orders of magnitude higher than those in the biota.

Three other projects involving the analysis of soils, sediments and water for most of the above radionuclides plus tritium were also on very tight schedules so that data could be used in Laboratory reports or open literature publications. Two of these projects were associated with ORNL burial grounds and trench areas. Concentrations of radionuclides in samples from trench-7 were found to be considerably higher than those we customarily find in most samples (see ORNL/TM-8839, "Chemical, Geological, and Hydrological Factors Governing Radionuclide Migration from a Formerly Used Sewage Trench: A Field Study"). Soils from the burial ground were analyzed primarily for strontium-90 to determine the distribution of radionuclides in the burial ground. Core samples from sites related to the Decontamination and Decommissioning (D and D) Program were analyzed to furnish information on strontium-90 and transuranic concentrations. A TM report titled "Radiological Characterization of Homogeneous Reactor Experiment No. 2 Facilities and Vicinity at ORNL" (in preparation) will present results of our efforts.

Some of the more unusual analyses and materials we have dealt with this year are carbon-14 and tritium in solids such as resin and charcoal; nickel-63 and iron-55 in similar solids and liquids; sulfur-35 in stable sulfur (at very low specific activity); phosphorus-32 in large sulfur wafers; radon-222 and radium-226 in a large variety of materials such as slag, mixed carbonates, and lead; and carbon-14 and tritium in a variety of waste organic materials.

A special project for NRC is nearing completion at this time. This project involved the bioassay of uranium, plutonium, and thorium in urine samples at very low concentrations. Our participation in the project was primarily concerned with "bead loading" for determining these elements by isotope dilution mass spectrometry. A prime goal was to determine uranium in urine at a concentration of 0.1 ng/ml with a 10% uncertainty. We reach this goal by taking extreme care to lower "blank" levels. This work is being published as an ORNL-TM report.

Even though we have had a larger variety of work this year, a major portion of our support effort continues to be devoted to the analysis of various environmental materials from monitoring and surveillance programs for statutory purposes. The materials normally analyzed are water, vegetation, soil, fish, small animals, and various types of filters and charcoal. The major radionuclides determined are iodine-131, strontium-90, cesium-137, cobalt-60, and the isotopes of uranium, thorium, and plutonium.

(L. D. Bible, P. S. Gouge, C. C. Granger, W. C. Massey, M. P. May, S. H. Prestwood, A. J. Weinberger)

SPECIAL PROJECTS

J. S. Eldridge

Activities in the Special Projects Group continue to focus on technical support and applied research in a variety of programs related to environmental surveillance and decontamination and decommissioning. Funding is provided mainly by the Department of Environmental Management from the Environmental and Occupational Safety Division.

Assistance during radiological emergency drills has been provided for three formal exercises during the past year. The Radiological Assistance Program (RAP) of the Department of Energy-Oak Ridge Operations (ORO) provides personnel and radiological measurement equipment for emergencies upon request from those states within the ORO jurisdiction. A simulated nuclear weapon accident exercise (Nuwax-83) was conducted at the Nevada Test Site in which the DOE-RAP team assisted the Commonwealth of Virginia in a two-week drill. Field and laboratory measurements of Ra-233 and Pd-103, simulants for the Pu-239 and Am-241, were made under accident conditions. Other federal agencies including DOD, FEMA, and EPA participated in the exercise. The second emergency response was performed at the Sequoyah Nuclear Plant annual exercise near Chattanooga, Tennessee. The DOE-RAP team performed field sampling for environmental materials (air, soil, vegetation, etc.) along with laboratory assays. The Sequoyah exercise lasted for two days and our participation was in support of the Tennessee State Health Department. The third emergency response by the DOE-RAP team was to the site of the Surrey Nuclear Plant near Newport News, Virginia. Again, both field sampling and laboratory assistance were provided to the Commonwealth of Virginia Health Department. Personnel from the Special Projects Group operated the onsite field laboratories during all these exercises and participated in a two-day emergency preparedness workshop at DOE-ORO.

Earlier studies on the levels of radioactivity in small animals were concentrated on road-killed deer for the most part. In those studies, nondestructive gamma-ray spectrometry provided data on Cs-137 concentrations in muscle and liver. The radioactivity levels in all road-killed deer were low; however, manure from deer found near a contaminated disposed site was found to contain moderate levels of Sr-90. Based on this observation, we collected rabbits in the vicinity of the suspected source that produced the contaminated manure. Cerenkov counting of wet-ashed bone samples was used for the quantitative determination of Sr-90 in tissues obtained at autopsy. Rabbits accumulated Sr-90 to levels of 3000-7000 picocuries per gram in bone. Future work will involve animal collections at variable radial distances from the contamination to determine the number of animals using the water source. Attempts to capture pregnant doe will be made in order to determine Sr-90 concentrations in rabbit fetuses.

Deer studies have been expanded to include the thyroid as a bioindicator for radioiodine. All road-killed deer thyroids from the Oak Ridge Reservation since May 1983 contained I-125 in concentrations of 3-100 pCi/g (freeze-dried weight). Since I-125 is no longer produced at ORNL, the source of the I-125 in the glands was not readily apparent. By plotting the location of each animal on an area map along with I-125 concentrations, it was found that those animals (5) containing the highest concentration of I-125 were killed near the east boundary of ORNL. Since the prevailing winds are from west to east, the I-125 was evidently originating from ORNL. Records of purchase requisitions showed that two shipments of 200 mCi each were delivered to ORNL on April 1 and June 1, 1983. Thus, the deer thyroids have served as useful bioindicators for this nuclide. In addition to the I-125 values, several glands collected from deer after a reported release of I-131 on August 22 showed concentrations of I-131 up to 200 pCi/g.

Decontamination and decommissioning plans for 16 facilities at ORNL require a determination of the overall extent of radioactive contamination at each facility or site. For this purpose, "walk-over" surveys, surface soil sampling, and core drilling for subsurface sampling were performed. Such activities produced about

800 individual samples, each requiring a determination of gross radioactivity levels. This gross level was necessary in order to select those samples requiring more detailed analyses. About 250 samples were selected on the basis of the gross screening method. These samples were processed for quantitative gamma-ray analysis as well as destructive analysis for Sr-90 and transuranic elements. The information provided by the survey will be incorporated into engineering plans for the actual clean-up procedures.

(N. A. Teasley, Peter Stegnar)*

*IAEA Visiting Scientist from Yugoslavia.

ACTIVATION ANALYSIS

J. F. Emery

The Activation Analysis Group provides general neutron activation analysis (NAA) services for a number of Laboratory divisions and programs.

Multielement NAA was used to establish the elemental content of soil samples from Hiroshima and Nagasaki to assist in the reassessment of atomic bomb radiation dosimetry in Hiroshima and Nagasaki. The number of determinations of uranium in soil samples from the FUSRAP program by the delayed neutron counting method totaled about 1700, down about 15% from last year. However, the determination of oxygen by 14 MeV neutron activation more than doubled this year. The materials analyzed for oxygen were mostly SiC, TiB_2, and coal derived hydrotreated napthas. Uranium and thorium determinations in semiconductor related materials increased substantially. The device-encapsulating or potting material, the polyimide starting materials, SiO_2, and aluminum were analyzed. It was necessary to develop a better separation procedure for U and Th from large quantities of Sb and Br. The final potting materials contains about 1% Sb and Br added along with Si. The U and Th content of this material was usually less than 0.5 ppb. Hair from a group of Y-12 employees, along with a similar group from ORNL, was analyzed for Hg by NAA and atomic absorption spectroscopy. In the area of fuel reprocessing, we provide gamma-ray spectrometric and NAA of fuel dissolver solutions and residues. We also provide assays of special and/or development radioisotope products produced by the Operations Division. An example is the determination of impurity activities and assay of Pa-233 and Pd-103 used in the Nuwax-83 exercise in Nevada.

Our "work for others" activities increased from 1/4 of a man-year of effort in 1982 to 1/2 of a man-year in 1983. The outside customers were Texas Instruments, Florida Power and Light Co., DuPont, Cominco Electronic Materials, Harbison-Walker, Sun Oil, UOP, Inc., University of Tennessee and Tennessee Nuclear Services.

One of the special projects we were involved in this year was the design of a radiotracer experiment to determine residence times in the liquid and gas phase in the reactor at the Wilsonville, Alabama solvent refined coal pilot plant. This was a collaborative effort with the Chemical Technology, Operations, and Instrumentation and Controls Divisions. We are also providing technical support to the Chemical Technology Division in a study, supported by NRC, of the deposition of fission products from aerosols. The fusion blanket experiment continued through June 1983. This experiment was an in-pile irradiation of $LiAlO_2$ to test the recovery of tritium. The irradiation began March 11, 1983 and ended June 13, 1983. Approximately 36 curies of tritium was produced and recovered. This was a collaborative effort with the Energy Technology Division of ORNL and Argonne National Laboratory.

(P. F. Dyer, L. C. Bate, and K. J. Northcutt)

6. QUALITY ASSURANCE, SAFETY, AND TABULATION OF ANALYSES

W. R. Laing
P. L. Howell
C. S. MacDougall
A. L. Harrod
R. E. Jones

QUALITY ASSURANCE

Responsibility for the quality of work done within the five sections of the Analytical Chemistry Division falls to the respective supervisors. Because of the diversity in types and scopes of work done in these sections, several means are used to assure quality. The annual quality assurance report (ORNL/CF-83/297) comprises a collection of statements from each group and/or laboratory, encompassing (1) scope of work, (2) quality assurance program and procedures, (3) quality assurance compliance information and data, and (4) standard reference materials and their sources. Included is a statement summarizing control samples prepared and distributed during the reporting period and the quality level obtained with these internal control (reference) standards. Table 6.1 shows the quality level for each of the participating laboratories within the division and compares the results with those from the previous year. Lists of the different control programs and the number of results reported for each are given in Tables 6.2 and 6.3. During 1983 control determinations increased by 16%; control programs increased 4%. Analytical work is summarized in table 6.4.

During this reporting period five internal quality assurance audits of ACD groups were conducted. External audits included one by the UCCND Environmental Programs Review Committee and four audits of the Nuclear Coatings Program by customers.

The Analytical Chemistry Division Quality Assurance Program manual and the Nuclear Coatings Program QA manual have been rewritten and issued.

Table 6.1 Distribution of control tests by service laboratory for Oct 1982 through Sept 1983

Laboratory	Number of control results Total	 Outside fixed limits	1982 Quality level	1983 Quality level (%)[a]
General and Environmental Analysis Laboratories				
Chemical and physical analysis	626	45	91%	93%
Environmental analysis	467	32	87%	93%
Radioactive Materials Analysis Laboratories				
Radioactive materials analyses	417	10	97%	98%
Transuranium analyses	278	11	88%	96%
Total	1788	98	91%	95%

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

Table 6.2 Control Samples Prepared for Oct 1982 through Sept 1983

Method	Number of control elements	Number of control solutions	Concentration range (mg/ml)
Atomic absorption spectrometry	14	16	0.002-0.250
Coulometry	1	4	8-12
Count, alpha	1	2	0.03-0.05
Fluorometry	1	4	0.001-0.010
Gravimetry	3	7	2-75%
Gravimetry (Leco)	2	4	100-800 μg/g
Ion chromatography	7	4	0.001-0.060
Inductively coupled plasma (ICP)	30	6	0.001-0.150
Infrared absorption spectrophotometry	1	4	0.004-0.015
Spectrophotometry	10	22	0.0001-5.0
Volumetric titrimetry	10	21	(acid)0.1 - 7 normal, 2-120
X-ray fluorescence spectrometry	7	13	0.50-150
Total	87	107	

Table 6.3 Distribution of control results by method for Oct 1982 through Sept 1983

Method of analysis	Number of control elements	Number of control results
Atomic absorption spectrometry	14	314
Coulometry	1	-
Count, alpha	1	123
Fluorometry	1	109
Gravimetry	3	20
Gravimetry (Leco)	2	66
Ion chromatography	7	103
Inductively coupled plasma (ICP)	30	349
Infrared absorption spectrophotometry	1	3
Spectrophotometry	10	226
Volumetric titrimetry	10	321
X-ray fluorescence	7	156
	87	1790

SAFETY

Employees of the division have accumulated 2,480,737 workday hours since the last lost-time accident in 1972. This record is possible because of the excellent support of the safety program within the division. Approximately ninety percent of employees attended a safety meeting each quarter.

Quarterly safety audits were made by the division safety committee and division safety officer. Over eighty five percent of the committee findings were corrected and the needed action was taken.

All members of the division's local emergency organization (squad) are trained in first aid and CPR. We conducted two in-house CPR recertification training classes and held one in-house workshop on laboratory emergency procedures. Housekeeping and safety awareness within the division continue to improve.

RADIATION SAFETY

During the year, three analytical chemistry facilities, buildings 2026, 3019-B and 2011 have been reviewed by the Radioactive Operations Committee.

The Instrumentation and Controls Division personnel have completed the calibration and maintenance of all sensors and controls for the ventilation system of building 2026. Engineering Division personnel have reviewed the existing ventilation system and have recommended modification and upgrading.

A caustic spray scrubber system has been installed on a glove box in building 2026. The system is used to remove nitric acid fumes generated as a result of sample preparation.

TRU Laboratory radiation exposure has decreased from 1500 mR/my in 1980 to 900 mR/my in 1983. The installation of shielded glove boxes for sample and waste handling which is planned for 1984 will further reduce exposure. Radioactive Materials Analytical Laboratory (RMAL) personnel exposure continues to be 90-100 mR/my.

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	982	4	506	98	39,295	40,885
Biology	247			12	8	267
Central Management			12		15,105	15,117
Chemical Technology	3,231	16,529	6,073	359	17,440	43,632
Chemistry	502	120	214		2,849	3,685
Energy					69	69
Engineering Physics	183				65	248
Engineering Technology	330		10	7	9,068	9,415
Environmental and Occupational Safety			16	3,020	21,522	24,558
Environmental Sciences		22	44	269	101,550	101,885
Finance and Materials			2		23	25
Fuel Recycle	271	224	2,155		945	3,595
Fusion Energy	542				58	600
Health	736		12	108	832	1,688
Health and Safety Research			1	566	1,993	2,560
Information					14	14
Instrumentation and Controls	1,021		4	2	2,486	3,513
Laboratory Protection				9	12	21
Metals and Ceramics	20,145	122	160		4,075	24,502
Operations	9,473	9,351	3,717		799	23,340
Physics	264	6	21		30	321
Plant and Equipment	207				1,342	1,549
Quality Assurance and Inspection	141				4	145
Solid State	2,879		1		1,214	4,094
Others						
Protective Coating Testing			657			657
K-25 and Y-12	4,763			1	849	5,613
Miscellaneous	6,699		39			6,738
Savannah River Laboratory	942					942
Work for Others		11				11
TOTAL	53,558	26,389	13,644	4,451	221,647	319,689

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 cycle for the division's Information Meeting has been extended to 18 months; the next meeting will be in January 1984. The 1983 Advisory Committee was composed of:

H. B. **Mark**, Chemistry Department, University of Cincinnati, Cincinnati, OH.
M. V. **Novotny**, Chemistry Department, Indiana University, Bloomington, IN.
J. W. **Taylor**, Chemistry Department, University of Wisconsin, Madison, WI.
J. G. **Grasselli**, Standard Oil Company, 4440 Warrensville Center Road, Cleveland, OH.

CONSULTANTS

The following specialists were brought to ORNL on short-term consulting basis this past year as part of our Seminar Program. Details of seminars are listed in Chapter 8.

J. **Guertin**, Electric Power Research Institute, Palo Alto, CA.
M. **Kaufman**, Emory University, Atlanta, GA.
P. **Stegnar**, Josef Stefan Institute, Ljublijana, Yugoslavia.
A. **Zlatkis**, University of Houston, TX.
D. E. **Leyden**, Colorado State University, Fort Collins, CO.
J. W. **Jorgenson**, University of North Carolina, Chapel Hill, NC.

