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Department of Chemistry • College of Liberal Arts
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(NOTICE: This is an application under DOE Program Solicitation No. DE-PS05-85OR21502 due 4:30 p.m., December 21, 1984. Date and time of receipt to be logged and also marked on this package.)

FROM: Dr. Gleb Mamantov
Department of Chemistry
University of Tennessee
Knoxville, TN 37996

TO: DOE University Research Instrumentation Program
Energy Programs and Support Division
U. S. Department of Energy
Oak Ridge Operations
200 Administration Road
Oak Ridge, Tennessee 37830

85-02-082

1076239

U.S. DEPARTMENT OF ENERGY
UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM

COVER PAGE

(THIS PAGE MUST BE THE FIRST PAGE OF THE APPLICATION)

85-02-082

1. Name of Institution: The University of Tennessee

2. Address: City Knoxville 3. State Tennessee 4. ZIP 37996-1600

5. Principal Investigator: Professor Gleb Mamantov

6. Department: Chemistry

7. Telephone: Area Code 615 Office: 974-3141 Home: ____

8. Title of Application: High Resolution Mass Spectrometer

9. Research Area: Health and Environmental; Advanced Materials; Catalysis; Geoscience

10. Total DOE Funding for Research in Selected Area, (During the last two calendar years): $ 931,000

11. Estimated Purchase Cost of Equipment: $ 592,000

12. Amount Requested from DOE: $ 492,000

List all Federal agencies which are currently considering proposals from the institution involving the same or similar equipment.

13. Agency: None Agency Proposal Number: ____
14. Agency: ____ Agency Proposal Number: ____

NOTE: *The institution is responsible for informing DOE if a proposal involving the same or similar equipment is submitted to a federal agency prior to the announcement of DOE's URI awards.*

15. List any federal agency which has provided funds to the institution during the past two years for the same or similar equipment.

Agency: None Amount of Funds: ____

16. Please check one of the following :

☒ I authorize external review of this proposal.

☐ I do not authorize external review of this proposal.

Signature of Principal Investigator: Gleb Mamantov Date: 12/19/84

Name and Title of Institutional Official (President or Designee)	Name and Title of Financial Officer
Thomas L. Bell	A. David Martin
Assistant Dean for Research	Treasurer
Signature: Thomas L Bell	Signature: A David Martin
Date: December 19, 1984	Date: December 19, 1984

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U.S. DEPARTMENT OF ENERGY
UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM

BUDGET PAGE

ESTIMATED COSTS

Instrumentation	Requested of DOE	Institution's Share *(1)*	Other Federal Funds *(2)*	TOTAL
A. Purchase Price *(3)*	492,000	100,000	0	592,000
B. Estimated Cost Sharing (Shipping, installation, etc.)	X X X X	19,000	-	19,000
C. TOTAL	492,000	119,000		611,000

NOTES: *(1)* *Non-Federal funds only*

(2) *Estimate funds to be obtained from other Federal agencies for purchasing the instrument, user charges, etc.*

(3) *Only the purchase price of the instrumentation is eligible for DOE funding through this program.*

A. Purchase Price (Detail)

Description	Quantity	Total Estimated Unit Price	Total
ZAB-E mass spectrometer, with high mass range, GC capability, jet separator, solids probe, positive/negative ions, reference inlet, alternate CI/EI source, FAB and MIKES capability; dedicated data system; PDP 1124/DEC RSX-11M multitasking system, with 80 Mbyte Winchester Hard Disk, 16 Mbyte removable, Printronix printer, DMA colar display	1	$592,000	$592,000
Subtotal:	1	$592,000	$592,000

B. Estimated Cost Sharing (Detail)

	Institution's Share	Other Federal Funds	Total
1. Shipping/Handling	--	--	--
2. Installation	--	--	--
3. Building/Laboratory Renovation	4,000		4,000
Subtotal:	4,000		4,000

DEPARTMENT OF ENERGY
UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM
CONTRACT SUMMARY FORM
of Participating Faculty

Contract/Subcontract No.	Principal Investigator	Title	Contract Dates FM MO	FM YR	TO MO	TO YR	Total Award Value	$ AMT Awarded for period 1984 to 1985	DOE Technical Monitor/Location
AS05-76ER02968	T. F. Williams	Studies of Radiation Produced Radicals and Radical Ions	1	84	12	87	318,000	96,000	ORO
AS05-83ER13113	S. Alexandratos	Synthesis of Polymeric Extractants	8	83	7	86	165,511	81,400	ORO
University of Calif. Subcontract 4502810	G. Mamantov	Studies of High Energy Cathodes and Anodes	4	84	3	85	15,921	15,921	LBL
AS05-80EV10363	G. Kabalka	Synthesis of Radio-pharmaceuticals	3	84	2	86	228,885	77,845	ORO
Union Carbide Sub Contract 7685 Proj. Auth x 61	G. Mamantov	Collaborative Research Program	10	84	9	85	40,000	40,000	ORNL
Union Carbide Sub Contract	G. Mamantov	Collaborative Research Program	12	84	11	85	45,000	45,000	ORNL
FG22-84PC70795	J. Kovac	Statistical Mechanics of Polymer Systems	12	84	10	87	272,000	82,354	ORO
FG05-84ER45114	J. Kovac	Macromolecular Chemistry of Coalification	7	84	7	87	174,904	67,580	ORO
AS05-81ER60006	G. Mamantov/ E. Wehry	Photochemistry of Polycyclic Organics on Coal Fly Ash	7	84	6	87	351,000	110,000	ORO
Union Carbide Sub Contract 19X-07248C	W. Bull	Collaborative Research Program	1	84	12	84	245,000	245,000	ORNL

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RELATED FEDERAL AGENCY CONTRACTS

Agency	Contract No.	Title	Contract FROM MO YR	Dates TO MO YR	Total Award Value
NSF	CHE-8317000	Fragmentation-Fluorescense Spectrometry	2/84	1/87	$336,362
NSF	CHE-8219210	Electroactive Polymers	7/83	12/86	182,500
NSF	CHE-8112965	Condensed Phase Isotope Effects	12/84	11/87	241,000
Army	DAA29-82-K-0115	Double Tailed Surfactants	4/82	9/85	180,000
NSF	CHE-8308362	Neutron Scattering from Micellar Systems	9/83	8/86	181,702
NSF	INST-8314066	Scattering from Biopolymer-Containing Reverse Micelles	7/84	12/87	13,835
NIH	CA33590-01	Early Breast Cancer Detection	2/83	1/86	263,551
NSF	RLL 8305855	New Rhodium Dimers	7/83	12/86	173,082
NSF	CHE-8411164	Ionic β-Elimination Reaction in the Gas Phase	12/84	11/87	154,000
NSF with ARO	DME8406825	Polymer Characterization by Electrohydrodynamic Ionization Mass Spectrometry	8/84	4/87	286,000

TABLE OF CONTENTS

SUMMARY

The Department of Chemistry seeks funding for a high resolution, high performance mass spectrometer, similar to the VG Ltd. ZAB-E, with features including high mass capabilities, maximum mass resolution of 100,000, an EI/CI source, positive/negative ions, FAB and FD ionization, GC/MS capability, and MS/MS in the form of the MIKES experiment. It will be capable of source interchangeability to permit the development of new ionization techniques.

This instrumentation will be used in several of the areas in the Notice of Program. Drs. WEHRY and MAMANTOV are studying photolytic processes involved in the degradation of pollutants on the surface of fly ash, the fate of these pollutants, and thus their health and environmental impact. Dr. SCHELL is interested in catalysis of hydride transfers in coal. Dr. KOVAC is interested in probing the mechanism of coal formation ("coalification"). Drs. BARNES and WOODS have synthesized and plan to characterize a number of organometallic compounds as catalysts. Dr. PAGNI seeks to better characterize the mechanism of photochemical reactions of PCB-like pollutants on natural (and model) surfaces. The work of Dr. CHAMBERS considers the mechanism of catalysis of electron transfer at functionalized polymer-coated electrodes. Dr. COOK would like to examine mass and charge distributions of polyelectrolytes, seeking correlations with their conductive properties. He also plans to examine natural polymers, developing analytical methodology (based on his unique electrohydrodynamic ionization source) for extracting both sequence information and characterization of the kinetics of enzymatic hydrolysis. His source may supplement FAB spectra to be obtained by Dr. ALEXANDRATOS, who needs a tool for characterizing the ion exchange polymers he has developed for selective scavenging and catalytic reduction of metal ions. Dr. BARTMESS is developing new ionization methods for use with compounds resistant to normal FAB techniques.

Dr. KABALKA is involved in the synthesis of radionuclides for medical applications. In addition to his work with coal, Dr. SCHELL is probing mechanisms of natural microbial action (e.g., in nitrogen fixation) and of natural inter-species recognition, including elucidation of synthetic routes to some of the products involved. Dr. ADCOCK is developing a synthetic route to fluoropolymers for use under conditions of high stress. Dr. COMPTON is interested in the fundamental stability of gas-phase, multiply charged negative ions.

This powerful spectrometer will facilitate research in virtually all areas of interest cited in the Notice of Program for the DOE University Research Instrumentation Program. This is particularly true because of our proximity and close collaborative ties with the Oak Ridge National Laboratory, which have led many of our faculty to be involved in DOE-sponsored research. A major aim of the new $36 million, five-year "Science Alliance" program is to foster cooperation between scientists at ORNL and the University of Tennessee, in order to enhance the quality of both.

This work involves more than half of the chemistry faculty at Tennessee. It will therefore involve a substantial fraction of our graduate students. While it is our intention that the equipment will be run by a full-time, qualified technician, students demonstrating sufficient need will be allowed to use the equipment, after an appropriate training period. There are currently a total of 60 graduate students in the groups mentioned in this proposal, of which 13 are supported all or in part by DOE funding. It would be expected that the research of more than half of these would be directly affected by the acquisition of the mass spectrometer.

NARRATIVE

Technical Merit and Departmental Capability.

The Department of Chemistry at The University of Tennessee, Knoxville, consists of 28 full-time faculty at the rank of Assistant Professor or above, plus four Adjunct Professors who are employed by the Oak Ridge National Laboratory (ORNL) and three part-time faculty. All of the faculty hold Ph.D.'s. The Department offers B.S. (ACS certified), M.S., and Ph.D. degrees, with programs in analytical, inorganic, organic, and physical chemistry, plus specializations in polymer and environmental chemistry, and in chemical physics. There are currently 99 graduate students and 15 postdoctoral researchers, plus nine staff members in the glass, electronics, and machine shops. The Department has traditionally been rated in the upper third of Ph.D. granting institutions in the country. Collaborative research efforts exist with colleagues in more than 11 foreign countries. We have a strong program in polymer chemistry, an extremely important discipline in which very few American universities maintain a degree program. This field of "new materials" plays a strong role in this proposal.

In addition, there have historically been strong ties between the Department and ORNL, due to the 30 mile proximity of the two institutions. This unique relationship has resulted in a great deal of collaborative research in energy-related topics, described below in the specific research projects. The Department has a number of research groups active in various areas of spectroscopy, including Raman, photoelectron, Fourier transform infrared, molecular fluorescence, and electron spin resonance, with a number of unique spectroscopic facilities within the Department. There has not in the past been active research in the field of mass spectrometry, however. This has been altered with the addition to the faculty in the past year of two people active in mass spectrometry and related topics: Dr. Kelsey D.

Cook, coming from the University of Illinois, and Dr. John E. Bartmess, from Indiana University. This will substantially enhance the Department's ability to use and maintain an instrument of the type proposed here.

This proposal seeks funding for a high resolution mass spectrometer, similar to the VG, Ltd. ZAB-E instrument, for energy-related research in the Department of Chemistry of the University of Tennessee. Such a spectrometer will facilitate research in virtually all areas of interest cited in the DOE Notice of Program. More than half of the faculty of the Chemistry Department are represented in this proposal as either major or minor users of such an instrument. The Department of Chemistry, in the years 1982-84, had funding from the Department of Energy of $931,000; our current fiscal year funding level from DOE sources, as noted in the faculty resumes, is $811,100, or approximately 37% of the total outside funding of $2.2 million.

Instrument Description.

