COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S)
(Indicate the most specific unit known, i.e. program, division, etc.)
Division of Undergraduate Education
Instrumentation for Laboratory Improvement

FOR NSF USE ONLY

NSF PROPOSAL NUMBER

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE
EHR/DUE ILI-IP (NSF #93-164) November 14, 1994

DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	FILE LOCATION

EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)

SHOW PREVIOUS AWARD NO. IF THIS IS:
☐ A RENEWAL OR
☐ AN ACCOMPLISHMENT-BASED RENEWAL

IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES_____ NO__✓__ IF YES, LIST ACRONYM(S)

NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE:
Youngstown State University

AWARDEE ORGANIZATION CODE (IF KNOWN)

ADDRESS OF AWARDEE ORGANIZATION, INCLUDING ZIP CODE
410 Wick Avenue
Youngstown, OH 44555-3663

NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE

PERFORMING ORGANIZATION CODE (IF KNOWN)

ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING ZIP CODE

IS AWARDEE ORGANIZATION(Check all that apply): ☐FOR-PROFIT ORGANIZATION ☐SMALL BUSINESS ☐MINORITY BUSINESS ☐WOMAN-OWNED BUSINESS
(See GPG For Definitions)

TITLE OF PROPOSED PROJECT
Integration of Automated GC-MS
into the Undergraduate Curriculum

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE
$ 40,859	12 months	1995

CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW:
- ☐ VERTEBRATE ANIMALS
- ☐ HUMAN SUBJECTS
- ☐ HISTORICAL PLACES
- ☐ BEGINNING INVESTIGATOR (See GPG SECTION I)
- ☑ GROUP PROPOSAL
- ☐ SMALL GRANT FOR EXPLANATORY RESEARCH (SGER)(SEE GPG SECTION II.C.12)
- ☐ NATIONAL ENVIRONMENTAL POLICY ACT
- ☐ PROPRIETARY AND PRIVILEGED INFORMATION
- ☐ DISCLOSURE OF LOBBYING ACTIVITIES
- ☐ FACILITATION FOR SCIENTISTS/ENGINEERS WITH DISABILITIES
- ☐ RESEARCH OPPORTUNITY AWARD
- ☐ INTERNATIONAL COOPERATIVE ACTIVITY: _____ Country/Countries

PI/PD Department
Chemistry

PI/PD Fax Number
(216) 742-1579

PI/PD Postal Address
410 Wick Avenue
Youngstown, OH 44555-3663

Names (Typed)	Social Security No.	High Degree, Yr	Telephone Number	Electronic Mail Address
PI/PD Name John A. Jackson, Chemistry	471-54-9574	Ph.D., 1990	216-742-1551	JAJACKSO@CC.YSU.EDU
Co-PI/PD Allen D. Hunter, Chemistry	293-94-4212	Ph.D., 1985	216-742-7176	ADHUNTER@CC.YSU.EDU
Co-PI/PD Steven M. Schildcrout	222-26-7673	Ph.D., 1968	216-742-7114	
Co-PI/PD Renee L. Falconer	171-64-9086	Ph.D., 1994	216-742-7100	
Co-PI/PD Timothy R. Wagner, Chemistry	396-74-0175	Ph.D., 1986	216-742-1960	

NOTE: THE FULLY SIGNED CERTIFICATION PAGE MUST BE SUBMITTED IMMEDIATELY FOLLOWING THIS COVER SHEET.

*SUBMISSION OF SOCIAL SECURITY NUMBERS IS VOLUNTARY AND WILL NOT AFFECT THE ORGANIZATION'S ELIGIBILITY FOR AN AWARD. HOWEVER, THEY ARE AN INTEGRAL PART OF THE NSF INFORMATION SYSTEM AND ASSIST IN PROCESSING THE PROPOSAL. SSN SOLICITED UNDER NSF ACT OF 1950, AS AMENDED.

CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

(1) the statements herein (excluding scientific hypotheses scientific opinions) are true and complete, and
(2) the text and graphics herein as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or individuals working under their supervision. I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this application

I understand that the willful provision of false information or concealing a material fact in this proposal or any other communication submitted to NSF is a criminal offense (U.S.Code, Title 18, Section 1001).

Names (Typed)	Signature	Date
PI/PD Name John A. Jackson		
Co-PI/PD Allen D. Hunter		
Co-PI/PD Steven M. Schildcrout		
Co-PI/PD Renee L. Falconer		
Co-PI/PD Timothy R. Wagner		

Certification for Authorized Institutional Representative or Individual Applicant:
By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt statue, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in the Grant Proposal Guide (GPG), NSF 92-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U.S.Code 1001).

Debt and Debarment Certifications (If answer "yes" to either, please provide explanation.)

Is the organization delinquent on any Federal debt? Yes ____ No X

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes ____ No X

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agrement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a materila representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

AUTHORIZED INSTITUTIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) Dr. Leslie H. Cochran, President		

TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS	FAX NUMBER
(216) 742-3101		(216) 742-1579

NATIONAL SCIENCE FOUNDATION
Division of Undergraduate Education

PROJECT DATA FORM

The instructions and codes to be used in completing this form begin on the next page.

1. Program to which the Proposal is Submitted: ILI-IP
2. Type of Submission: PR
3. Name of Principal Investigator/Project Director (as shown on the Cover Sheet):
   Dr. John A. Jackson
4. Name of Submitting Institution (as shown on the Cover Sheet)
   Youngstown State University
5. Other institutions involved in the project's operation:
   Hiram College, Mount Union College, Lake Erie College, Thiel College, Malone College, Westminster College

PROJECT CODES

A. Major Discipline Code: 1 2 Subfields: Org, Inorg, Poly, Anal/Envir, & Phys.
B. Academic Focus Level of Project: B O
C. Highest Degree Code: M
D. Category Code: ____ ____
E. Business/Industry Participation Code: ____ ____
F. Audience Code: W M H S
G. Institution Code: P U B L
H. Environmental Education Code: E N
J. Estimated Number of Undergraduate Students to be Directly Affected by the Activities of the Project During its Operation: 2000 over 5 years
K. Estimated Number of Pre-College Students to be Directly Affected by the Activities of the Project During its Operation: 50 over 5 years
L. Estimated Number of College Faculty to be Directly Affected by the Activities of the Project During its Operation: 60 (5 years)
M. Estimated Number of Pre-college Teachers to be Directly Affected by the Activities of the Project During its Operation: 25 (5 years)
N. Total Non-NSF Contribution: $40,859

Project Summary:

The Project Summary should be a concise description of the project limited to 22 lines of 12-point (standard pica type) or larger font on plain white paper.

PROJECT SUMMARY

The purpose of this proposal is to obtain seed funding for a robotic sample changer controlled GC-MS facility directed towards undergraduate education and student research courses at Youngstown State University. This facility will be available to the faculty and students of YSU and also to those of regional liberal arts colleges, especially the nine members of the YSU Public/Private Alliance. The requested robotic sample changer controlled GC-MS will enable unattended data collection on student samples overnight and on weekends. The GC-MS will be networked to a series of existing data stations, allowing student data processing, analysis, and use in lecture courses. The GC-MS results will be integrated with the results from other spectroscopic (especially multinuclear NMR) and crystallographic techniques. Laboratory studies in the sophomore through senior years will emphasize "hands on" research based laboratory experiences. The mass spectra and GC data will be made available to other users via INTERNET, in combination with NMR data for the same compound, and summer courses on advanced instrumentation operation and data analysis techniques will be offered to college faculty.

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1. Results from Prior NSF Support.

The PI/PD and other YSU co-applicants have not previously had NSF support except that T. R. Wagner, A. D. Hunter, and J. A. Jackson were notified on July 21, 1994, that they were awarded $71,199 from the NSF-Materials Division towards the purchase of a single crystal X-ray diffractometer ($191,199 in total including match). A. Hunter has since attended the American Crystallographic Association short course in X-ray crystallography at the University of Pittsburgh (August 1-12). Formal quotations have now been obtained, instruments are being evaluated, and we expect to order the diffractometer in late Fall for delivery during the Winter quarter. The quotations include site licenses for the X-ray diffraction analysis software for use on the computer networks of member colleges of the YSU public-private alliance.

2. Narrative.

Youngstown State University is an urban public institution serving, primarily, the "five-county" area that includes Northeast Ohio and Northwest Pennsylvania. We are a middle-sized, primarily undergraduate ($\approx$ 13,000 full and part time students pursuing 2- and 4-year technical and 4- and 5-year bachelor's level degrees) institution with M.S. programs in many departments ($\approx$ 1,200 students) but not offering Ph.D. degrees in Science or Engineering. Our student population is about one-half female (51.4%) and has a significant component of under-represented minority (9.0%) and non-traditional students that reflects the composition of our service area. We are currently attempting to increase the recruitment and especially retention of underrepresented groups as students and faculty. In particular, we are becoming increasingly involved with the Youngstown city schools, which have a substantial African-American enrollment, to encourage their students to attend the University and to help fund their education. We have found that "hands on" exposure to science research in the eighth through twelfth grades (e.g., through ACS Project SEED and Summer School) and close interaction with faculty mentors is particularly effective for this.

Youngstown State University's Chemistry Department has 17 faculty members (all having Ph.D.'s in Chemistry or Biochemistry). Of these faculty, 5 have been hired over the last 3 years

and 6 more are expected to be replaced over the next 2 years due to retirement (i.e., we have 4 openings for September 1995). We also have 3.8 full time support staff. This department has a very strong record of graduating well-educated chemistry majors. In a recent American Chemical Society survey (*Chemical & Engineering News*, August 9, 1993, pp. 24 to 33), we again ranked in the top 25 departments nationally in terms of the number of our Chemistry bachelor degree graduates (47 for 1991-92). Over the last several years we have averaged 46 bachelor graduates a year. Of those that we have been able to further track, typically: 21 proceed to professional postgraduate programs (e.g., Medical, Dental, and Law School); 5 proceed directly to graduate programs at other schools (e.g., The Ohio State University, Kent State University, The University of Akron, The University of Cincinnati, Penn State University, The University of Pittsburgh, and The University of Texas); 3 to 8 proceed to M.S. degrees here at YSU, often before proceeding to later Ph.D. programs. Our M.S. enrollment has, until recently, been around 15 students but we now have 22 students and are currently moving towards a new target enrollment of about 30 full time M.S. students by 1996. Most of the remainder of our graduates are working in local industries. Our department therefore has a relatively large role in university chemical education in this country. The nine private liberal arts colleges that are members of the YSU Public/Private Alliance (i.e., Hiram College, Mount Union College, Grove City College, Lake Erie College, Walsh University, Thiel College, Malone College, Geneva College, and Westminster College) and Lorain County Community College have more than 30 chemistry faculty, and a total enrollment of about 10,000 undergraduates. Together they have graduated over 100 chemistry majors over the last five years.