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

W. H. W. Triftshauser, Hochshule der Bundeswehr, Munich, FRG, worked as a guest scientist with L. D. Hulett and J. M. Dale from April to September, studying positron spectroscopy.

PARTICIPATION IN ORNL IN-HOURS PROGRAM

The following divisional people completed courses during the 1983 winter term of the Continuing Education Program for Scientific and Technical Personnel:

M-158D. Introduction to System 1022 Data Base Management System: J. S. Eldridge.
M-310J. Introduction to DECsystem-10: P. J. Mullins.
M-100F. Introduction to FORTRAN IV: T. G. Scott and N. A. Teasley.
M-300F. Intermediate FORTRAN IV: N. A. Teasley.

The following courses were completed during the spring 1982 term:

M-158E. Introduction to System 1022 Data Base Management System: C. S. Alley.
M-310K. Introduction to the DECsystem-10: C. S. Alley and D. A. Costanzo.
E-530. Personal Computers for Professional Use in R&D: J. S. Eldridge, R. W. Shaw, and W. D. Shults.

STUDENT ASSIGNMENTS

B. A. Tomkins served as "Dean" for the division's student guests during 1983. Two predoctoral students, Brisco Harward and Huston E. Howell continued their work in the Analytical Methodology Section as ORAU graduate research participants. Huston Howell completed his appointment in August.

The division maintains a subcontract with the University of Tennessee to enable advanced graduate students to participate in environmental analysis programs. Donna Taylor Dixon worked for a short period in 1983 with the Mass Spectrometry Section at Y-12 under this contract. Also under this contract, Chris P. Liebman worked with W. H. Griest in the Bio/Organic Analysis Section until he received a "Q" clearance. He then moved to Y-12 to work with P. J. Todd on organic SIMS studies.

John Vargo completed his appointment as an ORAU graduate research participant and received his Ph.D. December 1983. He worked with M. P. Maskarinec in the Bio/Organic Analysis Section.

SUMMER PROGRAM

During the summer, the division was host to a representative of the ORAU Undergraduate Research Program, which offers laboratory experience to exceptional college students. Perry Pellechia, St. Joseph's College, worked with M. P. Maskarinec in the Bio/Organic Analysis Section on applications of open-tubular liquid chromatography.

GLCA PROGRAM

During the fall semester, two students were assigned to the division. Sarah H. Fenton, Albion College, was assigned to the General and Environmental Analysis Section to assist in preparing human blood specimens and performing both inductively coupled plasma spectrometry (ICP) and neutron activation analysis (NAA) on the specimens. The Bio/Organic Analysis Section hosted Paul A. David, Monmouth College, who worked with M. P. Maskarinec on the development of advanced chromatographic methods.

ORNL CO-OP PROGRAM

Gregory B. Hurst, University of Tennessee, finished his final cooperative quarter working with the fossil fuel program.

SPECIAL AWARDS

W. S. Lyon was elected to the member grade of Fellow of the American Nuclear Society recognizing the many contributions he has made to nuclear knowledge and understanding. The official presentation was made at the annual awards luncheon on Tuesday, June 14, 1983, at the Westin Hotel in Detroit. Mr. Lyon also received the ASTM E-10 Honorary Member Award for his accomplishments in nuclear technology. This award was presented on June 28, 1983, in Colorado Springs, CO.

26th ORNL/DOE CONFERENCE ON ANALYTICAL CHEMISTRY IN ENERGY TECHNOLOGY

This year's conference was held at the Knoxville Hilton, October 11-12, 1983. The theme of the Conference was "Analytical Spectroscopy". Attendance was 225, with representatives from foreign countries, academia, industrial institutions, and other government agencies. There were 20 exhibits (41 representatives) and 26 booths. Topics emphasized during the meeting included lasers, mass spectrometry, and nuclear and plasma spectroscopy. Two poster sessions were conducted.

A. L. Harrod was Arrangements Chairman, W. S. Lyon was Technical Program Chairman, and M. L. Emery was Treasurer. Shirley Cates, Pat Mullins, and Sharon Ranney were Conference Secretaries. Other conference committee members included M. V. Buchanan, F. F. Dyer, D. R. Heine, W. R. Laing, J. M. Ramsey, W. D. Shults, and D. H. Smith. The Proceedings will be published in 1984: W. S. Lyon is editor and Gail Vineyard proceedings secretary.

ANALYTICAL CHEMISTRY DIVISION SEMINARS AT ORNL

Speaker	Title	Date
Guertin, J. Electric Power Research Inst., Palo Alto, CA	"Dark Suns and Moons"	Mar. 14, 1983
Kaufman, M. Emory Univ. Atlanta, GA	"Chemistry and Spectroscopy of Atomic Halogen Recombination Reactions"	Apr. 12, 1983
Stegnar, P. Josef Stefan Inst., Ljubljana, Yugoslavia	"Analytical Chemistry Applications in Environmental Reasearch"	Apr. 18, 1983

ANALYTICAL CHEMISTRY DIVISION
SEMINARS AT ORNL

Speaker	Title	Date
Zlatkis, A. Univ. of Houston, TX	"Ultra Trace G. C. Analysis by Use of Large On-Column Injection with Bonded Capillary Columns"	May 11, 1983
Leyden, D. E. Colorado State Univ., Fort Collins, CO	"Applications in X-Ray Spectrometry"	June 8, 1983
Jorgenson, J. W. Univ. of North Carolina, Chapel Hill, NC	"Capillary Zone Electrophoresis"	Nov. 9, 1983

ACD SUMMER LECTURE SERIES

The division sponsored a second summer lecture series to present in-depth lectures on current analytical techniques.

Speaker	Title	Date
Gedcke, D., Keller, J. M.	"Advances in X-Ray Spectroscopy and New Instrumentation for Highly Radioactive Samples"	June 24, 1983
Ramsey, J. M.	"New Laser Techniques for Analytical Chemistry"	July 8, 1983
Maskarinec, M. P.	"HPLC or What Is In an Acronym"	July 29, 1983
Todd, P. J.	"Organic Mass Spectrometry at ORNL"	Aug. 12, 1983

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

BOTTS, J. L.

Division Assistant Representative: Material Balance Area Representative for Nuclear Materials Management

BRAZELL, R. S.

Member: ACD Seminar Committee

BROOKSBANK, R. D.

Chairman: Task Group on Methods of Coatings Analysis, ASTM D-33

Member: ASTM Committee D-33, Protective Coating and Lining Work for Power Generation Facilities

BUCHANAN, M. V.

Member: Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, Oct. 11-13, 1983

CARTER, J. A.

Advisory Board: *Analytical Chemistry*

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

Laboratory Coordinator: ISPO Programs

Member: Committee C-26, Nuclear Fuel Cycle, and C-26:05, Test Methods, Task Group Leader, Micro Analytical Techniques, ASTM

Secretary: Subcommittee C-5:05, Analytical Task Group (Reactor Grade Graphite), Committee C-5, Manufacturer of Carbon and Graphite Products, ASTM

Symposium Organizer: Symposium on Analytical Chemistry of Nuclear Safeguards 184th National ACS Meeting, Kansas City, MO, Sept. 1982

CATON, J. E.

Co-Chairman: Vibrational Spectroscopy Subgroup of UCC Analytical Specialists' Group

Member: ACD Computer Utilization Committee
ACD Long Range Planning Committee

CHRISTIE, W. H.

Lecturer: ORAU Traveling Lecture Program

Member: ACD Long Range Planning Committee
ASTM Committee E-42, Surface Analysis

COOPER, J. H.		
	Member:	ORNL Management Information Committee
COSTANZO, D. A.		
	Member:	ASTM Committee C-26, Nuclear Fuel Cycle, and Subcommittee C-26:05, Methods of Test
DALE, J. M.		
	Co-organizer:	Symposium on Implementations of Monoenergetic Positrons in Fundamental and Applied Science, 1983 Annual Meeting of AAA, Detroit, Michigan, May 26-27, 1983
	Lecturer:	ORAU Traveling Lecture Program
	Member:	ACD Solids/Surfaces Characterization Team
DONOHUE, D. L.		
	Lecturer:	ORAU Traveling Lecture Program
	Member:	ACD Ad Hoc Committee on Computerization
DYER, F. F.		
	Member:	ACD Seminar Committee Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October 11-13, 1983
ELDRIDGE, J. S.		
	Member:	ACD Long Range Planning Committee Steering Committee, Environmental Radiation Section of Health Physics Society
EMERY, J. F.		
	Division Representative:	Laboratory Emergency Sample Coordinator Division Computer Systems Security Officer
FELDMAN, C.		
	Fellow:	American Society for Testing and Materials
	Member:	Atomic Absorption and Emission Spectroscopy Subgroup, Union Carbide Corporation 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:	UCCND Environmental Analysis Committee
GOERINGER, D. E.		
	Member:	ACD Ad Hoc Committee on Computerization ACD Ad Hoc Committee on Robotics

GRIEST, W. H.
Consultant: Department of Energy - BES
Electric Power Research Institute
Environmental Protection Agency - IERL/TSO
Member: DOE Oil Shale Working Group

GUERIN, M. R.
Advisor: NAS panel
Consultant: Department of Energy (OHER)
Brigham Young University Grant Review
Synfuels Chemistry Program Redirection
Federal Trade Commission
Cigarette Testing Methodology
National Academy of Sciences Panel
DOE Health and Environmental Effects Document
National Cancer Institute
American Health Foundation Grant Review
National Institute of Environmental Health Services
New York University Grant Review

HEINE, D. R.
Member: ACD Seminar Committee
Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October 11-13, 1983

HIGGINS, C. E.
ACD Ombudsman

HOLMBERG, R. W.
Coordinator: ACD Metric Coordinator

HULETT, L. D.
Coordinator: ACD Solids/Surfaces Characterization Team
Co-organizer: Symposium on Implementations of Monoenergetic Positrons in Fundamental and Applied Science, 1983 Annual Meeting of AAAS, Detroit, MI, May 26-27, 1983

JENKINS, R. A.
Consultant: National Institute of Drug Abuse - Exposure of Animals to Concentrated Smokes
Member: ORNL Speaker's Bureau

JONES, R. E.
Division Representative: ACD Radiation Control Officer

KELLER, J. M.
Member: ACD Ad Hoc Committee on Computerization
ACD Ad Hoc Committee on Robotics

KLATT, L. N.
Associate Editor: *Chemical Biomedical, and Environmental Instrumentation*
Member: Graduate Fellowship Committee of Division of Analytical Chemistry, ACS
UCCND Ph.D. Recruiting Team
ACD Long Range Planning Committee

LAING, W. R.
Chairman: Subcommittee C26:05, Test Methods, Nuclear Fuel Cycle, ASTM
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
Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October 11-13, 1983
UCCND Analytical Committee
Vice-chairman: ASTM Committee C26, Nuclear Fuel Cycle

LYON, W. S.
Advisory Board: *Analyst*
Chairman: Isotopes and Radiation Division, ANS
Honorary Member: Committee E-10, Nuclear Technology and Applications, ASTM
Member: Organizing Committee, 6th International Conference on Modern Trends in Activation Analysis
Scientific Committee 25 on Radiation Protection in the Use of Small Neutron Generators, NCRP
Technical Program Committee, 5th International Conference on Nuclear Methods in Environmental and Energy Research, Mayaquez, Puerto Rico
Session Chairman: "Chemical Information Flow: Present and Future," Seattle ACS Meeting, March 22, 1983
Regional Editor: *Journal of Radioanalytical and Nuclear Chemistry*
Technical Program Chairman: 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, Oct. 11-13, 1983

MASKARINEC, M. P.
Member: ASTM E-19 Committee on Chromatography
ASTM D-34 on Waste Disposal
ORNL Hazardous Waste Task Force
UCCND Gas Chromatography Specialists' Group
UCCND Liquid Chromatography Specialists' Group

McKOWN, H. S.
Division Representative: Interplant Computer Communications Committee

RAMSEY, J. M.
Member: ACD Seminar Committee
Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October 11-13, 1983

ROSS, H. H.
Chairman: ORNL Graduate Student Selection Panel
ORNL Post Doctorate Selection Panel
Member: ACD Seminar Committee
Editorial Advisory Board, *Journal of Radioanalytical and Nuclear Chemistry*
Fellowship Committee, ACS, Division of Analytical Chemistry
ORNL Proposal Review Committee
ORNL Technology Utilization Committee
Scientific Advisory Committee, International Conference on Scintillation Spectroscopy, Canada, 1982-1983

ROSSEEL, T. M.
Chairman: ACD Seminar Committee
Lecturer: ORAU Traveling Lecture Series
Member: Program Committee, 11th Annual FACSS Meeting
Scholarship Committee, Tennessee Valley Chapter, American Vacuum Society
ACD Solids/Surfaces Characterization Team

SCOTT, T. G.
Member: Committee D-19, Water, ASTM, and Subcommittee 4, Methods of Radiochemical Analysis

SHAW, R. W.
Member: ACD Solids/Surfaces Characterization Team

SHULTS, W. D.
Consultant: UCC 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, UCCND
President: Sigma Xi RESA, Oak Ridge Chapter

SMITH, D. H.
Coordinator: ACD PhD Recruiting
Member: Planning Committee, 26th ORNL/DOE Conference on Analytical Chemistry in Energy Technology, Knoxville, TN, October 11-13, 1983

STEWART, J. H., Jr.
Division Representative: ACD Environmental Protection Officer
Member: ACD Solids/Surfaces Characterization Team
ASTM C-26.02 Nuclear Fuel Cycle Task: C-26.05 X-Ray Fluorescence Methods
Manuscript Review Board for Analytical Chemistry Microbeam Analysis Society
Task Leader: International Working Group "Analytical Standards of Minerals, Ores and Rocks"

STOKELY, J. R.	
Coordinator:	ACD MS/BS Recruiting
TODD, P. J.	
Member:	ACD Seminar Committee
Coordinator:	ACD Awards
TOMKINS, B. A.	
Coordinator:	ACD University Relations
Member:	NBS/DOE Analytical Characterization Group
WALKER, R. L.	
Member:	ACD Long Range Planning Committee DOE/ISA Laboratory Advisory Group for Effluent Research (LAGER)
WHITTEN, W. B.	
Lecturer:	ORAU Traveling Lecture Program
YOUNG, J. P.	
Rapporteur:	"Spectroscopy of the Transplutonium Elements" Panel, Workshop on Future Directions in Transplutonium Element Research, National Research Council, Washington, DC, Feb. 2-March 3, 1983

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
Buchanan, M. V.	Buchanan, M. V.; Flanagan, J.*; Rubin, I. B.; Guerin, M. R. Effects of Hydrotreatment on the Composition of Mutagenic Fractions of a Coal-Derived Petroleum Substitute"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 211
	Buchanan, M. V.; Rubin, I. B.; Moneyhun, J. H. "Compositional Changes in Red and Violet Smoke Mixes After Combustion"	*Proc., Smoke/Obscurants Symp. VII*, Adelphi, MD, Apr. 26-28, 1983, p. 483
	Ho, C-h.; Guerin, M. R.; Buchanan, M. V. "Isolation and Identification of Bioactive Constituents in Synfuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 24
	Buchanan, M. V.; Guerin, M. R.; Kao, G. L.*; Rubin, I. B.; Caton, J. E. "Comparative Spectroscopic Characterization of Synthetic Fuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 286
	Dumont, J. N.*; Schultz, T. W.*; Buchanan, M. V.; Kao, G. L.* "Frog Embryo Teratogenesis Assay: Xenopus (FETAX). A Short Term Assay Applicable to Complex Environmental Mixtures"	*Short Term Bioassays in the Analysis of Complex Environ. Mixtures, III*, Waters, Sandhu, Lewtas, Claxton, Chernoff, and Nesnow, Eds., Plenum Press, 1983, p. 393
	Buchanan, M. V. "Differentiation of Isomeric Heteroatom-Substituted Aromatics Using Chemical Ionization"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, 1983, p. 708