The instrument requested is a high resolution mass spectrometer, similar to the ZAB-E instrument manufactured by VG, Ltd. It will be capable of a mass range of 3000 daltons at 10 kV accelerating potential and a maximum mass resolution of 100,000. It will be equipped with a number of ionization methods: electron impact, chemical ionization, positive/negative ion capability, fast atom bombardment, direct solids probe, and field ionization. There will be capability for GC/MS at a full range mass scan and return in approximately 1 sec, and will include a full multitask data system. The "reverse geometry" of the instrument will allow for the MS/MS experiment for determination of ion fragmentation patterns by the metastable ion kinetic energy method (MIKES). The instrument source will be capable of modification to allow for interchangeable use of other sources built in-house, including the electrohydrodynamic ionization technique and the electrochemical FAB probe described later in this proposal. The total purchase cost of such an instrument is $592,000.

This equipment represents the current state-of-the-art in an important field of analysis whose capabilities have expanded dramatically in the last five years. The mass range, speed of scan, flexibility of computer control, and, perhaps most importantly, flexibility of ionization methods, permit its utilization in problems of chemical characterization which would be virtually unsolvable without this new technology.

Justification of the Instrumentation.

The need for this equipment arises from the lack of suitable mass spectrometry facilities on-campus capable of carrying out the energy-related research described here. The mass spectrometric facilities of the Department of Chemistry currently consist of a Hewlett-Packard 5980 GC/quadrupole mass spectrometer that is 7 years old. This instrument, even when new and up to specifications, by reason of being a quadrupole instrument, is limited to a mass range of less than 800 daltons and a mass resolution of no better than 1000. It is thus incapable of the high resolution required for most of the proposals herein, or the high mass range needed for the many aspects of the polymer materials work. It does not have any of the newer volatilization techniques such as SIMS, FI, FD, or FAB needed to obtain spectra from most polymers and metal catalysts, due to their low volatility. Due to the lack of faculty on the staff who were involved in mass spectrometry research in the past, the department's instrumentation in this area has not been kept up to date. As a result, most investigators wishing to use mass spectrometry have had to rely on outside facilities, with concommitant time delays and inconvenience due to sample deterioration. Professor Kabalka alone has spent over $3000 in the last year for carbon-hydrogen analyses and exact mass determinations at a number of outside centers. Many of the other faculty have simply not used mass spectrometry in their research, even though it may have been the method of choice for analysis or experimentation, due to the lack of suitable in-house capabilities, and the quality of what was available. We note that while there are close ties with ORNL, this has not extended to include access to their mass spectrometry facilities on a routine basis. The majority of the mass spectrometric instrumentation at ORNL is at the Y-12 site where access is limited for security reasons. Many of the instruments there are designed for very specific uses, such as spark-source or isotope ratio, and are used extensively for certification work. These are neither applicable to much of the research described here, or available. The more general ORNL mass spectrometers are not usually free for use in outside work.

Research Projects.

The acquisition of such equipment would allow the many researchers involved in energy-related fields within the department to increase productivity, both in terms of time and money, and to perform experiments that would not be accessible at all if outside instrumentation were to be used. For example, Drs. Cook and Bartmess propose to do work involving temporary reconfiguration of the source area of the mass spectrometer, which is unlikely to be permitted at regional mass spectrometry centers; Drs. Wehry and Mamantov have a large number of analytical samples to be tested in work on PAH adsorption on fly ash; Dr. Barnes' research involves air sensitive organometallic catalysts that must be analyzed on-site to prevent decomposition; and Dr. Kabalka's work with radiopharmaceuticals likewise involves compounds with limited lifetimes.

Dr. Gleb Mamantov and Dr. E. L. Wehry: High Resolution Mass Spectrometric Studies of Polycyclic Organic Matter Adsorbed on Coal Fly Ash

We have been investigating the degradation of polycyclic aromatic hydrocarbons (PAHs) adsorbed on coal fly ash and other solid surfaces[1]; this research is supported by the Office of Health and Environmental Research of the Department of Energy[2]. Of particular concern is the photochemical reactivity of carcinogenic PAHs, such as benzo[a]pyrene, on airborne particulate substrates. Studies of reactions of gaseous co-pollutants, such as NO_2, with adsorbed PAHs also are in progress.[2] We have observed that PAHs are significantly less susceptible to photodecomposition when adsorbed on fly ash surfaces than when adsorbed on other solids (such as alumina or silica) or in the form of pure solids or in liquid solution. These results indicate that the atmospheric residence times of PAHs adsorbed on ash released from coal-fired steam plants may be significantly greater than has generally been believed. Different ashes stabilize PAHs to phototransformation with different efficiencies[2]; the various chemical and physical characteristics of ash surfaces responsible for these differences have yet to be fully elucidated.

Samples for photochemical study are prepared by depositing the PAH onto the ash from the vapor phase[3], as a means of simulating the actual environmental process whereby PAHs deposit on environmental particles. However, in order to analyze the extent of PAH photodecomposition with adequate precision, it has generally been necessary to deposit the PAHs at levels on the order of 50 μg PAH per g of ash, considerably larger than the concentrations of PAHs found in real samples of emitted ash. This situation has been brought about by inadequacies in the analytical techniques currently used for adsorbed PAHs. To be truly relevant to environmental considerations, these studies should use PAH concentrations of 1 μg(or less) of PAH per g of ash.

The analytical procedure currently used consists of Soxhlet extraction of an illuminated fly ash sample, followed by UV absorption or fluorescence analysis of the extract. This technique suffers from several shortcomings. First, recoveries of PAHs and photodecomposition products via extraction often are not quantitative[4,5]. Second, UV absorption and fluorescence spectrometry produce little, if any, information that can be used reliably to identify photoproducts. Moreover, many anticipated products of PAHs (e.g., quinones) are unlikely to be fluorescent. There is a need for analytical procedures with greater sensitivity and a higher information content for identifying unknown compounds.

In principle, gas chromatography/mass spectrometry (GC/MS) is an obvious choice for an analytical problem of this nature. In practice, however, our present mass spectrometric instrumentation provides neither the sensitivity nor the mass resolution required for this purpose. There have been numerous instances in which solvent extracts of illuminated fly ash samples have been colored (indicating the presence of one or more phototransformation products), yet we have been unable to obtain mass spectra of those products with our spectrometer. Acquisition of a more sensitive spectrometer should solve this problem, permitting identification and quantitation of photodegradation products using ash samples containing environmentally-realistic quantities of adsorbed PAHs.

It would be highly desirable in selected cases to be able to detect parent PAH and transformation products directly on the ash surface. Optical spectrometric techniques are unsuitable for this purpose because of the small concentrations of adsorbed PAHs in realistic samples and the strong background absorption and fluorescence of fly ashes. Most "surface spectroscopies" either are insufficiently sensitive (e.g., ESCA) or subject both the adsorbates and the ash surfaces themselves to unacceptable damage (e.g., SIMS). We have found that direct insertion probe mass spectrometry can on occasions provide indications of the presence of photodegradation products. Again, however, the extremely limited sensitivity and mass resolution of our present mass spectrometer are such that useful results cannot be obtained. A new mass spectrometer of greatly improved capabilities will improve the utility of direct-probe mass spectrometry for identification of photoproducts.

It is also important to examine the photoreactivity of PAHs in the presence of other gaseous species, such as NO_2 and O_3.[2,6] Nitro derivatives of some PAHs (which may be formed by reactions of adsorbed PAHs with HNO_3) are among the most potent known mutagens.[7] There are indications that nitro derivatives of PAHs are themselves unstable with respect to photodegradation,[8] and it is of interest to know how the photoreactivity of these very mutagenic compounds is influenced by adsorption on particulate surfaces. A major problem in these studies is that authentic samples of anticipated photoproducts are unavailable. Thus, analytical techniques which require comparisons of spectra of photoproducts with those of pure samples of reference compounds are not applicable to the problem. The ability to carry out mass spectrometric measurements with high mass resolution (and with exact mass capabilities for unambiguous assignments of empirical formulas to parent and fragment ions) is essential if meaningful progress is to be made in this very challenging endeavor.

REFERENCES

1. W. A. Korfmacher, E. L. Wehry, G. Mamantov, and D. F. S. Natusch, Environ. Sci. Technol. 1980, 14, 1094.
2. E. L. Wehry, G. Mamantov, A. A. Garrison, R. A. Yokley, and R. J. Englebach, Proceedings of the Ninth International Symposium on Polynuclear Aromatic Hydrocarbons, Battelle Press, Columbus, O., in press.
3. A. H. Miguel, W. A. Korfmacher, E. L. Wehry, G. Mamantov, and D. F. S. Natusch, Environ. Sci. Technol. 1979, 13, 1229.

4. W. H. Griest and J. E. Caton, in Handbook of Polycyclic Aromatic Hydrocarbons (A. Bjorseth, Ed.), Marcel Dekker, New York, 1983, p. 95.

5. W. H. Griest and B. A. Tomkins, Sci. Total Environ. 1984, 36, 209.

6. D. Grosjean, K. Fung, and J. Harrison, Environ. Sci. Technol. 1983, 17, 673.

7. L. C. King, K. Loud, S. B. Tejada, and M. J. Kohan, Environ. Mutagenesis 1983, 5, 577.

8. A. Yasuhara and K. Fuwa, Chem. Lett. 1983, 347.

Dr. Spiro D. Alexandratos: Characterization of Polymeric Metal Ion Extractants by Mass Spectrometry

Efforts to improve metal ion recovery by liquid-liquid extraction, especially by eliminating the problem of extractant entrainment during phase separation, have led to studies in which the extractant ligand is chemically supported on a polymer backbone allowing for solid-liquid extraction systems. Our research has emphasized the area of polymer supported extractants. We have made significant progress through our discovery of dual mechanism bifunctional polymers wherein phosphinic acid ligands selectively extract transition metal ions from aqueous solutions and then reduce those with a reduction potential greater than 0.8eV to the atomic state. In studying such polymers, important experimental variables in the metal ion extraction process include the number of phosphinic acid groups which coordinate with a metal ion after exchange occurs, the degree of polymer [illegible] of choice for controlling the degree of substitution (which must not be allowed to fall below 50% because that allows polystyrene's hydrophobic character to dominate). The linear analogues can be expected to form metal ion complexes similar to the beads, especially if we maintain the same polymer/water ratio (1g polymer to 3g water) in order to obviate the effect of dilution. The soluble polymers would be made with linear polystyrene having degrees of polymerization up to 50 (the approximate length of polymer unit between crosslinks in our most lightly crosslinked resin). The functionalized polymer would be dissolved in solutions of different metal ions, sufficient time allowed for equilibrium to be attained, and analysis carried out by mass spectrometry.

FAB-MS allows for the generation of gas phase ions from polymers. With the proposed mass range of 10^4, we can study polymers with degrees of polymerization of 50 - 60. After characterizing the uncomplexed polymers, we will study the ability of the polymer to complex with metal ions by identifying the number of metal ions with which a chain at a given level of substitution and polymerization can complex. We can then develop a simple test for metal ion selectivity by placing the polymer in a polar solution of a mixture of cations and quantifying any selectivity through analysis of the resulting mass spectrum. Our complexes are ideally suited to FAB analysis because they involve pre-formed ions in solution and FAB is particularly sensitive for such samples. The associated fragmentation, however, can be a disadvantage given the possiblity of splitting off the metal ion prior to ejection from solution and so disrupting the equilibrium mixture. The likelihood of obtaining an erroneous picture from the FAB-MS will be checked by parallel EHMS experiments. Given that EHMS does not involve molecular fragmentation (as illustrated in an accompanying proposal), the results will be complementary to the FAB experiments in that the latter will give the structural information that the former does not.

Information generated from the above-outlined experiments on selectivity as a function of degrees of polymerization and substitution will be used as a guide in the synthesis of future resins for the recovery of strategic metals.

Dr. Jeffrey D. Kovac: The Macromolecular Chemistry of Coalification

Coals are three dimensionally cross-linked macromolecular networks containing up to 20% (wt.) of dissolved organic molecules having a broad range of molecular weights.[1] The chemistry of the coalification process is poorly understood. It may be a condensation polymerization of multifunctional small molecules, a polymer degradation and modification, or both of these at different times.[2] Techniques have been developed which allow the estimation of the crosslink density (the number average molecular weight between crosslinks, $\overline{M}_c$) for coals.[3] It is also possible to obtain the molecular weight distribution of the dissolved molecules using gel permeation chromatography (GPC).[2] With an appropriate theoretical structure these two pieces of information can provide great insight into the geochemistry of the coalification process.