As with most chemistry departments, we serve chemistry majors, students with a minor in chemistry, and students whose programs have a chemistry requirement. In addition to traditional 4-year B.S. and 2-year M.S. degrees in chemistry we have just instituted a B.S. program in environmental science. We anticipate approval to offer an M.S. in environmental science in 1996. Our main service teaching loads are for students taking combined science, engineering,

nursing, medical technology, and pre-professional (e.g., pre-medical, pre-dental, pre-pharmacy) degrees.

Gas chromatography mass spectrometry (GC-MS) is an extremely important tool for establishing the structures of molecules and the composition of mixtures. Recent advances in instrumentation and computer technology, dramatically reduced maintenance requirements, and "menu driven" and "push button" software have simultaneously increased the power of GC-MS to help solve complex structural problems and the ease with which even novice users, such as undergraduates, can successfully collect and interpret such data. The speed of collecting GC-MS and the amount of easily interpretable spectral information obtained makes mass spectrometry very attractive for incorporation into the undergraduate curriculum. Unfortunately, the costs of obtaining a mass spectrometer has limited their purchase by primarily undergraduate, and especially 2- and 4-year liberal arts, institutions. Larger Ph.D. granting universities generally have multiple mass spectrometers in their departmental facilities, but they are almost exclusively used for graduate student, post-doctoral, and faculty research and undergraduates get little or no access, especially on a "hands on" basis in their laboratory courses. We are establishing a Regional Molecular Structure Center associated with the YSU Public/Private Alliance to allow the use of dedicated modern spectroscopic methods including GC-MS, high field NMR (400 MHz) and X-ray diffraction analysis in undergraduate education on a "hands on" basis. We will give priority in access to the GC-MS instrument described in this project to undergraduate students. It will enable us to integrate "research type" experiments into the labs where each student in a lab section does a separate, yet related, investigation and then the lab section jointly develops experimentally based theories to explain their observations. The large amount of spectral data obtained during these courses will be made available as a national educational resource through on-line access via the INTERNET.

a. Current Situation.

Youngstown State University has a Finnigan 1020 GC/MS obtained with University funding in 1984. This quadrupole instrument has EI and CI ion sources, mass range to 800 amu, and a

solids inlet probe. It has been used primarily for faculty and graduate-student research under the supervision of a co-PI (Schildcrout), but it is not suitable for regular use by undergraduates because of increasing maintenance problems, associated downtime and difficult operation. It is no longer supported by the manufacturer. Its data system is limited (data disk capacity only 10MB), slow, and difficult to use by modern standards. To adequately train undergraduates in its use would be prohibitively time consuming and frustrating both to the instructor and to the student, who needs to obtain and understand results but does not need to master the operation of such a complex, and now obsolete, instrument.

b. Development Plan.

To enable us to integrate this new gas chromatograph mass spectrometer into all four years of undergraduate chemistry education in a wide array of courses at both YSU and the 9 regional colleges, we require both the basic instrument and a robotic sample changer to increase sample throughput.

An explanation of how this new spectrometer would impact individual courses at YSU follows. In addition to published experiments from conventional texts and from journals such as *J. Chem. Ed*, specific new experiments or research based variations on more well known experiments are listed. In general, mass spectrometry will be used as a central tool in our chemistry program and its theory and use will be developed and expanded from the freshman to the senior years. In both lectures and labs we will have the students use empirical mass spectral data to derive important chemical concepts (e.g., in molecular weight determination, isotopic composition, molecular structure) from their data rather than memorize them from a lecture or a book. None of these experiments can be carried out with the current mass spectrometer. In the following section, the utilization of GC-MS in our new curriculum is illustrated with examples drawn from representative courses. Detailed listings of new experiments are contained in Appendix 6a (authorized by Dr. Susan Hixson, NSF Program Officer, on November 3, 1994).

Chemistry 515, 516, and 517, General Chemistry. Mass spectrometry offers the most direct method for determination of atomic weights of the elements, and is the most precise

method for determination of molecular weight. The existence of isotopes was first proven with mass spectrometry. The concept of charge, and formation of ions is critical in general chemistry. Mass spectrometry gives a real "hands on" method for students to explore these difficult text book concepts, in a manner that connects the lecture and laboratory more effectively than currently possible. These concepts will be introduced in the first quarter lecture in the context of the students' first exposure to the structure of the atom and molecules. Problem sets and lab/tutorials will be used to give students practice in determining different molecular weights, isotopic abundances and atomic weights in simple inorganic and organic molecules, predicting the expected isotope patterns, and using information from mass spectra on the PC network to check their predictions. The robotic sample changer would be essential to manage the large sample throughput.

Chemistry 603 and 604, Quantitative Analysis 1 and 2. GC-MS will be introduced as a method of determining relative concentrations of related volatile organics. Gas chromatography is already part of the laboratory sequence. The new GC-MS will allow students to compare the same sample by flame ionization detection (FID) and total ion count. Mass spectrometry will enable absolute identification of each component in the student's mixture. They will be able to evaluate the two methods and make there own conclusions as to the reliability of both methods.

Chemistry 719, 720, and 721, Organic Chemistry 1, 2, and 3. Organic Chemistry at YSU is being fundamentally reorganized away from the "classical" teaching approach to an approach that is more discovery based. In the lecture, the students will learn to deduce the structures and bonding of the fundamental organic functional groups and basic molecules from spectroscopic data, including GC-MS (along with FT-IR, ^{1}H and ^{13}C NMR) during the first month. Problem sets for lectures involving spectroscopic interpretation will be done by the students on the PC data stations using example data sets from the archives. The first quarter labs will introduce the main methods of purification and molecular identification (experiments 1 to 5, see Appendix 6a). The second quarter will be composed of two to four synthetic/mechanistic studies while the third quarter will be composed of one or two longer special projects. The emphasis in each quarter is

on student based "research problems" where they discover, from experimental data, some of the central concepts of organic chemistry. A major tool in this effort will be the use of GC-MS information in structure elucidation. The use of the gas chromatograph mass spectrometer will be discussed in class, demonstrated to the students in the lab, and learned via a "hands on" experiment (#1 in Appendix 6a). The students will make up their own GC-MS samples, and these will be run by the students under the supervision of a laboratory assistant during the lab period, or submitted for automated overnight collection (using the robotic sample changer) for more time consuming data collections. Students will plot their mass spectra at the spectrometer for the first experiments and subsequently the GC-MS data will be transferred to the computer data stations for them to examine and plot themselves. New experiments that are not currently possible and that have a substantial GC-MS component are included in Appendix 6a.

Chemistry 739, 740, and 741, Physical Chemistry 1, 2, and 3. The principles of mass spectrometry will be discussed, and various methods of ionization will be compared. Mass spectrometry will be used in the experimental determination of ionization energies, which will be compared to calculated values and literature values from other methods. Thermodynamic and kinetic principles will be applied to gas phase ion chemistry.

Chemistry 751 and 752, Water Quality Analysis 1 and 2. The use of GC-MS is one of the most important method to quantify and identify organic pollutants in aqueous solutions. Students will examine natural waters, drinking water, and waste water in the laboratory by GC-MS, relying extensively on the NIST database to identify as many environmental pollutants (and their relative concentration) as possible. There will be extensive lecture discussion of the use of GC-MS in environmental applications.

Chemistry 803 and 804, Chemical Instrumentation 1 and 2. This course is a detailed "hands on" course on the principles and operation of modern analytical instrumentation including GC-MS. The lab will have demonstrations and experiments on the practical aspects of GC-MS hardware, data systems, and spectrometer operation.

Chemistry 805, Applied Spectroscopy. This is a lecture course emphasizing the use of multiple types of spectroscopic data to identify and quantify organic compounds in analytical chemistry problems. The NIST data base will be used by the students to practice using mass spectral data in structure determinations.

Chemistry 822, Organic Analysis. This is a newly designed course based on modern instrumental methods, it will replace an antiquated course based on classical "wet methods." The lecture will introduce the practical aspects of carrying out mass spectral determinations and interpreting their results in complex structural identification problems. The lab will be totally "hands on" and will start where the sophomore organic sequence left off. Students will work individually and in groups collecting a range of GC-MS (in addition to multinuclear 1D and 2D NMR spectra and IR) data needed to assign the structures of a series of unknown organic compounds of increasing complexity (i.e., working up from simple functionalized alkanes and arenes to complex natural products such as di- and tri-terpenes, sugars, and "simple" steroids).

Chemistry 823, Organic Synthesis. In this course each student performs one or a few advanced synthesis projects, generally drawn out of journals such as *Organic Synthesis* or from advanced texts. Each project involves library research, followed by synthesis, purification, and product identification. Mass spectral methods are used "hands on" to identify reaction products and monitor reaction progress. Typically, each student carries out a different project. Projects used in 1992-93 and 1993-94 have included the synthesis of calix[n]arenes, triaryl phosphines and their derivatives, isomeric dialkyl benzene dicarboxylates, 2-methyl-1,3-cyclopentanedione, resolved bi-2-naphthols, and 3-butylcyclobutenone.

Chemistry 824 and 825, Polymer Chemistry Lecture and Lab. The lectures introduce students to the use of MS in polymer chemistry with an emphasis on the use of MS in prepolymer and polymer additive analysis. These methods will be applied by the students in the lab to prepolymers they have prepared and on additives they have extracted from commercial polymers. New experiments having a substantial MS component are listed in Appendix 6a.

