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CERTIFICATION PAGE

Certification for Principal Invest	igators and Co-Principal I	nvestigators				
I certify to the best of my knowledge that:				4		
 the statements herein (excluding scientifi the text and graphics herein as well as ar signatories or individuals working under their required progress reports if an award is made 	ny accompanying publications or othe supervision. I agree to accept respo	er documents, unless otherwise ind				
I understand that the willful provision of false criminal offense (U.S.Code, Title 18, Section	_	fact in this proposal or any other co	ommunication sul	bmitted to NSF is a		
Name (Typed)	Signature)ate		
PI/PD	3					
Dr. Allen D. Hunter						
Co-PI/PD	-					
Dr. Shane C. Brower						
Co-PI/PD Dr. Thomas D. Kim						
Co-PI/PD						
Dr. Daryl W. Mincey						
Co-PI/PD						
Dr. Timothy R. Wagner						
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 status, debarment and suspension, drug free workplace, and lobbying activities (see below), as set forth in the <i>Grant Proposal Guide (GPG)</i> , NSF 98-2. 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, Title 18, Section 1001). In addition, if the applicant institution employs more than fifty persons, the authorized official of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of <i>Grant Policy Manual Section</i> 510; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflicts which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF. Debt and Debarment Certifications (If answer "yes" to either, please provide explanation.) Is the organization delinquent on any Federal debt?						
Is the organization or its principals presently or voluntarily excluded from covered transact		•	Yes 🗌	No 🔀		
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 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 agreement, 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, and 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 of Lobbying Activities," 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 material representation certification is a prerequisite for making or en required certification shall be subject to a civi	tering into this transaction imposed t	by section 1352, title 31, U.S. Code	. Any person who			
AUTHORIZED ORGANIZATIONAL REPRI	ESENTATIVE	SIGNATURE		DATE		
NAME/TITLE (TYPED) Dr. Peter Kasvinsky, Dean of Graduat	e Studies and Research					
TELEPHONE NUMBER 330-742-3091	ELECTRONIC MAIL ADDRESS amgrad03@ysub.ysu.edu		FAX NUMBER 330-742-15			

Project Data and Summary Form (NSF Form 1295)

1. Program to which the Proposal is Submitted: <u>ILI-IP</u>
2. Type of Submission: PR
3. Name of Principal Investigator/Project Director (as shown on the Cover
Sheet): Dr. Allen D. Hunter
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
ATE and CETP only:
Preliminary Proposal Number (s) that led to this proposal
PROJECT CODES
A. Major Discipline Code: 1 2 Subfields: <u>Analytical, Biochemistry, Inorganic, Organic, Physical, Polymers, & Other (Materials)</u> and <u>Condensed Mater Physics</u>
B. Academic Focus Level of Project: <u>B</u> <u>O</u>
C. Highest Degree Code: M
D. Category Code:
E. Business/Industry Participation Code:
F. Audience Code: W M T H I
G. Institution Code: $\underline{P} \underline{U} \underline{B} \underline{L}$
H. Strategic Area Code:
Estimated number in each of the following categories to be directly affected by the activities of the project during its operation:
J. Undergraduate Students: 2,000 over 5 years
K. Pre-college Students: none
L. College Faculty: 50 over 5 years
M. Pre-college Teachers: 100 over 5 years
N. Total Non-NSF Contribution: \$44,600

Project Summary

Because of the growing scientific, technological, and economic importance of polymeric and solid state materials, many national science and technology organizations strongly encourage the integration of these topics into the curriculum for both majors and non-majors in science, engineering, and technology. At Youngstown State University, we have already integrated Materials Science lecture topics and qualitative lab experiments into many of our Chemistry and Physics courses. The acquisition of the equipment to be funded by this proposal will allow us to expand this coverage and introduce many new quantitative synthetic and biologically derived polymer and solid state materials experiments into our sophomore through senior level Chemistry lab classes, the condensed matter Physics lab classes, a proposed Materials Science lab course, and our professional development offerings for high school science teachers. We propose to purchase a thermogravimetric analyzer (TGA) and its data system and accessories, a constant temperature bath for viscometry studies, and a gel permeation/size exclusion chromatograph (GPC/SEC) and to upgrade our current differential scanning calorimeter (DSC). The thermal analysis equipment will allow our students to quantitatively evaluate phase changes in solid state, polymeric, and biologically relevant materials and to quantify the chemical reactions of solid state materials at elevated temperatures. The viscometry and GPC/SEC equipment will allow our students to quantify the molecular weights and related physical properties of synthetic and biologically derived polymers. These new quantitative experimental results will be related to both the underlying physical principles and the practical applications of these materials in lecture discussions. The proposed instrumentation project will directly impact over 400 students each year.

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1. Results From Prior NSF Support

In the past three years, Youngstown State University has implemented a number of curricular reforms in its Chemistry and Physics Programs, including six projects partially supported by NSF grants: a) an X-ray Diffractometer (DMR RUI DUE-9403889), b) a Gas Chromatograph-Mass Spectrometer (ILI-IP DUE 9551683), c) an Environmental Chemistry Lab (ILI-IP DUE 9751151), d) a Portable Mechanics Physics Lab (ILI-IP DUE-9552374), e) an Environmental Investigative Laboratory (ILI-IP DUE 9552347), and f) Enhancing Undergraduate Education Through Mossbauer Spectroscopy (ILI-IP DUE-9751236). The first five of these involved one or more of the principal investigators and will be discussed below.

a. NSF RUI DUE-9403889: X-ray diffractometer

Funds from this grant (\$71,199, matched by about \$200,000. Duration: 1994-96) were used to purchase 2 new Siemens P4 X-ray diffractometers, a low temperature setup, a multi-wire area detector, and a number of SGI and PC workstations for data processing. Acquisition of this instrumentation has allowed full integration of advanced diffraction methods into the Chemistry curriculum. A new 3 quarter hour course, Chemistry 832 "Solid State Structural Methods," that teaches crystallography to groups of about ten Chemistry, Geology, and Engineering majors, will be offered for the third time this year. The first offering of this course is resulting in several papers with undergraduate co-authors [Hunter et. al., 1997e, 1997g and 1997h and Cashman et. al., 1997]. A student laboratory manual (X-Ray Structure Determination by SHELXTL: A Beginners Introduction [Hunter, 1997c]) was written and is now being evaluated by crystallographers in about a dozen universities. This instrumentation has also allowed powder diffraction and single crystal diffraction methods to be integrated into four other upper level Chemistry courses. In addition, a new graduate course on advanced crystallographic methods,

Chemistry 993, as been developed and will be offered for the first time this year. Further detail on these courses and related curricular innovations can be found in upcoming publications in the *Journal of Chemical Education* [Hunter, et. al., 1997a, 1997b, 1997d and 1997f]. In addition, this instrumentation has contributed to chemical, materials, and geological research at YSU and three collaborating universities.

b. NSF ILI-IP DUE-9551683: GC-MS

This grant (\$34,450, matched by about \$40,000 from YSU. Duration: 1995-96) was used to purchase a Finnigan 1020 Gas Chromatograph-Mass Spectrometer. This instrument has been fully integrated into senior level organic synthesis, organic analysis, and inorganic lab courses serving about 50 students a year. These advanced courses operate on a largely collaborative learning, discovery-oriented model. It is also integrated into our sophomore organic lecture sequence which serves approximately 200 students each quarter, primarily from the natural sciences, engineering, and pre-medicine, where it has facilitated an ongoing conversion to a more research oriented laboratory approach.

c. NSF ILI-IP DUE 9751151: Environmental Chemistry Lab

Funds from this grant (\$78,350 matched by \$78,350 from YSU. Duration: 1997-98) have recently been used to purchase several items of equipment needed in the development of an integrated science course that exposes students to "real-life" techniques and procedures used in Phase I and Phase II property assessments of brownfields. This course will be offered for the first time during the Fall of 1998. Brownfields are previously used industrial sites that are presently not being fully utilized due to uncertainties in the cost of environmental remediation of the sites. The course is intended for students in environmental studies, chemistry, civil and environmental engineering, biology, and geology at Youngstown State University and ten other

colleges in the region. The course will present in an integrated format the dependence of an analysis protocol on size, type of sample collected, type of container and preservatives, collection procedure and method of sample preparation, and thus should provide students with an increased appreciation of the interconnections between what are often presented as independent functions. Equipment purchased includes a CEM Microwave Oven, a Varian Spectro-2000 Graphite Furnace Atomic Absorption Spectrometer, and a Varian Saturn Gas Chromatograph-Mass Spectrometer.

d. NSF-ILI DUE-9552374: Portable Mechanics Physics Lab

This grant (\$20,000, matched by \$25,038 from YSU. Duration: 1995-97) was used to purchase computing equipment and portable data collection equipment, and enabled the Department of Physics and Astronomy to reform its introductory mechanics laboratories (Physics 501L and 510L) for natural science majors. In these restructured courses, the number of experiments to be performed in the ten-week quarter has been reduced from nine to three. Each experiment focuses on one of the three fundamental approaches to mechanics: force and motion, energy, and momentum. Through a computer-assisted assessment, students are now able to target their own initial conceptions of each topic and decide how best to test their conceptions using portable data collection hardware funded through this grant. Over an extended three week period, students perform their tests using subjects and environments familiar from everyday experience, and report back to the laboratory to analyze results and repeat the assessment of their conceptions, comparing initial conceptions with final conclusions. The final NSF report on this effort will be submitted by December, 1997.

e. NSF-ILI DUE-9552347: Environmental Investigative Laboratory

Funds from this ILI grant (\$25,000, matched by \$46,300 from YSU. Duration: 1995 to 1997 with a one year extension to 1998.) were used to develop the laboratory for Fundamentals of Environmental Studies, the introductory two-quarter course sequence in the core curriculum of the Environmental Studies program. The course features a "discovery" type laboratory that emphasizes the scientific method, data management, understanding of accuracy, precision and error, critical thinking, teamwork, and communication skills. The course was first offered in Winter 1996, enrolling a total of 50 students, divided among two sections. An Investigative Laboratory Manual was also developed for the course, and includes exercises on the scientific method, team research and student-initiated projects. Equipment purchased with funds provided by this grant include: 6 analytical balances, 6 drying ovens, 6 spectrophotometers, 6 dissolved oxygen meters, 6 muffle furnaces, 6 centrifuges with rotors and buckets, and 6 computers.