With this in mind, we are measuring $\overline{M}_c$ and the molecular weight distribution of the soluble fraction of a series of geologically related coals of different ages in an attempt to better understand the chemistry of the coalification process. At the same time we are attempting to develop an appropriate theory of network formation to interpret the experimental results.

There are two potential problems with GPC separations of coal extracts. One arises because GPC separations are based on size. The relationship between size and molecular weight depends on the molecular shape, which may be very different for components of a mixture. The second is the possibility of specific interactions between the coal extract and the column packing which can significantly affect the separation mechanism. By contrast, mass spectrometry can provide a true molecular weight profile, and can therefore indicate whether our GPC separations are subject to either of these problems. Thus, the mass spectrometer proposed here will provide important check on the molecular weight distributions obtained from GPC.

The important features of the instrument for this project are its fast atom bombardment capability (for sampling and ionization of the labile nonvolatile coal extracts) and its extended mass range for detection of extract components with molecular weights of the order of 10,000.

REFERENCES

1. T. Green, J. Kovac, D. B. Brenner and J. Kovac, in "Coal Structure", R. A. Meyers, ed., Academic Press, N.Y., 1982, pp 299-382.

2. J. W. Larsen, M. Mohammadi, I Yiginsu, and J. Kovac, Geochim. Cosmochim. Acta., 48, 135 (1984).

3. T. K. Green, J. Kovac, and J. W. Larsen, Fuel, 63, 935 (1984).

Dr. George W. Kabalka: Radiopharmaceuticals

The objective of our DOE sponsored research is to develop new, rapid methods for incorporating short-lived radionuclides into agents for use in diagnostic nuclear medicine. During the initial phase of our program, we developed new methodology for incorporating iodine isotopes into long chain fatty acids which are currently used as heart imaging agents at a number of large medical research centers. Our methodology involves the intermediacy of organometallic reagents and their subsequent iodinations. One method we developed involves the iodination of organoborane compounds using no-carrier-added (very high specific activity) sodium iodide. The reaction is unique because it proceeds rapidly at room temperature in the presence of a variety of functional groups. Recently, we applied this new iodination methodology to the syntheses of a variety of radioiodinated agents which are of interest to our DOE supported medical collaborators at Oak Ridge National

Laboratory, Oak Ridge Associated Universities, and Massachusetts General Hospital. These new agents include tellurium substituted fatty acids, iodovinylestradiol (first synthesized at UTK) and iodovinylamino acid derivatives.

We are currently investigating the syntheses of oxygen-15 labeled alcohols in collaboration with Brookhaven National Laboratory. These are of value in positron emission studies of the human arterial system. The corresponding α-carbon-11 labeled alcohols are of even greater interest because of the longer half-life of carbon-11 (20 minutes) as compared to oxygen-15 (2 minutes). In addition, the new carbon insertion reaction can be utilized to synthesize more complex structures such as carbon-11 labeled estrone for use in receptor-site assays carried out in vivo.

The successful synthesis of reagents such as those outlined requires the synthesis of a large number of related (model) compounds in addition to the target molecules. As a general rule we synthesize dozens of related compounds in the course of a synthetic study. Most of these compounds have never been synthesized previously. These new reagents must be completely characterized before the results can be utilized. Currently we rely on NMR spectroscopy and quantitative elemental analysis for this characterization. The elemental analyses are carried out by commercial firms and are quite expensive. (Our average expenditures for analyses exceed $3,000 annually.) Even more important is the fact that many studies must be abandoned because of our inability to identify certain unknown products and reactive intermediates. The acquisition of a high resolution mass spectrometer would obviate these problems. The structural information obtained by employment of soft ionization techniques (especially FAB) should complement other data, and will be indispensable in cases where NMR has not been successful.

Dr. Robert N. Compton: Multiply Charged Negative Ions

Many of the properties of isolated singly charged negative ions are well understood and a number of text books have been written on the subject. The question of multiply charged negative ions in the gas phase, on the other hand, is controversial. Kiser[1] has summarized the evidence in favor of multiply charged negative ions with the opinion that such ions can exist for many microseconds and may be stable. We recently reviewed this evidence along with other reports and concluded that there is very little, if any, solid experimental evidence for such ions.[2] There are no theoretical calculations predicting stable multiply charged anions. However, Anbar and St. John[3] report that ions like SO_4^{2-}, FeF_6^{3-} and $RbBr_2^-$ can be field desorbed from surfaces containing these ions (e.g. SO_4^{2-} from H_2SO_4). In addition, we have presented some evidence, (albeit inconclusive), that AuF_6^{3-} can be produced at a surface.[2] In this experiment, ions of mass 103 ± 1 amu were produced from "burning" gold in fluorine gas. The mass is consistent with AuF_6^{3-}; unfortunately, the absolute mass calibration of the TOF mass spectrometer was insufficient to definitely ascribe the ion to AuF_6^{3-}. The metastability of AuF_6^{3-} was discussed in terms of a giant shape resonance in which two extra electrons reside in a potential well analogous to the Gamow model describing α-decay of the nucleus. Formation of multiply charged anions on surfaces overcomes the energetics problem of attaching an extra electron to a negative ion in the gas phase.

We propose to study the possible formation of multiply charged gas phase negative ions using fast atom bombardment of molecular surfaces. For example, fast atom bombardment of the salt $AuF_6{:}O_2$ might yield AuF_6^-, AuF_6^{2-} and AuF_6^{3-}. Alternatively, bombardment of H_2SO_4, Cs_3FeF_6, and RbBr might yield SO_4^{2-}, FeF_6^{3-} and $RbBr_2^-$. An understanding of multiply charged anions in the gas phase is important to many areas of liquid and surface

surface chemistry. Their production would be of tremendous importance to tandem heavy ion accelerator technology, where higher energy regions could be accessed with existing terminal voltages. The departmental mass spectrometer would be ideally suited for these experiments.

1. R. W. Kiser, Top Curr. Chemistry 101, 83, 89 (1979).
2. R. N. Compton in Photophysics and Photochemistry in the Vacuum Ultraviolet, ed. S.P.McGlynn, G. L. Firdley and K. H. Huebner, D. Reidel Publishing Company (in press).
3. M. Anbar and G. A. St. John, J. Amer. Chem. Soc. 97, 7195 (1975).

Dr. T. Ffrancon Williams: Studies of Radiation-Induced Chemical Reactions

A continuing research program on the fundamental chemistry of radiation effects in the condensed phase has been carried out in this laboratory for 23 years under a contract with the Department of Energy and its progenitor agencies (AEC & ERDA). The main focus of this work has been on the role of reactions intermediates (ions, free radicals, etc.) in photochemical and radiation-induced reactions. In particular, a considerable effort has been devoted to the characterization of radiation-produced radicals in solids by electron spin resonance (ESR) spectroscopy. Here we discuss ways in which the acquisition of a high resolution GC/MS instrument would both complement and supplement our present studies.

Although ESR studies provide useful data about the nature of the reactive intermediates in radiation-induced reactions, the study of reaction products by GC/MS would provide much-needed complementary information about the overall nature of the reactions. This is true of basic studies as well as investigations of complex systems which are frequently of technical interest to DOE. An illustrative example is furnished by our recent work on the radiation-induced generation of radical cations from three-membered ring compounds.[1-3] Thus, we have interpreted ESR results as showing that the ionized ethylene oxide molecule undergoes C•••C ring opening to give a

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symmetrical (C_{2v}) planar molecule.[1] Similarly, ESR studies of the radical cations derived from cyclopropane[2] and 1,1,2,2-tetramethylcyclopropane[3] also indicate that ring opening has occurred, although these two cations appear to adopt a twisted orthogonal structure rather than an edge-to-edge (C_{2v}) planar configuration. A GC/MS study of the reaction products would clearly be helpful in charting the detailed course of the ring-opening rearrangements in these systems. In fact, the analysis of reaction products has been used as evidence for ring opening in the electrochemical oxidation of cyclopropanes.[4]

Turning now to an example of a more complicated problem of crucial DOE importance in nuclear fuel reprocessing and waste disposal, the chemical analysis of tri-n-butyl phosphate (TBP) radiolysis products is of considerable interest with regard to the deleterious effects of these products on process efficiency. Radiation damage to the TBP extraction solvent is known to produce acidic esters[5] and these exhibit a strong complexing power toward plutonium, uranium, and certain fission products, particularly zirconium.[6] Recent ESR work in our group has shown the importance of McLafferty rearrangements in phosphate ester radical cations,[7] the radical cation of trimethyl phosphate undergoing a hydrogen atom transfer which brings about the protonation of the unique oxygen in the ester. Thus it appears that this step is implicated in acid phosphate production. The ability of GC/MS techniques to detect trace components of radiolysis products would clearly provide suplementary information on which to base a detailed reaction mechanism for the radiation decomposition of the TBP solvent. Moreover, GC/MS analysis would be very useful in conjunction with deuterium-labelling experiments, particularly where hydrogen-atom transfers are involved in the reaction sequence, as in this latter case.

REFERENCES

1. L. D. Snow, J. T. Wang, and F. Williams, *Chem. Phys. Letters*, **1983**, *100*, 193.
2. X.-Z. Qin and F. Williams, *Chem. Phys. Letters*, **1984**, *112*, 79.
3. X.-Z. Qin, L. D. Snow, and F. Williams, *J. Am. Chem. Soc.*, **1984**, *106*, 7640.
4. T. Shono and Y. Matsumura, *Bull. Chem. Soc. Japan*, **1975**, *48*, 2861.
5. F. Williams, R. W. Wilkinson, and T. Rigg, *Nature* (*London*), **1957**, *179*, 540; R. W. Wilkinson and F. Williams, *J. Chem. Soc.*, **1961**, 4098.
6. O. L. Keller, Jr., in *Proceedings of the Welch Foundation Conferences on Chemical Research*. XXII. *Chemistry of Future Energy Resources*, Houston, 1978, Chapter VI.
7. X.-Z. Qin, B. W. Walther, and F. Williams, *J. Chem. Soc., Chem., Commun.*, **1984**, in press.

Dr. Kelsey D. Cook: Mass Spectrometry of Polyelectrolytes and Natural Polymers

Studies in our laboratory have been aimed at understanding and ultimately enhancing the sensitivity of matrix assisted ionization. Our approach centers on the development, characterization, and application of electrohydrodynamic mass spectrometry (EHMS). This unique ionization methods relies on the action of an electric field to remove pre-formed ions from solution directly into the high-vacuum region of the spectrometer ion source. The resulting mass spectra can reflect the composition of complex solutions, including those characterized by competing equilibria.[1,2] Thus, the method is useful as a probe of solution *chemistry* as well as sample composition. Of particular interest are applications to the characterization of natural and synthetic polymers (including polyelectrolytes).[3-5]

Ionic conduction in polyelectrolytes is thought to proceed in some systems by charge migration along relatively immobile polymer backbones, rather than by molecular diffusion. The efficiency of such a process should depend on the charge density of the polyelectrolyte, among other factors.

Although average degrees of polymerization and overall charge can be readily determined by classical techniques, detailed information about the degree of dissociation and distribution of charge among various-sized n-mers is not generally available. EHMS has been shown to provide precisely this kind of information for some oligomer systems.[5] The spectrometer currently in use (an MS902) has a limited range (1,000 daltons/charge) and resolution (about 600 with the current EH source, although the instrument was capable of much better when it was new). Even so, it has been useful for characterization of up to quadruply charged ions of mass approaching 4,000 daltons. It remains to be established whether there is an intrinsic mass limitation to the EH sampling process. Thus, the extended mass range of the proposed equipment has obvious implications for advancing these studies to higher molecular weight systems which should be more representative models of true polymer systems. Equally important is the higher sensitivity and usable resolution of new-generation instrumentation, which will facilitate determination of charge distributions by allowing resolution of the peak in an isotope cluster. The spacing (in fractional mass units) of these peaks is inversely proportional to the charge on a detected ion, and can therefore be used to determine that charge. Resolving the peaks due to ^{13}C in an ion of mass 5,000 with a +5 charge requires a resolution of roughly 25,000. This is outside even the original specifications of our present equipment, but is within the capabilities of the equipment proposed.