Chemistry 831, Inorganic Lab. The students prepare and characterize a series of main group and transition-metal solid state, coordination, and organometallic complexes. The course emphasizes multi-technique characterization of the compounds synthesized, so that students are exposed to as many state-of-the art methods and techniques as possible. The characterization techniques currently utilized in the course include IR, NMR and X-ray diffraction. New experiments utilizing mass spectrometry as part of product characterization are listed in Appendix 6a.

Chemistry 650 and 850, Undergraduate Research. These courses are the primary vehicle by which our undergraduates become involved in research. Projects involve library studies, individual laboratory research study, and the writing of a thesis which often results in a formal presentation and/or publication. A related course, Chemistry 990, serves our M.S. research students. Projects are chosen from the research programs of our faculty in the areas of analytical, environmental, physical, theoretical, organic, polymer, and inorganic chemistry and biochemistry. A list of recent student results can be found in Appendix 6e.

c. Equipment

c.1. Equipment Request. To meet our needs for a large volume of mass spectral sample throughput, we require a robotic sample changer controlled GC-MS. The robotic sample changer will allow unattended spectrometer operation so that GC-MS data can be collected overnight and on weekends to meet the large volume teaching needs of our laboratory courses, detailed above. During "normal" school hours (i.e., Monday to Friday, 8 a.m. to 5 p.m.) students will run their GC-MS spectra "hands on" with the assistance of the undergraduate laboratory assistant(s) and the laboratory instructor (sophomore and junior labs) or under the supervision of the faculty instructor (senior labs). For the evenings and weekends, these "hands on" runs will be supplemented by the use of the robotic sample changer. Blocks of time (initially 2 or 3 mornings or afternoons), scheduled for their convenience, will be booked each week for students

and faculty from the regional colleges to run their own samples. They will also be able to submit samples by mail which will be run in the automatic mode on the sample changer and then the results sent by INTERNET to their school for processing. Each student will prepare the sample and load it into a numbered sample tray, use the "push button" mode on the GC-MS console, and the data will then be collected by the spectrometer in the unattended mode. This will allow us to collect the large numbers of basic mass spectra that the "research based" lab experiments described above require. YSU's teaching needs will be allocated 60% of the instrument's available time with 30% being dedicated to students from the regional colleges and 10% being available for instrumental maintenance, faculty research, and new experiment implementation.

The data system includes a small existing network of IBM compatible data stations, which we hope to expand in the near future with other proposals to the Dreyfuss Foundation, NSF-ILI, and internal YSU funds, so that all of the students in a lab can work in small groups at the same time during a lab on their data analyses and problems. Finally software for the workstations and for the IBM compatible computers already on faculty user desks is included. The department will also purchase software for other types of spectroscopic data analysis (i.e., IR, NMR) for single crystal X-ray data analysis (e.g., SHELXTL-PC), for molecular orbital/mechanics/modeling calculations (e.g., Chem-X) and, for AA, ICP, analytical instrument simulation. These programs will also be used on this network for these courses. The computer network will allow <u>each</u> student to practice interpreting real mass spectra for their lecture and lab courses, to practice GC-MS data manipulation and processing (i.e., selected ion searches, library comparisons, evaluate the effects of different chromatographic conditions, etc.), plot the spectrum, and to practice spectrometer operation (i.e., use the data stations as GC-MS simulators) in a "hands on" way. In addition, over several years a large library of GC-MS data files on compounds will be archived. This data will be available to YSU and regional college students and faculty for use in their classes, and nationally through INTERNET. This is especially useful for the schools lacking a GC-MS dedicated to <u>teaching</u>.

c.2. Equipment on Hand for the Project. A series of 4 data stations are available, and we are seeking other funding to supplement these with a network of 15 modern computers. The new GC-MS instrument will be integrated with this network. Other items of major equipment on hand for the labs described include a Varian Gemini-2000 400 MHz multinuclear NMR spectrometer, modern IR, UV-visible, X-ray diffraction, and chromatography systems. A complete list of departmental instruments is enclosed in Appendix 6b.

c.3. Implementation and Equipment Maintenance. YSU has a 4-person electronics maintenance staff available at no charge to Chemistry to help carry out routine maintenance. There is a full time SUN/PC network manager in the Computer and Information Science Department to help implement the data station network. The Chemistry Department has annual operating ($86,000) and maintenance ($25,000) budgets to fund consumables and repairs requiring outside assistance. The Chemistry Department receives ≈ $63,000 annually in "instructional" lab fees to help maintain and upgrade our instrumentation.

d. Faculty Expertise. The applicants have extensive experience in GC-MS operation since it is an integral part of their independent research, see Biographical Sketches.

e. Dissemination and Evaluation. The new discovery-based experiments, developed using the proposed instrumentation, will be presented at regional and national ACS and undergraduate education conferences, disseminated by electronic mail and through the Polymer Education Newsletter, and published in appropriate journals such as the *Journal of Chemical Education*. YSU will institute a summer program for faculty from predominately undergraduate institutions and liberal arts colleges designed to familiarize them with, and/or update them on, the "hands on" use of advanced instrumentation, including the gas chromatograph mass spectrometer, high field NMR spectrometer(s) and our new X-ray diffractometers. Instrument time will be made available to faculty and students from other predominately undergraduate institutions for curriculum development and student research. Importantly, the GC-MS spectra database collected by this spectrometer will be available via INTERNET to other institutions, especially to those lacking an instrument for use in teaching.

The evaluation of this project will occur in several stages. The individual and total frequencies of use and the number of users of the mass spectrometer, data stations, and on-line database will be tracked by network server system software packages. The knowledge and skills gained by the students will be tracked by "on-line" exams and "unknown" laboratory problems and by annual surveys of the students and faculty instructors. Finally, institutions where our students go to pursue Ph.D.'s, our local employers, and our graduates themselves will be surveyed at three-year intervals for feedback on how our program met their needs and could be improved. The results of these evaluations, particularly, the benefits of robotic sample changers to throughput, and the advantages (and problems!) of networked data stations and spectra distributions, will be disseminated to NSF, the ACS, and CUR, and through the INTERNET. Other schools may want to use any demonstrated benefits to (a) argue for the purchase of their own GC-MS and/or establishment of other regional centers dedicated to undergraduate instrumentation, (b) to argue for time on "research" GC-MS instruments , and/or (c) to argue for their own robotic sample changers and data station networks.

3. BIOGRAPHICAL SKETCH

Provide the following information for the senior personnel on the project. Begin with the Principal Investigator/Project Director.

DO NOT EXCEED 2 PAGES PER PERSON.

A. Vitae, listing professional and academic essentials and mailing address.

B. List up to 5 publications most closely related to the proposed project and up to 5 other significant publications, including those being printed. Patents, copyrights, or software systems developed may be substituted for publications. Do not include additional lists of publications, invited lectures, etc. Only the list of up to 10 will be used in merit review.

C. List of persons, other than those cited in the publication list, who have collaborated on a project or a book, article, report or paper within the last 48 months, including collaborators on this proposal. If there are no other collaborators, please indicate that fact.

D. Names of graduate and post-graduate advisors and advisees.

The information in C. and D. is used to help identify potential conflicts or bias in the selection of reviewers.

Biographical Sketch for John A. Jackson

Department of Chemistry, Youngstown State University, Youngstown, OH 44555

A. **Vitae.** John A. Jackson obtained his B.A. degree in Chemistry in 1982 from the University of Minnesota. In 1984, he started graduate school at the University of Iowa, receiving his Ph.D in Organic Chemistry in 1990, while working with Professor David F. Wiemer. The title of his dissertation was "New Chemistry of α-Phosphono Lactones". In the spring of 1990, John joined the laboratory of Professor Charles M. Thompson in the Chemistry Department at Loyola University Chicago as a postdoctoral research associate. While at Loyola, John worked on the synthesis of biologically active chiral organophosphorus compounds. In the fall of 1992, John accepted a Visiting Assistant Professor position in the Chemistry Department of Mansfield State University, in Mansfield Pennsylvania. John returned to Chicago during the summer of 1993, working again with Professor Charles M. Thompson at Loyola University. In the fall of 1993, John began his current position as an Assistant Professor in the Department of Chemistry at Youngstown State University. Dr. Jackson has used mass spectrometry as an integral part of all his research, and has extensive experience with Hewlett-Packard and VG Instruments mass spectrometers.

Dr. Jackson is a member of the American Chemical Society (Organic Division, Agrochemicals Division) and in 1994 has served on the Executive Committee of the Penn-Ohio Border Section. John is also a member of Sigma, Xi, The American Association for the Advancement of Science (AAAS), and The Council on Undergraduate Research (CUR).

B. **Refereed Journal Publications.** Five most relevant publications.

(1) Jackson, J. A.; Hammond, G. B.; Wiemer, D. F.: "Synthesis of α-Phosphono Lactones and Esters Via Phosphate-Phosphonate Rearrangement." *J. Org. Chem.* **1989**, *54*, 4750-4754.

(2) Ryu, S.; Jackson, J. A.; Thompson, C. M.: "Methanolysis of Phosphoramidates with Boron Trifluoride-Methanol Complex." *J. Org. Chem.* **1991**, *56*, 4999-5002.

(3) Jackson, J. A.; Berkman, C. E.; Thompson, C. M.: "Stereoselective and Chemoselective Oxidation of Phosphorothionates using MMPP." *Tetrahedron Lett.* **1992**, *33*, 6061-6064.

(4) Jackson, J. A.; Frick, J. A.; Thompson, C. M.: "Synthesis of Chiral Phosphorus Mustards Derived From Serine." *BioMed. Chem. Lett.* **1992**, *2*, 1547-1550.

(5) Thompson, C, M,; Suarez, A. I.; Lin, J.; Jackson, J. A.: "Synthesis of Phosphorylated Tripeptides Representing Poisoned Acetylcholinesterase." *Tetrahedron Lett.* **1993**, *34*, 6529-6532.