2. Project Narrative

a. Current Situation

1. Description of Youngstown State University

Youngstown State University is an urban primarily undergraduate institution serving ≈ 12,000 undergraduate and ≈ 900 MS students. We do not offer 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 which 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. We are closely involved with the Youngstown City and several other local school districts which have substantial African-American enrollments via curriculum and administrative support programs, in-service teacher training, and initiatives to encourage and support their students attending University. The Chemistry and Physics and Astronomy Departments also work closely with local high school science teachers and 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) as well as Lorain County Community College which have more limited laboratory facilities than we do.

The Departments of Chemistry and Physics and Astronomy at YSU have a total of 23 full time faculty members. Both Departments have very strong records of service teaching and of graduating well-educated majors. Over the last several years, we have averaged about 55 Chemistry and Combined Science, about 7 Physics and Astronomy, and about 7 MS Chemistry graduates a year {see Appendixes 6c and 6e}. The range, frequency of offering, and enrollment

in our upper division chemistry courses has substantially increased over the last five years as has the size of our MS program.

2. The Importance of Materials Science Topics in University Education

Advanced polymeric, solid state, and biochemical materials are of major and increasing scientific, technological, and economic importance. As a direct consequence, scientific and business publications such as Science, Nature, and Business Week present articles on related topics such as advanced plastics, high temperature superconductors, and designer proteins weekly, and these topics are also regularly discussed in general circulation newsmagazines and newspapers. Their importance has also recently been emphasized by national organizations such as the National Academies of Science and Engineering, the National Science Foundation, the American Chemical Society, the American Physical Society, and the American Association for the Advancement of Science. These bodies all agree that both Science, Engineering, and Technology majors and the wider student body needs greater exposure to Materials Science topics. Specialized Materials Science lecture and laboratory courses can help meet this need for our majors. However, only a minority of them, and very few non-majors, currently take such Therefore, professional organizations such as the American Chemical Society courses. Committee on Professional Training strongly recommend the integration of Materials Science topics throughout our programs and thermal analysis is one of the twelve instrumental methods whose use they monitor. The current NSF-ILI Instrumentation proposal seeks funding to help Youngstown State University meet this goal.

3. The Current Chemistry and Physics Curricula

As with most Science Departments, we serve majors, students with a minor in our disciplines, and students whose programs require Chemistry and/or Physics. Our main service

teaching loads are for students pursuing biology, environmental science, engineering, nursing, medical technology, education, and pre-professional (e.g., pre-medical, pre-dental, pre-pharmacy) degrees. The Chemistry Department offers an ACS certified BS degree in Chemistry (including options with an emphasis on Environmental Chemistry or Biochemistry) and a BA in Chemistry. Along with Biology, we also offer a Combined Science BS degree (this program has a Chemistry component similar to that required of our BA students). We also offer an MS degree in Chemistry (and are developing an option with an emphasis on Pre-College Chemical Education). The Department of Physics and Astronomy offers both a BS and a BA degree in Physics as well as a combined BS in Physics and Astronomy. In addition, the department is currently collaborating with the Department of Electrical Engineering in developing a BS degree in Engineering Physics and a MS degree in Optical Engineering. {See Appendix 6e for details.} Because of our excellent inventory of analytical, spectroscopic, molecular structure determination, and optics/laser equipment, these programs strongly emphasize the "hands on" use of this advanced instrumentation in their sophomore through senior level lab courses {See Appendix 6b} and in undergraduate research. For example, all Chemistry graduates now extensively use our 400 MHz NMR, our new X-ray diffractometers, and our GC-MS in their programs and even the students in "service" courses such as sophomore organic get extensive "hands on" exposure to FT-NMR, FT-IR, and GC-MS.

4. Resources for the Proposed Project

Our teaching programs have excellent internal support from the YSU administration. Over the last six years, this support has allowed us to: (a) replace 10 Chemistry and 4 Physics faculty, (b) hire two new technical support staff, (c) allocate a total of about 3 person years of faculty reassigned time from teaching to support research on curricular innovation, (d) increase

the graduate assistantships in Chemistry from 6 to 18, and (e) and provide internal funding of about three quarters of a million dollars towards the purchase of advanced instrumentation! This is all the more remarkable because it occurred at a time when many other units on campus have been significantly downsized. In addition, YSU recently established the related Center for Photon Induced Processes (CPIP). The internal seed funding for this center (i.e. over \$180,000) has provided the basic laser and optics infrastructure for the nonlinear optical (NLO) and photorefractive (PR) polymeric materials research programs of several faculty, including two of the PIs, Hunter and Brower. This instrumentation will also form an essential part of many of the upper division lab courses offered by the Departments of Chemistry and Physics & Astronomy.

5. Curricular Need for the Proposed Project

We have already integrated many aspects of materials synthesis and characterization into our lecture courses. This coverage begins with substantial discussion of polymers and solid state materials such as metal oxide superconductors in General Chemistry and continues through discussion of more advanced topics such as synthetic methods, reaction kinetics and thermodynamics, thermal analysis, viscosity, and GPC/SEC in the upper level classes {see Section 2-b-3 and Appendix 6b}. In the labs accompanying these classes, we prepare a variety of organic and inorganic polymers and solid state materials and isolate biological macromolecules. These materials are then characterized by their gross physical properties (e.g. color, melting point, and solubility) and their analytical and spectroscopic properties. These theoretical, synthetic, analytical, and spectroscopic studies are tightly integrated and substantially improve student learning. Within the physics curriculum, polymeric materials also receive extensive discussion in the thermodynamics and modern optics courses, in addition to the undergraduate research projects. In the associated labs, polymeric materials are utilized in a variety of

fundamental materials characterization projects as well as applied research topics, including the measurement of nonlinear optical susceptibilities in NLO polymers, characterization of the susceptibility decay in such materials, xerographic and time of flight measurements in photorefractive polymer composites, and fabrication of waveguide polymeric electro-optic modulators. Unfortunately, because we lack usable and appropriate thermal analysis, viscometry, and GPC/SEC equipment, we can not similarly integrate theory with quantitative aspects of these important materials characterization methods. As a result, the students can not properly characterize the molecular weights and thermal behaviors of the materials they make and/or isolate, can not develop structure/property relationships for these, and can not properly investigate the solid state reactivity of the materials they do study. We have made extensive efforts to integrate materials chemistry across the curriculum and have already integrated the appropriate characterization techniques for which we are equipped (e.g. X-ray diffraction of single crystals and powders, STM, TEM, and magnetic susceptibility). The requested equipment will allow us to fully integrate quantitative aspects of materials characterization across the chemistry and physics laboratory curricula.

b. Development Plan

1. Materials Characterization at Other Institutions and Literature Review

The theory of materials synthesis and characterization is discussed in the main texts we employ in our courses as well as in several excellent supplementary texts {see Appendix 6h}. Our current Analytical, Biochemistry Inorganic, Organic, and Physical Chemistry and Condensed Matter Physics lab manuals include well developed experiments involving materials characterization as do specialized polymer lab texts [Pearce, 1982 and POLYED]. The *Journal of Chemical Education* {see Appendix 6i} has published a range of appropriate experiments that

we could incorporate in our labs. The National Science Foundation Division of Undergraduate Education, Instruments and Laboratory Improvement Program has sponsored a few previous projects in this area (see Appendix 6j) which should have produced useful experiments. From these sources, we have tentatively identified a series of potential experiments for our adoption. In addition, we have developed several additional interesting new experiments of our own. Once the new equipment is in place, these promising leads will be evaluated in detail using "pilot sections" of students from the appropriate courses and the best examples will be incorporated into our continuing curricula. (See Appendix 6g for a list of some of the most promising experiments that we have developed and will be introduced and pilot tested in the first two years of this project. A range of the literature experiments describe above will also be evaluated.)

2. Revisions to Our Overall Curricula

With the provision of the proposed equipment our *chemistry curriculum* will take on an increased emphasis on the quantitative study of materials. There will be a significant increases in the lecture content on the topics, but the most important change will be the addition of at least one new quantitative experiment on materials characterization/properties in each of about a dozen chemistry courses. These lab changes are particularly important because of our continuing move towards a curriculum emphasizing "hands on" discovery based laboratory experiences and their integration with the "theory" taught in class. In particular the thermal analysis equipment will be used to study solid state reactions at elevated temperatures, phase changes, and stabilities of various materials and the viscometry and GPC/SEC equipment will be used to study the molecular weights of synthetic and biologically derived polymers.

The proposed instrumentation will facilitate the integration of materials science lab experiments and undergraduate research topics into the current *physics curriculum*, and will aid

in the development of the Engineering Physics BS and Optical Engineering MS degree programs. In particular, the TGA and DSC equipment will be used for materials characterization purposes in a variety of experiments in three separate physics lab courses. DSC and TGA measurements currently cannot be done on-site.

Both the Chemistry and Physics and Astronomy Departments offer extensive training to prospective teachers through our service courses and to current science teachers through a variety of in-service activities, short courses, and advanced professional development courses. These are often lab based and the purchase of this equipment will allow us to extend the "hands on" topics covered in our *teacher training activities* from small synthetic and biological molecules to synthetic and natural polymeric and solid state materials.