In applications to natural polymers, the softness of the EH process can be both a strength and a weakness. EH spectra are virtually free of fragment ions, except those resulting from chemical degradation in solution prior to sampling,[6] substantially reducing the structural information content of EH spectra. One approach to recovering this information has been to exploit the selectivity of enzymatically controlled hydrolysis, observing the evolution of chemically generated "fragments" as the reaction proceeds with time. This approach offers prospects of mass spectrometric characterization of the kinetics of these reactions, as well as sequencing information evident from the time-dependent diminution of the parent ion mass as peptides are sequentially cleaved. In this regard, the extended mass range of the requested equipment again offers obvious advantages for application to a wider range of high molecular weight samples. Furthermore, if equipment with metastable ion kinetic energy (MIKES) capability were available, an EH source for MS/MS experiments would allow extraction of structural information from each component of a mixture, regardless of its solution reactivity. This capability would enhance the analytical utility of EHMS for all samples, and may be especially valuable if efforts aimed at coupling an EH source to a liquid chromatograph are successful.

REFERENCES

1. K. W. Chan and K. D. Cook, J. Am. Chem. Soc. 104, 5031 (1982).
2. V. F. Man, J. D. Lin, and K. D. Cook, J. Am. Chem. Soc., submitted for publication.
3. S. T. F. Lai, K. W. Chan, and K. D. Cook, Macromolecules 13, 953 (1980).
4. K. W. Chan and K. D. Cook, Org. Mass Spectrom. 18, 423 (1983).
5. K. W. Chan and K. D. Cook, Macromolecules 16, 1736 (1983).
6. K. D. Cook and K. W. Chan, Int. J. Mass Spectrom. Ion Proc. 54, 135 (1983).

Dr. John E. Bartmess: Electrochemically Assisted Fast Atom Bmbardment

The Fast Atom Bombardment (FAB) technique, and the related Secondary Ion Mass Spectrometry (SIMS) technique, allow for volatilization and ionization of samples that had previously been resistant to mass spectrometric analysis. By dissolving the non-volatile material in a liquid matrix, typically glycerol, and then "sputtering" this solution with a beam of fast atoms or ions, both the solvent and any dissolved material is ejected into the gas phase where mass spectral analysis can occur. As a rough rule of thumb, however, these techniques result primarily in volatilization of any ions present, with only a lesser amount of ion formation. Thus, FAB has proved extremely useful for sampling biomolecules which are either ionic or highly polar, but has not been especially successful in use with nonpolar species such as lipids. Adjustment of pH, or Lewis acid/base chemistry, in the glycerol matrix can derivatize polar samples to produce ions, bu there is no similar method for non-polar ionization.

Glycerol is a reasonably polar solvent, where electrochemistry can occur. We have built and tested a FAB probe, with the tip modified to be a ring-disk electrode, capable of producing either oxidizing or reducing conditions, while floating at the mass spectrometer's source voltage. We have observed considerable enhancement of ion signals for non-polar aromatic compounds, triglycerides and other esters, and alkanes, using the MS-50 mass spectrometer at The Walter Reed Army Medical Center. The proposed instrument would be ideal to develop this technique further; the probe could be redesigned at minimal cost to be interchangeable with the FAB probe for the ZAB-E or equivalent. This technique would have obvious applications in energy related research, for analysis of very high mass petroleum mixtures or coal.

Dr. Fred M. Schell: Fossil Fuels and Other Natural Products

In conjunction with E. W. Hagaman (ORNL Chemistry Division) we are investigating the potential for hydride transfer to and from coal. Polycyclic aromatic ring systems in coal should be good hydride (or electron) acceptors in analogy with the reactions demonstrated by Ashby in simple systems. Coal should also have hydride donor sites capable of forming stable carbocation centers, e.g. benzylic methines, partially reduced polycyclic aromatics, and oxygen substituted aliphatic carbons in lower rank coals. Treatment of coal with a hydride abstractor followed by quenching with various nucleophiles (water, alcohol, cyanide, etc.) should label the sites responsible for hydride donation.

Mass spectrometry can play an important role in fully understanding the consequences of hydride addition/abstraction reactions. Solid state NMR analysis of our first experiments clearly shows that changes are taking place, but detailed analysis is difficult due to the continuum of resonances typical of coal. Mass spectrometry FAB experiments which contrast starting coal and treated material will give more specific information. Deuteride addition reactions will provide samples useful in fragmentation analysis; the extent of deuteride incorporation, and the site(s) of addition may be identified. Coals which donate hydride to catonic acceptors (e.g. triphenyl methyl carbenium ion) and subsequently incorporate nucleophiles can also be studied.

In an extensive investigation of the nitrogen fixing bacteria Rhizobium spp, Gary Stacey and his group (microbiology, UTK) are interested in chemicals important to the nodulation process. Rhizobium mutant strains are known that cannot nodulate soy beans, and therefore not fix nitrogen. An important observation is that the nature of the cell surface polysaccharides associated with the two types of Rhizobium vary considerably. Since these materials will be intimately involved with the interface between plant and bacteria during the nodulation process, they may contain a chemical required for successful symbiosis.

We have been actively engaged in characterizing some of the extracellular components such as glucans and lipopolysaccharides. Some contributions using high resolution proton and carbon NMR have been made, but the quantities of material available seriously limit our ability to carry out extensive degradative studies using only NMR for analysis. High resolution gc-ms facilities will open some important new avenues for identification of degradation products. Of particular interest is the possibility of degradative generation of oligosaccharides whose sequence could be ascertained using FAB-MS analysis. In some cases, FAB could be applied to isolated materials.

Other Faculty Members

In addition to the above users, there are a number of faculty who need high performance mass spectrometry for research in one of the energy-related areas. Dr. James Adcock is developing new perfluorinated polymers for use as coatings and sealants in high stress environments such as power plants. These are difficult to characterize due to their low volatility, but FAB ionization and thermal electron attachment would be ideal techniques for this purpose. Dr. Craig Barnes is involved in research on bimetallic homogeneous catalysts, and species with macrocyclic ligands. Their characterization by FAB-MS here is obvious. Dr. James Chambers has fabricated polymer-modified electrodes with catalytic sites in the polymers, for use in probing electron transfer mechanisms and in selective analysis. FAB-MS will be ideally suited to this investigation since the requirements for facile electron hopping in the polymer film are similar to those for good FAB substrates. Dr. Lee Magid is doing research on surfactants and microemulsions; FAB-MS would be a very useful technique in analyzing these ionic non-volatile species. Dr. Richard Pagni is studying catalysis of organic reactions by alumina surfaces; product distributions are profoundly affected by this surface catalysis and by pretreatment with various organics. Thermal desorption techniques and FAB in the mass spectrometer source will provide information on the nature of the physisorbed species. Dr. Pagni also has been studying photodegradation of PCBs adsorbed on clay in aqueous environments; similar mass spectrometric techniques will be useful here. Dr. Clifton Woods is involved in research on the catalytic properties of dimeric rhodium species, and in activating small molecules such as SO_2 and CO toward attack by other substrates. FAB-MS is again an obvious and needed tool for characterization.

Faculty Qualifications and Experience.

Until this year, while a considerable number of the faculty in the department had used the existing departmental mass spectrometry facilities, or sent samples to regional centers for exact mass determination, there was no member of the faculty whose principal research interest dealt with mass spectrometry. The long term effectiveness of an instrument as complicated as a double focusing mass spectrometer is clearly related to the presence of such expertise and commitment on the faculty. The recent additions of Professors Cook and Bartmess to the faculty have provided a strong base of qualified personnel to oversee, maintain, and modernize the department's facilities for mass spectrometry. Dr. Cook has an extensive background in high resolution and high mass range mass spectrometry, and in new ionization techniques, while Dr. Bartmess is utilizing ion cyclotron resonance mass spectrometry to investigate ion/molecule reactions. The proposed instrument will be housed in a departmental instrument laboratory immediately adjacent to their labs, to benefit both from the suitability and recent remodeling of that space for these new faculty, and from their expertise. Both of these faculty have a specific interest in keeping the proposed instrument operational, since they both will be users of it in their own research.

Cost Sharing.

A new State of Tennessee Center of Excellence program, the "Science Alliance" program is designed to foster cooperation between the science departments of The University of Tennessee and ORNL; it should enhance the quality of both institutions. Our "Alliance" with the scientific aims of DOE should become even stronger in the future. The Science Alliance will provide $119,000 in State-contributed matching funds to this proposal in the first year. A fee structure for users will be set up to defray operational costs, in conjunction with departmental funds.

The department currently has a technician as the operator of the HP 5980 GC/MS. This position will be upgraded to provide for the increase in complexity of instrumentation. In addition, those graduate students whose research is intensive and specific to the mass spectrometer will be trained as operators, both to utilize the instrument more efficiently and to provide these students training in this field as part of their graduate education. There have been, since 1980, 19 students who have obtained a Ph.D. and 13 M.S. degree graduates from the department, who have been supported all or in part by funding from DOE for the various research projects. At the present, DOE funding is supporting 13 graduate students and 4 postdoctoral researchers within the department. While not all of these would be expected to become operators of the mass spectrometer, several will be trained.

Based on experience with similar equipment elsewhere, with careful routine maintenance and operation, a ten year lifespan for this instrument is reasonable. While there are continually new developments in the state of the art in mass spectrometry instrumentation which are desirable to have available, this is a research quality instrument which can be upgraded as needed for specific experiments, either by commercial add-ons or in-house using the expertise of the mass spectroscopists on the faculty.

Other Major Research Instruments.

The department has a number of other shared instruments, as listed below. The operating costs for many of these are recovered from usage fees within the department. Outside users have had access to these instruments also. Thus, the NT-200 NMR has been used to obtain spectra for the Veterinary School of the University and for local technological firms, with a set fee structure. Both the NMR and the new ESCA spectrometer are scheduled for use by researchers at ORNL. The Textile Science Department has had samples run on the present GC/MS. Major items purchased in the last 15 years for more than $20,000 include:

Nicolet TT-14 FT ^{13}C NMR	1976	$103,000
Varian E109ES EPR Spectrometer	1977	44,000
Cary Model 17I Vis-UV Spectrometer	1973	$ 30,000
SpectraPhysics 166/366 Argon ion laser	1973	$ 28,000
Molectron DL14P/UV24 N2 pumped dye laser	1977	$ 36,000
Hewlett-Packard 5980 GC/quadrupole MS, HP 3954 data system	1978	$121,000
Digilab FTS-20C/D FT-IR, with Nova 3/12 data system	1974	$120,000
Raman Spectral System: Spex double monochromator, Scamp computer, and Coherent Argon ion and dye laser	1980	$ 94,000
JEOL FX-90Q NMR Spectrometer	1981	$100,000
Bruker ESR 200B-SRC	1982	$200,000
Nicolet FT-200 NMR	1982	$252,000
Perkin Elmer ESCA	1984	$180,000
Quanta Ray YAG laser	1984	$107,000
Retrofit to Digilab FT-IR	1984	$ 60,000

DOE Funded Major Accomplishments in the last five years:

Professors Mamantov and Wehry:

Elucidation of the chemical and physical factors affecting photo-transformation of polycyclic organics adsorbed on particulates.

Development of improved analytical techniques for detection and quantification of polycyclic organics in coal-derived materials.

Professor Kabalka:

Development of a new series of radioiodinated steroids, currently being evaluated in steroid receptor site studies at NIH.

Synthesis of the first oxygen-15 labeled alcohols for use in nuclear medicine imaging studies.

Development of a method for rapid incorporation of nitrogen-13 into organic molecules.

Development of new reactions useful for the conversion of α,β-unsaturated nitro compounds into ketones, oximines, hydroxylamines, and amines.

Professor Williams:

Elucidation of the radiation chemistry of phosphate esters, as it affects nuclear fuel reprocessing.

Characterization of haloalkane radical cations and anions in condensed phase by ESR techniques.

Professor Kovac:

Development of a computer simulation model to study the effects on entanglements on the dynamics of chain polymers.

Elucidation of the macromolecular topology of bituminous coals and development of experimental techniques to study the coalification process.

Professor Alexandratos:

Development and synthesis of dual mechanism bifunctional polymers, which exchange metal ions followed by reduction to the zero valent state, with very high capacities for mercury, silver, and gold.