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Carter, J. A.	Smith, D. H.; Walker, R. L.; Carter, J. A. "Sampling and Analysis of Radioactive Solutions"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 135
	Shimojima, H.*; Carter, J. A.; Walker, R. L.; Smith, D. H.; Musick, W. R.; Asakura, Y.*; Kagam, K.*; Irinouchi, J.*; Masui, J.*; Miyihara, K.*; Bure, J.*; Denon, S.*; Donohue. D. L. "Task J: Resin Bead Sampling and Analytical Technology"	*TASTEX: Advanced Safe. Techn. Exer. Tec. Rept.*, Series No. 213, IAEA, Vienna, 1982, p. 163
Caton, J. E.	Buchanan, M. V.; Guerin, M. R.; Kao, G. L.*; Rubin, I. B.; Caton, J. E. "Comparative Spectroscopic Characterization of Synthetic Fuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 286
	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H.; Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
	Griest, W. H.; Caton, J. E. "Extraction of Polycyclic Aromatic Hydrocarbons for Quantitative Analysis"	*Handbook of Polycyclic Aromatic Hydrocarbons*, A. Bjørseth, Ed., Marcel Dekker, NY, 1983, p. 95
Christie, W. H.	Anderson, R. L.*; Kollie, T. G.*; Christie, W. H.; Eby, R. E. "Decalibration of Sheathed Thermocouples"	*Temp. Its Meas. and Control in Sci. and Ind. 1982, Vol 5*, Ed., J. F. Schooley, Amer. Inst. of Phys., New York, NY, p. 977
	Christie, W. H. "SIMS: Simplified Investigations of Messy Samples"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 3
Dale, J. M.	Hulett, L. D.; Dale, J. M.; Dunn, H. W.; Murty, P. S.* "Characterization of Corrosion Scale from Nuclear Reactors: Approaching the Whole Problem"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 15

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Dale, J. M.	Hulett, L. D.; Dale, J. M.; Pendyala, S.* Chang, Y. K.*; Lyon, W. S. "Positron Spectroscopy Applied to the Analysis of Surfaces"	*Proc., Int. Symp. on Applied Technol. of Ionizing Radiation, Vol. 3*, King Saud Univ. Press, Riyadh, SAUDI ARABIA, 1983, p. 1443
Donohue, D. L.	Donohue, D. L.; Young, J. P. "Removal of Isobaric Interferences by Resonance Ionization Mass Spectrometry"	*Laser Based Ultrasensitive Spectrosc. and Detection*, R. A. Keller, Ed., Proc., SPIE 426, 1983, p. 8
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Resonance Ionization Mass Spectrometry"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 841
	Shimojima, H.*; Carter, J. A.; Walker, R. L.; Smith, D. H.; Musick, W. R.; Asakura, Y.*; Kagam, K.*; Irinouchi, J.*; Masui, J.*; Miyihara, K.*; Hure, J.*; Denon, S.*; Donohue, D. L. "Task J: Resin Bead Sampling and Analytical Technology"	*TASTEX: Advanced Safe. Techn. Exer. Tec. Rept.*, Series No. 213, IAEA, Vienna, 1982, p. 163
Dunn, H. W.	Hulett, L. D.; Dale, J. M.; Dunn, H. W.; Murty, P. S.* "Characterization of Corrosion Scale from Nuclear Reactors: Approaching the Whole Problem"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 15
	Stewart, J. H.; Dunn, H. W. "The Quantitative Determination of Chrysotile Asbestos by X-Ray Diffractometry"	*Proc., 1982 UCC-ND and GAT Environ. Prot. Semin.*, Gatlinburg, TN, Apr. 5-7, 1982 ORNL-CONF-820418, Apr. 1983 p.60
Eby, R. E.	Anderson, R. L.*; Kollie, T. G.*; Christie, W. H.; Eby, R. E. "Decalibration of Sheathed Thermocouples"	*Temp. Its Meas. and Control in Sci. and Ind. 1982, Vol 5*, Ed., J. F. Schooley, Amer. Inst. of Phys., New York, NY, p. 977
Eldridge, J. S.	Eldridge, J. S.; Oakes, T. W.*; Hubbard, H. M.*; Hibbitts, H. W.* Off-Site Response for Radiological Emergencies"	*Proc., 1982 UCC-ND and GAT Environ. Prot. Sem.*, Gatlinburg, TN, Apr. 5-7, 1982, ORNL-CONF-820418, Apr. 1983, p. 90

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Glish, G. L.	Glish, G. L.; Todd, P. J. "Cation Effects on SIMS MS/MS Spectra"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 136
	Glish, G. L.; Todd, P. J.; Busch, K. L.*; "MS/MS Spectra of Desorbed Ions"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 134
	Glish, G. L. "MS/MS and Thermal Desorption/ Ionization. The Ideal Combination?"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 191
	Todd, P. J.; Glish, G. L. "Applications of a SIMS MS/MS Device"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 207
Griest, W. H.	Griest, W. H.; Caton, J. E. "Extraction of Polycyclic Aromatic Hydrocarbons for Quantitative Analysis"	*Handbook of Polycyclic Aromatic Hydrocarbons*, A. Bjørseth, Ed., Marcel Dekker, NY, 1983, p. 95
	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H., Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
Guerin, M. R.	Guerin, M. R. Research Status Report: Mutagenicity Tests of Products and Wastes from Fossil Fuels	*Establishment of a Bioassay System for Cancer Risk Assess. in Energy Techn.: A Rept. on the Conf. Held in May 1982*, U.S. DOE, HERD, OHER, Div. of Biophys., School of Hygiene and Public Health, The Johns Hopkins Univ., Sept. 1983, p. 86

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Guerin, M. R.	Buchanan, M. V.; Flanagan, J.*; Rubin, I. B.; Guerin, M. R. Effects of Hydrotreatment on the Composition of Mutagenic Fractions of a Coal-Derived Petroleum Substitute"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 211
	Ho, C-h.; Guerin, M. R.; Buchanan, M. V. "Isolation and Identification of Bioactive Constituents in Synfuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 24
	Buchanan, M. V.; Guerin, M. R.; Kao, G. L.*; Rubin, I. B.; Caton, J. E. "Comparative Spectroscopic Characterization of Synthetic Fuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 286
	Dalbey, W.*; Lock, S.*; Garfinkel, S.*; Jenkins, R.; Holmberg, R.; Guerin, M. "Inhalation Exposures of Rats to Aerosolized Diesel Fuel"	*Proc., Symp. on Toxicol. of Pet. Hydrocarbons*, MacFarland, Holdsworth, MacGregor, Call, and Kane, Eds., Washington, DC, 1983, p. 13
Harmon, S. H.	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H.; Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
Ho, C.-h.	Ho, C-h.; Guerin, M. R.; Buchanan, M. V. "Isolation and Identification of Bioactive Constituents in Synfuels"	*Advanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 24
Holmberg, R. W.	Dalbey, W.*; Lock, S.*; Garfinkel, S.*; Jenkins, R.; Holmberg, R. Guerin, M. "Inhalation Exposures of Rats to Aerosolized Diesel Fuel"	*Proc., Symp. on Toxicol. of Pet. Hydrocarbons*, MacFarland, Holdsworth, MacGregor, Call, and Kane, Eds., Washington, DC, 1983, p. 13
	Holmberg, R. W.; Moneyhun, J. H. "A System for the Continuous Generation of Phosphorous Aerosols from Red Phosphorus-Butyl Rubber"	*Proc., Smokes/Obscurants Symp. VI, Vol. II*, Adelphi, MD, Apr. 27-29, 1982, p. 767

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Hulett, L. D.	Hulett, L. D.; Dale, J. M.; Pendyala, S.*; Chang, Y. K.*; Lyon, W. S. "Positron Spectroscopy Applied to the Analysis of Surfaces"	*Proc., Int. Symp. on Applied Technol. of Ionizing Radiation, Vol. 3*, King Saud Univ. Press, Riyadh, SAUDIA ARABIA, 1983, p. 1443
	Hulett, L. D.; Dale, J. M.; Dunn, H. W.; Murty, P. S.* "Characterization of Corrosion Scale from Nuclear Reactors: Approaching the Whole Problem"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 15
Jenkins, R. A.	Dalbey, W.*; Lock, S.*; Garfinkel, S.*; Jenkins, R.; Holmberg, R.; Guerin, M. "Inhalation Exposures of Rats to Aerosolized Diesel Fuel"	*Proc., Symp. on Toxicol. of Pet. Hydrocarbons*, MacFarland, Holdsworth, MacGregor, Call, and Kane, Eds.. Washington, DC, 1983, p. 13
Lyon, W. S.	Lyon, W. S. "Practical Applications of Activation Analysis and Other Nuclear Techniques"	*Proc., Int. Symp. on Applied Technol. of Ionizing Radiation, Vol. 2*, King Saud Univ. Press, Riyadh, SAUDIA ARABIA, 1983, p. 871
	Hulett, L. D.; Dale, J. M.; Pendyala, S.*; Chang, Y. K.*; Lyon, W. S. "Positron Spectroscopy Applied to the Analysis of Surfaces"	*Proc., Int. Symp. on Applied Technol. of Ionizing Radiation, Vol. 3*, King Saud Univ. Press, Riyadh, SAUDIA ARABIA, 1983, p. 1443
Maskarinec, M. P.	Maskarinec, M. P.; Brown, D. K.* "Batch and Column Extraction Procedures for Organics in Solid Wastes"	*Hazardous and Industrial Solid Waste Testing: 2nd Symp.*, Conway and Gulledge, Eds., ASTM-STP-805, 1983, p. 141
	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H.; Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
Moneyhun, J. H.	Holmberg, R. W.; Moneyhun, J. H. "A System for the Continuous Generation of Phosphorous Aerosols from Red Phosphorus-Butyl Rubber"	*Proc., Smokes/Obscurants Symp. VI, Vol. II*, Adelphi, MD, Apr. 27-29, 1982, p. 767
	Buchanan, M. V.; Rubin, I. B.; Moneyhun, J. H. "Compositional Changes in Red and Violet Smoke Mixes After Combustion"	*Proc., Smoke/Obscurants Symp. VII*, Adelphi, MD, Apr. 26-28, 1983, p. 483

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Musick, W. R.	Shimojima, H.*; Carter, J. A.; Walker, R. L.; Smith, D. H.; Musick, W. R.; Asakura, Y.*; Kagam, K.*; Irinouchi, J.*; Masui, J.*; Miyihara, K.*; Hure, J.*; Denon, S.*; Donohue, D. L. "Task J: Resin Bead Sampling and Analytical Technology"	*TASTEX: Advanced Safe. Techn. Exer. Tec. Rept.*, Series No. 213, IAEA, Vienna, 1982, p. 163
Pritchard, C. A.	Smith, D. H.; Walker, R. L.; Pritchard, C. A. "Evaluation of Internal Standards in Uranium and Plutonium Isotopic Ratio Measurements"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 847
Ramsey, J. M.	Ramsey, J. M.; Hieftje, G. M.* "Signal-to-Noise Considerations in Fluctuation Analysis Spectroscopic Techniques (FAST)"	*New Directions in Molecular Luminescence*, D. Eastwood, Ed., ASTM Pub. 822, Philadelphia, PA, 1983, p. 82
Reagan, R. R.	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H.; Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
Rubin, I. B.	Buchanan, M. V.; Rubin, I. B.; Moneyhun, J. H. "Compositional Changes in Red and Violet Smoke Mixes After Combustion"	*Proc., Smoke/Obscurants Symp. VII*, Adelphi, MD, Apr. 26-28, 1983, p. 483
	Buchanan, M. V.; Flanagan, J.*; Rubin, I. B.; Guerin, M. R. Effects of Hydrotreatment on the Composition of Mutagenic Fractions of a Coal-Derived Petroleum Substitute"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 211
	Buchanan, M. V.; Guerin, M. R.; Kao, G. L.*; Rubin, I. B.; Caton, J. E. "Comparative Spectroscopic Characterization of Synthetic Fuels"	*Avanced Techn. in Synthetic Fuels Analysis*, Wright, Weimer, and Felix, Eds., 1983, p. 286
Smith, D. H.	Smith, D. H.; Walker, R. L.; Pritchard, C. A. "Evaluation of Internal Standards in Uranium and Plutonium Isotopic Ratio Measurements"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 847
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Resonance Ionization Mass Spectrometry"	*Proc., 31st Annu. Conf. on Mass Spectrom.*, Boston, MA, May 8-13, 1983, p. 841

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Smith, D. H.	Smith, D. H.; Walker, R. L.; Carter, J. A. "Sampling and Analysis of Radioactive Solutions"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., Washington, DC, 1983, p. 135
	Shimojima H.*; Carter, J. A.; Walker, R. L.; Smith, D. H.; Musick, W. R.; Asakura, Y.*; Kagam, K.*; Irinouchi, J.*; Masui, J.*; Miyihara, K.*; Hure, J.*; Denon, S.*; Donohue, D. L. "Task J: Resin Bead Sampling and Analytical Technology"	*TASTEX: Advanced Safe. Techn. Exer. Tec. Rept.*, Series No. 213, IAEA, Vienna, 1982, p. 163
Stewart, J. H.	Stewart, J. H.; Dunn, H. W. "The Quantitative Determination of Chrysotile Asbestos by X-Ray Diffractometry"	*Proc., 1982 UCC-ND and GAT Environ. Prot. Sem.*, Gatlinburg, TN, Apr. 5-7, 1982, ORNL-CONF-820418, Apr. 1983, p. 60
Todd, P. J.	Danis, P. O.*; Todd, P. J.; Gallene, J. C.*; Ray, J. C.*; Carpenter, B. K.*; McLafferty, F. W.* "Neutralization-Reionization Mass Spectrometry"	*Proc, 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983, p. 50
	Todd, P. J.; McLefferty, F. W.* "Collisionally Activated Decompositions of High Kinetic Energy Ions"	*Tandem Mass Spec.*, F. W. McLafferty, Ed., John Wiley and Sons, 1983, p. 149
	Todd, P. J.; McGilvery, D. C.*; Baldwin, M. A.*; McLafferty, F. W. "Tandem High Resolution Mass Spectrometry"	*Tandem Mass. Spec.*, F. W. McLafferty, Ed., John Wiley and Sons, 1983, p. 271
	Glish, G. L.; Todd, P. J. "Cation Effects on SIMS MS/MS Spectra"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983 p. 136
	Glish, G. L.; Todd, P. J.; Busch, K. L.*; "MS/MS Spectra of Desorbed Ions"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983 p. 134
	Todd, P. J.; Glish, G. L. "Applications of a SIMS MS/MS Device"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983 p. 207

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Tomkins, B. A.	Tomkins, B. A.; Reagan, R. R.; Maskarinec, M. P.; Harmon, S. H.; Griest, W. H.; Caton, J. E. "Analytical Chemistry of Polycyclic Aromatic Hydrocarbons Present in Coal-Fired Power Plant Fly Ash"	*Polynucl. Aromatic Hydrocarbons*, M. Cooke and A. J. Dennis, Eds., Battelle Press, Columbus, OH, 1983, p. 1173
Walker, R. L.	Smith, D. H.; Walker, R. L.; Pritchard, C. A. "Evaluation of Internal Standards in Uranium and Plutonium Isotopic Ratio Measurements"	*Proc., 31st Annu. Conf. on Mass Spectrom. and Allied Topics*, Boston, MA, May 8-13, 1983 p. 847
	Smith, D. H.; Walker, R. L.; Carter, J. A. "Sampling and Analysis of Radioactive Solutions"	*The Anal. Approach*, J. G. Grasselli, Ed., Amer. Chem. Soc., 1983, p. 135
	Shimojima, H.*; Carter, J. A.; Walker, R. L.; Smith, D. H.; Musick, W. R.; Asakura, Y.*; Kagam, K.*; Irinouchi, J.*; Masui, J.*; Miyihara, K.*; Hure, J.*; Denon, S.*; Donohue, D. L. "Task J: Resin Bead Sampling and Analytical Technology"	*TASTEX: Advanced Safe. Techn. Exer. Tec. Rept.*, Series No. 213, IAEA, Vienna, 1982, p. 163
Young, J. P.	Donohue, D. L.; Young, J. P. "Removal of Isobaric Interferences by Resonance Ionization Mass Spectrometry"	*Laser Based Ultrasensitive Spectrosc. and Detection*, R. A. Keller, Ed., Proc., SPIE 426, 1983, p. 8
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Resonance Ionization Mass Spectrometry"	*Proc., 31st Annu. Conf. on Mass Spectrom.*, Boston, MA, May 8-13, 1983, p. 841