C. **List of Other Collaborators**

None

D. **Names of Mentors.**

(1) Ph.D. Advisor. Dr. David F. Wiemer, Department of Chemistry, The University of Iowa, Iowa City, IA 52242-1294.

(2) Postdoctoral Advisor. Dr. Charles M. Thompson, Department of Chemistry, Loyola University Chicago, Chicago, IL 60626. Current Address: Department of Chemistry, University of Montana, Missoula, MT 59812-1006.

Biographical Sketch for Allen D. Hunter.

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555.

A. **Vitae.** Allen Hunter received his Honors B.Sc. in Chemistry in 1981 from the University of British Columbia in Canada with a graduating thesis under Dr. E.E. Burnell entitled "A NMR Structural Determination of Azulene Oriented in a Nematic Liquid Crystal". Allen obtained his Ph.D. degree from the University of British Columbia in 1985 under Dr. P. Legzdins with a thesis entitled "Aspects of the Organometallic Nitrosyl Chemistry of Cr, Mo, and W". He worked as a postdoctoral fellow with Dr. M. Bennett of the Research School of Chemistry at the Australian National University in Canberra, Australia, doing phosphine and iron phosphine chemistry (1985-86) and with Dr. M. Cowie at the University of Alberta in Canada carrying out single crystal X-ray diffraction studies for Dr. D. Seyferth of M.I.T. (1987). From 1987 to 1992 Allen was an Assistant Professor of Chemistry at the Chemistry Department of the University of Alberta where he currently holds an Adjunct appointment. On September 15th of 1992 he joined Youngstown State University as an Associate Professor of Chemistry and he currently holds a Research Professorship there. He is a member of the American Chemical Society and the American Association for the Advancement of Science. Dr. Hunter has extensive experience in the use of mass spectrometry in inorganic and organometallic chemistry. He is very experienced with small PC networks including mixtures of Apple and IBM systems.

Allen received a Izaak Walton Killam Memorial Postdoctoral Fellowship and a NSERC Postdoctoral Fellowship for 1985-87 and he held a Natural Sciences and Engineering Research Council of Canada, NSERC, Graduate Scholarship for 1981-85. He received the Governor General's Gold Medal in Arts and Sciences, the Lefevre Medal and Prize in Honors Chemistry, and the Society of Chemical Industry Merit Award in 1981. Allen held a NSERC Undergraduate Summer Research Award in 1980 and 1981. He was awarded the Chemical Institute of Canada Prize in 1980 and Charles A. and Jane C.A. Banks Foundation Scholarships for 1978-80.

During the 1990-93 period Allen received over $400,000 (US), excluding overhead, in external funding at the University of Alberta from the Canadian federal science granting agency, NSERC, and US and Canadian Industry for his work on organometallic polymers and biologically active organometallics.

B. **Refereed Journal Publications,** Five Most Relevant (1 - 5) and Five Other Significant (6 - 10) Publications.

(1) Sturge, K.C.; Hunter, A.D.; McDonald, R.; Santarsiero, B.D.: "Organometallic Polymer and Linear Mono-, Bi-, and Trimetallic Octafluoro-p,p'-biphenylene-Bridged Complexes of Bis(methyldiphenylphosphine)nickel: X-ray Crystal Structures of $Ni(PMePh_2)_2(4,4'\text{-}C_{12}F_8H)Br$ and $Ni(PMePh_2)_2(4,4'\text{-}C_{12}F_8H)_2$," *Organometallics,* **1992**, *11*, 3056-3062.

(2) McDonald, R.; Sturge, K.C.; Hunter, A.D.; Shilliday, L.: "Synthesis and Spectroscopic Characterization of Linear Mono-, Bi- and Trimetallic Bis(methyldiphenylphosphine)-nickel Complexes having 1,4-Tetrafluorophenylene Bridges," *Organometallics*, **1992**, *11*, 893-900.

(3) Macdonald, P.M.; Hunter, A.D.; Lesley, G.; Li, J.: "Solid State Distortions of Linear Mono-, Bi-, and Trimetallic Bis(Tri-n-ButylPhosphine) Nickel and Palladium Complexes Having 1,4-Tetrafluorophenylene Bridges as Observed Via ^{31}P CP/MAS NMR Spectroscopy," *Solid State Nuclear Magnetic Resonance,* **1993**, *2*, 47-55.

(4) Hunter, A.D.; Burnell, E.E.; Wong, T.C. " Vibrationally Averaged Structure of Azulene Partially Oriented in a Nematic Phase," *J. Molec. Struct.* **1983**, *99*, 159-164.

(5) Guo, X.A.; Hunter, A.D.: "Polyesters, Polycarbonate, and Polyurethanes from a Novel Monomer: α,α,α',α'-Tetramethyl-1,4-tetrafluorobenzenedimethanol," *J. Polym. Sci., Part A*, **1993**, *31*, 1431-1439.

(6) Guo, X.A.; Hunter, A.D.; Chem, J.: "Preparation and Characterization of Acrylates and Polyacrylates Having Variable Fluorine Contents and Distributions," *J. Polym. Sci., Part A*, **1994**, *32*, 47-56.

(7) Hunter, A.D.; Mozol, V.; Tsai, S.D.: "Non-linear Substituent Interactions and the Electron-Richness of Substituted (η^6-Arene)$Cr(CO)_3$ Complexes: The Role of σ-Donor and π-Acceptor Interactions," *Organometallics*, **1992**, *11*, 2251-2262.

(8) Hunter, A.D.; Szigety, A.B.: "Phenylene-Bridged Organometallic Complexes of Iron and Manganese," *Organometallics*, **1989**, *8*, 2670-2679.

(9) Hunter, A.D.; McLernon, J.L.: "Arene-Bridged Polymetallic Clusters: σ,π Complexes of $CpFe(CO)_2$ or $Cp'Fe(CO)_2$ and $Cr(CO)_3$, $Mo(CO)_3$ or $W(CO)_3$," *Organometallics*, **1989**, *8*, 2679-2688.

(10) Hunter A.D.; Ristic-Petrovic, D.; McLernon, J.L.: "Biphenyl-, Terphenyl-, Naphthalene-, and Anthracene-Bridged Bimetallic Complexes of Iron and Chromium," *Organometallics*, **1992**, *11*, 864-871.

C. **List of Other Collaborators.**

(1) Dr. M. Williams, Department of Chemical Engineering, University of Alberta, Edmonton, Alberta, Canada

D. **Names of Mentors.**

(1) B.Sc. Honors Thesis Advisor: Dr. E.E. Burnell, Department of Chemistry, University of British Columbia, Canada.

(2) Ph.D. Advisor. Dr. P. Legzdins, Department of Chemistry, University of British Columbia, Canada.

(3) Postdoctoral Advisors. Dr. M. Bennett, Research School of Chemistry, Australian National University, Canberra, Australia. Dr. M. Cowie, Department of Chemistry, University of Alberta, Canada.

Biographical Sketch for Steven M. Schildcrout

Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555

A. **Vitae.** Steven M. Schildcrout received his B.S. degree in Chemistry from the University of Chicago in 1964 with a senior project on kinetics of alkene hydrogenation under the supervision of Edgar W. Garbisch, Jr. He received his Ph.D. degree in Physical Chemistry at Northwestern University in 1968 with his dissertation, "Studies of Metal Complexes by Electron-Impact Mass Spectrometry," under the supervision of Fred E. Stafford and partially in collaboration with Ralph G. Pearson. The research was carried out with a Nuclide magnetic sector instrument. While at Northwestern he taught undergraduate physical chemistry laboratory and was an NIH Predoctoral Fellow. During 1968-69 he spent 20 months as a postdoctoral research associate with Joe L. Franklin at Rice University in Houston, where he studied ion-molecule reactions of small molecules in electrical discharges and under "high"-pressure electron ionization using a "home-made" quadrupole mass spectrometer.

Since 1969 Dr. Schildcrout has been a faculty member at Youngstown State University, where he has been full Professor since 1981 and a Distinguished Member of the Graduate Faculty. At YSU he has used a DuPont 21-491 double-focusing mass spectrometer (since replaced), funded by the University and with an ACS-PRF grant, and the present Finnigan 1020 GC/MS to carry out research in gaseous ion chemistry of organic and metal coordination compounds. He has supervised and performed the operation and maintenance of these instruments. He has done collaborative research recently with John Masnovi, an organic chemist at Cleveland State University. He teaches general and physical chemistry, including a graduate special-topics course on mass spectrometry. He has been named several times as research professor and was awarded a distinguished professorship for his scholarship.

He is a member of the American Society for Mass Spectrometry, Sigma Xi, and the American Chemical Society, for which he has served in all offices of the Penn-Ohio Border Section and in which he is now Councilor for the local section and an associate of the national Constitution & Bylaws Committee.

B. **Refereed Journal Publications.** Five most relevant (1-5) and five other significant (6-10) publications.

(1) Schildcrout, S. M.; Krafcik, R. B.; Masnovi, J. "Gas Phase Reactivities and Interchromophoric Effects in 1,n-Dicarbazolylalkane Cations and Related Species" *J. Org. Chem.* **1991,** *56*, 7026-7034.

(2) Schildcrout, S. M.; Besozzi, L.M. "Chemical-Ionization and Electron-Ionization Mass Spectra of Dimethylglyoxime and Its Complexes with Nickel(II), Palladium(II), and Platinum(II)" *Inorg. Chem.* **1990**, *29*, 1054-1057.

(3) Schildcrout, S. M.; Geidner, R. M. "Comparative Chemical-Ionization Mass Spectra of Tricyclic Antidepressant Amines and Related Compounds," *Org. Mass Spectrom.* **1989**, *24*, 241-245.

(4) Schildcrout, S. M. "Electron-Ionization Mass Spectra of Fluorinated Diketonate Complexes of Cerium(IV)," *Inorg. Chem.* **1985**, *24*, 760-762.