Professor Schell (with Dr. E. Hagaman - Chemistry Division at ORNL)

Characterization of the sites of hydride donors and acceptors in coal by solid state magic angle nmr.

Major accomplishments of other Federally funded research in the designated areas in the last two years:

Professor Mamantov:
Molten salt catalysis of the hydrogenation of carbon monoxide (with Professor Pagni).

Electroreduction of carbon dioxide in molten chloroaluminates.

Professor Wehry
Detection and quantification of non-fluorescent compounds from fluorescent fragments formed by electron impact or laser photolysis.(NSF)

Professor Kabalka
Synthesis of ^{11}C and ^{15}N labeled species for human blood flow analysis and receptor site tracing.(NIH)

Professor Chambers
Demonstrated proton- and electron-coupled charge transport in electroactive polymer films.

Professor Bartmess
Ionic hydrogen bond strengths are a quantitative function of acid/base character and electronegativity in the gas phase.(NIH)

Slow proton transfer between anions in the gas phase is due to structural barriers, but the solution phase analogs are also affected by solvation requirements.(NSF)

Professor Cook
Development of electrohydrodynamic ionization as a source technique for mass spectrometry.(NSF)

Professor Pagni
Photochemistry of haloaromatics in water results in halogen replacement by hydroxy groups, not hydrogen as previously believed.(EPA)

Estimated Cost and Budget

ZAB-E mass spectrometer, with high mass range, GC capability, jet separator, solids probe, positive/negative ions, reference inlet, alternate CI/EI source	$410,000
Dedicated Data System: PDP 1124/DEC RSX-11M multitasking system, with 80 Mbyte Winchester Hard Disk, 16 Mbyte removable, Printronix printer, DMA color display	$137,000
Fast Atom Bombardment	$ 27,000
Mass Analyzed Ion Kinetic Energy Accessory	$ 18,000
Shipping/Packing	included
Training of Operator	included
Installation	included
	$592,000
University of Tennessee Cost Sharing on purchase	$100,000
Amount requested from DOE	$492,000

University of Tennessee support for five years:

Site Preparation	$ 4,000
First year supplies, spare parts, tools	$ 15,000
Second year supplies	$ 10,000
Third year supplies	$ 11,000
Fourth year supplies	$ 11,000
Fifth year supplies	$ 12,000

U.S. DEPARTMENT OF ENERGY

ASSURANCE OF COMPLIANCE

Nondiscrimination in Federally Assisted Programs

Gleb Mamantov (Hereinafter called the "Applicant")
(Name of Applicant)

HEREBY AGREES to comply with Title VI of the Civil Rights Act of 1964 (Pub. L. 88-352), Section 16 of the Federal Energy Adminstration Act of 1974 (Pub. L. 93-275), Section 401 of the Energy Reorganization Act of 1974 (Pub. L. 93-438), Title IX of the Education Amendments of 1972, as amended, (Pub. L. 92-318, Pub. L. 93-568, and Pub. L. 94-482), Section 504 of the Rehabilitation Act of 1973 (Pub. L. 93-112), the Age Discrimination Act of 1975 (Pub. L. 94-135), Title VIII of the Civil Rights Act of 1968 (Pub. L. 90-284), the Department of Energy Organization Act of 1977 (Pub. L. 95-91), and the Energy Conservation and Production Act of 1976, as amended, (Pub. L. 94-385). In accordance with the above laws and regulations issued pursuant thereto, the Applicant agrees to assure that no person in the United States shall, on the ground of race, color, national origin, sex, age, or handicap, be excluded from participation in, be denied the benefits of, or be otherwise subjected to discrimination under any program or activity in which the Applicant receives Federal assistance from the Department of Energy.

Applicability and Period of Obligation

In the case of any service, financial aid, covered employment, equipment, property, or structure provided, leased, or improved with Federal assistance extended to the Applicant by the Department of Energy, this assurance obligates the Applicant for the period during which Federal assistance is extended. In the case of any transfer of such service, financial aid, equipment, property, or structure, this assurance obligates the transferee for the period during which Federal assistance is extended. If any personal property is so provided, this assurance obligates the Applicant for the period during which it retains ownership or possession of the property. In all other cases, this assurance obligates the Applicant for the period during which the Federal assistance is extended to the Applicant by the Department of Energy.

Employment Practices

Where a primary objective of the Federal assistance is to provide employment or where the Applicant's employment practices affect the delivery of services in programs or activities resulting from Federal assistance extended by the Department, the Applicant agrees not to discriminate on the ground of race, color, national origin, sex, age, or handicap, in its employment practices. Such employment practices may include, but are not limited to, recruitment, recruitment advertising, hiring, layoff or termination, promotion, demotion, transfer, rates of pay, training and participation in upward mobility programs, or other forms of compensation and use of facilities.

Subrecipient Assurance

The Applicant shall require any individual, organization, or other entity with whom it subcontracts, subgrants, or subleases for the purpose of providing any service, financial aid, equipment, property, or structure to comply with laws cited above. To this end, the subrecipient shall be required to sign a written assurance form, however, the obligation of both recipient and subrecipient to ensure compliance is not relieved by the collection or submission of written assurance forms.

Data Collection and Access to Records

The Applicant agrees to compile and maintain information pertaining to programs or activities developed as a result of the Applicant's receipt of Federal assistance from the Department of Energy. Such information shall include, but is not limited to, the following: (1) the manner in which services are or will be provided and related data necessary for determining whether any persons are or will be denied such services on the basis of prohibited discrimination; (2) the population eligible to be served by race, color, national origin, sex, age and handicap; (3) data regarding covered employment including use or planned use of bilingual public contact employees serving beneficiaries of the program where necessary to permit effective participation by beneficiaries unable to speak or understand English; (4) the location of existing or proposed facilities connected with the program and related information adequate for determining whether the location has or will have the effect of unnecessarily denying access to any person on the basis of prohibited discrimination; (5) the present or proposed membership by race, color, national origin, sex, age and handicap, in any planning or advisory body which is an integral part of the program; and (6) any additional written data determined by the Department of Energy to be relevant to its obligation to assure compliance by recipients with laws cited in the first paragraph of this assurance.

The Applicant agrees to submit requested data to the Department of Energy regarding programs and activities developed by the Applicant from the use of Federal assistance funds extended by the Department of Energy. Facilities of the Applicant (including the physical plants, buildings, or other structures) and all records, books, accounts, and other sources of information pertinent to the Applicant's compliance with the civil rights laws shall be made available for inspection during normal business hours on request of an officer or employee of the Department of Energy specifically authorized to make such inspections. Instructions in this regard will be provided by the Director, Federally Assisted Programs Division, Office of Equal Opportunity, U.S. Department of Energy.

This assurance is given in consideration of and for the purpose of obtaining any and all Federal grants, loans, contracts (excluding procurement contracts), property, discounts or other Federal assistance extended after the date hereto, to the Applicant by the Department of Energy, including installment payments on account after such date of application for Federal assistance which are approved before such date. The Applicant recognizes and agrees that such Federal assistance will be extended in reliance upon the representations and agreements made in this assurance and that the United States shall have the right to seek judicial enforcement of this assurance. This assurance is binding on the Applicant, its successors, transferees, and assignees, as well as the person whose signature appears below and who is authorized to sign this assurance on behalf of the Applicant.

December 19, 1984
(Date)

Gleb Mamantov
(Name of Applicant)

Department of Chemistry
University of Tennessee
Knoxville, TN 37996-1600
(Address)

Thomas L. Bell
(Authorized Official) Thomas L. Bell, Assistant Dean for Research

(615) 974-3141
(Applicant's Telephone Number)

Attachment 1. Resumes of Participating Faculty

Gleb Mamantov, Professor and Head, Department of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Electrochemistry, solutes in molten halides, batteries, inorganic fluorine chemistry, matrix isolation spectroscopy.

PROFESSIONAL EXPERIENCE:

Research Chemist, Electrochemicals Department, du Pont, Niagara Falls, N.Y., 1957-58.
2nd and 1st Lt., USAF, Directorate of Rocket Propulsion, Edwards AFB, California, 1958-60.
Project scientist, Directorate of Rocket Propulsion, Edwards AFB, California, 1960.
Instructor and project associate (with Professor J. L. Margrave), University of Wisconsin, 1960-61.
Assistant Professor of Chemistry, University of Tennessee, 1961-66.
Associate Professor of Chemistry, University of Tennessee, 1966-71.
Professor of Chemistry, University of Tennessee, 1971-present.
Head, Department of Chemistry, University of Tennessee, 1979-present.
Consultant, Oak Ridge National Laboratory, 1962-present.

CURRENT RESEARCH SUPPORT

Department of Energy, Contract No. DE-AS-05-81 ER 60006 07/01/84 - 06/30/87 $351,000 (jointly with Professor E. L. Wehry).
University of California Subcontract No. 4502810 (Department of Energy), 04/01/84 - 03/31/85, $15,921.
Atlantic-Richfield Company; 07/01/84 - 06/30/85 $160,000
Martin-Marietta Grant 05/01/84 - 04/30/85, $25,000 (jointly with Professor J. Q. Chambers).

RECENT PUBLICATIONS

E. L. Wehry, G. Mamantov, A. A. Garrison, R. A. Yokley, and R. J. Engelbach, "Chemical Transformation of Polycyclic Aromatic Hydrocarbons Vapor-Adsorbed on Coal Stack Ash", in Proceedings of Ninth International Symposium on Polynuclear Aromatic Hydrocarbons, W. M. Cooke and A. J. Dennis, eds. (in press).

H. E. Howell, G. Mamantov, E. L. Wehry, and R. W. Shaw, "Photoacoustic Spectroscopy of Matrix-Isolated Polycyclic Aromatic Compounds", Anal. Chem., 1984, 56, 821.

D. M. Chapman, G. P. Smith, M. Sϕrlie, C. Petrovic, and G. Mamantov, "Electrochemical Properties of the Solvent $SbCl_3$-AlCl-N-(1-butyl)-pyridinium Chloride and Electrochemical and Spectroelectrochemical Studies of Arlene Solutes], J. Electrochem. Soc., 131, 1609 (1984).

G. Mamantov and J. Hvistendahl, "Rechargeable High Voltage Low Temperature Molten Salt Cell Na/β"-Alumina/SCl_3^+ in $AlCl_3$-NaCl," J. Electroanal. Chem., 168, 451 (1984).

Gleb Mamantov, Professor and Head, Department of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Electrochemistry, solutes in molten halides, batteries, inorganic fluorine chemistry, matrix isolation spectroscopy.

PROFESSIONAL EXPERIENCE:

Research Chemist, Electrochemicals Department, du Pont, Niagara Falls, N.Y., 1957-58.
2nd and 1st Lt., USAF, Directorate of Rocket Propulsion, Edwards AFB, California, 1958-60.
Project scientist, Directorate of Rocket Propulsion, Edwards AFB, California, 1960.
Instructor and project associate (with Professor J. L. Margrave), University of Wisconsin, 1960-61.
Assistant Professor of Chemistry, University of Tennessee, 1961-66.
Associate Professor of Chemistry, University of Tennessee, 1966-71.
Professor of Chemistry, University of Tennessee, 1971-present.
Head, Department of Chemistry, University of Tennessee, 1979-present.
Consultant, Oak Ridge National Laboratory, 1962-present.

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Atlantic-Richfield Company; 07/01/84 - 06/30/85 $160,000
Martin-Marietta Grant 05/01/84 - 04/30/85, $25,000 (jointly with Professor J. Q. Chambers).

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Earl L. Wehry, Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Fluorescence and phosphorescence spectroscopy, analytical laser spectroscopy, chemical degradation of environmental pollutants, low-temperature molecular spectroscopy, photochemistry.

PROFESSIONAL EXPERIENCE:

Assistant Professor, Department of Chemistry, Indiana University, 1965-70.
Assistant Professor, Department of Chemistry, University of Tennessee, 1970-72.
Associate Professor, Department of Chemistry, University of Tennessee, 1972-77.
Professor, Department of Chemistry, University of Tennessee, 1977-.

CURRENT RESEARCH SUPPORT

"Characterization and Environmental Fate of Polycyclic Aromatic Compounds Adsorbed on Coal Fly Ash and Related Solid Surfaces", DOE (OHER), 7/81-6/87; total support for period $681,000.
"High Resolution Fragmentation-Fluorescence Spectrometry", NSF, 2/84-1/87; total support for period $336,362.