3. Examples of Revisions to Specific Courses

As described above, acquisition of the requested equipment will allow us to integrate new quantitative materials experiments into a wide variety of our courses along with appropriate supporting revisions to the lecture classes. Below are outlined the current status and proposed changes to specific individual courses and groups of courses. {Details on specific new and revised experiments are given in Appendix 6g.}

In our four core Analytical Chemistry Courses (Chemistry 603/604: Quantitative Analysis and Chemistry 803/804: Chemical Instrumentation) the basic principles of thermal analysis, viscometry, and gel permeation/size exclusion chromatography (GPC/SEC) are introduced and the net results of thermal decomposition reactions (e.g. of metal hydrates and carbonates) are studied in lab. The new equipment will allow the quantitative study of the thermodynamics and kinetics of such decomposition reactions. Similarly, the provision of the GPC/SEC will allow the investigation of the fundamental chromatographic technique. { \approx 170 students per year}

In our sophomore organic courses (especially Chemistry 721: Organic Chemistry III) polymers are discussed extensively and one condensation and one addition polymer are prepared in the lab. The provision of the GPC/SEC will allow our student to quantify the effects of molecular weights (which vary as a function of reaction conditions) and how these correlated with visually observable differences in materials properties (e.g. in each lab section, the polystyrene samples typically range from gummy oils to hard brittle solids due to varying degrees of polymerization). {~170 students per year}

In our physical chemistry classes (Chemistry 739/740/741: Physical Chemistry I/II/III and Chemistry 801/802: Biophysical Chemistry) the underlying principles of calorimetry, viscosity, and macromolecular solution behavior are developed in detail and the semiquantitative phase diagram of a binary Pb/Sn alloy are determined in the lab from the melting points of a range of compositions. The provision of the upgraded DSC will allow these students to study the phase diagrams of a much wider range of lower melting systems (e.g. organics and inorganics) much more precisely (at least one order of magnitude improvement), to routinely obtain heat capacities and heats of phase transitions (which can't be done now), and to study more complex/relevant phase diagrams (e.g. liquid crystalline phase transitions of biologically relevant materials such as cholesterol). Similarly, the viscometry apparatus will be used in conjunction with the GPC/SEC to study the properties of solutions of biologically relevant macromolecules such as carbohydrates, DNA, and proteins. { ≈40 students per year}

In the inorganic and structural methods courses (Chemistry 831: Inorganic Lab and Chemistry 832: Solid State Structural Methods) we currently prepare solid state materials (e.g. the copper oxide supper conductors) and characterize them by methods such as STM and powder X-ray diffraction. The provision of the TGA will allow us to monitor the kinetics and

mechanisms of these high temperature syntheses and the upgraded DSC will be used to provide information on the complex phase transition characteristics. The viscometry and GPC/SEC equipment will be used to study the molecular weight distributions of the inorganic polymers prepared (e.g. polysiloxanes). { \approx 20 students per year}

The Polymer Chemistry Lab course (Chemistry 825) will make the most extensive use of all of this equipment, in specialized experiments on thermal analysis and molecular weight determination, to characterize the polymers the students prepare, and to establish structure property relationships. {≈3-5 students per year}

The acquisition of DSC and TGA instrumentation will allow the inclusion/modification of several new experiments into the condensed matter physics labs (Physics 710L: Thermodynamics Laboratory and Physics 722L: Physical Optics Laboratory), including measurements of amorphous materials including thermal decomposition temperature, glass transition temperature, enthalpy, etc., measurement of NLO susceptibility vs. structure and glass transition temperatures for NLO polymeric materials, and fabrication of polymeric waveguide electro-optic modulators complementing lecture discussion of these topics. { \approx 44 students per year}

In both Chemistry and Physics this new instrumentation will be used extensively for undergraduate research (Chemistry 850: Undergraduate Research and Physics 805: Undergraduate Physics Research). This will include the study of new inorganic solid state materials with Wagner, new organic and organometallic polymers with Hunter, isolation and characterization of biopolymers with Kim, and NLO materials physics with Brower as well as other projects with the other faculty members listed in Appendix 6f. {≈10-15 students per year}

4. Adaptation to Programs at Other Institutions

We continue our ongoing program of adapting new experiments we develop to other institutions. We are using our relationship with regional colleges to facilitate this process. In particular, Dr. John Andrews at Hiram College has been intimately involved in the current dissemination of our new X-ray crystallography experiments [Hunter 1997b and 1997c] and will continue this role in the future. Indeed, his expertise in thermal analysis will be invaluable during the implementation phase of this project at YSU.

c. Equipment

1. Equipment Request

We propose to purchase a TA Instruments model 2950 Thermogravimetric Analyzer, TGA, a new Model 3200 data system, and associated minor components (e.g. a capsule press). This robust system is ideal for use by large numbers of students since its "user friendly" software allows a beginner to use it after a few minutes of training. We currently have a DuPont Model 9900 Differential Scanning Calorimeter, DSC. Although the DSC module itself is fully functional, its data system is obsolete and unreliable and software is not "user friendly." It therefore can not be routinely used by undergraduates in our large enrollment courses. The budget will allow us to upgrade this DSC and interface it with the new data system so that undergraduates can also use it routinely. Approximately 220 students will use this thermal analysis instrumentation each year.

The proposed Cannon Instruments CT-1000 constant temperature bath is digitally controlled which allows its temperatures to be set to ± 0.01 degrees over a range of 20° to 100° and ± 0.03 degrees above 100°. Changing this temperature is very quick and easy and therefore different lab classes can use it the same day (e.g. the polymer lab at 30.00° in the morning and the

biophysical lab at 20.00° in the afternoon). Approximately 60 students will use this viscometry equipment each year.

The proposed GPC/SEC from Polymer Laboratories will allow us to determine molecular weights in solvents ranging from water to aromatics. We have specified an integrated GPC data system to make the students learning curve on the software easier. The autosampler is required to handle the large number of samples to be produced in several of these courses, particularly the sophomore organic class. A column oven is needed to ensure reproducible and reliable results. Most courses involve organic polymers where the refractive index, RI, detector is generally much more sensitive and appropriate. However, the Biophysical course requires an Ultra-Violet Visible, UV-Vis, detector for the study of its biological macromolecules. Approximately 220 students will use this chromatography equipment each year.

The equipment we have chosen is the most reasonably priced that meets the diverse needs of our classes. Each of these items provides complementary information needed for the *quantitative* characterization of solid state and polymeric materials. Since the conceptual purpose and rationale of each of these items is similar (indeed, many are used in the same experiments) we decided to include them in a common application.

2. Equipment on Hand for the Project

The Departments currently have excellent facilities for the synthesis of polymers, for the preparation of solid state materials, and for the isolation of biological macromolecules such as proteins. We also have excellent facilities for the characterization of molecular structures and properties and for the study of the optical properties of solids. {See Appendix 6a}

3. Implementation and Equipment Maintenance

The principal investigators and other faculty users (See Appendix 6f) have all of the knowledge and experience to ensure that the proposed curricular innovations will be fully implemented. Our current maintenance budgets (\$24,000 and \$5,000), the recently hired Electronic Instrumentation Service Specialist (with 10 years experience servicing advanced scientific instrumentation at Tulane University), and the soon to be hired Coordinator of Technical Services (to maintain, coordinate, and supervise our computer equipment and laboratories) will ensure that all new instrumentation will be fully maintained. A total of 12 quarter hours of reassigned time (i.e. 1/3 of a faculty member's annual teaching load) has been committed by YSU for the implementation of this project. {See section 5, Budget}

d. Faculty Expertise

As noted in the attached biographical sketches, the PIs are experts in materials science and in thermal analysis (SB, ADH, DWM, and TRW), viscometry (ADH and TDK), and GPC/SEC (ADH and DWM) and have strong track records of curriculum innovation.

e. Dissemination and Evaluation

Data generated by students at YSU will be made available through Web pages of individual courses and faculty. New laboratory experiments will be presented at local, regional, and national ACS and CUR (Council on Undergraduate Research) meetings, disseminated by electronic mail, and published in appropriate journals such as the *Journal of Chemical Education*. In addition, Dr. John Andrews of Hiram College will assist us in first evaluating and disseminating these results to the ten cooperating two and four years colleges, and then nationally. This will be done by seminars and workshops at YSU and they by taking the experiments "on-site" to other schools.

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- Hunter, A. D.; Kwolek, K.; Leslie, K.: "Advanced Spectroscopic and Structural Methods: A Professional Development Course for High School Chemistry Teachers. Why Shouldn't They Join the Fun?," manuscript in preparation for the *Journal of Chemical Education* (expected submission date: January, 1998). (1997f)
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- pages + ≈80 pages of supplementary material, manuscript in preparation for the *Journal of Organometallic Chemistry* (expected submission date: December, 1997). (1997g)
- Hunter, A. D.; Pollack, J. E.; Zaworotko, M. J.; Furey, W. S.: "Donor/Acceptor Interactions in four (η⁶-1,4-C₆H₄(Donor)(Acceptor))Cr(CO)₃ Complexes: X-Ray Crystallographic Study of (η⁶-1,4-C₆H₄(NH₂)(CO₂Me))Cr(CO)₃, (η⁶-1,4-C₆H₄(NMe₂)(CO₂Me))Cr(CO)₃, (η⁶-1,4-C₆H₄(OMe)(CO₂Me))Cr(CO)₃, and (η⁶-1,4-C₆H₄(NH₂)(CF₃))Cr(CO)₃," 49 pages + ≈100 pages of supplementary material, manuscript in preparation for the *Journal of Organometallic Chemistry* (expected submission date: January, 1998). (1997h)
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4. Biographical Sketches

Biographical Sketch for Allen D. Hunter.

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

Vitae. Allen Hunter received his Honors B.Sc. in Chemistry in 1981 from the University Α. 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. He is a member of the American Chemical Society, the American Association for the Advancement of Science, The American Crystallographic Association, The Council of Undergraduate Research and three other professional associations. Dr. Hunter has extensive experience in the use of mass spectrometry, nuclear magnetic resonance spectrometry and X-ray crystallography in inorganic and organometallic chemistry. He has extensive experience with polymer synthesis and characterization including the use of combinations of thermal analysis (including DSC and TGA), viscometry, and GPC/SEC data to characterize new polymers. He is one of two designated faculty coordinators of YSU's new Gemini-2000 400 MHz NMR and of our Siemens X-ray diffractometers. He is also the director of the YSU Structure Center and serves as the representative for YSU and other predominantly undergraduate institutions in Ohio on State wide coordinating committees for NMR and X-ray consortia.

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. Since coming to YSU he has been PI or co-PI on instrumentation grants totaling over \$500,000 which have supported the YSU Chemistry Department's innovative teaching program.