(5) Schildcrout, S. M. "Temperature-Dependent Single vs. Double Ionization in the Mass Spectra of Phthalocyanine and Its Metal(II) Complexes," *J. Amer. Chem. Soc.* **1983**, *105*, 3852-3855.
(6) Schildcrout, S. M. "High Pressure Mass Spectra and Gaseous Ion Chemistry of Metal Diketonates with Bulky Substituents," *Inorg. Chem.* **1980**, *19*, 224-227.
(7) Schildcrout, S. M. "High-Pressure Mass Spectra and Gaseous Ion Chemistry of Metal Acetylacetonates," *J. Phys. Chem.* **1976**, *80*, 2834-2838.
(8) Schildcrout, S. M. "High-Pressure Mass Spectra and Gaseous Ion Chemistry of Ferrocene," *J. Amer. Chem. Soc.* **1973**, *95*, 3846-3849.
(9) Schildcrout, S. M.; Gebelein, C. G. "Electron-Impact-Induced Ion Fragmentation of Polyfunctional *N*-Cyclohexylcarbamates," *Org. Mass Spectrom.* **1972**, *6*, 485-491.
(10) Schildcrout, S. M.; Collins, J. G.; Franklin, J. L. "Mass Spectrometric Study of Ion-Neutral Reactions in Radio-Frequency Discharges in Carbon Dioxide," *J. Chem. Phys.* **1970**, *52*, 5767-5774.

C. **List of Other Collaborators.**

None.

D. **Names of Mentors.**

(1) Undergraduate Project: Dr. E. W. Garbisch, Jr., Department of Chemistry, University of Chicago, Chicago, Illinois (retired).
(2) Ph.D. Advisor: Dr. F. E. Stafford, Department of Chemistry, Northwestern University, Evanston, Illinois (Now at Office of Research, University of Chicago).
(3) Postdoctoral Supervisor: Dr. J. L. Franklin, Department of Chemistry, Rice University, Houston, Texas (deceased).

Biographical Sketch for Renee L. Falconer

Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555

A. **Vitae.** Renee L. Falconer obtained her B.S. degree in Chemistry in 1990 from Grove City College. She immediately started graduate work at the University of South Carolina and earned her Ph.D. in Analytical Chemistry in 1994 under the direction of Dr. Terry F. Bidleman. While there, Renee received the Joseph Bouknight Award for Excellence in Teaching (Fall 1990 and Spring 1991) and the Patricia R. Harris Graduate Fellowship (U.S. Dept. of Education, Fall 1991-Spring 1992). The title of her dissertation was "Physico-chemical Properties and Partitioning of Organochlorine Compounds in Air and Water". From 1992-94 she was employed as a contractor by Atmospheric Environment Service, Environment Canada to study vapor-particle partitioning of Polychlorinated Biphenyls (PCBs) and to develop separation techniques for different PCB congeners. In June 1994, Renee won the International Association for Great Lakes Research Hydrolab Award for Best Student Paper. Both her dissertation work and contract work entailed the use of mass spectrometry for analysis of trace contaminants. In September 1994, Renee began her current position as Assistant Professor in the Department of Chemistry at Youngstown State University.

Dr. Falconer is a member of the American Chemical Society, the International Association for Great Lakes Research and the Society for Environmental Toxicology and Chemistry and is presently serving on the Executive Committee of the Penn-Ohio Border Section of ACS.

B. **Refereed Journal Publications**. Five most relevant publications.

(1) Falconer, R. L.; Bidleman, T. F.: "Vapor Pressures and Predicted Particle/Gas Distributions of Polychlorinated Biphenyl Congeners as Functions of Temperature and Ortho-chlorine Substitution." *Atmos. Environ.* **1994**, *28*, 547-554.

(2) Falconer, R. L.; Bidleman, T. F., Gregor, D. J.: "Air-Water Gas Exchange and Evidence for Metabolism of Hexachlorocyclohexanes in Resolute Bay, N.W.T." *Sci. Total Environ.* (in press).

(3) Falconer, R. L.; Bidleman, T. F., Gregor, D. J., Semkin, R.: "Enantioselective Breakdown of α-Hexachlorocyclohexane in a Small Arctic Lake and its Watershed." *Environ. Sci. Technol.* (in press).

(4) Falconer, R. L.; Bidleman, T. F., Cotham, W. E.: "Preferential Sorption of Non- and Mono-ortho Polychlorinated Biphenyls to Urban Aerosols." *Environ. Sci. Technol.* (submitted).

(5) Bidleman, T. F.; Falconer, R. L.; Walla, M. D.: "Toxaphene and Other Organochlorine Compounds in Air and Water at Resolute Bay, N.W.T., Canada." *Sci. Total Environ.* (in press).

C. **List of Other Collaborators.**

None

D. **Names of Mentors.**

Ph.D. Advisor. Dr. Terry F. Bidleman, Environment Canada, Ontario, Canada, M3H 5T4; Adjunct Professor, University of South Carolina, Columbia, SC, 29208

Biographical Sketch for Timothy R. Wagner

Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555

A. **Vitae.** Timothy R. Wagner received his B.S. degree in Chemistry from the University of Wisconsin-River Falls in May, 1981. He then enrolled in the chemistry graduate program at Arizona State University in the Fall of that year, and completed his Ph.D. thesis in Solid State Chemistry under the supervision of Professor Michael O'Keeffe in May 1986. His thesis topic was: Electron Microscopy and Crystal Chemistry of Compounds Related to β-Alumina and Magnetoplumbite. Following graduate school, Dr. Wagner worked in the Radar Systems Group at Hughes Aircraft Company, El Segundo, California. His duties there involved development and testing of software to be used for airborne radar signal processing and software/hardware integration of programs.

In the spring of 1988, Dr. Wagner joined Professor Lawrence Marks' group in the Department of Materials Science at Northwestern University, Evanston, Illinois, as a postdoctoral fellow. At Northwestern University, Dr. Wagner conducted HREM studies of electron and ion-stimulated surface reactions & damage in oxides. He spent the summer of 1990 as a supporting laboratory scientist at the Pharmaceutical Products Division, Abbott Labs, North Chicago, Illinois. This project involved programming and documentation of robotics software for chemical analysis. In the Fall of 1990, Dr. Wagner then joined the faculty of the Chemistry Department at the Illinois Institute of Technology, Chicago, Illinois, at a Visiting Assistant Professor. He remained at IIT for two years, and began his current position as Assistant Professor of Chemistry at Youngstown State University in the Fall of 1992.

Dr. Wagner is a member of the Sigma Pi Sigma National Physics Honor Society, Phi Lamda Upsilon National Chemistry Honor Society and Sigma Xi. He is also a member of the American Chemical Society, and is currently chair of the Penn-Ohio Border section of the ACS.

B. **Refereed Journal Publications.** Five most relevant publications.

(1) T. Wagner and M. O'Keeffe, "Electron Microscopy of Defects and Disorder in Barium Hexagallate," *Acta Cryst.* **1985**, *B41*, 108-112.

(2) T. Wagner and M. O'Keeffe, "A Structural Model for Barium Hexagallate," *J. Solid State Chem.*, **1988,** *73*, 19-26.

(3) T. Wagner and M. O'Keeffe, "Bond Lengths and Valences in Aluminates with the Magnetoplumbite and β-Alumina Structures," *J. Solid State Chem.* **1988,** *73*, 211-216.

(4) M.I. Buckett, S.R. Singh, H. Fan, T. Wagner and L.D. Marks, "Electron-Stimulated Damage Processes in Oxides Under Ultra High Vacuum (UHV) Conditions," Proc. 47th Ann. Mtng. of the Electron Mic. Soc. of America, **1989**, 636-7.

(5) T. Wagner, "HREM of Electron-Beam-Induced Damage in L-Ta_2O_5," *J Solid State Chem.* **1991**, *91*, 189-203.

C. **List of Other Collaborators.**

(1) S. M. Hues, Surface Chemistry Branch, Naval Research Labs, Washington, D.C., 20375-5000. Ph. 202-767-2671

D. **Names of Mentors.**

(1) Ph.D. Advisor. Michael O'Keeffe, Department of Chemistry, Arizona State University, Tempe, Arizona, 85287.

(2) Postdoctoral Advisor. Lawrence Marks, Department of Materials Science, Northwestern University, Evanston, Illinois, 60208.

4. ILI-IP DETAILED BUDGET (EQUIPMENT LIST) FORMAT

Item (Descriptive name, probable brand and model)	How Many	Unit Price (List)	Unit Price (Discounted)	Total Cost (Discounted)
HP 5972A Mass Selective Detector (MSD) High Performance Bundle with MSD, MS Software, HP Vectra 486, 16MB RAM, 450MB hard disk, 17" Monitor and LaserJet 4	1	47,600	47,600	47,600
HP Ion Gauge Controller for MSD	1	1,545	1,545	1,545
Installation of MSD High Performance Bundle	1	238	238	238
GC-columns	2	400	400	800
Chemical Ionization for HP 5972A MSD	1	7,730	7,730	7,730
Installation of Chemical Ionization for HP 5972A MSD	1	950	950	950
HP 5890 Series II Plus Gas Chromatograph with Electronic Pressure Control (EPC)	1	7,830	7,830	7,830

4. ILI-IP DETAILED BUDGET (EQUIPMENT LIST) FORMAT

Item (Descriptive name, probable brand and model)	How Many	Unit Price (List)	Unit Price (Discounted)	Total Cost (Discounted)
MSD Bundle Split/Splitless inlet	1	3,710	3,710	3,710
Auxiliary EPC flow control/gas saver	1	805	805	805
HP 5890 Series Autosampler	1	8,760	8,760	8,760
NIST MS Library	1	1,750	1,750	1,750

Total project cost:	81,718
Non-NSF contribution (including any overmatch):	40,859
NSF request:	40,859

Use additional page(s) if needed.