RECENT PUBLICATIONS

E. L. Wehry, V. B. Conrad, J. L. Hammons, J. R. Maple, and M. B. Perry, "Characterization of Complex Samples by Laser-Excited Matrix Isolation Fluorescence Spectrometry", *Opt. Eng.*, *22*, 558 (1983).

M. B. Perry, E. L. Wehry, and G. Mamantov, "Determination of Polycyclic Aromatic Hydrocarbons in Unfractionated Solid Solvent-Refined Coal by Matrix Isolation Fluorescence Spectrometry", *Anal. Chem.*, *55*, 1893 (1983).

E. L. Wehry, "Laser-Induced Low-Temperature Fluorescence Spectroscopy", *Trends Anal. Chem.*, *2*, 143 (1983).

V. B. Conrad, W. J. Carter, E. L. Wehry, and G. Mamantov, "Matrix Isolation Fluorescence Spectrometric Detection in Gas Chromatography", *Anal. Chem.*, *55*, 1340 (1983).

E. L. Wehry, "Optical Spectrometric Techniques for Determination of Polycyclic Aromatic Hydrocarbons", in *Handbook of Polycyclic Aromatic Hydrocarbons* (A. Bjϕrseth, ed.), Marcel Dekker, New York, p. 323 (1983).

V. B. Conrad and E. L. Wehry, "Laser-induced Matrix Isolation Fluorescence Spectrometry of Methyl and Methoxy Derivatives of Benzo[a]pyrene", *Appl. Spectrosc.*, *37*, 46 (1983).

G. Mamantov, A. A. Garrison, and E. L. Wehry, "Analytical Applications of Matrix Isolation Fourier Transform Infrared Spectroscopy", *Appl. Spectrosc.*, *36*, 339 (1982).

Spiro D. Alexandratos, Assistant Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Polymer supported reagents, metal ion recovery, chelating and ion exchange resins, optically active polymeric catalysts and resolving reagents.

PROFESSIONAL EXPERIENCE:

Rohm and Haas Co.; Philadelphia, PA; Senior Research Chemist, 1977-1981.
University of Tennessee, Assistant Professor of Chemistry, 1981-present.
Oak Ridge National Laboratory, Guest Scientist, 1982-present.
Argonne National Laboratory, Guest Scientist, 1984-present.

CURRENT RESEARCH SUPPORT:

Department of Energy (DE-AS05-83ER13113: Synthesis of Polymeric Extractants) 1983-1986; $82,400
University of Tennessee Research Incentive Proposal (Co-PI: Membrane Osmometry), 1983.

MOST RECENT DOE PUBLICATIONS:

Dual-Mechanism Bifunctional Polymers: A New Class of Ion Exchange Resins S. D. Alexandratos and D. L. WQilson, J. Am. Chem., submitted.

Metal Ion Extraction Capability of Phosphinic Acid Resins, S. D. Alexandratos, D. L. Wilson, M. A. Strand, D. R. Quillen, A. J. Walder, and W. J. McDowell, Macromolecules, in press (1985).

Synthesis and Characterization of Bifunctional Phosphinic Acid Resins, S. D. Alexandratos, M. A. Strand, D. R. Quillen, and A. J. Walder, Macromolecules, in press (1985).

Polymeric Bifunctional Extractants and Method of Making Same, S. D. Alexandratos, United States Patent Application filed May 25, 1984.

Polymeric Bifunctional Extractants with Synergistic Possibilities, S. D. Alexandratos and W. J. McDowell, Separation Sci. Technol. 18, 1715 (1983).

The Asymmetric Synthesis of Carboxylic Acids, S. D. Alexandratos in Optical Resolution Procedures for Chemical Compounds, Vol. II edited by P. Newman, Optical Resolution Information Center (1981).

Ab Initio Modeling of Substituent Effects in Hammett Correlations, E. R. Vorpagel, A. Streitwieser, Jr., and S. D. Alexandratos, J. Am. Chem. Soc., 103, 3777 (1981).

George W. Kabalka, Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Organometallic Chemistry, Synthetic Organic Chemistry, Radiopharmaceutical Syntheses, Nuclear Magnetic Resonance.

PROFESSIONAL EXPERIENCE:

Postdoctoral Research, Purdue University, W. Lafayette, IN, 1970.
Assistant Professor, University of Tennessee, 1970-1976.
Associate Professor, University of Tennessee, 1976-1981.
Professor of Chemistry, University of Tennessee, 1981-.
Head of Basic Research, Department of Radiology, University of Tennessee Memorial Research Hospital, 1984-.

CURRENT RESEARCH SUPPORT:

"Synthesis of Radiopharmaceuticals Containing Short-Lived Radionuclides," D.O.E. (Human Health Assessments Division), 3/84-2/86; Total Support: $228,885.
"Early Breast Cancer Detection: A Unique Approach," National Cancer Institute, 2/83-1/86; Total Support: $263,551.

MOST RECENT DOE PUBLICATIONS:

"Incorporation of Stable and Radioactive Isotopes Via Organoborane Chemistry," G. W. Kabalka, Acc. Chem. Res, 17, 215 (1984).

"Synthesis of Dialkylamines Via The Reaction Organoboranes With N-Chloroalkylamines," G. W. Kabalka, G. W. McCollum, and K. A. R. Sastry, J. Org. Chem., 49, 1656 (1984).

"Crystalline Organomercuric Acetates via Organoboranes," S. A. Kunda, R. R. S. Varma, G. W. Kabalka, Synth. Commun., 14, 755 (1984).

"The Effect of Tellurium Position on the Myocardial Specificity of Radioiodinated 18-Iodo-tellura-17-octadenoic Acid Analogs," F. F. Knapp, P. C. Srivastava, A. P. Callahan, and E. B. Cunningham, G. W. Kabalka, and K. A. R. Sastry, J. Med. Chem., 27, 57 (1984).

"Synthesis and Evaluation of 18-[^{125}I]-Iodo-17-octadenoic Acid," M. M. Goodman, F. F. Knapp, G. W. Kabalka, and K. A. R. Sastry, J. Med. Chem. 27, 94 (1984).

"Synthesis of Carbon-13 Labeled Aldehydes, Carboxylic Acids, and Alcohols, Via Organoborane Chemistry," G. W. Kabalka, M. C. Delgado, U. S. Kunda, S. A. Kunda, J. Org. Chem., 49, 174 (1984).

"Myocardial Imaging Agents: Synthesis, Characterization and Evaluation of cis-(Z) and trans-(E) 18-Bromo-[^{82}Br]-5-tellura-17-octadecenoic Acid," P. C. Srivastava, F. F. Knapp, A. P. Callahan, B. A. Owen, G. W. Kabalka, and K. A. R. Sastry, J. Med. Chem., 27, 94 (1984).

Jeffrey D. Kovac, Associate Professor of Chemistry

EDUCATI

[redacted]

PROFESSIONAL EXPERIENCE:

University of Tennessee, Assistant Professor of Chemistry, 1976-1983.
Associate Professor 1983-
Oak Ridge National Laboratory, Consultant 1984-

CURRENT RESEARCH SUPPORT

"Computer Studies pf Cubic Lattice Models for Polymer Chains", Petroleum Research Fund; $52,500, June 1984-August 1987
"Statistical Mechanics of Polymer Systems" Department of Energy, $272,000, September 1984-August 1987.
"The Macromolecular Chemistry of Coalification", Department of Energy, $174,904, July 1984-July 1987.

RECENT PUBLICATIONS

J. Kovac, "Modified Gaussian Model for Rubber Elasticity," Macromolecules 11, 363 (1978).

J. W. Larsen and J. Kovac, "Polymer Structure of Bituminous Coals," in The Organic Chemistry of Coal, ACS Symposium Series No. 71, J. W. Larsen, editor (1978).

J. Kovac, "Non-Equilibrium Thermodynamics of Interfacial Systems II, Boundary Conditions for Fluids with Spin," Physica 107A, 280 (1981).

J. Kovac, "Equilibrium Thermodynamics of the Glass Transition," J. Phys. Chem. 85, 2060 (1981).

J. Kovac and C. C. Crabb, "Modified Gaussian Model for Rubber Elasticity II The Wormlike Chain," Macromolecules 15, 537 (1982).

T. Green, J. Kovac, D. Brenner and J. W. Larsen, "The Macromolecular Structure of Coals," in Coal Structure, R. A. Meyers, Ed. Academic Press, N.Y., 1982 pp. 299-382.

M. T. Gurler, C. C. Crabb, D. M. Dahlin and J. Kovac, "Effect of Bead Movement Rules on the Relaxation of Cubic Lattice Models of Polymer Chains," Macromolecules, 16, 398 (1983).

J. W. Larsen, M. Mohammadi, I. Yiginsu and J. Kovac, "The Molecular Weight Distribution of Coal Extracts. Coal is Not a Condensation Polymerization." Geochim. Cosmochim. Acta, 48, 135 (1984).

T. K. Green, J. Kovac and J. W. Larsen, "A Rapid and Convenient Method for Measuring the Swelling of Coals by Solvents," Fuel, 63, 935 (1984).

J. Kovac, "Molecular Size and Raoult's Law," submitted to J. Chem. Educ.

C. C. Crabb and J. Kovac, "Dynamics of Cubic Lattice Models of Polymer Chains at High Concentrations," submitted to Macromolecules.

T. Ffrancon Williams, Professor of Chemistry

EDUCATION:

[redacted].,

MAJOR RESEARCH INTEREST:

ESR studies of radical cations and anions; spin delocalization; quantum mechanical tunneling; radiation chemistry; ionic polymerization

PROFESSIONAL EXPERIENCE:

Scientific Officer, AERE Harwell (UK), 1949-55; Senior Scientific Officer, AERE Harwell (UK) 1955-57 and 1959-61; Research and Teaching Associate, Northwestern University, 1957-59; Research Scientist, Armlur Research Foundation, Ill. Inst. of Tech. 1961; Assistant Professor, University of Tennessee, 1961-63; Associate Professor, University of Tennessee, 1963-67; Professor, University of Tennessee, 1967-present; Alumni Distinguished Service Professor, University of Tennessee, 1974-present

CURRENT SUPPORT:

DOE DE-AS05-76ER02968, 1/85-12/87, $318,000, "Studies of Radiation Produced Radicals and Radical Ions"

PUBLICATIONS:

(with B. W. Walther) "Trigonal-^{13}C Hyperfine Coupling in CF_3CCl_2," *J. Chem. Phys.*, **79**, 3167 (1983).

(with L. D. Snow) "Long-Range Proton Hyperfine Couplings in Radical Cations of Carbonyl Compounds," *J. Chem. Soc., Chem. Commun.*, 1090 (1983).

(with B. W. Walther and D. M. Lemal) "The Octafluorocyclooctatetraene Radical Anion. Identification and Proof of Aromaticity by Electron Spin Resonance," *J. Am. Chem. Soc.*, **106**, 548 (1984).

(with J. A. Aikins) "The Radiation-Induced Cationic Polymerization of Limonene Oxide, α-Pinene Oxide, and β-Pinene Oxide," *ACS Symposium Series* (Ring-Opening Polymerization: Kinetics, Mechanisms, and Synthesis, ed. J. E. McGrath), in press.

(with L. D. Snow) "Spin Delocalization in Radical Cations of Organic Oxygen Compounds As Revealed by Long-Range Hyperfine Interactions and Solvent Effects," *Faraday Discussions Chem. Soc.*, No. 78, in poress (September 4-6, 1984).

(with Xue-Zhi Qin and B. W. Walther) "An ESR Study of the Trimethyl Phosphate Radical Cation - Trichlorofluoromethane σ* Complex and Its Dissociation," *J. Chem. Soc., Chem. Commun.*, in press.

(with Xue-Zhi Qin and L. D. Snow) "Electron Spin Resonance Evidence for the Ring-Closed and Ring-Opened Forms of a Substituted Cyclopropane Radical Cation", *J. Am. Chem. Soc.*, **106**, 7640 (1984).

(with Xue-Zhi Qin) "ESR Evidence for the Formation of the Trimethylene Radical Cation $\cdot CH_2CH_2CH_2^+$ from Cyclopropane", *Chem. Phys. Letters*, **112**, 79 (1984).