B. Refereed Journal Publications, Allen has had 36 refereed journal publications, generally in American Chemical Society Journals, including 17 since 1992. A selection

- of publication which are related to this proposal is presented below (1 to 5 are the five most relevant).
- 1. Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *Journal of Chemical Education*, in press, 9 pages (accepted September 9th, 1997).
- Hunter, A. D.; Bianconi, L. J.; DiMuzio, S. J.; Braho, D. L.: "Synthesis and Structure/Property Relationships in (η⁶-Arene)Cr(CO)₃ Chemistry: from Guided Experiments to Discovery Research. Physical Properties, IR, MS, and Multinuclear NMR Spectra, and Cyclic Voltammetry," *Journal of Chemical Education*, 52 pages in press (accepted October 4th, 1997).
- 3. Guo, X. A.; Sturge, K. C.; Hunter, A. D.; Williams, M. C.: "Molecular Weight Determination and Establishment of a Rod-Like Structure for Organonickel Polymers [Ni(PR₃)₂Ar^F]_n-," *Macromolecules*, **1994**, 27, 7825-7829.
- 4. Hunter, A. D.; Guo, X. A.: "Organometallic Polymers, Fluoroarylene Bridged (Rigid Rods to Segmented Chains)," *The Polymeric Materials Encyclopedia, Volume 6*, CRC Press, **1996**, 4813-4822.
- 5. Guo, X. A.; Hunter, A. D.: "Polyfluoroacrylates (Effects of Side-Chain H/F Variations)," *The Polymeric Materials Encyclopedia, Volume 8*, CRC Press, **1996**, 6138-6144.
- 6. Guo, X. A.; Hunter, A. D.; Chen, J.: "Synthesis and Characterization of Novel Organonickel-Organosilicon Alternating Copolymers," *J. Polymer Science, Part A*, **1994**, *32*, 2859-2866.
- 7. Guo, X. A.; Hunter, A. D.; Chen, J.: "Preparation and Characterization of Acrylates and Polyacrylates Having Variable Fluorine Contents and Distributions," *J. Polym. Sci., Part A*, **1994**, 32, 47-56.
- 8. 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.
- 9. 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(PMePh₂)₂(4,4'-C₁₂F₈H)Br and Ni(PMePh₂)₂(4,4'-C₁₂F₈H)₂," Organometallics 1992, 11, 3056-3062.
- 10. 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.
- C. Other Collaborators: None.
- D. Graduate Students: X. Andrew Guo, Ph.D. 1994 (University of Alberta), Xiaochung Wang, MS 1994 (Youngstown State University), Larry J. Bianconi, MS 1994 (Youngstown State University), Stanislaus Tsai, Ph.D. 1995 (University of Alberta), Dianne Braho, MS 1995 (Youngstown State University), Steven DiMuzio, MS 1996 (Youngstown State University), and Bev Smith-Papa, MS 1997 (Youngstown State University).
- E. Advisors: Detailed in Section A, above.

Biographical Sketch for Shane C. Brower Department of Physics and Astronomy, Youngstown State University

A. VITAE

Education:

Ph. D.

1996 University of Maryland Baltimore County, Baltimore, MD

Research Advisor: Professor L. Michael Hayden

Thesis Title: Activation Volumes Associated With Chromophore Motion in

Poled Polymer Systems: Their Physical Significance and

Relationship to Stability

MS 1993 University of Maryland Baltimore County, Baltimore, MD

Research Advisor: Professor L. Michael Hayden

Thesis Title: A Technique for Measuring the Pressure Dependence of the

Second Order Non-Linear Optical Susceptibilities in Poled

Polymers

BS 1991 Bucknell University, Lewisburg, PA (Summa Cum Laude)

Professional Experience:

9/96-present: Assistant Professor, Department of Physics and Astronomy, Youngstown State University (YSU). I am currently collaborating with another first-year member of the department in developing and implementing new teaching techniques in undergraduate physics utilizing collaborative and inquiry based learning techniques. Together with three other members of the department of Physics and Astronomy and one member of the department of Chemistry, I am forming the YSU Center for Photon Induced Processes, wherein I will investigate the orientational stability of photorefractive and electro-optic organic and polymeric materials using second harmonic generation and a unique delay-trigger pressure technique. Finally, I am part of a collaborative effort with the dept. of Electrical Engineering to develop a BS degree program in engineering physics and a MS degree program in optical engineering.

1995-1996 Director of Grants and Instructor (Physical Sciences Department), Villa Julie College, Stevenson, MD.

1995, 1996 Instructor (Summer), Department of Physics, University of Maryland Baltimore County (UMBC), Baltimore, MD

1992-1996 Graduate Research Assistant, Department of Physics, UMBC

1992-1995 Instructor/Director of Physics Tutoring, Meyerhoff Scholarship Program, UMBC

1992-1993 Instructor, Horizons Exploration Program, Center for Educational Research and Development, UMBC

B. PUBLICATIONS

Five most relevant publications:

(1) "Nonlinear optical studies of the pressure dependence of transitions in glass forming polymers", L. M. Hayden, S. C. Brower, and S. J. Strutz, Macromolecules, 30, 2734 (1997).

- (2) "Activation volumes associated with chromophore reorientation in corona poled guest host and side chain polymers", **S. C. Brower** and L. M. Hayden, J. Poly. Sci. Part B, **33**, 2391 (1995).
- (3) "Synthesis of a Stable NLO-Polymer: In-Situ Poling and Cross-linking of Polymers by the use of 'NLO-Tweezers'", Michael E. Wright, Isabel McFarland, S. C. Brower, and L. M. Hayden, Macromolecules, 28, 8129 (1995).
- (4) INVITED PAPER "Advances in Mainchain Syndioregic Nonlinear Optical Polymers", J. D. Stenger-Smith, R. A. Henry, A. P. Chafin, L. H. Merwin, R. A. Nissan, R. Y. Yee, M. P. Nadler, G. A. Lindsay, L. M. Hayden, S. C. Brower, D. Kokron, N. Mokal*, W. N. Herman, and P. Ashley, *Polymers for Second-Order Nonlinear Optics*, G. A. Lindsay and K. D. Singer, eds., ACS Symp. Ser. 601, 181 (American Chemical Society, Washington, D.C., 1995).
- (5) "Activation volume associated with the relaxation of the second order nonlinear optical susceptibility in a guest host polymer", S. C. Brower and L. M. Hayden, Applied Physics Letters, 63, 2059 (1993).

Other publications:

- (6) "Nonlinear Optical Studies of the Pressure Dependence of Transitions in Glass Forming Polymers," L. M. Hayden, S. C. Brower, and S. J. Strutz, *Journal of Polymer Science*, in press.
- (7) "Temperature Dependence of the Activation Volume in a Nonlinear Optical Polymer: Evidence for Chromophore Reorientation Induced by Sub-Tg Relaxations," S. J. Strutz, S. C. Brower, and L. M. Hayden, *Journal of Polymer Science*, in press.

C. OTHER COLLABORATORS: None

D. GRADUATE ADVISEES: None

E. GRADUATE ADVISOR: Dr. L. Michael Hayden

^{*} Undergraduate Co-author

Biographical Sketch for Thomas D. Kim

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

A. Vitae

Thomas D. Kim received his BS degree in Chemistry from Loyola College in Maryland in May of 1987 while pursuing research on the synthesis of novel organometallic compounds. He then began graduate studies in the Department of Chemistry at the University of Wisconsin-Madison. He completed his Ph.D. in Bio-inorganic chemistry in December, 1993 under the supervision of Professor Judith N. Burstyn. As the first student in the Burstyn, he was instrumental in initiating studies on the mechanism of activation of soluble guanylyl cyclase by nitric oxide. The title of his thesis was "Identification and Characterization of an Endogenous Inhibitor of Soluble Guanylyl Cyclase from Bovine Lung".

Immediately following graduate school, Dr. Kim began work as a postdoctoral associate in the Department of Pharmacology at Cornell University, Ithaca, NY under the supervision of Professor Clare Fewtrell. While at Cornell, Dr. Kim studied the role of intracellular calcium ion in the stimulus-response pathway in mucosal mast (immune) cells. In 1995, he was awarded the Arthritis Foundation and American Heart Association Postdoctoral Fellowships to continue his work at Cornell. He began his current position as Assistant Professor of Biochemistry in the Department of Chemistry at Youngstown State University in the Fall of 1995. In addition to his collaborative research on glycosidase transition state analogs, Dr. Kim is also investigating the role of the nitric oxide-cyclic GMP signaling pathway in mucosal mast cells. He is also interested in the incorporation of computer technologies in the undergraduate chemistry and biochemistry curriculum

Dr. Kim is a member of the American Chemical Society (Division of Biological Chemistry), the Council on Undergraduate Research (CUR) and the National Association of Advisors for the Health Professions (NAAHP).

B. Refereed Journal Publications

- 1. Thomas D. Kim, Timothy J. McNeese, Arnold L. Reingold, "Preparation and X-ray Crystal Structure Analysis of the Hydroxo-Bridged, Dinuclear (p-Arene)ruthenium(II) Cation in [Ru(h⁶-C₆H₆)₂(m-OH)₃]Cl^o3H₂O", *Inorganic Chemistry*, **1988**, 27, 2554.
- 2. Thomas D. Kim and Judith N. Burstyn, "Identification and Partial Purification of an Endogenous Inhibitor of Soluble Guanylyl Cyclase from Bovine Lung", *Journal of Biological Chemistry*, **1994**, 269, 15540-15545.

C. List of Other Collaborators

1. Dr. Peter Norris, Department of Chemistry, Youngstown State University

D. Names of Mentors

- 1. Ph.D. Advisor: Dr. Judith N. Burstyn, Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin, 53706
- 2. Postdoctoral Advisor: Dr. Clare Fewtrell, Department of Pharmacology, College of Veterinary Medicine, Cornell University, Ithaca, New York, 14853

Biographical Sketch for Daryl W. Mincey

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

A. Vitae.

Daryl W. Mincey received his BS degree in Chemistry from the University of Cincinnati in June, 1972. He then continued his education at the University of Cincinnati under the direction of Dr. Joseph A. Caruso. He received his MS in Analytical Chemistry in June, 1974. His research dealt with the synthesis of various non-aqueous solvents and studying their physical properties. Dr. Mincey continued working with Dr. Caruso and received his Ph.D. in Bioanalytical Chemistry in June of 1979. His thesis described the first time an electrochemical reaction was monitored by nuclear magnetic resonance spectrometry directly within the probe of the instrument. While receiving his Ph.D., Dr. Mincey was the graduate student operator of all NMR instruments at the University of Cincinnati.

In the winter of 1978, Dr. Mincey took a temporary position at Youngstown State University as a sabbatical replacement. In the fall of 1978, he was employed as an Assistant Professor of Chemistry. The following year Dr. Mincey returned to Youngstown State University, where he earned the ranks of Assistant Professor in 1980, Associate Professor in 1985, and Professor in 1991. He was selected Assistant Dean of Arts and Sciences in 1993 and was elected Chairperson of Chemistry in 1995. While at Youngstown State University his duties have included teaching graduate courses in analytical and clinical environmental chemistry and undergraduate courses in introductory, analytical, biological, and environmental chemistry. Three new courses were developed to reflect changes in the direction of analytical chemistry. They are Chemical Toxicology, Chemical Instrumentation Interfacing and Chemical Literature. The direction of undergraduate and graduate research has been a significant responsibility. Thirty-one master students our of a departmental total of eighty have received degrees under his direction.