Articles

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Bate, L. C.	Christie, N. T.*; Gosslee, D. G.*; Bate, L. C.; Jacobson, F. B.* "Quantitative Aspects of Metal Ion Content And Toxicity In Drosophila"	*Toxicol.*, **26**, 295, 1983
Bostick, D. A.	Bostick, D. A.; Strain, J. E.; McCue, D. D.*; Harper, R. E.*; Bauer, M. L.* "A New In-Line Fiber Optic Spectrometer for Remote Analysis and Process Control"	*Trends in Anal. Chem.*, 2(9), 12, 1983
Buchanan, M. V.	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. "The Preparative Scale Separation and the Identification of Constituents of Anthraquinone-Derived Dye Mixtures. Part 3. Products from the Combustion of Red and Violet Smoke Mixtures"	*Anal. Chim. Acta*, 155, 151, 1983
	Buchanan, M. V.; Kao, G. L.*, Barkenbus, B. D.*; Ho, C.-h.; Guerin, M. R. "Chemical Characterization of the Mutagenic Neutral Aromatic Polar Fractions of Petroleum Substitutes"	*Fuel*, **62**, 1177, 1983
Carter, J. A.	Smith, D. H.; Walker, R. L.; Pritchard, C. A.; Carter, J. A. "Experimental Evaluation of Lutetium for Tank Calibration by Isotope Dilution Mass Spectrometry"	*Anal. Chem.*, 55, 143, 1983
Caton, J. E.	Yeatts, L. B.; Hurst, G. B.*; Caton, J. E. "Determination of Hydroxybenzenes in Fossil Fuel Derived Liquids and in Associated Process Waters"	*Anal. Chim. Acta*, 151, 349, 1983
	Barkenbus, B. D.*; MacDougall, C. S.; Griest, W. H.; Caton, J. E. "Methodology for the Extraction and Analysis of Hydrocarbons and Carboxylic Acids in Atmospheric Particulate Matter"	*Atmos. Environ.*, 17, 1537, 1983
	Higgins, C. E.; Griest, W. H.; Caton, J. E.; Harmon, S. H. "Thermal-Desorption Gas Chromatographic Procedure for Screening Coal Fly Ash for Volatile Organic Compounds"	*Anal. Chim. Acta*, 154, 173, 1983
Christie, W. H.	Loundes, D. H.*; Cleland, J. W.*; Christie, W. H.; Eby, R. E.; Jellison, G. E.*; Narayan, J.*; Westbrook, R. D.*; Wood, R. F.*; Nilson, J. A.*; Dass, S. C.* "Pulsed Excimer Laser Annealing of Ion Implanted Silicon: Characterization and Solar Cell Fabrication"	*Appl. Phys. Lett.*, 41(10), 938, 1982
	Young, R. T.*; Narayan, J.*; Christie, W. H.; Vander Leeden, G. A.*; Levatter, J. I.*; Cheng, L. J.* "Semiconductor Processing with Excimer Lasers"	*Solid State Techn.*, 26(11), 183, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Dale, J. M.	Dale, J. M.; Hulett, L. D., Jr.; Pendyala, S.* "The Interaction of Monoenergetic Positrons with Solid Surfaces"	*Appl. Spectros. Rev.*, 19(1), 105, 1983
Donohue, D. L.	Young, J. P.; Dononhue, D. L. "Ionization Spectra of Neodymium and Samarium by Resonance Ionization Mass Spectrometry"	*Anal. Chem.*, **55**, 86, 1983
	Donohue, D. L.; Young, J. P. "Detection of of Plutonium by Resonance Ionization Mass Spectrometry"	*Anal. Chem.*, **55**, 378, 1983
Eby, R. E.	Loundes, D. H.*; Cleland, J. W.*; Christie, W. H.; Eby, R. E.; Jellison, G. E.*; Narayan, J.*; Westbrook, R. D.*; Wood, R. F.*; Nilson, J. A.*; Dass, S. C.* "Pulsed Excimer Laser Annealing of Ion Implanted Silicon: Characterization and Solar Cell Fabrication"	*Appl. Phys. Lett.*, 41(10), 938, 1982
Eldridge, J. S.	Lyon, W. S.; Eldridge, J. S. "Weapons-Accident Drill Puts Virginia Town and ORNL Staff in Nevada Dessert"	*ORNL LAB NEWS*, July 1983, p. 4
	Eldridge, J. S.; Oakes, T. W.* "Radionuclide Migration from Shallow Land Burial Sites"	*Health Phys.*, **45**, 214, 1983
	Burkhardt, W. A.*; Voshell, J. R.*; Eldridge, J. S.; Oakes, T. W.* "Dispersal of Radionuclides from a Contaminated Pond by Emerging Aquatic Insects"	*Health Phys.*, **45**, 222, 1983
Feldman, C.	Feldman, C. "Behavior of Traces of Refractory Minerals in the Lithium Metaborate Fusion - Acid Dissolution Procedure"	*Anal. Chem.*, **55**, 2451, 1983
Glish, G. L.	Glish, G. L.; Smith, D. H. "Thermal Ionization of Quaternary Ammonium Salts"	*Int. J. Mass Spectrom. Ion Phys.*, **50**, 143, 1983
	Cooks, R. G.*; Busch, K. L.*; Glish, G. L. "Mass Spectrometry: Analytical Capabilities and Potentials"	*Sci.*, **222**, 273, 1983
	Glish, G. L.; McBay, E. H.; Goodman, M. M.*; Knapp, F. F.* "The Fragmentation of Chalcogen Containing Fatty Acids and Their Methyl Esters"	*Biomed. Mass Spectrom.*, **10**, 572, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Griest, W. H.	Higgins, C. E.; Griest, W. H.; Olerich, G. "Application of Tenax Trapping to the Analysis of Gas Phase Organic Compounds in Ultra-Low Cigarette Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**(5), 1074, 1983
	Barkenbus, B. D.*; Griest, W. H.; Huntzicker, J. J.*; Heyerdahl, E. K.*; MacDougall, C. S. "Recovery of Organic Carbon from Atmospheric Particulate Matter Using Soxhlet Extraction with the Benzene/Methanol Azeotrope"	*J. Environ. Sci. and Health*, **A18**(2), 297, 1983
	Barkenbus, B. D.*; MacDougall, C. S.; Griest, W. H.; Caton, J. E. "Methodology for the Extraction and Analysis of Hydrocarbons and Carboxylic Acids in Atmospheric Particulate Matter"	*Atmos. Environ.*, **17**, 1537, 1983
	Higgins, C. E.; Griest, W. H.; Caton, J. E.; Harmon, S. H. "Thermal-Desorption Gas Chromatographic Procedure for Screening Coal Fly Ash for Volatile Organic Compounds"	*Anal. Chim. Acta*, **154**, 173, 1983
Guerin, M. R.	Buchanan, M. V.; Kao, G. L.*; Barkenbus, B. D.*; Ho, C.-h.; Guerin, M. R. "Chemical Characterization of the Mutagenic Neutral Aromatic Polar Fractions of Petroleum Substitutes"	*Fuel*, **62**, 1177, 1983
	Ma, C. Y.; Ho, C.-h.; Quincy, R. B.; Guerin, M. R.; Rao, T. K.*; Allen, B. E.*; Epler, J. L.* "Preparation of Oils for Bacterial Mutagenicity Testing"	*Mutat. Res.*, **118**, 15, 1983
	Ho, C.-h.; Ma, C. Y.; Walton, B. T.*; Guerin, M. R. "Identification of a Potent Acridine-Related Insect Teratogen"	*The Toxicol.*, **3**(1), 29, 1983
Harmon, S. H.	Higgins, C. E.; Griest, W. H.; Caton, J. E.; Harmon, S. H. "Thermal-Desorption Gas Chromatographic Procedure for Screening Coal Fly Ash for Volatile Organic Compounds"	*Anal. Chim. Acta*, **154**, 173, 1983
Higgins, C. E.	Higgins, C. E.; Griest, W. H.; Caton, J. E.; Harmon, S. H. "Thermal-Desorption Gas Chromatographic Procedure for Screening Coal Fly Ash for Volatile Organic Compounds"	*Anal. Chim. Acta*, **154**, 173, 1983
	Higgins, C. E.; Griest, W. H.; Olerich, G. "Application of Tenax Trapping to the Analysis of Gas Phase Organic Compounds in Ultra-Low Cigarette Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**(5), 1074, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Ho, C.-h.	Buchanan, M. V.; Kao, G. L.*; Barkenbus, B. D.*; Ho, C.-h.; Guerin, M. R. "Chemical Characterization of the Mutagenic Neutral Aromatic Polar Fractions of Petroleum Substitutes"	*Fuel*, **62**, 1177, 1983
	Ma, C. Y.; Ho, C.-h.; Quincy, R. B.; Guerin, M. R.; Rao, T. K.*; Allen, B. E.*; Epler, J. L.* "Preparation of Oils for Bacterial Mutagenicity Testing"	*Mutat. Res.*, **118**, 15, 1983
	Walton, B. T.*; Ho, C.-h.; Ma, C. Y.; O'Neill, E. G.*; Kao, G. L.* "Benzoquinolinediones: Activity as Insect Teratogens"	*Sci.*, **222**, 422, 1983
	Ho, C.-h.; Ma, C. Y.; Walton, B. T.*; Guerin, M. R. "Identification of a Potent Acridine-Related Insect Teratogen"	*The Toxicol.*, **3**(1), 29, 1983
	Goerdeler, J.*; Ho, C.-h. "Cyclic and Linear Adducts from Carbonic Ester Isothiocyanates and Imines of Different Types"	*Chem. Ber.*, **116**, 1297, 1983
Holladay, S. K.	White (Holladay), S. K.; Bondietti, E. A.* "Removing Uranium by Current Municipal Water Treatment Processes"	*Am. Water Works Assoc. J.*, 374, 1983
Hulett, L. D.	Dale, J. M.; Hulett, L. D., Jr.; Pendyala, S.* "The Interaction of Monoenergetic Positrons with Solid Surfaces"	*Appl. Spectros. Rev.*, 19(1), 105, 1983
Jenkins, R. A.	Manni[illegible] D. L.; Maskarinec, M. P.; Jenkins, R. A.; Marshall, A. H. "High Performance Liquid Chromatographic Determination of Selected Gas Phase Carbonyls in Tobacco Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**, 8, 1983
Laing, W. R.	Laing, W. R. "Test Methods for the Nuclear Fuel Cycle"	*Standardization News*, March 1983
Lyon, W. S.	Lyon, W. S. "Coincident Readings Re Scientific Success"	*Radiochem. and Radioanal. Letts.*, 57, 131, 1983
	Lyon, W. S.; Roberts, P. P.* "Technical Oral Publications: What Happens to Them"	*Anal. Proc.*, **20**, 374, 1983
	Lyon, W. S.; Eldridge, J. S. "Weapons-Accident Drill Puts Virginia Town and ORNL Staff in Nevada Dessert"	*ORNL LAB NEWS*, July 1983, p. 4
	Lyon, W. S. "Radiation Hazards from Ear Studs and Neckwear"	*Radiochem. Radioanal. Letts.*, **59**, 3, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Lyon, W. S.	Lyon, W. S. "NUWAX-83 - Nucleonics in the Desert"	*Radiochem. Radioanal. Letts.*, **58**, 133, 1983
Ma, C. Y.	Ma, C. Y.; Ho, C.-h.; Quincy, R. B.; Guerin, M. R.; Rao, T. K.*; Allen, B. E.*; Epler, J. L.* "Preparation of Oils for Bacterial Mutagenicity Testing"	*Mutat. Res.*, **118**, 15, 1983
	El-Sohly, M. A.*; Adawadkar, P. D.*; Ma, C. Y.; Turner, C. E.* "Separation and Characterization of Poison Ivy and Poison Oak Urushiol Components"	*J. Nat. Products*, **45**, 532, 1983
	Walton, B. T.*; Ho, C.-h.; Ma, C. Y.; O'Neill, E. G.*; Kao, G. L.* "Benzoquinolinediones: Activity as Insect Teratogens"	*Sci.*, **222**, 422, 1983
	Ho, C.-h.; Ma, C. Y.; Walton, B. T.*; Guerin, M. R. "Identification of a Potent Acridine-Related Insect Teratogen"	*The Toxicol.*, **3**(1), 29, 1983
MacDougall, C. S.	Barkenbus, B. D.*; Griest, W. H.; Huntzicker, J. J.*; Heyerdahl, E. K.*; MacDougall, C. S. "Recovery of Organic Carbon from Atmospheric Particulate Matter Using Soxhlet Extraction with the Benzene/Methanol Azeotrope"	*J. Environ. Sci. and Health*, **A18**(2), 297, 1983
	Barkenbus, B. D.*; MacDougall, C. S.; Griest, W. H.; Caton, J. E. "Methodology for the Extraction and Analysis of Hydrocarbons and Carboxylic Acids in Atmospheric Particulate Matter"	*Atmos. Environ.*, **17**, 1537, 1983
Manning, D. L.	Manning, D. L.; Maskarinec, M. P. "Determination of Low Molecular Weight Carboxylic Acids in Water by HPLC with Conductivity Detection"	*J. Liq. Chromatogr.*, 6, 705, 1983
	Manning, D. L.; Maskarinec, M. P.; Jenkins, R. A.; Marshall, A. H. "High Performance Liquid Chromatographic Determination of Selected Gas Phase Carbonyls in Tobacco Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**, 8, 1983
Marshall, A. H.	Manning, D. L.; Maskarinec, M. P.; Jenkins, R. A.; Marshall, A. H. "High Performance Liquid Chromatographic Determination of Selected Gas Phase Carbonyls in Tobacco Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**, 8, 1983
Maskarinec, M. P.	Manning, D. L.; Maskarinec, M. P. "Determination of Low Molecular Weight Carboxylic Acids in Water by HPLC with Conductivity Detection"	*J. Liq. Chromatogr.*, 6, 705, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Maskarinec, M. P.	Maskarinec, M. P.; Vargo, J. D.*; Sepaniak, M. J.* "Characterization of Phenolic Compounds by Open Tubular Liquid Chromatography"	*J. Chromatogr.*, **261**, 245, 1983
	Browman, M. G.*; Maskarinec, M. P. "Environmental Aspects of Organics in Selected Coal Conversion Solid Wastes"	*J. Environ. Sci. and Health*, **A17**(5), 737, 1982
	Manning, D. L.; Maskarinec, M. P.; Jenkins, R. A.; Marshall, A. E. "High Performance Liquid Chromatographic Determination of Selected Gas Phase Carbonyls in Tobacco Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**, 8, 1983
McBay, E. H.	Todd, P. J.; Warmack, R. J.*; McBay, E. H. "The Angular Distribution of Fragment Ions Produced from Polyatomic Ion Collisions"	*Int. J. Mass Spectrom. Ion Phys.*, **50**, 299, 1983
	Glish, G. L.; McBay, E. H.; Goodman, M. M.*; Knapp, F. F.* "The Fragmentation of Chalcogen Containing Fatty Acids and Their Methyl Esters"	*Biomed. Mass Spectrom.*, **10**, 572, 1983
McKown, H. S.	McKown, H. S.; Smith, D. H.; Sherman, R. L. "A Thermal Ion Source for Quadrupole Mass Spectrometers"	*Int. J. Mass Spectrom. Ion Phys.*, **51**, 39, 1983
Moneyhun, J. H.	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. "The Preparative Scale Separation and the Identification of Constituents of Anthraquinone-Derived Dye Mixtures. Part 3. Products from the Combustion of Red and Violet Smoke Mixtures"	*Anal. Chim. Acta*, 155, 151, 1983
Olerich, G.	Higgins, C. E.; Griest, W. H.; Olerich, G. "Application of Tenax Trapping to the Analysis of Gas Phase Organic Compounds in Ultra-Low Cigarette Smoke"	*J. Assoc. Off. Anal. Chem.*, **66**(5), 1074, 1983
Pritchard, C. A.	Smith, D. H.; Walker, R. L.; Pritchard, C. A.; Carter, J. A. "Experimental Evaluation of Lutetium for Tank Calibration by Isotope Dilution Mass Spectroscopy"	*Anal. Chem.*, **55**, 578, 1983
Quincy, R. B.	Ma, C. Y.; Ho, C.-h.; Quincy, R. B.; Guerin, M. R.; Rao, T. K.*; Allen, B. E.*; Epler, J. L.* "Preparation of Oils for Bacterial Mutagenicity Testing"	*Mutat. Res.*, **118**, 15, 1983
Rubin, I. B.	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. "The Preparative Scale Separation and the Identification of Constituents of Anthraquinone-Derived Dye Mixtures. Part 3. Products from the Combustion of Red and Violet Smoke Mixtures"	*Anal. Chim. Acta*, **155**, 151, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Sherman, R. L.	McKown, H. S.; Smith, D. H.; Sherman, R. L. "A Thermal Ion Source for Quadrupole Mass Spectrometers"	*Int. J. Mass Spectrom. Ion Phys.*, 51, 39, 1983
Smith, D. H.	McKown, H. S.; Smith, D. H.; Sherman, R. L. "A Thermal Ion Source for Quadrupole Mass Spectrometers"	*Int. J. Mass Spectrom. Ion Phys.*, 51, 39, 1983
	Smith, D. H. "Closing the Accountability Gap"	*Nature*, 301, 292, 1983
	Smith, D. H.; Walker, R. L.; Pritchard, C. A.; Carter, J. A. "Evaluation of Lutetium for Volumetric Calibration by Isotope Dilution Mass Spectrometry"	*Anal. Chem.*, 55, 578, 1983
	Glish, G. L.; Smith, D. H. "Thermal Ionization of Quaternary Ammonium Salts"	*Int. J. Mass Spectrom. Ion Phys.*, 50, 143, 1983
Strain, J. E.	Bostick, D. A.; Strain, J. E.; McCue, D. D.*; Harper, R. E.*; Bauer, M. L.* "A New In-Line Fiber Optic Spectrometer for Remote Analysis and Process Control"	*Trends in Anal. Chem.*, 2(9), 12, 1983
Todd, P. J.	Todd, P. J.; Warmack, R. J.*; McBay, E. H. "The Angular Distribution of Fragment Ions Produced from Polyatomic Ion Collisions"	*Int. J. Mass Spectrom. Ion Phys.*, 50, 299, 1983
Walker, R. L.	Smith, D. H.; Walker, R. L.; Pritchard, C. A.; Carter, J. A. "Evaluation of Lutetium for Volumetric Calibration by Isotope Dilution Mass Spectrometry"	*Anal. Chem.*, 55, 578, 1983
Whitten, W. B.	Whitten, W. B. "Time Domain Optical Spectrometry With Fiber Optic Waveguides"	*Appl. Spectrosc. Revs.*, 19, 325, 1983
Yeatts, L. B.	Yeatts, L. B.; Hurst, G. B.*; Caton, J. E. "Determination of Hydroxybenzenes in Fossil Fuel Derived Liquids and in Associated Process Waters"	*Anal. Chim. Acta*, 151, 349, 1983
Young, J. P.	Donohue, D. L.; Young, J. P. "Detection of of Plutonium by Resonance Ionization Mass Spectrometry"	*Anal. Chem.*, 55, 378, 1983
	Young, J. P.; Dononhue, D. L. "Ionization Spectra of Neodymium and Samarium by Resonance Ionization Mass Spectrometry"	*Anal. Chem.*, 55, 38, 1983