Robert N. Compton, Part-time Professor of Chemistry

EDUCATION: [redacted]

PROFESSIONAL EXPERIENCE:

Senior Research Scientist, Group Leader, Oak Ridge National Lab. 1966-Present.

Ford Foundation Professor of Physics, University of Tennessee, 1970-1973.

Visiting Scientist, FOM-Institute, Amsterdam, Holland, 1978.

Adjunct Professor of Chemistry, University of Tennessee, 1984-Present.

CURRENT RESEARCH SUPPORT:

"Basic Studies in Chemical Physics", DOE, 1984-1985, $192,000 per year.

RECENT PUBLICATIONS:

R. N. Compton, J. A. D. Stockdale, and C. D. Cooper, X. Tang and P. Lambropoulos, "Photoelectron Angular Distributions from Multiphoton Ionization of Cesium Atoms", Phys. Rev. A 30, 1766 (1984).

W. Christian, R. N. Compton, J. A. D. Stockdale, J. C. Miller, C. D. Cooper, S. Trang and P. Lamboropoulos, "Near-infrared Multiphoton Ionization of Cesium", Physical Review A 30, 1775 (1984).

R. N. Compton, "Electron Attachment to Molecules" in Electron and Atomic Collisions, N. Oda and K. Takayanagi, eds., North Holland Publishing Co.; pp. 252-262 (1984).

Kelsey D. Cook, Assistant Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Analytical mass spectrometry for characterization of interactions in polymer (and related) solutions. Fundamentals of matrix-assisted ionization. Mechanisms underlying surfactant applications in analysis.

PROFESSIONAL EXPERIENCE:

Assistant Professor, University of Illinois, 1978-1984. Assistant Professor, University of Tennessee, 1984-.

CURRENT RESEARCH SUPPORT

"Polymer Characterization by Electrohydrodynamic Ionization Mass Spectrometry," N.S.F., Division of Materials Research (funded jointly by the U.S. Army Research Office), 8/84-4/87; Total support: $286,000.

RECENT PUBLICATIONS

G. J. Klopf and K. D. Cook, "Surfactant Effects on the Spectroscopy of the Gadolinium-Chrome Azurol S Complex," Anal. Chim. Acta 162, 293 (1984).

J. H. Callahan and K. D. Cook, "Mechanism of Surfactant Induced Changes in the Visible Spectroscopy of Metal-Chrome Azurol S Complexes," Anal. Chem. 56, 1632 (1984).

S. L. Murawski and K. D. Cook, "Sampling Ions from Volatile Solutions by Electrohydrodynamic Mass Spectrometry," Anal. Chem. 56, 1015 (1984).

K. D. Cook and K. W. C. Chan, "Energy Deposition in Desorption Ionization," Int. J. Mass Spectrom. Ion Proc. 54, 135 (1983).

K. W. C. Chan and K. D. Cook, "Extended Mass Range by Multiple Charge: Sampling Quadruply Charged Quasimolecular Ions of Poly(ethylene Glycol) 4000," Org. Mass Spectrom. 18, 423 (1983).

K. W. C. Chan and K. D. Cook, "Mass Spectrometric Study of Interactions Between Poly(ethylene Glycols) and Alkali Metals in Solution," Macromolecules 16, 1736 (1983).

K. W. C. Chan and K. D. Cook, "Factors Affecting Mass Spectral Sensitivity for Ions Sampled by Field Evaporation from a Liquid Matrix," Anal. Chem. 55, 1306 (1983).

K. W. C. Chan and K. D. Cook, "Chemical Reactivity of Glycerol as a Mass Spectrometric Matrix," Anal. Chem. 55, 1422 (1983).

K. W. C. Chan and K. D. Cook, "Observation of some Transition Metal Complexes in Solution by Electrohydrodynamic Ionization Mass Spectrometry," J. Amer. Chem. Soc. 104, 5031 (1982).

John E. Bartmess, Assistant Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Ion/molecule chemistry, organic reaction mechanisms, solvation effects, solution calorimetry, molecular orbital calculations

PROFESSIONAL EXPERIENCE:

Instructor, Organic Chemistry, Norwestern University, 1974-1975
Postdoctoral Research, University of California Irvine, Irvine, CA, 1975-77
Assistant Professor, Department of Chemistry, Indiana University, 1977-84
Assistant Professor, Department of Chemistry, University of Tennessee, 1984-

CURRENT RESEARCH SUPPORT

"Mechanism of the Ionic β-Elimination Reaction in the Gas Phase", NSF, 12/84-11/87; total support for the period $154,000
"Compilation of Anionic Thermochemistry", NBS, yearly contract, 10/84-9/85, $3000

RECENT PUBLICATIONS

G. Caldwell, M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess "Anion-Alcohol Hydrogen Bond Strengths in the Gas Phase" J. Am. Chem. Soc. 1984, 106, 4660.

J. E. Bartmess and J. Kester, "Gas Phase Ion Chemistry of Zinc Atoms and Ions", Inorg. Chem. 1984, 23, 1877.

J. E. Bartmess and R. D. Burnham "Effect of Central Substituents on the Gas Phase Acidities of Propenes", J. Org. Chem. 1984, 49, 1382.

M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess, "The Anionic Cope Rearrangement: Structural Effects in the Gas Phase and in Solution" J. Am. Chem. Soc. 1984, 106, 1025.

G. Caldwell, M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess, "Displacement, Proton Transfer, or Hydrolysis? Mechanistic Control of Acetonitrile Reactivity by Stepwise Solvation", J. Am. Chem. Soc. 1984, 106, 809.

J. E. Bartmess, G. Caldwell, and M. D. Rozeboom "Dipole Stabilized Carbanions in the Gas Phase" J. Am. Chem. Soc. 1983, 105, 340.

J. E. Bartmess "Gas Phase Ion Chemistry of 5-Methylene-1,3-Cyclohexadiene (o-Isotoluene) and 3-Methylene-1,4-Cyclohexadiene (p-Isotoluene)" J. Am. Chem. Soc. 1982, 104, 335-7.

G. Caldwell and J. E. Bartmess "Bimolecular Ion-Molecule Addition Reactions in the Gas Phase. Alcohols and Alkoxides" J. Phys. Chem. 1981, 85, 3571-7.

John E. Bartmess, Assistant Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Ion/molecule chemistry, organic reaction mechanisms, solvation effects, solution calorimetry, molecular orbital calculations

PROFESSIONAL EXPERIENCE:

Instructor, Organic Chemistry, Norwestern University, 1974-1975
Postdoctoral Research, University of California Irvine, Irvine, CA, 1975-77
Assistant Professor, Department of Chemistry, Indiana University, 1977-84
Assistant Professor, Department of Chemistry, University of Tennessee, 1984-

CURRENT RESEARCH SUPPORT

"Mechanism of the Ionic β-Elimination Reaction in the Gas Phase", NSF, 12/84-11/87; total support for the period $154,000
"Compilation of Anionic Thermochemistry", NBS, yearly contract, 10/84-9/85, $3000

RECENT PUBLICATIONS

G. Caldwell, M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess "Anion-Alcohol Hydrogen Bond Strengths in the Gas Phase" J. Am. Chem. Soc. 1984, 106, 4660.

J. E. Bartmess and J. Kester, "Gas Phase Ion Chemistry of Zinc Atoms and Ions", Inorg. Chem. 1984, 23, 1877.

J. E. Bartmess and R. D. Burnham "Effect of Central Substituents on the Gas Phase Acidities of Propenes", J. Org. Chem. 1984, 49, 1382.

M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess, "The Anionic Cope Rearrangement: Structural Effects in the Gas Phase and in Solution" J. Am. Chem. Soc. 1984, 106, 1025.

G. Caldwell, M. D. Rozeboom, J. P. Kiplinger, and J. E. Bartmess, "Displacement, Proton Transfer, or Hydrolysis? Mechanistic Control of Acetonitrile Reactivity by Stepwise Solvation", J. Am. Chem. Soc. 1984, 106, 809.

J. E. Bartmess, G. Caldwell, and M. D. Rozeboom "Dipole Stabilized Carbanions in the Gas Phase" J. Am. Chem. Soc. 1983, 105, 340.

J. E. Bartmess "Gas Phase Ion Chemistry of 5-Methylene-1,3-Cyclohexadiene (o-Isotoluene) and 3-Methylene-1,4-Cyclohexadiene (p-Isotoluene)" J. Am. Chem. Soc. 1982, 104, 335-7.

G. Caldwell and J. E. Bartmess "Bimolecular Ion-Molecule Addition Reactions in the Gas Phase. Alcohols and Alkoxides" J. Phys. Chem. 1981, 85, 3571-7.

Fred M. Schell, Associate Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Natural product chemistry: development of new synthetic methods, total synthesis, isolation and structure determination; coal chemistry.

PROFESSIONAL EXPERIENCE:

Assistant Professor, Chemistry, University of Tennessee, 1972-1980.
Associate Professor, Chemistry, University of Tennessee, 1980-
Consultant, Oak Ridge National Laboratory, 1976.
Part-time employee, Oak Ridge National Laboratory, 1978-

CURRENT RESEARCH SUPPORT

Biological Nitrogen Fixation, Host Recognition in the Nitrogen-Fixing *Rhizobium japonicum*-Soybean Symbiosis,
F. M. Schell, co-PI, Gary Stacey, PI, USDA, 9-1-83 to 8-31-84, $90,000.

RECENT PUBLICATIONS

F. M. Schell, P. M. Cook, "Intramolecular Photochemistry of a Vinylogous Amide and Some Transformations of the Photoproduct", *J. Org. Chem.* 1984, *49*, 4067.

P. J. Weldon, F. M. Schell, "Responses by Kingsnakes (*Lampropeltis getulus*) to Chemicals from Colubrid and Croataline Snakes", *J. Chem. Ecol.* 1984, *10*, 1509.

E. W. Hagaman, F. M. Schell, D. C. Cronauer, Oil Shale Analysis by CP/MAS-13C NMR Spectroscopy. *Fuel*, 1984, *63*, 915.

F. M. Schell and A. M. Smith, N-Chloramine Rearrangements. The Use of Cyclobutylamine as a Pyrrolidine Precursor. *Tetrahedron Lett.*, 1983, 1883.

F. M. Schell and P. R. Williams, Jr., Synthesis of N-Benzoyl-4-oxo-1,2,3,4-tetrahydrapyridine and its Ethylene Ketal. *Syn. Commun.*, 1982, *12*, 755.

F. M. Schell, R. N. Ganguly, Silver Ion Induced Rearrangement of N-Chloramines. Isolation of an Ionic Product in High Yield, *J. Org. Chem.*, 1980, *45*, 4069.

James L. Adcock, Associate Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Reactions of elemental fluorine, synthetic and mechanistic aspect of fluorinated compounds, aerosol fluorination.

PROFESSIONAL EXPERIENCE:

Assistant Professor, Department of Chemistry, University of Tennessee, 1974-79
Associate Professor, Department of Chemistry, University of Tennessee, 1979-
Research participant/consultant, Oak Ridge National Laboratory, 1980-

CURRENT RESEARCH SUPPORT:

"Aerosol Direct Fluorination and Synthesis", 3M Co., $34,997, 4/84-4/85
"Aerosol Fluorination", Sun Oil Co., $30,000, 11/84-10/86

MOST RECENT DOE PUBLICATIONS:

"Aerosol Direct Fluorination: Alkyl Halides II, Chlorine Shifts and the Stability of Radicals," James L. Adcock and Wm. D. Evans, J. Org. Chem., 1984, 49, 2719-2723.

"Aerosol Direct Fluorination: Syntheses of the Highly Branched Ketones, F-Pinacolone and 'F-Provolone'," J. L. Adcock and M. L. Robin, J. Org. Chem., 1984, 49, 1442-1445.

"Aerosol Direct Fluorination - Indirect Syntheses of Perfluorocycloketones," James L. Adcock and Mark L. Robin, J. Org. Chem., 1984, 49, 191-193.

"Aerosol Direct Fluorination Synthesis: Alkyl Halides I, Neopentyl Chlorides and Bromides - Free Radicals Versus Carbocations," James L. Adcock, Wm. D. Evans and Lilly H. Grossman, J. Org. Chem., 1983, 48, 4953-4957.