Dr. Mincey is a member of the American Chemical Society, Penn-Ohio Border Section. He served as Treasurer 1980-1981, Chairperson-elect 1981-1982, and Chairperson 1982-1983. He is also a member of Sigma Xi, the honorary research society. He served as Chairperson-elect 1990-1991, and Chairperson 1991-1992. Dr. Mincey was the founding Director of the District 15 of the Ohio Junior Academy of Science, an organization dedicated to the promotion of science education through hands-on research. The District 15 Science Fair has a yearly attendance of 400 students. Many district winners have also been highly successful at the Ohio State Science Fair.

Dr. Mincey has received two Youngstown State University recognitions, Research Professor in 1983-1984 and Distinguished Professor in 1985-1986. He either independently or in collaboration with others has received grants from various state and national agencies. He received an Education for Economic Security Act 207C grant of \$60,000 for his work in promoting science fair involvement in 1988. Dr. Mincey was awarded a \$32,000 grant from the Ohio Board of Regents' Research Challenge Program in 1989 to study the interaction between various drugs and model lipid membrane systems by ATR-FTIR. Also in 1989, he cooperated with Dr. L. Spiegel, R. Varma, and F. Bharudi in a \$32,000 study of the correlation between vitamin C and zinc concentrations and sickle cell anemia. Dr. Mincey, with Drs. G. Sutton, S. Martin, L. Schroeder, and I. Khan, have received two grants of \$78,000 in 1986 and \$72,000 in 1988. These grants developed techniques to model pollutant transport in the Mahoning River.

Drs. Schroeder, Martin, and Mincey have worked with the Youngstown State University Technology Development Corporation on a \$372,000 Ohio Department of Development Grant titled: "The Mahoning River Corridor Redevelopment Project." Drs. Martin (PI), Mincey, and Schroeder received a National Science Foundation College Science Instrumentation Grant Program grant of \$68,000 in 1989, another of \$25,000, Schroeder (PI) in 1995, and another of \$78,350 Mincey (PI) in 1997. Equipment was acquired to enhance the recently development environmental science curriculum both minor and major.

B. Referred Journal Publications

- 1. <u>Monitoring of Electrochemical Reactions by Nuclear Magnetic Resonance Spectrometry,</u> **Daryl W. Mincey**, Marc J. Popovich, Patrick J. Faustino, Marilyn M. Hurst, and Joseph A. Caruso, <u>Analytical Chemistry</u>, **1990**, 62, 1197-1200.
- 2. <u>A Microprocessor Regulated Constant Voltage, Current, Wattage and Temperature Electrophoresis Power Supply, Daryl W. Mincey, Kenneth J. Kuzior, Leslie H. Allen III, Jennine S. Frease, and Irene N. Strasser, Analytical Chemistry, 1991, 193, 168-172.</u>
- 3. The Analysis of Steel Samples Employing Ion Chromatography/Sequential Inductively Coupled Plasma Atomic Emission Spectroscopy, Jeffrey J. Giglio, Daryl W. Mincey, and James H. Mike, Analytica Chemica Acta, 1991, 254, 1-2, 109-112.
- 4. <u>Temperature Controlled Microwave Oven Digestion System</u>, **Daryl W. Mincey**, Richard C. Williams, Jeffrey J. Giglio, Gale A. Graves, and Anthony J. Pacella, <u>Analytica Chemica Acta</u>, **1992**, 264, 97-100.

C. List of Other Collaborators

1. Dr. Kenneth Rosenthal, Department of Physiology, Northeastern Universities College of Medicine, Rootstown, Ohio.

D. Names of Mentors

1. Ph.D. thesis advisor, Dr. Joseph A. Caruso, Department of Chemistry, University of Cincinnati,

Biographical Sketch for Timothy R. Wagner

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

A. Vitae. Timothy R. Wagner received his BS 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. In the Fall of 1990, Dr. Wagner joined the faculty of the Chemistry Department at the Illinois Institute of Technology, Chicago, Illinois, as 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.

Since Joining the chemistry department at YSU, Dr. Wagner has focused much effort on establishing a departmental infrastructure for solid state structure analysis. He located two donor high resolution transmission electron microscopes, and combined them into one functional instrument. He also played a major role in establishing the department's state-of-the-art x-ray facility, which includes two single crystal diffractometers, and one multi-wire area detector. He is currently the designated faculty operator of the YSU transmission electron microscope and one of two designated faculty operators of the X-ray diffractometers.

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 a past chair of the Penn-Ohio Border section of the ACS.

B. Refereed Journal Publications.

- (1) Wagner, T and O'Keeffe, M.: "Electron Microscopy of Defects and Disorder in Barium Hexagallate," *Acta Cryst.* **1985**, *B41*, 108-112.
- (2) Wagner T. and O'Keeffe, M.: "A Structural Model for Barium Hexagallate," J. Solid State Chem., 1988, 73, 19-26.
- Wagner T. and O'Keeffe, M.: "Bond Lengths and Valences in Aluminates with the Magnetoplumbite and β-Alumina Structures," J. Solid State Chem. 1988, 73, 211-216.
- (4) Wagner, T.: "HREM of Electron-Beam-Induced Damage in L-Ta₂O₅," *J Solid State Chem.* **1991**, 91, 189-203.

C. Submitted Publications

- (5) Wagner T.: "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type Barium Hexagallate" J. Solid State Chem., accepted August 1997.
- (6) Wagner T. and Styranec, T., : "Preparation and Crystal Structure Analysis of Ba₂BiGa₁₁O₂₀", J. Solid State Chem., submitted Sept. 1997.

D. List of Other Collaborators.

None.

E. Names of Mentors.

- (1) Ph.D. Advisor. Michael O'Keeffe, Department of Chemistry, Arizona State University, Tempe, AZ 85287.
- (2) Postdoctoral Advisor. Lawrence Marks, Department of Materials Science, Northwestern University, Evanston, IL 60208.

5. ILI Detailed Budget

a. Equipment List

Item	Quantity	Unit Price	Unit Price	Total Cost
(Descriptive name, probable brand, and model)		(list)	(discounted)	(discounted)
(1) Thermal Analysis Equipment (TA Instruments)	1 system	61,575	43,200	43,200
(a) TGA 2950 Thermogravimetric Analyzer	1	37,100	26,000	26,000
(b) Thermal Analyst 3200 (including: data system, software, and upgrade of our Dupont 9900 DSC)	1 each	20,525	14,400	14,400
(c) Accessories (including: metering system for DSC/TGA purge gasses, DSC sample press, and quench cooling reservoir)	1 each	3,950	2,800	2,800
(2) Viscometry Equipment (Cannon Instruments model CT-1000 from Fischer Scientific)	1	4,800	3,900	3,900
(3) GPC/SEC Equipment (Polymer Laboratories)	1 system	44,691	42,100	42,100
(a) K1001 LC Pump	1	6,995	6,650	6,650
(b) K2300 Refractive Index Detector	1	6,950	6,600	6,600
(c) LC1200 UV-Vis Detector	1	6,995	6,650	6,650
(d) PL-GPC 110 Autosampler	1	8,000	7,600	7,600
(e) Column Oven	1	2,325	2,200	2,200
(f) PL Logical GPC/SEC Data Station and	1	9,550	9,100	9,100
Software				
(g) GPC columns (in THF)	2	893	760	1,520
(h) SEC columns (in water)	2	1045	890	1,780

Total Project Cost: \$89,200

Non-NSF contribution: \$44,600

(including any overmatch)

NSF request: **\$44,600**

The requested materials characterization equipment will be housed in a dedicated lab adjacent to the current advanced synthesis lab in the Chemistry Department (i.e. Ward-Beecher Science Hall room 5011).

To ensure the timely integration of the proposed instrumentation into our curricula, the Dean of Arts and Sciences, Dr. B. Brothers, and the Department of Chemistry are committing reassigned time from teaching to support the implementation of this project. This reassigned

time will total 12 quarter hours (i.e. 1/3 of a faculty member's annual workload) over the 1998/99 and 1999/2000 school years.

b. Budget Justification

Because we do not currently have a functioning DSC, any GPC/SEC or TGA equipment, or an appropriate constant temperature bath for viscometry, we can not currently do the proposed experiments at Youngstown State University.

For the thermal analysis system, we chose TA instruments because of the quality, robustness, and user friendliness of their systems. The requested TGA system has a purge system so that the measurements can be done under a controlled atmosphere which is critical for many TGA and high temperature synthesis experiments. It is usable for temperatures of up to 1,000° which we require for the inorganic lab experiments. The price for the data system¹ includes the upgrade of our currently non-usable Dupont Instruments model 9900 DSC module to modern specifications. We have no other DSC/TGA equipment available.

We chose a constant temperature bath for viscometry studies that has digital controls. For the CT-1000, this allows the routine change of operating temperature in under one half of an hour. This system is stable to $\pm 0.01^{\circ}$ up to 100° and to $\pm 0.03^{\circ}$ at over 100° . Our current "constant" temperature bath is fully utilized for current experiments, takes almost a week of "readjustments" to equilibrate at a new temperature, is only usable to about 70° , and its temperature fluctuates by at least $\pm 0.2^{\circ}$ even on its good days.

This data system will be available in a Windows NT version by next summer and will be able to simultaneously control both the DSC and TGA instruments.

For the GPC/SEC system, we chose the package from Polymers Labs. The other manufacturers either quoted significantly higher prices (e.g. Waters) or had systems that were comparably priced but did not integrate GPC/SEC software. The LC pump specified is a basic model but does have a gradient capability (this added only about \$1,500 to the cost and we hope to use it in our advanced organic synthesis lab if sufficient time is available). We specify both RI and UV-Vis detectors because most of the synthetic organic polymers we require are best (or can only be) detected by the former while the latter is much superior for biopolymers such as proteins. With the large number of users on this instrument (i.e. we will often be collecting data for one or more lab sections of 20 to 27 students in an overnight run for subsequent processing by students in our computer lab the next class) and the fact that GPC/SEC separations routinely take about one half hour, we are requesting funds for an autosampler. The column oven is required for reproducible separations. The data station and software allows easy data processing and the ready integration of the chromatographic data with that from other techniques (e.g. with viscometry data in universal calibration experiments). We currently only have two functioning liquid chromatographs in the department, none is equipped with GPC/SEC software, and they are both fully utilized for student research and for the teaching of conventional liquid chromatography in the analytical chemistry labs.

The with previous instrumentation purchases, the Departments will fund all consumable supplies for these systems over their lifetimes.