AUTHOR	AUTHOR(S) AND TITLE	PUBLISHED IN
Young, J. P.	Haire, R. G.*; Hellwege, H. E.*; Hobart, D. E.*; Young, J. P "Syntheses, Lattice Parameters and Solid State Absorption Spectra of the First Five Transplutonium Orthophosphates"	*J. of the Less-Common Met.*, **93**, 358, 1983
	Haire, R. G.*; Young, J. P.; Peterson, J. R.* "X-Ray Diffraction and Absorption Spectrophotometric Studies of AmI and AmOI"	*J. of the Less-Common Met.*, **93**, 339, 1983

Reports

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Bostick, D. T.	Bostick, D. T.; Strain, J. E. *The Photometric Determination of Plutonium in Organic Purex Solutions*	ORNL/TM-8286 (Mar. 1983)
	McCue, D. D.*; Harper, R. E.*; Bostick, D. T.; Strain, J. E. *A Bench Test of the Multiwavelength Photometer on Aqueous Uranium Solutions*	ORNL/CFRP-83/8 (July 1983)
	Bostick, D. T.; Strain, J. E. *The Electroreduction and Photometric Detection of Low-Level Uranium in Aqueous Purex Solutions*	ORNL/TM-8646 (Apr. 1983)
	Strain, J. E.; Bostick, D. T. *The Evaluation of the Spectrophotometric Determination of Plutonium in Aqueous Reprocessing Streams*	ORNL/TM-8101 (Mar. 1983)
Botts, J. L.	Walker, R. L.; Botts, J. L.; Cooper, J. H.; Adair, H. L.*; Bigelow, J. E.*; Raman, S.* *Characterization of Actinide Physics Specimens for the US/UK Joint Experiment in the Dounreay Prototype Fast Reactor*	ORNL-5986 (Oct. 1983)
Brazell, R. S.	Brazell, R. S. *Report of Foreign Travel of R. S. Brazell, Research Associate, Bio/Organic Analysis Section, Analytical Chemistry Division*	ORNL/FTR-1654 (Oct. 20, 1983)
Brooksbank, R. D.	Bayne, C. K*; Brooksbank, R. D.; Howell, P. L. *The Calibration of Uranium and Plutonium in Nitric Acid Solutions for X-Ray Fluorescence Analysis*	ORNL/TM-8981 (Dec. 1983)
	Brooksbank, R. D. *Quality Assurance Plan for the Nuclear Coating Testing Program, Analytical Chemistry Division, Oak Ridge National Laboratory*	ORNL/QA-AC-101 (Mar. 1983)
Buchanan, M. V.	Olerich, G.; Buchanan, M. V. *Compilation of Mass Spectra of Nitrogen-Containing Aromatics*	ORNL/TM-8855 (Sept. 1983)
	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: Chemical Characterization of Combusted Inventory Red and Violet Smokes Mixes*	ORNL/TM-8810 (July 1983)
	Rubin, I. B.; Buchanan, M. V. *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures - Chemical Characterization of Army Colored Smokes: Inventory Smoke Mixes (Red, Violet, Yellow and Green)*	ORNL/TM-8956 (Oct. 1983)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Carter, J. A.	Carter, J. A. *Analytical Chemistry Division Research and Development Summary: Mass and Emission Spectrometry Section*	ORNL/CF-83/207 (June 1, 1983)
	Lambert, S. J.*; Carter, J. A. *Uranium-Isotope Disequilibrium in Brine Reservoirs of the Castile Formation, Northern Delaware Basin, Southeastern New Mexico, I: Principles and Methods*	SAND83-0144 (Apr. 1983)
	Carter, J. A. *Analytical Chemistry Division Research and Development Summary: Mass and Emission Spectrometry Section*	ORNL/CF-83/18 (Feb. 1, 1983)
	Carter, J. A.* *Analytical Chemistry Division Research and Development Summary: Mass and Emission Spectrometry Section*	ORNL/CF-83/287 (Oct. 1, 1983)
	Carter, J. A. *Report of Foreign Travel to Ispra, Italy*	ORNL/FTR-1683 (Nov. 22, 1983)
Cooper, J. H.	Walker, R. L.; Botts, J. L.; Cooper, J. H.; Adair, H. L.*; Bigelow, J. E.*; Raman, S.* *Characterization of Actinide Physics Specimens for the US/UK Joint Experiment in the Dounreay Prototype Fast Reactor*	ORNL-5986 (Oct. 1983)
Eldridge, J. S.	Alexander, W. A.*; Huang, S.*; Oakes, T. W.*; Hubbard, H. M.*; Eldridge, J. S. *Radionuclide Characterization of Subsurface Soil on the Site of Building 3505 at Oak Ridge National Laboratory*	ORNL/TM-8479 (Dec. 1982)
Emery, J. F.	Jolley, R. F.*; Begovich, J. M.*; Brashear, H. R.*; Case, N.*; Clark, T. G.*; Emery, J. F.; Patton, B. D.*; Rodgers B. R.*; Villers-Fisher, J. F.; Watson, J. S.* *Plan for Radionuclide Tracer Studies of the Residence Time Distribution in the Wilsonville Dissolver and Preheater*	ORNL/TM-8777 (Dec. 1983)
Goeringer, D. E.	Goeringer, D. E. *A Macro-11 Intersystem Communication Program for Terminal Emulation and File Transfer Operations*	ORNL/TM-8943 (Nov. 1983)
Griest, W. H.	Cushman, R. M.*; Suter, G. W.*; Brown, D. K.*; Griest, W. H.; Stewart A. J.*; Strand, R. H.* *Environmental Evaluation of the University of Minnesota-Duluth Coal Gasifier*	ORNL/TM-8552 (Mar. 1983)
	Griest, W. H.; Giddings, J. M.*; Klein, J. A.* *Effects of Hydrotreatment on the Properties of Coal-Derived Liquid Products: A Status Report*	ORNL/TM-8836 (Aug. 1983)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Griest, W. H.	Jenkins, R. A.; White (Holladay), S. K.; Griest, W. H.; Guerin, M. R. *Chemical Characterization of the Smokes of Selected U.S. Commercial Cigarettes: Tar, Nicotine, Carbon Monoxide, Oxides of Nitrogen, Hydrogen Cyanide, and Acrolein*	ORNL/TM-8749 (May 1983)
	Griest, W. H. *Report of Foreign Travel of W. H. Griest, Group Leader, Bio/Organic Analysis Section, Analytical Chemistry Division*	ORNL/FTR-1621 (Sept. 27, 1983)
Guerin, M. R.	Jenkins, R. A.; White (Holladay), S. K.; Griest, W. H.; Guerin, M. R. *Chemical Characterization of the Smokes of Selected U.S. Commercial Cigarettes: Tar, Nicotine, Carbon Monoxide, Oxides of Nitrogen, Hydrogen Cyanide, and Acrolein*	ORNL/TM-8749 (May 1983)
	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; February, 1983, Bio/Organic Analysis Section*	ORNL/CF-83/40 (Mar. 1, 1983)
	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; June, 1983, Bio/Organic Analysis Section*	ORNL/CF-83/229 (July 1, 1983)
	Guerin, M. R. *Analytical Chemistry Division Research and Development Summary; October, 1983, Bio/Organic Analysis Section*	ORNL/CF-83/322 (Nov. 1, 1983)
Holladay, S. K.	Jenkins, R. A.; White (Holladay), S. K.; Griest, W. H.; Guerin, M. R. *Chemical Characterization of the Smokes of Selected U.S. Commercial Cigarettes: Tar, Nicotine, Carbon Monoxide, Oxides of Nitrogen, Hydrogen Cyanide, and Acrolein*	ORNL/TM-8749 (May 1983)
Holmberg, R. W.	Holmberg, R. W.; Moneyhun, J. H.; Gayle, T. M.* *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: Generating, Monitoring and Controlling Petroleum Aerosols for Inhalation Chamber Studies*	ORNL/TM-8903 (Oct. 1983)
Howell, P. L.	Bayne, C. K*; Brooksbank, R. D.; Howell, P. L. *The Calibration of Uranium and Plutonium in Nitric Acid Solutions for X-Ray Fluorescence Analysis*	ORNL/TM-8981 (Dec. 1983)
Jenkins, R. A.	Jenkins, R. A.; White (Holladay), S. K.; Griest, W. H.; Guerin, M. R. *Chemical Characterization of the Smokes of Selected U.S. Commercial Cigarettes: Tar, Nicotine, Carbon Monoxide, Oxides of Nitrogen, Hydrogen Cyanide, and Acrolein*	ORNL/TM-8749 (May 1983)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Jenkins, R. A.	Jenkins, R. A. *Report of Foreign Travel of R. A. Jenkins, Research Staff Member, Bio/-Organic Analysis Section, Analytical Chemistry Division*	ORNL/FTR-1477 (Mar. 29, 1983)
Keller, J. M.	Keller, J. M.; Sparks, C. J. Jr.* *Evaluation of a Wavelength Dispersive X-Ray System for the Determination of Uranium and Plutonium in Highly Radioactive Solutions*	ORNL-5971 (Sept. 1983)
	Rivers, A. L.*; Keller, J. M. *Initial Studies in the Development of Advanced Processes and Equipment for the Management of the Wastewaters Generated During the Washing of the Gel Spheres Produced by Internal Gelation*	ORNL/CFRP-84/16 (Dec. 1983)
Laing, W. R.	Laing, W. R. *Analytical Chemistry Division Monthly Report for March, 1983, Radioactive Materials Analysis Section*	ORNL/CF-83/61 (Apr. 1, 1983)
	Laing, W. R. *Analytical Chemistry Division Monthly Report for July, 1983, Radioactive Materials Analysis Section*	ORNL/CF-83/248 (Aug. 1, 1983)
	Laing, W. R. *Analytical Chemistry Division Monthly Report for November, 1983, Radioactive Materials Analysis Section*	ORNL/CF-83/330 (Dec. 1, 1983)
	Laing, W. R. *Quality Assurance Report of the Analytical Chemistry Division, October 1982 Through September 1983*	ORNL/CF-83/297 (Oct. 1, 1983)
Lyon, W. S.	Lyon, W. S. *Analytical Chemistry Division Research and Development Summary for August, 1983, Analytical Methodology Section*	ORNL/CF-83/277 (Sept. 1, 1983)
	Lyon, W. S. *Analytical Chemistry Division Research and Development Summary for April, 1983, Analytical Methodology Section*	ORNL/CF-83/84 (May 2, 1983)
	Lyon, W. S. *Analytical Chemistry Division Research and Development Summary for December, 1982, Analytical Methodology Section*	ORNL/CF-82/332 (Jan. 1, 1983)
Maskarinec, M. P.	Brown, D. K.*; Maskarinec, M. P.; Larimer, F. W.*; Francis, C. W.* *Mobility of Organic Compounds from Hazardous Wastes*	EPA/600/S4-83-001 (Mar. 1983)
	White, C. M.*; et al.*; Maskarinec, M. P. *Development of an Analytical Method for the Determination of Organic Compounds in Fossil Fuel Aqueous Leachates*	DOE/PETC/TR-84/1 (Oct. 1983)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Moneyhun, J. H.	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: Chemical Characterization of Combusted Inventory Red and Violet Smokes Mixes*	ORNL/TM-8810 (July 1983)
	Holmberg, R. W.; Moneyhun, J. H.; Gayle, T. M.* *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: Generating, Monitoring and Controlling Petroleum Aerosols for Inhalation Chamber Studies*	ORNL/TM-8903 (Oct. 1983)
Olerich, G.	Olerich, G.; Buchanan, M. V. *Compilation of Mass Spectra of Nitrogen-Containing Aromatics*	ORNL/TM-8855 (Sept. 1983)
Rubin, I. B.	Rubin, I. B.; Buchanan, M. V.; Moneyhun, J. H. *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures: Chemical Characterization of Combusted Inventory Red and Violet Smokes Mixes*	ORNL/TM-8810 (July 1983)
	Rubin, I. B.; Buchanan, M. V. *Chemical Characterization and Toxicological Evaluation of Airborne Mixtures - Chemical Characterization of Army Colored Smokes: Inventory Smoke Mixes (Red, Violet, Yellow and Green)*	ORNL/TM-8956 (Oct. 1983)
Smith, D. H.	Smith, D. H. *Report of Foreign Travel*	ORNL/FTR-1541 (July 6, 1983)
Stokely, J. R.	Stokely, J. R. *Analytical Chemistry Division Summary Report: General and Environmental Analysis Section*	ORNL/CF-82/333 (Jan. 3, 1983)
	Stokely, J. R. *Analytical Chemistry Division Summary Report: General and Environmental Analysis Section*	ORNL/CF-83/91 (May 1, 1983)
Strain, J. E.	Bostick, D. T.; Strain, J. E. *The Electroreduction and Photometric Detection of Low-Level Uranium in Aqueous Purex Solutions*	ORNL/TM-8646 (Apr. 1983)
	Strain, J. E.; Bostick, D. T. *The Evaluation of the Spectrophotometric Determination of Plutonium in Aqueous Reprocessing Streams*	ORNL/TM-8101 (Mar. 1983)
	Bostick, D. T.; Strain, J. E. *The Photometric Determination of Plutonium in Organic Purex Solutions*	ORNL/TM-8286 (Mar. 1983)