"A Simple Photochemical Conversion of Perfluoroalkyl Hydrides to Perfluoroalkyl Bromides Using Interhalogen Compounds," J. L. Adcock and W. D. Evans, J. Org. Chem., 1983, 48, 4122-4125.

"Aerosol Direct Fluorination - Synthesis of Perfluoroadamantane - The Penultimate Step," James L. Adcock and Mark L. Robin, J. Org. Chem., 1983, 48(18), 3128-3130.

"Aerosol Direct Fluorination-Syntheses of Perfluoroketones," James L. Adcock and Mark L. Robin, J. Org. Chem., 1983, 48, 2437-2439.

"Feasibility Studies for Improving Gas Insulation by Coating Contaminating Particles, M. O. Pace, J. L. Adcock, L. C. Frees and L. G. Christophorou, Gaseous Dielectrics, Proc. Int. Symp., 3rd, 307-314 (1982).

Craig E. Barnes, Assistant Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTERESTS:

Transition metal catalysis, development of electrochemical catalytic methods, fuel cells, olefin metathesis models.

PROFESSIONAL EXPERIENCE:

Assistant Professor, Department of Chemistry, University of Tennessee, 1984-

CURRENT RESEARCH SUPPORT:

Petroleum Research Foundation Type G Starter Grant, $15,000, 1984-

MOST RECENT PUBLICATIONS:

W. A. Herrmann, C. E. Barnes, R. Serrano and B. Koubouris, "LII. Synthesekonzepte zum Aufbau Heterodinuclearer Metall - Metall Mehrfachbindungen" (Synthetic Approaches to the Construction of Heterometallic Metal-Metal Multiple Bonds), J. Organomet. Chem., 256, C30 (1983).

J. P. Collman, C. E. Barnes, P. J. Brothers, T. J. Collins, T. Ozawa, J. C. Gallucci, and James A. Ibers, "Oxidation of Ruthenium(II) and Ruthenium(III) Porphyrins. Crystal Structures of μ-Oxobis p-methylphenoxo-(meso-tetraphenyl=porphyrinato)-ruthenium(IV) and Ethoxo-(meso-tetraphenyl=porphyrinato)-ruthenium(III)-bisethanol", J. Am. Chem. Soc., in press.

J. P. Collman, C. E. Barnes and L. Keith Woo, "Systematic Variation of Metal-Metal Bond Order in Metalloporphyrin Dimers," Proc. Nat. Acad. Sci., in press.

J. P. Collman, C. E. Barnes, P. N. Swepston and J. A. Ibers, "Synthesis, ^{1}H NMR and Structural Characterization of Binuclear Ruthenium Porphyrin Dimers," J. Am. Chem. Soc., in press.

J. P. Collman, F. C. Anson, C. E. Barnes, C. S. Bencosme, T. Geiger, E. R. Evitt, R. P. Kreh, K. Meier and R. Pettman, "Further studies of the Dimeric β-Linked "Face-to-Face Four" Porphyrin: FTF4", J. Am. Chem. Soc., 105, 2694 (1983).

J. P. Collman, C. S. Bencosme, C. E. Barnes and B. D. Miller, "Two New Members of the Dimeric Beta-Linked Face-to-Face Porphyrin Series: FTF4* and FTF3," J. Am. Chem. Soc., 105, 2704 (1983).

J. P. Collman, C. E. Barnes, T. J. Collins, P. J. Brothers, "Binuclear Ruthenium(II) Porphyrins: A Reinvestigation of their Preparation, Characterization and Interactions with Molecular Oxygen," J. Am. Chem. Soc., 103 7030 (1981).

1076291

James Q. Chambers, Professor of Chemistry

EDUCATION: [redacted]

MAJOR RESEARCH INTEREST:

Electrochemistry, Polymeric Modified Electrodes, Enzyme Electrodes, Multisulfur Electron Donors.

PROFESSIONAL EXPERIENCE:

Assistant Professor, Department of Chemistry, University of Colorado, 1964-1969
Assistant Professor, Department of Chemistry, University of Tennessee, 1969-1971
Associate Professor, Department of Chemistry, University of Tennessee, 1971-1979
Professor, Department of Chemistry, University of Tennessee, 1979-

CURRENT RESEARCH SUPPORT:

"Synthesis and Electrochemistry of Electroactive Polymers," NSF, 7/83 - 12/86; $182,500 (3 year total support).
"Polymer Modified Electrodes," Martin Marietta Corp., 4/84 - 3/85; $25,000 (Co-PI with Gleb Mamantov).

RECENT PUBLICATIONS:

Q. Chambers and G. Inzelt, "Temperature Dependence of the Voltammetric Response of Thin Electroactive Polymer Films," submitted for publication.

M. A. Lange and J. Q. Chambers, "An Amperometric Enzyme Electrode for the Oxidation of Glucose Based on Redox Mediation and Entrapment in a Polyacrylamide Gel," submitted for publication.

P. Joo and J. Q. Chambers, "Solvent Effects on the Electrochemistry of Tetracyanoquinodimethane Polymer Modified Electrodes," submitted for publication.

G. Inzelt, J. Q. Chambers, J. F. Kinstle and R. W. Day, "Protonation Equilibria and Charge Transport in Electroactive Tetracyanoquinodimethane Polymer Filsm," J. Am. Chem. Soc., 1984, 106, 3396-3401.

G. Inzelt, J. Q. Chambers, J. F. Kinstle, M. A. Lange, "Metal Substrate Effect on pH Response of Tetracyanoquinodimethane Modified Electrodes," Anal. Chem., 1984, 56, 301-302.

G. Inzelt, R. W. Day, J. F. Kinstle and J. Q. Chambers, "Spectroelectrochemistry of Tetracyanoquinodimethane Modified Electrodes," J. Electroanal. Chem., 1984, 161, 147-161.

G. Inzelt, J. Q. Chambers, and F. B. Kaufman, "Electrochemistry of Tetrathiafulvalene Polymer. Electric Spin Resonance of Polymer Film Electodes," J. Electroanal. Chem., 1983, 159, 443-448.

J. Q. Chambers, "Electrochemistry in the General Chemistry Curriculum," J. Chem. Ed., 1983, 60, 259-262.

Richard M. Pagni, Professor of Chemistry

EDUCATION

[redacted]

MAJOR RESEARCH INTERESTS

The Chemical and Physical Properties of Biradicals and Carbenes. Electrocyclic Reactions of Radical Cations and Anions. Environmental Photochemistry. Organotransition Metal Chemistry. Organic Reactions on Solid Surfaces. Organic Reactions in Superacids.

PROFESSIONAL EXPEDRIENCE

Assistant Professor, University of Tennessee, 1969-76;
Associate Professor, UT, 1976-81
Professor, UT, Sept. 1981-present.
Consultant/Part-time Employee, Oak Ridge National Laboratory, 1984-present.
Consultant, Tennessee Valley Chemical Company, 1984-present.

CURRENT RESEARCH SUPPORT

Inorganic and Organic Reactions in Molten Salts (with G. Mamantov): $180,000; ARCO; July 1, 1984-June 30, 1985.

RECENT PUBLICATIONS

H. M. Hassaneen, A. O. Abdelhamid, A. S. Shawali and R. Pagni, A Study of the Effect of Nitro Group in the Synthesis of Pyrazoles and Thiadiazolines from Hydrazidoyl Halides, *Heterocycles*, *19*, 319 (1982).

R. J. Smith, T. Moore Miller and R. M. Pagni, Studies on the Protonation of Stable π-Carbocations. Requirements for the Reaction of Two Positively Charged Species with Each Other in Solution. *J. Org. Chem.*, *47*, 4181 (1982).

G. S. Sayler, M. C. Reid, B. K. Perkins, R. Pagni, R. L. Smith, T. K. Roa, J. L. Epler, W. D. Morrison and R. DuFrain, Evaluation of the Mutagenic Potenntial of Bacterial, PCB Biodegration Products, *Arch. Environm. Contam. Toxicol.*, *11*, 577 (1982).

W. P. Cofino, S. M. van Dam, G. P. Hoornweg, C. Gooijer, C. MacLean, N. H. Velthorst and R. M. Pagni, Highly Resolved Optical Spectra of the Biradical 1,4-Perinaphthadiyl, *Spectrochim. Acta*, *40A*, 251 (1984).

R. M. Pagni, Multiple Charged Carbocations and Related Species in Solution, *Tetrahedron*, *40*, 0000 (1984).

K. Gaetano, R. M. Pagni, G. W. Kabalka, P. Bridwell, E. Walsh, J. True and M. Underwood, The Reaction of Organic Molecules on Solid Surfaces. II. AEfficient Method for the Preparation of Deuterated Alumina, *J. Org. Chem.*in press.

R. M. Pagni, Organic and Organometallic Reactions in Molten Salts, Advances in Molten Salt Chemistry, manuscript in preparation.

R. Varma, G. W. Kabalka, L. Evans and R. M. Pagni, Aldol Condensations of Alumina; The Facile Syntheses of Chalcones and Enones in a Solvent-Free Medium, *Syn. Commun.*, submitted.

Clifton Woods, Associate Professor of Chemistry

EDUCATION:

[redacted]

MAJOR RESEARCH INTEREST:

Synthesis, characterization, and electrochemistry of organorhodium complexes; interaction of metal complexes with biological molecules.

PROFESSIONAL EXPERIENCE:

Instructor, North Carolina State University, 1970-71
Interim Assistant Professor of Chemistry, University of Florida, 1971-73
Visiting Assistant Professor of Chemistry, Bowling Green State University, 1973-74
Assistant Professor of Chemistry, University of Tennessee, 1974-82
Associate Professor of Chemistry, University of Tennessee, 1983-present

CURRENT SUPPORT:

National Science Foundation, "Synthesis, Electrochemistry and Catalysis of New Rhodium Dimers" $173,081, 7/1/83-6/30/86.

PUBLICATIONS:

P. D. Enlow and C. Woods, "Synthesis and Characterization of Some Rhodium(I) Dimers Containing (Diphenylarsino)(diphenylphosphino)methane as the Bridging Ligand," Organometallics. 1983, 2, 64-68.

D. W. Abbott and C. Woods, "Synthesis and Infrared and Magnetic Resonance Studies of Organohodium Complexes of Guanosine, Inosine, 1-Methylinosine, Purine, Adenine, and Adenosine," Inorg. Chem. 1983, 22, 597-602.

D. W. Abbott and C. Woods, "Carbon-13 and Phosphorus-31 NMR Studies of Interactions of Organorhodium Complexes with Guanosine, Inosine, 6-Mercaptoguanosine, and 8-Mercaptoguanosine in Neutral and Basic Dimethyl-d_6 Sulfoxide Solutions," Inorg. Chem. 1983, 22, 1918-1924.

D. R. Womack, P. D. Enlow and C. Woods, "Electrochemical Studies of Tetrakis(isocyanide) Rhodium(I) Dimers Containing Bis(diphenylphosphine)methane as the Bridging Ligand," Inorg. Chem. 1983, 22, 2653-2656.

D. W. Abbott and C. Woods, "Interactions of the Carbonylbis(triphenylphosphine)rhodium(I) Cation with Purine-Pyrimidine Base Pairs as Studied by Carbon-13 Phosphorus-31, and Protn NMR," Inorg. Chem. 1983, 22, 2918-2923.

D. W. Abbott and C. Woods, "Carbon-13, Phosphorus-31 and Proton NMR Studies of the Interactions of the carbonylbis(triphenylphosphine)-rhodium(I) Cation with Base Pairs of s^6 Guanosine and s^8 Guanosine with Cytidine," Inorg. Chem. 1984, 23, 3626-3629.

P. D. Enlow and C. Woods, "The Effect of Nitrogenous Bases on the Electrochemical Oxidation of a Diphosphine-Bridged Tetrakis(isocyanide) Rhodium(I) Dimer," Inorg. Chem. in press.

C. Woods and C. Daffron, "A Study of the Trans Influence in Some Rhodium(I) Complexes Using Infrared Spectroscopy," Inorg. Chim. Acta in press.

Proposal Acknowledgment Cards

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Address one card to the Institution's official authorized to sign cover sheet)

Institution University of Tennessee

Project Director Gleb Mamantov

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Institution University of Tennessee

Project Director Gleb Mamantov

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