6. Appendices

a. Appendix 6a: Major Equipment

The YSU Chemistry and Physics and Astronomy Departments are equipped with a wide range of modern instrumentation and additional equipment is available in other campus departments. Examples of the most relevant major instruments are tabulated below:

Item	Year	Estimated
	Purchased/	Purchase
A 1 Fl 1 ' 7 . M .	Last Upgraded	Cost
Analyzer, Electrophoresis, Zeta-Meter	07/24/85	7,530
Analyzer, Mercury, Buck Scientific Model	07/14/88	3,000
Analyzer, DSC, DuPont 9900 (to be upgraded with this proposal)	07/29/85	80,181
Centrifuge, (3)	1983-87	16,000
Chromatograph, Gas with FID, Hewlett Packard	1994	10,000
Chromatograph, Gas with ECD detector, Varian	1995	30,000
Chromatograph, Gel Permeation, Various Components	1992-94	8,000
Chromatograph, Liquid, with ultraviolet, refractive index, fluorescence and electrochemical detectors (1), IBM LC/9533	08/06/84	41,000
Chromatograph, HPLC, Model 338, Beckman (2)	1990	30,000
Chromatograph, Ion, Dionex 2000i	06/10/84	9,170
Computer Lab and Computerized Lecture Halls (40 PCs, Server, Printers, etc., scheduled for installation January of 1998)	1998	≈200,000
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
Glove Box, Vacuum/Atmosphere	1980	15,000
Hydrogenation and medium pressure reaction apparatus, Parr	02/12/87	4,279
Incubators, Percival, Lighted, Model I-25LLVL (3)	06/14/85	13,641
Instrumental Impact System, Tinius 620	09/06/84	18,515
Microscope, Scanning Tunneling	1994	12,000
Microwave Digestion CEM	07/01/97	23,200
Potentiostat/galvanostat, EG&G PAR, Model 273	09/24/84	8,860
Shear Apparatus, Direct (2), Hogentogler S6564	08/07/84	9,716
Spectrofluorometer, Model RF-50000, Shimadzu	1985	17,000
Spectrometer, Atomic absorption, (4)	1983-85, 97	101,000
Spectrometer, FT-IR, (3), Digilab FTS 40, IBM-IR-32, PE-1600	1984-88	120,000
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-GCQ	1996	95,000
Spectrometer, Nuclear magnetic resonance, IBM NR/80	02/07/83	120,692
Spectrometer, Nuclear magnetic resonance, Varian 400 MHz Gemini 2000 with VT, Multinuclear, and PFG capabilities and 4 probes	1994-97	320,000

Spectrometer, Nuclear magnetic resonance, Anasazi Instruments EFT-60 (currently equipped for ¹ H NMR with the installation of ¹³ C capabilities due this Fall) This is an upgrade of our 1973 Varian EM-360 magnet.	1996/97	50,000
Spectrometer, Ultraviolet, (7), Beckman, Shimadzu, DU	1977-87	80,000
Spectrometer, Ultraviolet-visible, Diode array, Hewlett Packard HP8452A (2)	03/06/87	25,000
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
Furnace, Linberg High Temp. Tube	06/94	5,000
Microscope, Electron, Transmission	1992	used
Diffractometers, X-ray, single crystal (2) with powder capabilities	1994-95	260,000
Continuum EPO-5000 Q-switched, diode pumped Nd:YAG laser	6/97	\$27,000
Stanford Research Systems dual-phase Lock-in Amplifier	6/97	\$7,000
Tektronix 400 MHz digital oscilloscope	6/97	\$4,500
Newport Scientific Optical Bench (4'x12'x12")	6/97	\$10,000
2 Boxcar Averagers, 1 computer interface module, 1 power supply	6/97	\$10,000
Products for Research photomultiplier detection system	6/97	\$1,500

The most relevant equipment we have available includes: IR and UV-Visible spectrometers, two new GC-MS systems, two new single crystal diffractometers (one suitable for powder diffraction measurements), two new FT NMR spectrometers (a 400 MHz broad-banded system for use in upper level classes and a 60 MHz 1 H/ 13 C instrument for use in lower level classes). In addition, the physics department is fully equipped to perform the optical measurements required to study structure-property relationships in polymeric materials, including: a Continuum EPO-5000 Q-switched, diode pumped Nd:YAG laser; a Stanford Research Systems data collection system including two boxcar averagers, a computer interface module, and a power supply; a Tektronix 400 MHz digital oscilloscope, a Stanford Research Systems dual-phase lock-in amplifier, a Products for Research photomultiplier detection system, a Newport Scientific Vibration Isolation Table (4'x12'x12"), and numerous optical components such as mirrors, filters, polarizers, posts, etc.

b. Appendix 6b: Course Descriptions

Chemistry 603, 604: Quantitative Analysis 1 and 2. Chemical equilibrium, stoicheometry, 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 592H for 603. 5 + 5 q.h. {approximately 100 and 40 students, respectively, per year}

Chemistry 719, 720, 721: Organic Chemistry 1, 2, and 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 q.h. {approximately 250, 230, and 170 students, respectively, per year}

Chemistry 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 q.h. {approximately 40, 30, and 20 students, respectively, per year}

Chemistry 801: Elements of Physical Chemistry. An introduction to thermodynamics, spectroscopy, chemical structure, reaction rates, and other physical properties of physical systems. Four hours lecture and three hours laboratory. Prereq.: CHEM 604 and 721; PHYS 603 or 611; and PHYS 611L, and MATH 674 (may be concurrent). 5 q.h. {approximately 10 students per year}

Chemistry 802: Biophysical Chemistry Principles of chemical thermodynamics, spectroscopy, and kinetics as specifically applied to biological systems. Four hours lecture and three hours laboratory. Prereq.: CHEM 801 or 740. 5 q.h. {approximately 10 students per year}

Chemistry 803, 804: Chemical Instrumentation 1 and 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 CHEM 741 or 802.4 + 3 q.h. {approximately 15 students per year for each course}

Chemistry 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 q.h. {approximately 10 students per year}

Chemistry 822: Organic Analysis. 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 q.h. {approximately 7 students per year}

Chemistry 823: Organic Synthesis. Preparations of organic compounds and applicable instrumental techniques. One hour lecture and six hours laboratory with discussion. Prereq.: CHEM 721. 3 q.h. {approximately 15 students per year}

Chemistry 824: Polymer Chemistry. Polymerization processes and polymer structure-property relationships. Prereq.: CHEM 720. 3 q.h. {approximately 5 students per year}

Chemistry 825: Polymer Chemistry Laboratory. Preparation and characterization of some polymers. One hour lecture and six hours laboratory. Prereq.: CHEM 824. 3 q.h. {approximately 3 students per year}

Chemistry 831: Inorganic Chemistry Laboratory. Preparation of typical inorganic compounds and their characterization. Six hours laboratory-discussion. Prereq. or concurrent: CHEM 729, 740. 2 q.h. {approximately 10 students per year}

Chemistry 832: Solid State Structural Methods. Structure determination for single-crystal and multi-phase organic and inorganic solids by techniques such as single crystal and powder diffraction, electron microscopy, and X-ray microanalysis. Integration of theoretical and practical perspectives through laboratory exercises. Two hours lecture and three hours laboratory-discussion. Prereq.: CHEM 721 and CHEM 741 or 802. 3 q.h. {approximately 10 students per year}

Chemistry 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 q.h. {approximately 30 students per year} Note: as of the 1998/99 school year, this course will be required of all Chemistry majors as a capstone experience.

Chemistry 991/997: Structural Methods for High School Chemistry Teachers These two classes were taught as special sections of Chemistry 805 and 822 optimized to meet the professional development needs of pre-college science teachers. Thus, the content was somewhat more focused (avoiding the more esoteric spectroscopic methods but giving more information on the most relevant methods) and the relationship of each topic to the pre-college curriculum was discussed in detail. {approximately 10 students in each alternate year}

Physics 710L: Thermodynamics Laboratory. Experimental work designed to supplement the corresponding lecture course. Three hours per week. Prereq. or concurrent: Physics 710. {approximately 4 students per year}

Physics 722L: Physical Optics Laboratory. Experimental work designed to supplement the corresponding lecture course. Three hours per week. Prereq. or concurrent: Physics 722. {approximately 40 students per year}

Physics 805: Undergraduate Physics Research. Research conducted under the direction of a faculty member. May be repeated to a maximum of 6 q.h. Prereq.: Intermediate Classical Mechanics (Physics 702), Introduction to Modern Physics (Physics 705). {approximately 4 students per year}

c. Appendix 6c: Subject Area Majors

		Undergraduates Sent To	Undergraduates Sent To	Graduate Schools Our Chemistry	MS Degrees Granted By The
Year	Combined Science Majors Graduated	Graduate	Professional Schools	Majors Have Attended	YSU Chemistry Department
1996-97	51	9	32	*	7
1995-96	62	7	20	*	8
1994-95	50	4	24	*	7

* 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, as well as to our own MS program from which many subsequently went on to do Ph.D. degrees at the above universities.

The Department of Physics and Astronomy is relatively small in terms of majors with a present number of 14 at all levels, having graduated an average of three per year over the past five years. A similar number of minors has been served over this same period. The department has provided quality education to majors and minors and approximately one half of graduates have gone on to graduate studies. Two former students received PhDs during 1995-96. The remaining graduates have obtained technical employment. Notable graduates include Ronald Parise, Space Shuttle Payload Specialist, and Chris Dulya, who will receive the Ph.D. from CERN in 1996.

d. Appendix 6d: Student Research

CHEMISTRY UNDERGRADUATE RESEARCH

1990-present

Hunter

- * "Fun With Inert Atmosphere Techniques", Lisa Bernard, 1993
- "Organometallic Compounds Using Inert Atmosphere Techniques", Lisa Bernard, 1993
- * "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
- * "Synthesis and Characterization of the Chromium Complexed Aromatic Polymers from Polymerizations of p-Phenylenediamine Chromium Tricarbonyl and m-Phenylenediamine Chromium Tricarbonyl", Steven J. DiMuzio, 1994

Mike

- ❖ "The Effect of Methanol on the Activity of the Enzyme Choloylglycine Hydrolase", Laura A. Lyden, 1990
- * "Chololylglycine Hydrolase: The Effect of Pore Size on Enzymic Activity", Francine A. Byrdy, 1991
- ❖ "Determination of Palmitic Acid by Solvent Extraction, Michael J. McKee, 1991
- * "Choloylglycine Hydrolase: Glycocholic Acid Salt", Thomas Smith II, 1991
- ❖ "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
- "Immobilization of Glucose Oxidase with 2-amino-4,6-dichloro-S-Triazine", Paul Bassett, 1992
- * "Detection of Formaldehyde Using 4-Amino-5 Hydrazino-4H-1,2,4-Triazole-3-Thiol", Michael J. Patrick, 1992
- ❖ "Determination of Mirex in Soil Samples", Kevin Lawrence, 1993
- * "Packard Electric Research Project", Joseph Potkonicky, 1993
- * "Experiments in Ion Exchange", Michael Simonsic, 1993
- ❖ "Synthesis of Calixarene for Use as a Stationary Phase in HPLC", Shannon Phillips, 1996