AUTHOR	AUTHOR(S) AND TITLE	REPORT NO. AND DATE
Strain, J. E.	McCue, D. D.*; Harper, R. E.*; Bostick, D. T.; Strain, J. E. *A Bench Test of the Multiwavelength Photometer on Aqueous Uranium Solutions*	ORNL/CFRP-83/8 (July 1983)
Walker, R. L.	Walker, R. L.; Botts, J. L.; Cooper, J. H.; Adair, H. L.*; Bigelow, J. E.*; Raman, S.* *Characterization of Actinide Physics Specimens for the US/UK Joint Experiment in the Dounreay Prototype Fast Reactor*	ORNL-5986 (Oct. 1983)

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	AUTHOR(S) AND TITLE	PRESENTED AT
Attrill, J. E.	Attrill, J. E. "Problems Associated with the Environmental Analysis at ORNL"	4-Lab Anal. Infor. Meet. Paducah, KY, Nov. 15, 1983
Bacarella, A. L.*	Bacarella, A. L.*; Dale, J. M.; Hulett, L. D. "An Electrochemical and ESCA Study of Titanium Dissolution in Acidic Sulfate Solutions Containing CrII/CrIII Ions"	Electrochem. Soc. Meet., San Francisco, CA, May 8-13, 1983
Brazell, R. S.	Brazell, R. S.; Moneyhun, J. H.; Holmberg, R. W. "Chemical Characterization of Selected Military Obscurants"	Chem. Systems Lab. Conf. on Obscuration and Aerosol Res., Aberdeen Proving Ground, MD, June 20-24, 1983
	Brazell, R. S.; Holmberg, R. W. "Application of HPLC/FIA for the Determination of Polyphosphoric Acids in Phosphorous Smokes"	Invited, Int. Symp. on Adv. in Chromatogr., AMSTERDAM, Oct. 3-6, 1983
Brooksbank, R. D.	Brooksbank, R. D. "The Decontamination Factor Test as Currently Performed at ORNL	Subcom. D-33.1i on Decontamination, ASTM Vista, FL, Nov. 17, 1983
Buchanan, M. V.	Buchanan, M. V. "Isomeric Discrimination Using Chemical Ionization Mass Spectrometry"	NBS/DOE Anal. Charac. Grp. Meet., Ames, IA, Nov. 2, 1983
	Buchanan, M. V. "Compositional Changes in Red and Violet Smoke Mixes After Combustion"	Smoke/Obscurants Symp. VII, Adelphi, MD, April 26-28, 1983
	Buchanan, M. V. "Differentiation of Isomeric Heteroatom-Substituted Aromatics Using Chemical Ionization"	Am. Soc. for Mass Spectrom. Meet., Boston, MA, May 8-13, 1983
Budjoso, E.*	Budjoso, E.*; Lyon, W. S. "Mapping the Information Flow of Analytical Chemistry"	Invited, Am. Chem. Soc. Meet., Seattle, WA, Mar. 20-25, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Busch, K. L.*	Busch, K. L.*; Cooks, R. G.*; Glish, G. L.; Todd, P. J. "MS/MS of Desorbed Ions;	Pittsburgh Conf. and Expo. on Anal. Chem. and Applied Spectros., Atlantic City, NJ, Mar. 7-12, 1983
Carter, J. A.	Carter, J. A. "Mass Spectrometry Developments"	CFRP Info. Meet. for HEDL and AGNS, Oak Ridge Nat. Lab., Oak Ridge, TN, Jan. 5, 1983
	Carter, J. A. "Use of Lutetium for Tank Volume Calibration and SNM Verification"	Invited, ESARDA Workshop Deter. of the Vol. of Reprocess. Input Solutions by Tracer Mass Spectrom. Techn., Joint Res. Centre, Ispra (Varese), Italy, Nov. 8-10, 1983
	Carter, J. A.; Glish, G. L. "Detection of Organic Vapors by MS/MS Technique"	Invited, USDOE-OSS, Washington, DC, June 29, 1983
	Carter, J. A.; Walker, R. L. "Review and Status of Resin-Bead/Mass Spectrometry"	Invited, USDOE-OSS, Washington, DC, Aug. 2-3, 1983
Caton, J. E.	Caton, J. E.; Guerin, M. R. "Fingerprinting the Chemical Characteristics of Fossil Fuel Derived Liquids"	CONFAB 83, Government, Industry, and Academic Tech. Conf. on Fossil Fuel Chem., Saratoga, NY, Aug. 2-5, 1983
Christie, W. H.	Christie, W. H. "Quantitative Aspects of SIMS as a Depth Profiling Technique: Some Applications in Energy Research Programs"	Invited, 25th Rocky Mountain Conf., Denver, CO, Aug. 14-19, 1983
	Christie, W. H.; Eby, R. E.; Taylor, D. H.*; Pavone, D.* "SIMS Study of Compositional Changes Observed in a PuO_2 Heat Source Cladding Alloy"	26th Oak Ridge Nat. Lab. Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Oct. 11-13, 1983
Costanzo, D. A.	Costanzo, D. A. "Status of the Breeder Reactor Engineering Test, Anal. Chem. Requirements at ORNL"	ORNL/HEDL/AGNS Infor. Exchange Meet., ORNL, May 12 and June 24, 1984
	Costanzo, D. A. "Analytical Chemistry Problems in Criticality Experiments with Plutonium"	CFRP Tech. Sem. June 16, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Costanzo, D. A.	Costanzo, D. A. "Analytical Chem. Develop. for CFRP"	CFRP Prog. Rev. Meet. July 12, 1983
	Costanzo, D. A. "Anal. Chem. for Bldg. 2026 and 3019-B - An Overview"	1983 ORNL Radioactive Operations Com. Review Meet., July 15, 1983
	Costanzo, D. A. "Anal. Chem. Develop. for the Consolidated Fuel Reprocessing Program - An Overview"	ORNL/HEDL CFRP Infor. Exchange Meet., ORNL, Jan. 5, 1983
	Costanzo, D. A. "Determination of Free Acid in the Presence of Uranium and Plutonium"	ORNL/HEDL/PNL Inf. Exchange Meet., Richland, WA, Dec. 7, 1983
	Costanzo, D. A. "Anal. Chem. for the Breeder Reprocessing Engineering Test"	Consolidated Fuel Reprocessing Eng. Test, ORNL, Dec. 15, 1983
Dale, J. M.	Dale, J. M.; Hulett, L. D.; Miller, P. D., Jr.*; Moak, C. D.* "Low Energy Monoenergetic Positron Generation and Spectrometry"	3rd Annu. Tenn. Valley AVS Symp., Knoxville, TN, May 9-11, 1983
	Dale, J. M.; Hulett, L. D.; Pendyala, S.* "Some Techniques for the Generation, Detection, and Spectrometry of Monoenergetic Positrons and Scattering Studies from Solids and Gases"	Invited, Annu. Meet. of the Am. Assoc. for the Adv. of Sci., Detroit, MI, May 26-27, 1983
David, P. A.*	David, P. A.* "Capillary Zone Electrophoresis with Non-Aqueous Solvents"	ORNL-GLCA/ACM Science Semester Presentation, Oak Ridge, TN, Dec. 16, 1983
Donohue, D. L.	Donohue, D. L.; Young, J. P. "Resonance Ionization Mass Spectrometry"	Invited, Chem. Phys. Sem. ORNL, Oak Ridge, TN, May 23, 1983
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Isotopic Measurements of Uranium and Plutonium by Resonance Ionization Mass Spectrometry"	26th Oak Ridge Nat. Lab. Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Oct. 11-13, 1983
	Donohue, D. L.; Young, J. P.; Smith, D. H. "Resonance Ionization Mass Spectrometry"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Donohue, D. L.	Young, J. P.; Donohue, D. L.; Smith, D. H. "Recent Advances in Resonance Ionization Mass Spectrometry"	Invited, DOE Contractors' Workshop on "Advanced Laser Technol. for Chem. Measure.", Livermore, CA, June 8-9, 1983
	Donohue, D. L. "Isotope Ratio Measurements by Resonance Ionization Mass Spectrometry"	Invited, ORAU Traveling Lecture Program, Univ. of VA, Charlottesville, VA, Mar. 21, 1983
	Donohue, D. L. "Nuclear Safeguards,"	Invited, ORAU Health Phys. and Radiation Prot. Course, Oak Ridge, TN, Mar. 28, 1983
	Donohue, D. L. "New Laser Techniques for Analytical Chemistry"	ORNL/ACD Sum. Sem. Ser., Oak Ridge Nat. Lab., July 8, 1983
Dyer, F. F.	Dyer, F. F.; Clemmer, R. G.*; Finn, P. A.*; Billone, M. C*; Misra, B.*; Aroust, R. M.*; Paeppel, R. B.*; Dudley, I. T.; Bate, L. C.; Clemmer, E. D.*; Scott, J. L.*; Watson, J. S.*; and Fisher P. W.* "The TRIO-01 Experiment: In-Situ Tritium Recovery Results"	3rd Topical Meet. on Fusion Reactor Mate., Albuquerque, NM, Sept. 19-22, 1983
Eldridge, J. S.	Eldridge, J. S. "Laboratory and Sample Preparation Techniques"	DOE Radiological Emergency Preparedness Workshop, Oak Ridge, TN, Oct. 14, 1983
	Eldridge, J. S.; Oakes, T. W.* "Radionuclide Migration from Shallow Land Burial Sites"	28th Annu. Meet. Health Phys. Soc., Baltimore, MD, June 19-23, 1983
	Eldridge, J. S. "Toxicology of Radioactivity"	Univ. of Tenn., Special Topics in Environ. Toxicol., Knoxville, TN, Nov. 22, 1983
Feldman, C.	Feldman, C. "The Behavior of Traces of Refractory Minerals (Including Monazite) in the Lithium Metaborate Fusion"	LABCON Central 1983 Meet., Chicago, IL, Sept. 20-22, 1983
Francis, C. W.*	Francis, C. W.*; Maskarinec, M. P. "Short-Term Leaching of Solid Wastes from the H-Coal Liquefaction Process"	2nd Conf. on Municipal, Hazardous, and Coal Wastes Manage., Miami Beach, FL, Dec. 5-7, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Glish, G. L.	Glish, G. L.; Todd, P. J.; Busch, K. L.* "MS/MS Spectra of Desorbed Ions"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
	Glish, G. L.; Todd, P. J. "Cation Effects on SIMS MS/MS Spectra"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
	Glish, G. L. "MS/MS and Thermal Desorption/ Ionization. The Ideal Combination?"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
	Glish, G. L. "Desorption Ionization and MS/MS: A Valuable Combination"	Invited, The UpJohn Co. Kalamazoo, MI, Dec. 1, 1983
	Glish, G. L.; Todd, P. J.; Busch, K. L.*; Cooks, R. G.* "MS/MS: A Necessity with Desorption Ionization?"	Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 28-Sept. 2, 1983
Goeringer, D. E.	Goeringer, D. E. "ACD Data Logger System"	Invited, ORNL Course "Professional Use of Personal Computers in R&D", Oak Ridge, TN May 23, 1983
Griest, W. E.	Griest, W. H.; Tomkins, B. A. "Carbonaceous Particles in Coal Combustion Stack Ash and Their Interaction with Polycyclic Aromatic Hydrocarbons"	2nd Int. Conf. on Carbonaceous Part. in the Atmos., Linz, AUSTRIA, Sept. 11-14, 1983
Guerin, M. R.	Guerin, M. R.; Griest, W. H.; Yeatts, L. B.; Harvey, R. W. "Synfuels Research Materials Facility"	3rd Int. Congr. on Toxicol., San Diego, CA, Aug. 28-Sept. 3, 1983
	Guerin, M. R.; Caton, J. E.; Rubin, I. B.; Epler, J. L.*; Buchanan, M. V. "Toxicological Characterization of Petroleum Substitutes in Terms of Composite Chemical Parameters"	3rd Int. Congr. on Toxicol., San Diego, CA, Aug. 28-Sept. 3, 1983
	Ho, C.-h.; Ma, C. Y.; Walton, B. T.*; Guerin, M. R. "Identification of a Potent Acridine-Related Insect Teratogen"	Soc. of Toxicol. Annu. Conf., Las Vegas, NV, Mar. 6-8, 1983
	Guerin, M. R. "Toxicologically Relevant Chemical Descriptions of Complex Mixtures"	Soc. of Environ. Toxicol. and Chem., 4th Annu. Meet., Crystal City, VA, Nov. 6-9, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Haire, R. G.*	Haire, R. G.*; Young, J. P.; Peterson, J. R. "Absorption Spectrophotometric and X-Ray Diffraction Studies of AmI_3 and AmOI"	16th Rare Earth Res. Conf., Tallahassee, FL, Apr. 18-21, 1983
	Haire, R. G.*; Hellwege, H. E.*; Hobart, D. E.*; Young, J. P. "Syntheses, Lattice Parameters, and Solid State Absorption Spectra of the First Five Transplutonium Orthophosphates"	16th Rare Earth Res. Conf., Tallahassee, FL, Apr. 18-21, 1983
Harward, B.*	Harward, B.*; Klatt, L. N.; Mamantov, G.* "Multipass Spectroelectrochemistry"	35th Southeastern Reg. Meet. of the Am. Chem. Soc., Charlotte, NC, Nov. 9-11, 1983
Ho, C.-h.	Ho, C.-h.; Ma, C. Y.; Caton, J. E.; Buchanan, M. V.; Maskarinec, M. P.; Rubin, I. B.; Guerin, M. R. "Chromatographic and Spectroscopic Analysis of Acridine Isomers"	Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 28-Sept. 2, 1983
Hulett, L. D.	Hulett, L. D., Jr.; Dale, J. M.; Miller, P. D., Jr.*; Moak, C. D.*; Pendyala, S.*; Triftshauser, W.*; Howell, R. H.*; Alvarez, R. A. "The Generation of Monoenergetic Positrons"	Invited, North Atlantic Treaty Organization Advanced Res. Workshop, "Positron Scattering in Gases," Surrey, UK, July 19-23, 1983
	Hulett, L. D.; Dale, J. M. "Discussion of Low-Pass High-Pass Charged Particle Spectrometer Designs"	Chem. Phys. Sem., Oak Ridge Nat. Lab., Oak Ridge, TN, Jan. 24, 1983
	Hulett, L. D.; Dale, J. M. "The Generation and Spectrometry of Monoenergetic Positrons"	Invited, Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 28-Sept. 2, 1983
	Hulett, L. D. "Review of the Properties of Amorphous and Crystalline Phases in Fly Ash"	Invited, 1983 Annu. Meet. of Mate. Res. Soc., Boston, MA, Nov. 13-18 1983
	Hulett, L. D. "Scanning Electron Microscopy"	Invited, Southeastern Louisiana State Univ., Hammond, LA, Dec. 5, 1983