5. **CURRENT AND PENDING SUPPORT**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: John A. Jackson

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Acquisition of a Single Crystal X-ray Diffractomer (with T. R. Wagner*, A. D. Hunter, and R. E. Beiersdorfer)

Source of Support: NSF - Materials Research Division

Award Amount (or Annual Rate): $ 71,199 Period Covered: 1994

Location of Research: Youngstown State University

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Supramolecular Host-Guest Chemistry of Calix[n]Arenes and Its Application to Molecular Affinity Liquid Chromatography (with A. D. Hunter, J.H. Mike, M.A. Serra, and T.R. Wagner)

Source of Support: NSF-C-RUI

Award Amount (or Annual Rate): $ 755,391 Period Covered: 48 months (1995-99)

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ: 10 (in total)

Support ☐ Current ☐ Pending ☑ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Acquisition of a High Field NMR for Solids and Solutions, (with 5 others)

Source of Support: NSF, Ohio Board of Regents, YSU, Dreyfus Foundation

Award Amount (or Annual Rate): $ ≈550,000(total) Period Covered: 1996

Location of Research:

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Robotic Sample Changer and NMR Data Stations for Integration of 400 MHz NMR into the Undergraduate Curriculum (with A.D. Hunter* and others)

Source of Support: NSF-ILI and The Camile and Henry Dreyfus Foundation

Award Amount (or Annual Rate): $ 179,845 (Total) Period Covered: 1995

Location of Research:

Person-Months Committed to the Project. Cal: 2 (in total) Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

5. **CURRENT AND PENDING SUPPORT**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Allen D. Hunter | Other agencies (including NSF) to which this proposal has been/will be submitted.

Support ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Acquisition of a Single Crystal X-ray Diffractomer (with T.R. Wagner*, J. A. Jackson, and R. E. Beiersdorfer)

Source of Support: NSF - Materials Research Division

Award Amount (or Annual Rate): $ 71,199 Period Covered: 1994

Location of Research: Youngstown State University

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Integration of High Field Multinuclear NMR into the Undergraduate Curriculum: Establishment of a Regional NMR Facility

Source of Support: The Camille & Henry Dreyfus Foundation and NSF-ILI

Award Amount (or Annual Rate): $ 179,000 Period Covered: 1995

Location of Research: Youngstown State University

Person-Months Committed to the Project. Cal: 3(in total) Acad: Summ:

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Supramolecular Host-Guest Chemistry of Calix[n]Arenes and Its Application to Molecular Affinity Liquid Chromatography (with J.A. Jackson, J.H. Mike, M.A. Serra, and T.R. Wagner)

Source of Support: NSF-C-RUI

Award Amount (or Annual Rate): $ 755,391 Period Covered: 48 months (1995-99)

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ: 10 (in total)

Support ☐ Current ☐ Pending ☑ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title: Acquisition of a High Field NMR for Solids and Solutions, (with 5 others)

Source of Support: NSF, Ohio Board of Regents, YSU, Dreyfus Foundation

Award Amount (or Annual Rate): $ ≈550,000(total) Period Covered: 1996

Location of Research:

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support
Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ (total) Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

5. **CURRENT AND PENDING SUPPORT**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Steven M. Schildcrout

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: None

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

5. **CURRENT AND PENDING SUPPORT**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Renee L. Falconer

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: Chiral Pesticides as Tracers of "Old" vs. "New" Atmospheric Sources. (with T.F. Bidleman)

Source of Support: EPA-AREAL (Atmospheric Research and Exposure Assessment Laboratory)

Award Amount (or Annual Rate): $ 42,000 Period Covered: 1995

Location of Research: YSU

Person-Months Committed to the Project. Cal: Acad: Summ: 2

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

5. **CURRENT AND PENDING SUPPORT**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Timothy R. Wagner

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support ☑ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: Acquisition of a Single Crystal X-ray Diffractomer (with A. D. Hunter, J. A. Jackson, and R. E. Beiersdorfer)

Source of Support: NSF - Materials Research Division

Award Amount (or Annual Rate): $ 71,199 Period Covered: 1994

Location of Research: Youngstown State University

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☑ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: Supramolecular Host-Guest Chemistry of Calix[n]Arenes and Its Application to Molecular Affinity Liquid Chromatography (with A.D. Hunter, J.A. Jackson, J.H. Mike, and M.A. Serra)

Source of Support: NSF-C-RUI

Award Amount (or Annual Rate): $ 755,391 Period Covered: 48 months (1995-99)

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ: 10 (in total)

Support ☐ Current ☐ Pending ☑ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: Acquisition of a High Field NMR for Solids and Solutions, (with 5 others)

Source of Support: NSF, Ohio Board of Regents, YSU, Dreyfus Foundation

Award Amount (or Annual Rate): $ ≈550,000(total) Period Covered: 1996

Location of Research:

Person-Months Committed to the Project. Cal: 6 (in total) Acad: Summ:

Support ☐ Current ☐ Pending ☑ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title: Robotic Sample Changer and NMR Data Stations for Integration of 400 Mhz NMR into the Undergraduate Curriculum (With A.D. Hunter, J.A. Jackson, J.H. Mike, and P.M. Mullins)

Source of Support: The Camille & Henry Dreyfus Foundation and NSF-ILI

Award Amount (or Annual Rate): $ 179,845(total) Period Covered: 1995

Location of Research:

Person-Months Committed to the Project. Cal: 2 (in total) Acad: Summ:

Support ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Appendix 6a. REPRESENTATIVE NEW EXPERIMENTS*

Chemistry 603 and 604, Quantitative Analysis 1 and 2.

1. "Determination of Organic Molecule Concentrations by GC-MS" where the concentrations of organic compounds in organic solvents will be determined by the integration of total ion count of the mass spectrum, comparison to the relative peak intensities from GC with a FID, and the method of internal standards and multiple dilution.. The student will learn how to prepare samples for GC-MS, operate the spectrometer with the help of the instructor and laboratory assistants, and interpret integration results. Each student in the class will be given a different unknown containing multiple analytes of environmental relevance (e.g., a polycyclic aromatic hydrocarbon (PAH) and a polychlorinated biphenyl (PCB)) whose differing GC retention time allow simultaneous determination of the concentrations of two molecular species.

Chemistry 719, 720, and 721, Organic Chemistry 1, 2, and 3.

1. "Introduction to the Gas Chromatograph Mass Spectrometer" where the students will learn basic spectrometer operation and data processing.

2. "Assignment of Spectra of Known Organics" where each student will learn to assign the mass spectra (and IR, NMR) of a series of 5 to 10 related organic molecules having the same functional groups (e.g., alkanes, alkenes, alkyl halides, ethers, alkyl aromatics, alcohols, amines, carboxylic acids, esters, and amides). Mass spectra will be collected for two compounds of known structure and spectra for related compounds will be drawn from the "archived" data base. Their assignments will be discussed with their peers, and this will be followed by a practical lab exam of "unknowns" on the PC data stations. The spectroscopic data from this and subsequent experiments will be stored on an archival data base for use in other experiments, in the lecture "problem sets", and to compare to unknown starting materials and products.

3. "Spectroscopic Analysis of Unknown Organics" where each student will be given two compounds, each having a different combination of functional groups, and will use Mass Spectrometry, IR and, ^{1}H and ^{13}C NMR data to identify their structures.

*This appendix was authorized by Dr. Susan Hixson, NSF Program Officer, on November 3, 1994.

4. "Separation and Identification of Liquid Unknowns" where each student will be given a different mixture of two liquid organic compounds to separate by distillation. They will "separate" them by distillation and identify them by spectroscopic methods including GC-MS, NMR, and IR. The composition of the starting mixture and of the two "purified" distillation fractions will be determined by GC-MS. The dependence of the "sharpness" of the separation as a function of the lengths of the distillation column and the difference in boiling points of the components will be evaluated by comparing the class results.

5. "Separation and Identification of Solid Unknowns" where each student will be given a mixture of two organic compounds and two inorganic impurities (e.g., salt and sand). They will separate these by extraction and crystallization and identify and evaluate the purity of the resulting two organic solids by spectroscopic methods, including GC-MS, ^{1}H and ^{13}C NMR.

6. "Evaluation of the Orientation of Electrophillic Aromatic Substitution Reactions" in which each student in a lab section will carry out an EAS substitution using a different combination of electrophile (i.e., HNO_3/H_2SO_4 or $Br_2/FeBr_3$) and aromatic substrate. GC-MS will be utilized to determine the degree of substitution by molecular weight determination of the product mixtures. The students will propose rational mechanisms to explain fragmentation differences observed in isomeric products. ^{1}H NMR will be used by the students to evaluate the products as to the degree and orientation of addition and the relative yields of o-, m-, and p-isomers. Class results will be pooled so that the students can experimentally determine the o/p- vs m- directing character of various aromatic substituents and to experimentally determine if the identity of the electrophile or the reaction conditions (e.g., temperature and solvent) affects the orientations.

7. "Carbocation Generation, Rearrangements, and Reactions" in which students will carry out Friedel Crafts alkylations of benzene with an $AlCl_3$ catalyst and each student in a lab section will use a different alkyl halide (i.e., R-X where X = Cl, Br, or I) potentially capable of carbocation rearrangements (i.e., R = isomeric C3, C4, C5, and C6 alkyls). The alkylaromatic products will be isolated and their GC-MS, ^{1}H and ^{13}C NMR data used to identify their

structures. Pooled class data will be used to evaluate any effects of the halide and the structure of the R group on the nature and degree of alkyl group isomerization of the carbocations which give rise to the products. Mass spectrometry will be extremely important in determining the amounts of di-, and trisubstitution obtained in the Friedel Crafts alkylations.

8. "Dehydrohalogenation of Alkyl Halides" where students will use GC-MS, ^{1}H and ^{13}C NMR to identify the isolated dehydrohalogenation product(s) from their unique combination of R-X, base, solvent, and temperature. They will evaluate the regioselectivity of their reaction and the cis/trans isomer distributions. Comparison of the classes' results will be done to evaluate the affects of these variables.

9. "Orientation of Addition Reactions on Cyclohexene" where each student will use GC-MS and ^{1}H NMR to characterize the isolated 1,2-dibromide or 1,2-dihydroxide addition products that they have prepared from cyclohexene. The isotope patterns observed in the bromination reaction will be compared to predicted values.

10. "Ester Synthesis" where each student must identify their unique combination of the acid chloride and alcohol starting materials they are given based on the structure determined by GC-MS, ^{1}H and ^{13}C NMR for the ester products (e.g., Ar-CO_2R and RCO_2Ar where R = alkyl and Ar = aryl) that they prepare from them.