Jackson

- "Synthesis of Phosphorus Mustards Derived from Terpenoids", Diana R. Arnett, 1994
- * "Synthesis of α-Amino Phosphonic Acids", David S. Bronson, 1994-95
- * "Synthesis of α-Phosphonolactones", Jason Smulik, 1994-96
- "Synthesis of Chiral Phosphorus Mustards", Todd Emch, 1996
- "Purification of Chiral Phosphorus Mustards", Joe Kopcash, 1996
- * "New Methods in Peptide Synthesis", Tim Styranec, 1996

Mincey

❖ "Trace Metal Analysis Employing Ion Chromatography - Inductively Coupled Plasma Atomic Emission Spectrometry", Jeff Giglio, 1990

- ❖ "A Square Wave Voltammetric Detection System for Anion Chromatography", Terri Rulick, 1990
- "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
- ❖ "Determination of the Extent of Contamination of Soils for the Mahoning River Redevelopment Project", Kathy Scott, 1993

"Structure Determination of Carbohydrate Dithioacetals", Bruce Jeffries, 1996

Schildcrout

* "Recycling & Reconditioning of Heavy Duty Diesel Engine Coolant", William F. Booher, 1995

Serra Wagner

Norris

- "O-acetylation of Gly-Tyr, Stephen Ray, 1996
- "Perovskite Synthesis", Angella Ferrett, 1993
- * "Perovskites and Oxide Superconductors", Mario Petrino, 1993
- ❖ "Syntheses to Precursors of Fluoride Analogues to Layered Oxide Structures", Sharlene Barb, 1994
- ❖ "Synthesis of Compounds Related to Magnetoplumbite and Beta-alumina Phases and Characterization by X-ray Powder Diffraction, Amy Cecil, 1994
- * "Attempted Synthesis of BaSc₁₂O₁₉ as a Model", Vincent Lucarelli, 1996

The recent thrust of the Department of Physics has provided increased opportunities for students to become involved in research at the undergraduate level. Over the past four years a project has emerged under the direction of Prof. W. G. Sturrus for laser spectroscopy of Rydberg states of neutron atoms. This project has been sponsored externally by Research Corporation and internally by matching funds and faculty release time. Both majors and minors have been involved in the construction and testing of experimental equipment including a vacuum system, spectrometer and associated laser source, and neutral beam source. In related educational efforts, students are involved in the production and in the construction of a CO₂ laser. Presently one major and three minors are participating.

Undergraduate students in the Department of Physics and Astronomy are encouraged to participate in one-quarter research programs at other institutions and then review their work in the "Quest" meeting, held on campus every spring. Recently, Michael Schueller spent a quarter at the FermiLab Cyclotron (Fall 1993), William Goebel spent the Summer of 1995 at the

Pennsylvania State University, and Robert Kamara spent the summer of 1997 at the University of Chicago. All three students have presented talks at Quest.

This is only SCB's second year at YSU, however, one undergraduate is currently working under his supervision, designing and fabricating instrumentation for the NLO polymeric materials research laboratory (e.g. corona poler, heating stages, etc.). In the past, SCB has clearly demonstrated the ability to supervise undergraduates in research, overseeing three undergraduate research projects in NLO polymers, one of which resulted in a paper co-authored by the student.

e. Appendix 6e: Current Chemistry and Physics Curriculum Sheets

Please find attached a list of seven curriculum sheets for our major current Chemistry and Physics undergraduate programs.

- 1. BS in Chemistry
- 2. BA in Chemistry
- 3. BS in Combined Science in Chemistry and Biology
- 4. BS in Chemistry with a Biochemistry Option
- 5. BS in Physics
- 6. BA in Physics
- 7. BS in Physics and Astronomy

f. Appendix 6f: Other Faculty Users of this Equipment for their Teaching

Youngstown State University's Chemistry and Physics and Astronomy Departments have 16 and 7 faculty members, respectively, (all having PhD's in Chemistry, Biochemistry, Physics, or Astronomy) and five full time support staff positions. In addition, faculty from other campus departments and from neighboring institutions will use the requested equipment to teach their classes and for their undergraduate research projects. The currently identified faculty include:

Dr. Larry Curtin, Analytical Chemistry, YSU

Dr. Renee Falconer, Environmental Chemistry, YSU

Dr. John Jackson, Organic Chemistry, YSU

Dr. Sherri Lovelace, Inorganic Chemistry, YSU

Dr. Howard Mettee, Physical Chemistry, YSU

Dr. Jim Mike, Analytical Chemistry, YSU

Dr. Peter Norris, Organic Chemistry, YSU

Dr. Steve Schildcrout, Physical Chemistry, YSU

Dr. Mike Serra, Biochemistry, YSU

Dr. Jef Smiley, Biochemistry, YSU

Dr. Jim Andrews, Condensed Matter Physics, YSU

Dr. Greg Sturrus, Condensed Matter Physics, YSU

Dr. Ray Beiersdorfer, Geology, YSU

Dr. John Andrews, Physical Chemistry, Hiram College

g. Appendix 6g: Examples of Experiments

i. Chemistry 603: Quantitative Analysis

The students in this course currently do several pyrolysis experiments in which inorganic compounds are heated until decomposition and the difference in weight before and after heating is used to evaluate the analytes. For example, metal hydrate complexes are heated and from the weight loss the total number of water molecules in the initial complexes are calculated. With the addition of TGA, such experiments can be made much more valuable because the water loss is seen to occur in a step wise fashion as the temperature is raised. The students can therefore readily distinguish between water molecules in the metal salts inner coordination sphere (which may come off in several stages) and more weakly bound water in the outer hydration sphere. This exercise directly relates to the coordination chemistry taught in the first year General Chemistry course and in the first Inorganic course as well as to fundamental analytical problems such a matrix effects and the need to pre-dry analytes to remove physically adsorbed water.

ii. Chemistry 721: Organic Chemistry III

In this class the students currently prepare two polymers, polystyrene by free radical addition polymerization, and a network polymer by condensation. In each lab section that does the polystyrene synthesis, the students notice that some products are gummy liquids while others range up to hard brittle solids and we explain that this is due to differences in the molecular weight. By having the students' samples characterized by GPC, the students will be able to correlate these gross physical properties with the observed molecular weight and molecular weight distributions (i.e. they will determine structure/property correlations). This new equipment will also allow us to modify this experiment to the discovery oriented approach where each student in the class with prepare their polymer under different conditions (i.e. varying

reaction temperature, time, and solvent) and correlate this with the observed molecular weights to find the optimum reaction conditions. In addition, with this equipment we will also introduce new polymer experiments as options for their capstone organic experience. Hunter is currently working on two examples, one explores the mechanisms of free radical polymerizations and the other involved the synthesis of Nylon copolymers. Both projects require both the GPC and the DSC.

iii. Chemistry 739/740/741: Physical Chemistry I/II/III

The students in this course currently do an experiment on phase equilibria of the binary liquid-solid lead-tin system, which gives a single eutectic. Students measure cooling curves using a thermistor or thermocouple, which gives only semiquantitative results for the resulting phase diagram, including the eutectic point and enthalpies of fusion. Using the computerized DSC to enhance such an experiment would permit a wider variety of systems to be studied (including organics and inorganics), with much smaller sample sizes, less waste, and greater safety. Better quality data and results could be obtained. Heat capacities and second order phase transitions could be studied also.

iv. Chemistry 801/2: Biophysical Chemistry I/II

Size exclusion determination of proteins: By the use of gel permeation chromatography, students will assess the solvation radius of standard and unknown proteins. Different model systems will be based on proteins with shapes known to deviate from spheroidal and these determinations will be used to relate the concept of Stokes radius to the students.

Viscosity determination of bio-polymers: Viscosity analysis will be used in a complimentary experiment to determine molecular weights of proteins. Comparison of results

from chromatographic, sedimentation and viscosity experiments will serve as a combined unit in the treatment of transport properties of bio-polymers.

v. Chemistry 803: Chemical Instrumentation

Although thermal analysis, viscometry, and GPC/SEC are all covered in the lecture and are central to Analytical Chemistry, we do not currently do labs on them because of the lack of suitable instrumentation. If this grant is funded, we will introduce new experiments:

The thermogravimetric analysis of metal carbonates. The weight loss thermograms of carbonates such as $CaCO_3$ and $MgCO_3$ will be studied. The first is observed to decompose directly to the metal oxide at $\approx 700^\circ$ while the second proceeds through an intermediate oxide/carbonate at $\approx 120^\circ$ before forming the final oxide at $\approx 400^\circ$. Experience with thermal analysis experiments such as this one is one of the widely requested skills from our industrial advisors.

Viscometry analysis of polymer solutions. From viscometry data on commercial polymer samples, the students will determine their molecular weights by the Mark-Houwink-Sakurada relationship.

Size exclusion chromatography. The students will study the principles of chromatography by relating the theory of chromatographic separations to experimental SEC data. Calibration with commercial standards and the universal calibration procedure will also be introduced.

vi. Chemistry 825: Polymer Lab

In this discovery orient lab course the student carry out several technique oriented initial experiments and then study one polymer system in detail. New experimental components will be introduced to ensure all students know how to apply TGA and DSC methods, viscometry, and

GPC to the characterization of commercial polymer samples (a different one for each student) and to relate these results to materials properties (this will take four weeks including about 1/2 of their time spent on currently available techniques such as powder diffraction and TEM analysis). In the final six weeks, the students will carry out an in depth study of one polymer system, typically one that has not been previously reported. The provision of this equipment will allow them to characterize the thermal and molecular weight properties of the new polymers they synthesize.

vii. Chemistry 831: Inorganic Lab

"Monitoring the formation of 123 High T_c Superconductor Using TGA" An experiment currently performed in the inorganic lab course which could benefit from TGA equipment is one involving the synthesis of the 123 High T_c superconductor (i.e. YBa₂Cu₃O_{7-x}). The procedure is a multi-step process in which a stoichiometric pre-ceramic mixture of the metal hydroxides, carbonates or oxalates (obtained by homogeneous co-precipitation) are first calcined in air at 900 °C. The utilization of TGA at this point would allow students to monitor the loss of CO₂ and H₂O, and help them to better understand the transformation occurring during the solid-state synthesis.