	Hulett, L. D.; Dale, J. M.; Pendyala, S.* "Implementations of Monoenergetic Positrons in Fundamental and Applied Science"	1983 Annu. Meet. of AAAS, Detroit, MI, May 26-27, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Hulett, L. D.	Hulett, L. D., Jr.; Dale, J. M.; Pendyala, S.* Triftshauser, W.* "New Developments of Positron Moderators for Materials Analysis"	1983 Annu. Meet. of the Mate. Res. Soc., Boston, MA, Nov. 13-18, 1983
Jenkins, R. A.	Jenkins, R. A.; Guerin, M. R. "Analytical Chemical Methods for the Detection of Ambient Tobacco Smoke Constituents"	Invited, Int. Workshop on Environ. Tobacco Smoke, Geneva, SWITZERLAND, Mar. 14-17, 1983
	Jenkins, R. A.; White, S. K.; Griest, W. H.; Guerin, M. R. "'Tar', Nicotine, and Carbon Monoxide Deliveries of Commercial Cigarettes from Selected Nations"	5th World Conf. on Smoking and Health, Winnipeg, CANADA, July 10-15, 1983
Keller, J. M.	Keller, J. M. "Determination of Uranium and Plutonium in Nuclear Fuel Reprocessing Solutions"	Tech. Rev. of CFRP Process and Eng. R/D Act., ORNL, Oak Ridge, TN, Dec., 1981
	Keller, J. M. "WDS-XRF System for the Determination of Uranium and Plutonium in Highly Gamma-Active Solutions"	CFRP Tech. Sem., ORNL, Oak Ridge, TN, Dec. 2, 1982
	Keller, J. M. "An XRF System for the Analysis of Highly Radioactive Samples"	ORNL/HEDL CFRP Info. Exchange Meet., ORNL, Oak Ridge, TN, Jan. 5, 1983
	Keller, J. M. "X-Ray Fluorescence Application"	Annu. CFRP Process R/D Tech. Review Meet., ORNL, Oak Ridge, TN, Apr. 20, 1983
	Keller, J. M. "X-Ray Fluorescence for Highly Radioactive Samples"	ACD Summer Seminar Series, ORNL, Oak Ridge, TN, June 24, 1983
Klatt, L. N.	Klatt, L. N. "Intelligent Instruments and Chemical Analysis in a High Radiation Environment"	Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 28-Sept. 2, 1983
Laing, W. R.	Laing, W. R. "Upgrade of ORNL Analytical Chemistry Radioactive Materials Facilities"	Workshop on Anal. Chem. Related to Canada's Ind., Helca Is. Manitoba, CANADA, Oct. 24-25, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Lee, D. A.	Lee, D. A. "Separation of Lithium Ions by Chromatography"	Southeastern Reg. Am. Chem. Soc. Meet., Charlotte, NC, Nov. 9-12, 1983
	Lee, D. A. "Separation of Lithium Ions by Chromatography"	Southeastern Reg. Am. Chem. Soc. Meet., Charlotte, NC, NOv. 9-11, 1983
Ma, C. Y.	Ma, C. Y.; Ho, C.-h.; Walton, B. T.*; Caton, J. E.; Guerin, M. R. "On the Nature of Cricket Teratogens in a Coal Oil"	Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 28-Sept. 2, 1983
Maskarinec, M. P.	Maskarinec, M. P. "HPLC or What is in an Acronym"	Oak Ridge Nat. Lab., New Directions in Anal. Chem. Sum. Sem. Ser., Oak Ridge, TN, July 29, 1983
	Vargo, J. D.*; Maskarinec, M. P.; Sepaniak, M. J.* "The Determination of Polar Compounds in a Coal-Derived Fuel Oil by Open Tubular Liquid Chromatography"	Pittsburgh Conf. and Exposition on Anal. Chem. and Applied Spectrosc., Atlantic City, NJ, Mar. 7-12, 1983
May, M. P.	May, M. P.; Walker, R. L.; Scott, T. G.; Dyer, F. F.; Stokely, J. R. "The Determination of Uranium in Urine by Isotope Dilution Mass Spectrometry Using Resin Bead Loading"	26th Oak Ridge Nat. Lab. Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Oct. 11-13, 1983
Raman, S.*	Alton, G. D.*; Broadhead, B. L.*; Cole, D. R.*; Kolasinski, W. A.*; Rosseel, T. M.; Raman, S.*; Tombrello, T. A.*; Vane, C. R.*; Walker, R. L. "Nuclear Science Applications"	Phys. Div. Info. Meet., Oak Ridge Nat. Lab., Oak Ridge, TN, Dec. 12-13, 1983
	Rosseel, T. M.; Dale, J. M.; Dunn, H. W.; Hulett, L. D.; Kahane, S.*; Krause, H. F.*; Raman, S.*; Slaughter, G. G.*; Vane, C. R.*; Young, J. P. "Chemical Effects in X-Ray Satellites of Molybdenum Compounds and Alloys"	3rd Int. Conf. on Particle Induced X-Ray Emis. (PIXE), Max-Planck-Insti. fur Kernphysik, Heidelberg, W. GERMANY, July 18-22, 1983
	Vane, C. R.*; Hulett, L. D.; Kahane, S.*; McDaniel, F. D.*; Milner, W. T.*; O'Kelley, G. D.*; Raman, S.*; Rosseel, T. M.; Slaughter, G. G.*; Varghese, S. L.*; Young, J. P. "Chemical Effects in High-Resolution Sulfur K X-Ray Spectra"	3rd Int. Conf. on Particle Induced X-Ray Emis. (PIXE), Max-Planck-Insti. fur Kernphysik, Heidelberg, W. GERMANY, July 18-22, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Raman, S.*	O'Kelley, G. D.*; Auble, R. L.*; Hulett, L. D.; Kim, H. J.*; Milner, W. T.*; Raman, S.*; Shahal, O.*; Vane, C. R.*; Young, J. P.; Lapicki, G.* "Production of Vanadium, Copper, Niobium, Tantalum, and Platinum"	3rd Int. Conf. on Particle Induced X-Ray Emis. (PIXE), Max-Planck-Insti. für Kernphysik, Heidelberg, W. GERMANY, July 18-22, 1983
Ramsey, J. M.	Ramsey, J. M. "Laser Intracavity Absorption with Phase Conjugate Optics"	Invited, ORNL Chem. Phys. Sem., Oak Ridge, TN, July 25, 1983
	Ramsey, J. M. "Time-Domain Spectrochemical Analysis"	Invited, Dept. of Chem., Univ. of New Mexico, Albuquerque, NM, Nov. 18, 1983
	Ramsey, J. M. "Phase Conjugate Optics and Chemical Analysis?"	Invited, Los Alamos Nat. Lab., Los Alamos, NM, Nov. 17, 1983
	Ramsey, J. M.; Whitten, W. B. "New Laser Techniques for Analytical Chemistry"	ACD/ORNL Summer Lecture Series, Oak Ridge Nat. Lab., July 8, 1983
	Ramsey, J. M.; Whitten, W. B. "Optical Absorbance Through Temporal Measurements"	Invited, 30th Annu. Conf. of the Spectros. Soc. of Canada, British Columbia, CANADA, Oct. 6-8, 1983
	Ramsey, J. M.; Whitten, W. B. "A Field Correlation Technique for Microwave Spectrometry"	Pittsburgh Conf. and Exposition on Anal. Chem. and Applied Spectros., Atlantic City, NJ, Mar. 7-12, 1983
	Ramsey, J. M.; Whitten, W. B. "Delayed Lasing with Tunable Gain Media"	Pittsburgh Conf. and Exposition on Anal. Chem. and Applied Spectros., Atlantic City, NJ, Mar. 7-12, 1983
	Ramsey, J. M.; Whitten, W. B. "Laser Intracavity Absorbance by Time Domain Measurements"	Invited, DOE Contractors' Workshop on "Advanced Laser Technol. for Chem. Measure.", Livermore, CA, June 8-9, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Ramsey, J. M.	Ramsey, J. M. "Chemical Analysis by Time-Domain Measurements"	Invited, Dept. of Chem., Ohio State Univ., Columbus, OH, Jan. 25, 1983
	Ramsey, J. M."New Laser Techniques for Analytical Chemistry"	Anal. Chem. Div. Summer Lecture Series, Oak Ridge Nat. Lab., July 8, 1983
	Ramsey, J. M. "Picosecond Phase Fluorimetry with A Self-Modulated Argon-Ion Laser"	Invited, Pittsburgh Conf. on Anal. Chem. and Applied Spectros., Atlantic City, NJ, Mar. 7-12, 1983
Ross, H. H.	Ross, H. H. "Scintillation Counting: An Extrapolation into the Future"	Invited, Advances in Scintillation Counting, Banff, Alberta, CANADA, May 15-18, 1983
Rosseel, T. M.	Rosseel, T. M.; Dale, J. M.; Hulett, L. D. Krause, H. F.*; Raman, S.*; Vane, C. R.*; Young, J. P. "Heavy-Ion Induced X-Ray Fluorescence as a Chemical Probe"	10th Fed. of Anal. Chem. and Spectros., Soc. Meet., Philadelphis, PA, Sept. 25-30, 1983
	Rosseel, T. M. "The Scanning Electron Microscope"	Sci. Minimester; Prof. Training Semin., Oak Ridge Assoc. Univ., Oak Ridge, TN, May 27, 1983
	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.*; Raman, S.*; Vane, C. R.*; Young, J. P. "Analytical Potential of Heavy-Ion Induced X-Ray Satellite Emission"	Invited, Rohm & Haas, Spring, House, PA, Sept. 28, 1983
	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.*; Raman, S.*; Vane, C. R.; Young, J. P. "Heavy-Ion Induced X-Ray Satellite Emission as a Chemical Probe"	26th Oak Ridge Nat. Lab. Conf. on Anal. Chem. in Energy Technol, Knoxville, TN, Oct. 11-13, 1983
	Rosseel, T. M. "The Scanning Electron Microscope"	Oak Ridge Assoc. Univ. Training Lecture, Oak Ridge, TN, Jan. 17, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Rosseel, T. M.	Rosseel, T. M. "Apple II Control of an X-Ray Diffractometer"	ORNL Course on Prof. Use Personal Computers in R/D, Oak Ridge, TN, May 23, 1983
	Rosseel, T. M.; Dale, J. M.; Hulett, L. D.; Krause, H. F.*; Raman, S.*; Vane, C. R.*; Young, J. P. "Heavy-Ion Induced X-Ray Fluorescence - A Chemical Probe of Materials"	3rd Annu. Tenn. Valley AVS Symp., Knoxville, TN, May 9-11, 1983
Scott, T. G.	Scott, T. G. "Data Management and Report Writer Programs Developed by Use of System 1022"	4-Lab Anal. Infor. Meet. Paducah, KY, Nov. 15, 1983
	Scott, T. G. "Sequential Analysis of Strontium-90, Uranium and Plutonium Isotopes in Ashed Fish"	29th Annu. Conf. on Bioassay, Anal. and Environ. Chem., Seattle, WA, Oct. 12-13, 1983
Shaw, R. W.	Shaw, R. W.; Howell, H. E.*; Mamantov, G.*; Wehry, E. L.* "Matrix Isolation Photoacoustic Spectroscopy"	26th Oak Ridge Nat. Lab. Conf. on Anal. Chem. in Energy Technol., Knoxville, TN, Oct. 11-13, 1983
Smith, D. H.	Smith, D. H.; Walker, R. L.; Pritchard, C. A. "Evaluation of Internal Standards in Uranium and Plutonium Isotopic Ratio Measurements"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
	Smith, D. H.; Walker, R. L.; Carter, J. A. "Sampling and Assaying Radioactive Solutions for Plutonium and Uranium"	185th Am. Chem. Soc. Meet., Seattle, WA, March 20-25, 1983
	Smith, D. H. "Thermal Ionization Quadrupole Mass Spectrometer for On-Site Isotopic Analysis"	Invited, Seminar, IAEA, Vienna, Austria, June 27, 1983
	Smith, D. H. "Application of Internal Standards to Uranium Isotopic Ratio Measurements	Invited, 17th Union Carbide Corp. Nucl. Div. and Goodyear Atomic Plant Anal. Chem. Forum, ORGDP, Oak Ridge, TN, July 26, 1983
Stegnar, P.*	Stegnar, P*, Eldridge; Teasley, N. A.; Oakes, T. W.* "Environmental Applications for an Intrinsic Germanium Well Detector"	26th ORNL-DOE Conf. on Anal. Chem. in Energy Tech., Knoxville, TN, Oct. 11-13, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Stewart, J. H.	Stewart, J. H., Jr. "Status and Use of Inductively Coupled Plasma Spectroscopy Within the Union Carbide Nuclear Division"	Invited, Am. Soc. for Test. and Mater., Lake Buena Vista, FL, Jan. 17-21, 1983
	Stewart, J. H., Jr. "Multidisciplinary Analytical Coordination"	Invited, 16th Union Carbide Corp. Nucl. Div. Anal. Services Forum, Y-12 Plant, Oak Ridge, TN, Mar. 22, 1983
Todd, P. J.	Todd, P. J. "Applications of a SIMS-MS/MS Device"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
	Danis, D. O.*; Todd, P. J.; Gellene, J. C.*; Ray, J. C.*; Carpenter, B. K.*; McLafferty, F. W.*; "Neutralization-Reionization Mass Spectrometry"	31st Annu. Conf. on Mass Spectrom. and Allied Topics, Boston, MA, May 8-13, 1983
Tomkins, B. A.	Tomkins, B. A. "Applications of Combined HPLC/HPLC and HPLC/GC to the Characterization of Coal-Derived Products"	Invited, 7th Annu. Meet. on the Charac. of Coal-Derived Materials, Pittsburgh, PA, May 19-20, 1983
	Tomkins, B. A ; Brazell, R. S. "Determination of Nitro-Derivatives of Polycyclic Aromatic Hydrocarbons in Particulate Matter Using a Thermal-Energy Analyzer"	Am. Chem. Soc. Nat. Meet., Washington, DC, Aug. 26-Sept. 2, 1983
Vargo, J. D.*	Vargo, J. D.*; Sepaniak, M. J.*; Maskarinec, M. P. "An Efficient Ultraviolet and Laser Fluorescence Detector Cell for Use in Open Tubular Liquid Chromatography"	Pittsburgh Conf. and Exposition and Anal. Chem. and Applied Spectrosc. Atlantic City, NJ, Mar. 7-12, 1983
Walker, R. L.	Walker, R. L. "Resin Bead Technique of Nd Analysis for Burn-up Estimation"	Workshop on Anal. Chem. Related to Canada's Ind., Helca Is., Manitoba, CANADA Oct. 24-26, 1983
Young, J. P.	Young, J. P.; Haire, R. G.*; Peterson, J. R.* Ensor, D. D.* "Chemical and Physical Consequences of Alpha and Beta-Decay in the Solid State	Invited, Am. Chem. Soc. Meet., Seattle, WA, Mar. 20-25, 1983