11. "Identification of Fats and Oils" where each student analyzes by GC-MS, ^{1}H and ^{13}C NMR a sample of an oil or fat (e.g., various brands and grades of commercial oils, shortenings, lard and animal fat) to determine, as fully as possible, the structures of the lipids that make it up (i.e., average fatty acid chain lengths, % unsaturation, % cis vs trans fatty acids, % conjugated fatty acids). Molecular weight determination will be aided greatly by GC-MS.

Chemistry 739, 740, 741, Physical Chemistry.

1. "Isotopic Abundances of an Element," where mass spectra of mono or polychlorinated or brominated organic compounds are obtained. The peaks are assigned, and the Cl or Br isotope distribution ratios are used to determine isotopic abundances using the binomial coefficients and

to calculate the average atomic mass of the halogen. Results are compared with accepted values, and an error analysis is made.

2. "Energetics of Ion Formation and Fragmentation," where mass spectra are obtained as a function of ionizing-electron energy for a series of simple hydrocarbons (e.g. methane, ethane, propane). By extrapolation to zero ion current, ionization energies and appearance energies may be estimated. Using known heats of formation of the neutral gases, bond energies may be estimated by Hess's Law. Students will recognize the limitations in accuracy of this method.

Chemistry 822, Organic Analysis.

1. "GC-MS and 1-Dimensional ^{1}H and ^{13}C NMR Spectroscopy of Substituted Alkane, Alkenes, and Arenes" in which each student collects and assigns the GC-MS, ^{1}H and ^{13}C NMR of a series of related organic molecules and the class then pools and uses this data to identify a series of more complex unknowns containing similar structural fragments.

2. "Natural Products" where students work as a group employing the full range of instrumental techniques to identify unknown natural products of moderate complexity (e.g., terpenes, steroids).

3. "Fragmentation Patterns" where students examine by GC-MS a series of structurally related compounds and make correlation's between the observed fragmentation's and the known structure.

Chemistry 824, Polymer Chemistry Lab.

1. "Siloxane Elastomers" where the students will each synthesize and characterize (including by ^{1}H, ^{13}C, and ^{29}Si NMR) a series of siloxane oligimers and polymers made from a different ratio of Me_3SiCl, Me_2SiCl_2, and $MeSiCl_3$. The effects of the degree of crosslinking (due to $MeSi\text{-}(O)_3\text{-}$ units) on the physical and mechanical properties of the siloxane elastomers will be evaluated by comparing the different student's results. MS will be used to evaluate the low molecular weight oligimers and polymers.

2. "Polymer Additives" where the students will Soxhlet extract, using organic solvents, samples of commercial plastics brought from home. The low molecular weight organic additives extracted will be quantified and identified by MS, IR, and ^{1}H, ^{13}C, and ^{31}P NMR and by comparison to authentic samples.

Chemistry 831, Inorganic Lab.

1. "Synthesis of SnR_yCl_{4-y} compounds" where the students react various ratios of $SnCl_4$ and RMgX and obtain products of mixed compounds which are difficult to separate. Mass spectrometry is especially useful in these compounds, since one can take advantage of the large number of stable isotopes of Sn in the assignment of peaks to ion fragments containing Sn.

2. "Synthesis of $(\eta^6$-Arene$)M(CO)_3$ Complexes" where the students each react a different arene (e.g., $C_6H_{6-n}R_n$) with $Cr(CO)_6$ or $Mo(CO)_6$ to produce an $(\eta^6$-Arene$)M(CO)_3$ complex. Trends in complex electron richness as a function of arene structure (from cyclic voltametry and ^{13}C NMR data) are evaluated by comparison of the students' data. Fragmentation patterns in the mass spectra of the differing isomeric complexes will be evaluated and compared to those for the uncomplexed arene.

3. "Steric and Electronic Effects in the Synthesis of Molybdenum Carbonyl Phosphines" where each student reacts $Mo(CO)_6$ with a different PR_3 ligand and the identity and ratios of the organometallic product(s) (i.e., $Mo(CO)_5(PR_3)$, cis and trans-$Mo(CO)_4(PR_3)_2$, and fac- and mer-$Mo(CO)_3(PR_3)_3$) are determined by MS, IR and by ^{13}C and ^{31}P NMR. The students' results are then compared to evaluate the effects of phosphine steric and electronic parameters on the rates of the reactions and the isomeric identities of the products.

4. "Synthesis and Derivative Chemistry of Bimetallic Iron Complexes" where the students thermally react $Fe(CO)_5$ with dicyclopentadiene, dimethylcyclopentadiene, or indene to produce $\left[(\eta^5-\text{ligand})\text{Fe(CO)}(\mu-\text{CO})\right]_2$ complexes. These are in turn reacted with HCl/air, Br_2, or I_2 to give $(\eta^5-\text{ligand})\text{Fe(CO)}_2X$ (where X = Cl, Br, or I, respectively), with $Ph_2PCH_2CH_2PPh_2$ to

give $(\eta^5 - \text{ligand})_2 Fe_2(CO)_2(\mu_2, \eta^2 - Ph_2PCH_2CH_2PPh_2)$, or with a phosphine to give $(\eta^5 - \text{ligand})Fe_2(CO)(PR_3)X$. Spectroscopic data, including MS, ^1H, ^{13}C, and ^{31}P NMR, will be used to establish molecular structures and non-rigidity in the bimetallic complexes will be investigated by variable temperature NMR. The mass spectra of the bimetallic products with and without phosphine bridges will be compared to evaluate the metal-metal bond energies.

5. "Synthesis and Characterization of Organosiloxanes" where each student will react their own alcohol or phenol with Me_3SiCl, Me_2SiCl_2, $MeSiCl_3$, and $SiCl_4$ in the presence of a base to prepare a series of four related silicon compounds. These will be isolated and characterized, especially by GC-MS, along with ^1H, ^{13}C, and ^{29}Si NMR, and the effect of Me vs OR substitutions on the metal's electron richness evaluated and compared with the trends from the other students.

Environmental Chemistry

1 "Determination of Polyaromatic Hydrocarbons in Street Runoff" in which students will collect and extract samples and use mass spectrometry to determine the concentrations of individual compounds. The most probable source of the PAHs (automobile exhaust, lubricating oils, etc.) will be determined from the types of PAHs present in each sample. The results will be compared to analysis by fluorescence spectrometry which is often used for estimating petroleum levels in sediments and seawater.

2 "Determination of Polyaromatic Hydrocarbons in Ambient Air" where students will again collect and extract samples and use mass spectrometry to determine concentrations and sources of PAHs to the atmosphere. These results will be compared to those for Street Runoff and will lead to discussions on transport and fate of pollutants through different media in the environment.

6b MAJOR EQUIPMENT

The YSU chemistry department is equipped with a wide range of instrumentation and additional equipment is available in other campus departments. Examples of major instrumentation are listed below:

Equipment	Year Purchased	Estimated Cost
Analyzer, Differential thermal/thermogravimetric, Fisher Model 370 and 500	12/12/75	6,428
Analyzer, Electrophoresis, Zeta-Meter	07/24/85	7,530
Analyzer, Mercury, Buck Scientific Model	07/14/88	3,000
Analyzer, Thermal-mechanical with TMA, DMA, and DSC modules, DuPont 9900	07/29/85	80,181
Calorimeter, Oxygen bomb, Parr, Model 2611 (2)	09/01/71	5,400
Centrifuge, (3)	1983-87	16,000
Chromatograph, Gas with FID, Hewlett Packard	1994	10,000
Chromatograph, Gas with TC detector, IBM GC/9630	12/26/84	8,085
Chromatograph, Gel Permiatation, Various	1992-94	8,000
Chromatograph, Liquid, Isco 2350/60	07/22/87	6,357
Chromatograph, Liquid, with ultraviolet, refractive index, fluorescence and electrochemical detectors (2), IBM LC/9533	08/06/84	41,000
Chromatograph, gas, Shimadzu, Model GC9AP	01/16/84	8,515
Chromatograph, HPLC, Model 338, Beckman (2)	1990	30,000
Chromograph, Ion, Dionex 2000i	06/10/84	9,170
Delivery System, Solvent, Millipore, Model M600	03/30/87	11,468
Detector, Photodiode array, Millipore, Model 990	03/30/87	20,468
Electrochemistry Programmer, Princeton Applied Research Model 175	06/15/84	3,700
Electrochemistry System, Bioanalytical Systems CV-27	06/28/84	2,968
Furnace, Graphite, Perkin-Elmer HGA-300	06/05/85	7,502
Gamma Counter (4), EG & G Ortec	06/14/84	14,124
Gamma Counting system, Beckman Gamma 8000	08/10/79	19,400
Gamma Spectrometer (7), The Nucleus Model 2010	09/09/82	9,359
Glove Box, Vacuum/Atmosphere	1980	15,000
GPC Columns (5)	1993-94	5,000
Hydrogenation and medium pressure reaction apparatus, Parr	02/12/87	4,279
Incubators, Percival, Lighted, Model I-25LLVL (3)	06/14/85	13,641
Incubators, (3)	1980-88	7,000
Instrumental Impact System, Tinius 620	09/06/84	18,515
Microscope, Scanning Tunneling	1994	12,000