"Preparation of BaTiO₃ and Characterization by DSC" This is a new experiment for our course, and it is designed to teach students about structure/property relationships in the inorganic solid state, while at the same time adding DSC analysis to the repertoire of experimental methods that they learn in course. The experiment involves the preparation of BaTiO₃, which is widely used in capacitors because of its high dielectric constant. The samples could be made through a variety of methods (e.g. sol-gel, hydrothermal, or ceramic), so that students could gain experience in a new synthesis technique as well. BaTiO₃ has the perovskite structure with a tetragonal distortion, but adopts a perfect cubic structure above 120 °C (i.e. the Curie temperature). Therefore students

would use the DSC to characterize their BaTiO₃ samples by determining the Curie temperature, and in the process would learn the significance of the Curie temperature as related to the ferroelectric properties of their samples.

The preparation and Characterization of Polysiloxanes. Polysiloxanes are fun and easy to prepare. The GPC and viscometry equipment will allow the students to determine the molecular weights of the materials they prepare and relate these to macroscopic properties.

viii. Chemistry 832: Solid State Structural Methods

The students will carry out DSC studies of crystalline and powdered materials and relate these to the multiple phases observed in single crystal and powder diffraction analyses of many of the materials they study.

ix. Chemistry 850: Undergraduate Research

The study of solid state, polymeric, and protein and DNA materials are amongst the most popular of our undergraduate research projects. The proposed equipment will be heavily used in these projects.

x. Chemistry 991/994: Structural Methods for High School Science Teachers

In the lab portions of these courses the students currently use NMR, FT-IR, UV-Visible, and X-ray crystallographic instrumentation and GC-MS will be introduced this year. With the provision of the thermal analysis and GPC equipment, the students will also get a chance to use these methods which we already discuss in lecture.

xi. Chemistry 100: Investigative Approaches to Chemistry

This is a proposed in course to meet the general science requirements of non-science and technology majors and will be fully introduced with our conversion to semesters in the year 2000. It is a discovery oriented course and one topic that has been proposed is for the students to study the synthesis, characterization, and recycling of polymers. It is expected that once this course is in operation these students will make significant use of the proposed instrumentation.

xii. Physics 710L: Thermodynamics Laboratory.

DSC and TGA instrumentation will be used to teach the principles of materials characterization measurements of amorphous materials including thermal decomposition temperature, glass transition temperature, enthalpy, etc., complementing lecture discussion of these topics. {4 students per year}

xiii. Physics 722L: Physical Optics Laboratory.

DSC and TGA instrumentation will allow the inclusion/modification of several experiments including: (1) measurement of NLO susceptibility vs. structure for NLO polymeric materials, (2) measurement of rate of decay of NLO susceptibility vs. glass transition temperature in NLO polymeric materials, and (3) fabrication of polymeric waveguide electro-optic modulator. {30 students per year}

xiv. Physics 805: Undergraduate Physics Research.

DSC and TGA instrumentation will be used in undergraduate research projects being carried out with faculty within the NLO polymeric materials research laboratory of the CPIP. Currently, DSC and TGA measurements must be done off-site. This is both inconvenient and time consuming for students, significantly impacting the pace of their research. {4 students per year}

h. Appendix 6h: Recent Texts on Polymer Characterization

Over the last several decades there have been a series of excellent texts on polymer/materials characterization, all of which give excellent ideas for materials characterization experiments. Some of the best include:²

- 1. A. C. Woodward and F. A. Bovey, Editors, "Polymer Characterization by ESR and NMR", ACS Symposium Series #142, 1980, American Chemical Society, Washington, D. C.
- 2. A. R. Cooper, Editor, "Determination of Molecular Weight", 1989, John Wiley & Sons, NY.
- 3. B. Chu, "Laser Light Scattering: Basic Principles and Practice", Second Edition, 1991, Academic Press, NY.
- 4. B. Wunderlich, "Thermal Analysis", 1990, Academic Press, NY.
- 5. D. Braun, "Simple Methods for Identification of Plastics", 1995, Hanser, NY.
- 6. D. Campbell and J. R. White, "Polymer Characterization: Physical Techniques", 1989, Chapman and Hall, NY.
- 7. E. D. Craver and T. Provder, Editors, "Polymer Characterization: Physical Property, Spectroscopic, and Chromatographic Methods", Advances in Chemistry Series, 1990, American Chemical Society, Washington, D. C.
- 8. E. Schroder, G. Muller, and K. F. Arndt, "Polymer Characterization", 1989, Hanser, NY.
- 9. E. Schroder, G. Muller, and K.-F. Arndt, "Polymer Characterization", 1989, Hanser Publishers, NY.

Note: all of these are available in Hunter's personal library and/or in the YSU campus library for both student and faculty use.

- 10. F. A. Bovey, "High Resolution NMR of Macromolecules", 1972, Academic Press, NY.
- 11. H. G. Barth and J. W. Mays, "Modern Methods of Polymer Characterization", 1991, John Wiley & Sons, NY.
- 12. H. Saechtling, "International Plastics Handbook: for the Technologist", 1995, Hanser, NY.
- 13. H. Ulrich, "Introduction to Industrial Polymers", 1993, Hanser, NY.
- 14. H. Ulrich, "Raw Materials for Industrial Polymers", 1988, Hanser, NY.
- 15. J. D. Randall, Editor, "NMR and Macromolecules: Sequence, Dynamics, and Domain Structure", ACS Symposium Series #247, 1984, American Chemical Society, Washington, D. C.
- J. L Koenig, "Spectroscopy of Polymers", 1992, American Chemical Society, Washington,
 DC.
- 17. K. S. Schmitz, "An Introduction to Dynamic Light Scattering by Macromolecules", 1990, Academic Press, NY.
- 18. K. Schmidt-Rohr and H. W. Spiess, "Multidimensional Solid-State NMR and Polymers", 1994, Academic Press, NY.
- 19. M. E. Brown, "Introduction to Thermal Analysis: Techniques and Applications", 1988, Chapman and Hall, NY.
- 20. T. R. Crompton, "Analysis of Polymers: An Introduction", 1989, Pergamon Press, NY.
- 21. W. W. Wendlandt, "Thermal Analysis", 1986, Wiley, NY.

i. Appendix 6i: Relevant Journal of Chemical Education Experiments

The *Journal of Chemical Education* is an excellent resource for new experiments. Below is a list of experiments that have been recently published there that are relevant to this proposal. If the requested equipment is funded, these experiments will be tested here at YSU and those that prove useful will be incorporated into our curricula.

JCE thermal analysis experiments that merit testing at YSU include:

- 1) Wynne, A. M., "The Thermal Decomposition of Urea," *Journal of Chemical Education*, 1987, 64, 180.
- 2) Temme, S. M., "Determination of Heats of Fusion," *Journal of Chemical Education*, 1995, 72, 916.
- 3) Crumpton, D. M.; Laitinten, R. A.; Smieja, J.; Cleary, D. A., "Thermal Analysis of Carbon Allotropes: An Experiment for Advanced Undergraduates," *Journal of Chemical Education*, 1996, 73, 590.
- 4) Williams, D. R., "The Modern Student Laboratory: Analysis of Ethylene-Vinyl Acetate Copolymers: A Combined TGA/FTIR Experiment," *Journal of Chemical Education*, **1994**, 71, A195.
- 5) Brown, M. E., Determination of purity by differential Scanning calorimetry (DSC)," *Journal of Chemical Education*, **1979**, *56*, 310.
- 6) Tanaka, H.: Koga, N., "The thermal decomposition of basic copper(II) sulfate: An undergraduate thermal analysis experiment," *Journal of Chemical Education*, **1990**, 67, 612.
- 7) Burrow, H. D.; Ellis, H. A.; Odilora, C. A., "The Dehydrochlorination of PVC: An Introductory Experiment in Gravimetric Analysis," *Journal of Chemical Education*, **1995**, 72, 448.

JCE viscometry experiments merit testing at YSU include:

- 1) Richards, J. L., "Viscosity and the shapes of macromolecules: A physical chemistry experiment using molecular-level models in the interpretation of macroscopic data obtained from simple measurements," *Journal of Chemical Education*, **1993**, 70, 685.
- 2) Rosenthal, L. C., "A polymer viscosity experiment with no right answer," *Journal of Chemical Education*, **1990**, 67, 78.
- 3) Mathias, L. J., "Evaluation of a viscosity-molecular weight relationship: an undergraduate-graduate polymer experiment," *Journal of Chemical Education*, **1983**, *60*, 422.
- 4) Perrin, J. E.; Martin, G. C., "The viscosity of polymeric fluids," *Journal of Chemical Education*, **1983**, 60, 516.

5) Belliveau, J. F.; O'Leary, Jr., G. P.; Hajian, H., "The biochemistry of the muscle contraction process: An undergraduate laboratory experiment using viscosity to follow the progress of a reaction," *Journal of Chemical Education*, **1981**, 58, 442

JCE GPC/SEC experiments merit testing at YSU include:

- 1) Hardgrove, G. L.; Tarr, D. A.; Miessler, G. L., "Polymers in the Physical Chemistry Laboratory," *Journal of Chemical Education*, 1993, 70, 685.
- 2) McLoughlin, D. J., "Size exclusion chromatography: Separating large molecules from small," *Journal of Chemical Education*, **1992**, *69*, 993.

j. Appendix 6j: Recent NSF DUE-ILI Grants

The National Science Foundation has recently funded a number of related grants for Polymer Chemistry Incorporation into the Curriculum and for Thermal Analysis, Viscometry, and GPC/SEC Equipment. If the requested equipment is funded, we will contact these institutions for information on new thermal analysis, viscometry, and GPC/SEC experiments that they have developed using their NSF funded equipment, but have not yet published. These will be tested at YSU and those that prove useful will be incorporated into our curricula. Five recent NSF funded projects that seem very relevant include:

- 1) "Thermal Analysis in the Undergraduate Curriculum," 9650084.
- 2) "Size Exclusion Chromatography and Thermal Analysis as Teaching Tools in Polymer.

 Biophysical, and Physical Chemistry," 9650197.
- 3) "Incorporating Polymer Chemistry Across the Curriculum," 9552098.
- 4) "Polymeric Characterization Via GPC and DSC in an Undergraduate Chemistry Curriculum," 9650218.
- 5) "Gel Permeation and Viscosity Equipment for Studies in Polymer Chemistry," 9251242.