SPEAKER	AUTHOR(S) AND TITLE	PRESENTED AT
Young, J. P.	Young, J. P.; Donohue, D. L.; Smith, D. H. "Analytical Applications of Resonance Ionization Mass Spectrometry"	185th Am. Chem. Soc. Meet., Seattle, WA, March 20-25, 1983
	Donohue, D. L.; Young, J. P. "Removal of Isobric Interferences by Resonance Ionization Mass Spectrometry"	Invited, SPIE's 27th Annu. Int. Tech. Symp., San Diego, CA, Aug. 21-26, 1983
	Young, J. P. "Spectral Characterization Concerned with Several Research Frontiers"	Invited, Symp. on Chem. Measure. and Charac., Indiana Univ., Bloomington, IN, Oct. 21-22, 1983

ARTICLES REVIEWED OR REFEREED FOR PERIODICALS

	Anal. Chem.	*Anal. Chim. Acta*	*Anal. Lett.*	*Health Physics*	*J. Radioanal. Chem.*	*ORNL Reports*	*Proposals*	*Radiochem. Radioanal. Lett.*	*Others*	*Total*
Brazell, R. S.	4						1			5
Brooksbank, R. D.									1	1
Buchanan, M. V.	2						1		1	4
Carter, J. A.	2						1			3
Caton, J. E.		1					1		1	3
Christie, W. H.	3						1			4
Costanzo, D. A.						3			1	4
Dale, J. M.							1			1
Donohue, D. L.	2									2
Eldridge, J. S.				1						1
Feldman, C.	4						3			7
Glish, G. L.	1	1					2			4
Goeringer, D. E.							1			1
Griest, W. H.	4					1			5	10
Guerin, M. R.							2		5	7
Holmberg, R. W.									1	1
Hulett, L. D.							1		1	2
Jenkins, R. A.						1			2	3
Keller, J. M.						1			1	2
Klatt, L. N.	1	1				1				3
Laing, W. R.					1				4	5
Lee, D. A.					1				4	5
Lyon, W. S.	1	4	1		1		6	3	2	20
Manning, D. L.	4									4
Maskarinec, M. P.	4						1			5
Shaw, R. W.							2			2
Shults, W. D.	1									1
Stewart, J. H.									1	1
Stokely, J. R.	1						2			3
Tomkins, B. A.	10									10
Whitten, W. B.							1			1
Young, J. P.	4						3		3	10
Total	48	7	1	1	3	7	32	3	33	135

DIVISIONAL MAN-POWER AND FINANCIAL SUMMARY
FY 1983

Source	$K	PY
DOE programs		
Health and Environmental Research	896	7.8
Basic Energy Sciences	1,291	11.8
Nuclear Energy	202	3.3
Fossil Energy	345	3.6
Safeguards and Security	60	0.5
Total DOE programs	2,794	27.0
Work for others - federal agencies		
Department of Defense (U.S. Army)	784	6.4
National Cancer Institute	467	3.9
Environmental Protection Agency	300	2.3
National Regulatory Commission	131	0.9
Miscellaneous	55	0.6
Total work for others - federal agencies	1,737	14.1
Work for others - nonfederal agencies		
Electric Power Research Institute	162	1.4
Protective Coating Companies	150	2.2
DuPont (SRL)	90	1.3
Westinghouse	70	1.0
Miscellaneous	241	2.8
Total work for others - nonfederal agencies	713	8.7
Support/Services		
ORNL divisions	4,120*	67.4
Other clients	596	9.8
	4,716*	77.2
Total financial plans	9,960	127.0

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

December 31, 1983

ANALYTICAL CHEMISTRY DIVISION

W D SHULTS, DIRECTOR
S J RANNEY, SECRETARY
D A FORD, SECRETARY

TECHNICAL SUPPORT

W R LAING, QUALITY ASSURANCE COORDINATOR[1]
J F EMERY, EMERGENCY SAMPLES COORDINATOR[1]
L D HULETT, SOLIDS/SURFACES CHARACTERIZATION COORDINATOR[1]
R E JONES, *RADIATION CONTROL OFFICER*[1]
H H ROSS, TECHNOLOGY UTILIZATION OFFICER[1]
J H STEWART, JR, ENVIRONMENTAL PROTECTION OFFICER[1]
J F EMERY, COMPUTER SYSTEMS SECURITY OFFICER[1]

ADMINISTRATIVE SUPPORT

J M HOLLADAY, FINANCE OFFICER[FM]
A L HARROD, ADMINISTRATIVE ASSISTANT[1]
A L HARROD, SAFETY OFFICER[1]
C E HIGGINS, OMBUDSMAN[1]
S D CATES, *AFFIRMATIVE ACTION REPRESENTATIVE*[1]

BIO/ORGANIC ANALYSIS

M R GUERIN, SECTION HEAD
P J MULLINS, SECRETARY
H C CASON, SECRETARY
C K BAYNE, STATISTICS[CS]

ANALYTICAL CHROMATOGRAPHY

- W H GRIEST, GROUP LEADER
- C E HIGGINS[1]
- D L MANNING
- M P MASKARINEC
- M J SEPANIAK[2]
- B A TOMKINS
  - S H HARMON
  - R W HARVEY
  - R R REAGAN

SEPARATIONS AND SPECTROSCOPY

- J E CATON, GROUP LEADER
- M V BUCHANAN
- B R CLARK
- C-H HO
- A R JONES
- C Y MA
- R B QUINCY, JR
- I B RUBIN
  - G OLERICH

SPECIAL PROJECTS

- R W HOLMBERG, GROUP LEADER
- R S BRAZELL
- T M GAYLE[IC]
- S K HOLLADAY
- R A JENKINS
- J H MONEYHUN
  - G M HENDERSON
  - D O PAIR

ANALYTICAL METHODOLOGY

W S LYON, JR, SECTION HEAD
N G VINEYARD, SECRETARY

ANALYTICAL INSTRUMENTATION

- H H ROSS, GROUP LEADER[1]
- D A BOSTICK
- C FELDMAN
- L N KLATT
- G MAMANTOV[2]
- J M RAMSEY
- J E STRAIN
- W B WHITTEN
- J P YOUNG
  - B L HARWARD[3]

ANALYTICAL PHYSICS

- L D HULETT, JR, GROUP LEADER[1]
- J M DALE
- T M ROSSEEL

GENERAL AND ENVIRONMENTAL ANALYSIS

J R STOKELY, SECTION HEAD
S D CATES, SECRETARY[1]

CHEMICAL AND PHYSICAL ANALYSIS

J H STEWART, JR, GROUP LEADER[1]

- J E ATTRILL, TASK LEADER
  - B PHILPOT
  - K I WEBB

- H G DAVIS, TASK LEADER
  - C S ALLEY
  - J H HACKNEY
  - W I ROGERS

- H W DUNN
- C S MacDOUGALL
- J C PRICE

ENVIRONMENTAL ANALYSIS LABORATORIES

- N M FERGUSON, GROUP LEADER
- W R MUSICK
- J W WADE
  - I S BARRINGER
  - S J MORTON

ACTIVATION ANALYSIS

- J F EMERY, GROUP LEADER[1]
- L C BATE
- F F DYER
  - K J NORTHCUTT

ENVIRONMENTAL RADIOCHEMISTRY

SPECIAL PROJECTS

- J S ELDRIDGE, TASK LEADER
  - N A TEASLEY, JR

LOW-LEVEL RADIOCHEMICAL ANALYSIS

- T G SCOTT, GROUP LEADER
- M P MAY
- L M ROSEBERRY
- A J WEINBERGER
  - L D BIBLE
  - P S GOUGE
  - C C GRANGER
  - W C MASSEY
  - S H PRESTWOOD

MASS AND EMISSION SPECTROMETRY

J A CARTER, SECTION HEAD
R L WALKER, GROUP LEADER[1]
D C SMITH, SECRETARY

ACTINIDES AND ISOTOPIC MASS SPECTROMETRY

- R L WALKER, TASK LEADER[1]
- L K BERTRAM
- C A PRITCHARD
- J R SITES
  - L QUINN
  - M M HONAKER
  - E G MILLER
  - H C SMITH
  - C L WATSON
  - D I WHALEY

ELEMENTAL SPECTROCHEMISTRY AND SECONDARY ION MASS SPECTROMETRY

- W H CHRISTIE, TASK LEADER
- R E EBY
- G S GROENEWOLD[5]
- L LANDAU
- S A MacINTYRE
- P J TODD
  - R C BRYANT
  - G I GAULT
  - E H WATERS

R&D PROGRAMS AND PROJECTS

- D H SMITH, TASK LEADER
- D L DONOHUE
- G L GLISH
- D E GOERINGER
- E H McBAY
- H S McKOWN
- S A McLUCKEY[6]
- T R MUELLER[5]

RADIOACTIVE MATERIALS ANALYSIS

W R LAING, SECTION HEAD[1]
L K PLEMONS, SECRETARY

RADIOACTIVE MATERIALS ANALYTICAL LABORATORY

- D A COSTANZO, GROUP LEADER[1]
- J L BOTTS, TASK LEADER
- R D BROOKSBANK[1]
- R E JONES[1]
- F L LAYTON
  - R BURNS
  - W M CALDWELL
  - L R HALL
  - P I HOWELL
  - P W PAIR
  - J K THOMPSON
  - S C WELLS

TRANSURANIUM ANALYTICAL LABORATORY

- J H COOPER, GROUP LEADER
- J M PEELE, TASK LEADER
  - E C FEARNOW — A SHIFT
  - M E PETERS, JR
  - C C FOUST — B SHIFT
  - R A JONES — C SHIFT
  - V G McCLUNG
  - J D PENDLETON — D SHIFT
  - C P BAKER

PROGRAMS AND PROJECTS

- D A COSTANZO, GROUP LEADER[1]
- R D BROOKSBANK[1]
- J M KELLER
- D A LEE

[CS] *COMPUTER SCIENCES DIVISION*
[FM] *FINANCE AND MATERIALS DIVISION*
[IC] *INSTRUMENTATION AND CONTROLS DIVISION*

[1] *MULTIPLE ASSIGNMENT*
[2] *ADJUNCT RESEARCH PARTICIPANT, THE UNIVERSITY OF TENNESSEE*
[3] *PREDOCTORAL STUDENT, THE UNIVERSITY OF TENNESSEE*
[4] *LEAVE OF ABSENCE*
[5] *ORAU POST-DOCTORAL APPOINTMENT*
[6] *WIGNER FELLOWSHIP APPOINTMENT*

ORNL-6039
Distribution Category UC-4

INTERNAL DISTRIBUTION

1. J. E. Attrill
2. H. Adair
3. S. I. Auerbach
4. S. M. Babcock
5. J. B. Ball
6. D. A. Bostick
7. R. S. Brazell
8. R. D. Brooksbank
9. M. V. Buchanan
10. W. D. Burch
11. J. A. Carter
12. J. E. Caton, Jr.
13. W. H. Christie
14. D. A. Costanzo
15. J. M. Dale
16. D. L. Donohue
17. J. Dorsey
18. F. F. Dyer
19. J. S. Eldridge
20. J. F. Emery
21. K. Erb
22. D. Eyman
23. C. Feldman
24. N. M. Ferguson
25. J. C. Franklin
26. W. Fulkerson
27. T. M. Gayle
28. D. E. Goeringer
29. R. A. Griesemer
30. W. H. Griest
31-36. M. R. Guerin
37. R. L. Hahn
38. C.-h. Ho
39. R. W. Holmberg
40. L. D. Hulett
41. D. W. Jared
42. R. A. Jenkins
43. P. R. Kasten
44. S. V. Kaye
45. J. M. Keller
46. L. N. Klatt
47. E. H. Krieg
48. W. R. Laing
49. C. E. Lamb
50. F. L. Layton
51. D. A. Lee
52-53. W. S. Lyon
54. F. C. Maienschein
55. T. Malinauskas
56 G. Mamantov
57. D. L. Manning
58. M. P. Maskarinec
59. L. E. McNeese
60. R. Morrow
61. W. R. Musick
62. F. R. Mynatt
63. T. W. Oakes
64. G. W. Oliphant
65. D. C. Parzyck
66 J. M. Peele
67. J. J. Pinajian
68. H. Postma
69. M. L. Poutsma
70. J. M. Ramsey
71. C. R. Richmond
72. D. E. Reichle
73. P. S. Rohwer
74. L. M. Roseberry
75. H. H. Ross
76. T. M. Rosseel
77. T. H. Row
78. I. B. Rubin
79. T. G. Scott
80. R. W. Shaw
81-100. W. D. Shults
101. J. R. Sites
102. D. H. Smith
103. J. H. Stewart
104. J. R. Stokely
105. P. J. Todd
106. J. H. Swanks
107. B. A. Tomkins
108. H. E. Trammell
109. C. W. Weber
110. J. R. Weir, Jr.
111. R. Wiltshire
112. J. C. White
113. W. B. Whitten
114. M. K. Wilkinson
115. P. Woolridge
116. R. G. Wymer
117. J. P. Young
118. A. Zucker
119. Biology Library
120. Laboratory Shift Supv.
121. ORNL-Y-12 Library,
  Document Reference
122. Laboratory Records,
  ORNL-RC
123. ORAU Technical Library
  (MERT)
124. ORAU/UPD
  Beth Jinkerson
125. PGDP Library
  (B. Barbre)
126-127. Central Research
  Library
128-131. Laboratory Records
132-134. Technical Publication

EXTERNAL DISTRIBUTION

135. D. A. Coffin, Health Effects Research Laboratory, MD-52, EPA, Research Triangle Park, NC 27711
136. Paul Cunningham, Analytical Chemistry Division, Los Alamos National Laboratory, CMB-1, MS G740, Los Alamos, NM 87545
137. P. Duhamel, Pollutant Characterization & Safety Research, Office of Health & Environmental Research, GTN, DOE, Washington, DC 20545
138. G. Goldstein, Pollutant Characterization & Safety Research, Office of Health & Environmental Research, GTN, DOE, Washington, DC 20545
139. J. A. Goleb, DOE, Division of Safeguards and Security, Washington, DC 20545
140. J. Grasselli, Standard Oil Company (Ohio), 4420 Warrensville Center Road, Cleveland, OH 44128
141. David W. Green, Chemical Technology Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439
142. J. Lamb, Processes & Techniques Branch, ER-162, Division of Chemical Sciences, Office of Basic Energy Sciences, U.S. Department of Energy, Mail Station J-309, GTN, Washington, DC 20545
143. B. C. Musgrave, Measurement Science Division, L-310, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550
144. R. B. Neel, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, 5650 Nicholson Lane, Washington, DC 20555
145. M. Novotny, Chemistry Department, Indiana University, Bloomington, IN 47401
146. Office of Assistant Manager, Energy Research and Development, DOE, Oak Ridge Operations Office, Oak Ridge, TN 37830
147. T. B. Owen, National Cancer Institute, Bethesda, MD 20014
148. Institute for Energy Analysis, P.O. Box 117, Oak Ridge, TN 37830
149. E. S. Pierce, Division of Chemical Sciences, GTN, DOE, Washington, DC 20545
150. Vassilis C. Stamoudis, Energy & Environment System, Bldg, 362, Argonne National Lab, Argonne, IL 60439
151. D. Stevenson, Processes & Techniques Br., Division of Chemical Sciences, Office of Basic Energy Sciences, DOE, Washington, DC 20545
152. James W. Taylor, Chemistry Dept., Univ. of Wisconsin, 1101 W. University Avenue, Madison, WI 53706
153. USDA SEA-TIS National Agricultural Bldg., Current Serial Records, Beltsville, MD 20705
154. Donald E. Walsh, University Research, University of Mississippi, University, MS 38677
155. R. W. Wood, Pollutant Characterization & Safety Research, Office of Health & Environmental Research, GTN, DOE, Washington, DC 20545
156. D. J. Wynn, USATHAMA, DRX TH-TE-A, Bldg. E4585, Aberdeen Proving Ground, MD 21010

157-311. Distribution as shown in TID-4500 under Chemistry category (25 copies--NTIS)

☆U.S. GOVERNMENT PRINTING OFFICE: 1983-746-081/4006