Microwave Digestion CEM	09/02/86	7,190
Potentiostat/galvanostat, EG & G PAR, Model 273	09/24/84	8,860
Scintillation System, Liquid w/teletype, Beckman, Model LS-133	02/02/70	9,441
Shear Apparatus, Direct (2), Hogentogler S6564	08/07/84	9,716
Spectrofluorometer, Model RF-50000, Shimadzu	1985	17,000
Spectrofluorometer, Turner 430	04/08/75	4,863
Spectrometer, Atomic absorption, (3)	1983-85	60,000
Spectrometer, FTIR, (3), Digilab FTS 40, IBM-IR-32, PE-1600	1984-88	120,000
Spectrometer, Inductively-coupled plasma, Allied Analytical Plasma 200	07/20/84	42,225
Spectrometer, Inductively-coupled plasma, ARL Model 3410	1985	60,000
Spectrometer, Laser-Raman, Spex DM-3000	05/10/88	42,318
Spectrometer, Mass with GC, Finnigan-MAT 1020	07/09/84	128,900
Spectrometer, Nuclear magnetic resonance, IBM NR/80	02/07/83	120,692
Spectrometer, Nuclear magnetic resonance, Varian 400 MHz Gemini 2000 with VT and 5mm switchable probe, 10 mm broadband probe	1994	166,000
Spectrometer, Nuclear magnetic resonance, Varian EM-360	06/01/73	55,000
Spectrometer, Ultraviolet, (7), Beckman, Shimadzu, DU	1977-87	80,000
Spectrometer, Ultraviolet-visible, Diode array, Hewlett Packard HP8452A	03/06/87	7,127
Sterilizer, Laboratory/isothermal, AMSCO, 2300	10/07/85	42,188
Timer, Mercury drop and controller, Princeton Applied Research, 264A-3	05/01/87	5,769
Ultracentrifuge, Beckman L-8	10/08/79	23,657
Washer apparatus, Activator & Spiral (2), MTS	02/08/85	16,694
Weight apparatus, Molecular, Perkin Elmer Model 115	09/01/67	3,250
Weight apparatus, Osomatic molecular, Wescan Recording Osmometer	10/30/78	7,250
Furnace, Linberg High Temp. Tube	06/94	5,000
Microscope, Electron, Transmission	1992	used
Diffractometers, X-ray, single crystal (2)	1994-95	200,000

6c. COURSE DESCRIPTIONS

515, 516, 517 General Chemistry 1, 2, 3. The fundamental principles and the more important elements and compounds; qualitative analysis. Intended for majors in the natural sciences and engineering. Three hours lecture and three hours laboratory-discussion. Prereq.: Three units of high school algebra and geometry (or Math. 511 and 510 or their equivalents), and one unit of high school chemistry or CHEM 501 or 505. 4+4+4 qh.

603, 604 Quantitative Analysis 1, 2. Chemical equilibrium, stoichiometry, theory of errors, and volumetric and gravimetric procedures as applied to quantitative determinations. Introduction to electroanalytical and spectrophotometric methods. Emphasis on development of technique. Three hours lecture and six hours laboratory. Prereq.: CHEM 517 or 592 for 603. 5 + 5 qh.

650 Introduction to Undergraduate Research. An introduction to the methods of chemical research under the direction of a faculty member. This may include literature searching and analysis, instructional laboratory development, and/or original basic or applied research. May be repeated for a maximum of six q.h. Prereq. or concurrent: CHEM 516 or equivalent and approval of department chair. 1 or 2 qh.

719, 720, 721 Organic Chemistry 1, 2, 3. Organic compounds, reactions, and theories. Typical preparations and procedures of analysis. Three hours lecture and three hours laboratory. Prereq.: CHEM 517 or 592. 4+4+4 qh.

739, 740, 741 Physical Chemistry 1, 2, 3. Principles and applications of physical chemistry. Three hours lecture and three hours laboratory. Prereq.: CHEM 603; PHYS. 610, 611, 610L, 611L or Phys. 650, 502L, 503L. Prereq. or concurrent: Math. 674. 4+4+4 qh.

751 Water Quality Analysis 1. An introduction to physical, chemical, and biological measurements of water quality. Provides laboratory experience in the analysis of natural waters, drinking water, and wastewater. Emphasizes procedures for the collection and interpretation of data on current environmental problems. Two hours lecture and six hours laboratory. Identical to CEEGR 751 and BIOL 751. Prereq.: CHEM 603. 4 qh.

752 Water Quality Analysis 2. Advanced analytical techniques for evaluation of environmental problems. Topics include pollutant transport in natural waters, toxic contaminants in drinking water, and advances in wastewater treatment. Experience with several modern laboratory instruments is provided. Two hours lecture and six hours lab. Identical to CEEGR 752 and BIOL 752. Prereq.: CHEM 751. 4 qh.

796, 797; 798,799 Biochemistry 1, 2. The chemistry and metabolism of living organisms, with laboratory work to illustrate modern biochemical methods. Primarily designed for Biology and Medical Technology majors. Two hours lecture and three hours laboratory-discussion. Prereq.: CHEM 603 or 692; CHEM 721 or 793; and Biol. 506, 507, 508 or equivalent. 3 + 3 qh.

803, 804 Chemical Instrumentation 1, 2. The theoretical foundations of instrumental procedures and use of instruments in analytical work. CHEM 803: Two hours lecture and six hours laboratory. CHEM 804: Two hours lecture and three hours laboratory. Prereq.: CHEM 604 and 741. 4 + 3 qh.

805 Applied Spectroscopy. Infrared, ultraviolet, nuclear magnetic resonance, electron spin resonance, mass spectrometry, and methods of current interest as applied to chemical systems. Three hours lecture. Prereq.: CHEM 721; Prereq. or concurrent: CHEM 740 or permission of instructor. 3 qh.

822 Organic Analysis. "Current": Qualitative and functional-group analysis of organic compounds. Laboratory exercises and discussion of underlying principles. "New Content": Analysis of the structures of complex organic molecules using advanced instrumental methods, including: IR, NMR, and MS. One hour lecture and six hours laboratory-discussion. Prereq.: CHEM 721. 3 qh.

823 Organic Synthesis. Preparations of organic compounds and applicable instrumental techniques. One hour lecture and six hours laboratory with discussion. Prereq.: CHEM 721. 3 qh.

824 Polymer Chemistry. Polymerization processes and polymer structure-property relationships. Prereq.: CHEM 720. 3 qh.

825 Polymer Chemistry Laboratory. Preparation and characterization of some polymers. One hour lecture and six hours laboratory. Prereq.: CHEM 824. 3 qh.

831 Inorganic Chemistry Laboratory. Preparation of typical inorganic compounds and their characterization. Six hours laboratory-discussion. Prereq. or concurrent: CHEM 729, 740. 2 qh.

850 Undergraduate Research. Research participation under the direction of a faculty member. May be repeated to a maximum of nine q.h. Prereq.: CHEM 603 or 719 and approval of department chair. 2 or 3 qh.

6d. SUBJECT AREA MAJORS

Year	Total	To Graduate School*	To Medical, Dental, Law School	MS Obtained or in Progress	Ph.D. Obtained	Ph.D. in Progress	Graduate School Attended
1993-94	45	3	13	21	none	none	**
1992-93	35	2	19	18	none	none	**
1991-92	47	6	22	15	none	none	**
1990-91	30	5	6	7	none	none	**
1989-90	49	7	28	13	none	none	**
1988-89	62	6	31	11	none	none	**
1987-88	52	4	21	15	none	none	**
1986-87	49	8	21	23	none	none	**

* Does not include students proceeding to our MS program.

** Over the last several years, our BS graduates have gone on do to Ph.D. degrees at The Ohio State University, Kent State University, The University of Akron, The University of Cincinnati, Penn State University, University of Pittsburgh, The University of Texas, as well as to our own MS program from which many subsequently went on to do Ph.D. degrees at the above universities.

6e. STUDENT RESEARCH

CHEMISTRY 850: UNDERGRADUATE RESEARCH 1988-present

Mettee, H.	*"Photodynamics of $Ru(bipy)_3^{2+}$||MeV^{2+} in Dowex"*, Art Bain, 1988
Mettee, H.	*"Transition Metal Catalysts in Dowex"*, Jeanette Cho, 1988
Mettee, H.	*"Ion Exchange Kinetics"*, Pam Toth, 1988
Mincey, D.	*"Ion Chromatography"*, Ted Chrobak and Tom Kukura, 1988
Dobbelstein, T.	*"The Preparation and Study of Doped Bakelites"*, Althea Peloquin, 1989
Jackson, J	*"Synthesis of Phosphorus Mustards Derived from Terpenoids"*, Diana R. Arnett, 1994
Jackson, J	*"Synthesis of α-Amino Phosphonic Acids"*, David S. Bronson, 1994
Mike, J.	*"An Electrochemical Reactor for Post-Column Fluorescence Detection of Catecholamines HPLC"*, Brigitte Ramos, 1989
Mike, J.	*"The Effect of Methanol on the Activity of the Enzyme Choloylglycine Hydrolase"*, Laura A. Lyden, 1990
Mincey, D.	*"Trace Metal Analysis Employing Ion Chromatography - Inductively Coupled Plasma Atomic Emission Spectrometry"*, Jeff Giglio, 1990
Mincey, D.	*"A Square Wave Voltammetric Detection System for Anion Chromatography"*, Terri Rulick, 1990
Mike, J.	*"Chololylglycine Hydrolase: The Effect of Pore Size on Enzymic Activity"*, Francine A. Byrdy, 1991
Mike, J.	*"A pH Study of the Mobile Phase to be Utilized in the Detection of Conjugated Bile Acids Using HPLC and Immobilized Choloylglycine Hydrolase"*, Gina Terrago, 1991
Mike, J.	*"Choloylglycine Hydrolase: Glycocholic Acid Salt"*, Thomas Smith II, 1991
Mincey, D.	*"The Determination of Zinc, Iron, and Copper Concentrations in the Blood of Sickle Cell Disease (SCD) Children by Way of Inductively Coupled Plasma (ICP) Emission Spectrometry"*, Melissa Spin, 1992
Hunter, A.	*"Synthesis and Characterization of the Chromium Complexed Aromatic Polymers from Polymerizations of p-Phenylenediamine Chromium Tricarbonyl and m-Phenylenediamine Chromium Tricarbonyl"*, Steven J. DiMuzio, 1993
Hunter, A.	*"Organometallic Compounds Using Inert Atmosphere Techniques"*, Lisa Bernard, 1993
Hunter, A.	*"Fun With Inert Atmosphere Techniques"*, Lisa Bernard, 1993
Spiegal, L.	*"Sickle Cell Anemia: Analysis of Trace Elements"*, Dianne Braho, 1993
Spiegal, L.	*"Lipid Content of an Italian Macaroni Product by Thin Layer Chromatography*, Dawn Skala, 1994