COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 01-2

NSF 00-144

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)

CHE - CHE - Chemical Instrumentation (continued)

FOR NSF USE ONLY

NSF PROPOSAL NUMBER

0130968

DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION
				073131237	

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

341011998

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

IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES ☐ NO ☒ IF YES, LIST ACRONYMS(S)

NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE

Youngstown State University

AWARDEE ORGANIZATION CODE (IF KNOWN)

0031450000

ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE

Youngstown State University
One University Plaza
Youngstown, OH. 445550001

NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE

ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING 9 DIGIT ZIP CODE

PERFORMING ORGANIZATION CODE (IF KNOWN)

IS AWARDEE ORGANIZATION (Check All That Apply)
(See GPG II.C For Definitions) ☐ FOR-PROFIT ORGANIZATION ☐ SMALL BUSINESS ☐ MINORITY BUSINESS ☐ WOMAN-OWNED BUSINESS

TITLE OF PROPOSED PROJECT **RUI - Purchase of Glove Box and Vacuum Line Systems for Materials Synthesis & Characterization**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE
$ 131,779	36 months	01/01/02	

CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW

☐ BEGINNING INVESTIGATOR (GPG I.A)
☐ DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C)
☐ PROPRIETARY & PRIVILEGED INFORMATION (GPG I.B, II.C.6)
☐ NATIONAL ENVIRONMENTAL POLICY ACT (GPG II.C.9)
☐ HISTORIC PLACES (GPG II.C.9)
☐ SMALL GRANT FOR EXPLOR. RESEARCH (SGER) (GPG II.C.11)
☐ VERTEBRATE ANIMALS (GPG II.C.11) IACUC App. Date
☐ HUMAN SUBJECTS (GPG II.C.11)
Exemption Subsection or IRB App. Date
☐ INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED
☐ HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.E.1)

PI/PD DEPARTMENT
Department of Chemistry

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CO-PI/PD				

Electronic Signature

CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

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

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

Name (Typed)	Signature	Social Security No.*	Date
PI/PD **Allen D Hunter**	**Signature Not Required**		
Co-PI/PD **Larry S Curtin**	**Signature Not Required**		
Co-PI/PD **Sherri R Lovelace-Cameron**	**Signature Not Required**		
Co-PI/PD **Timothy R Wagner**	**Signature Not Required**		
Co-PI/PD			

SSN's are confidential and are not displayed *ON FASTLANE SUBMISSIONS*

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 01-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuring 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 Grant Policy Manual Section 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. Conflict which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Debarment Certification

(If answer "yes", please provide explanation.)

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

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, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, ''Disclosure Form to Report Lobbying,'' in accordance with its instructions.

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

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

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) **Peter Kasvinsky**	**Electronic Signature**	**Jul 9 2001 11:45AM**

TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS	FAX NUMBER
330-742-3091	**amgrad03@ysub.ysu.edu**	**330-742-1580**

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

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) - continued from page 1
(Indicate the most specific unit known, i.e. program, division, etc.)

CHE - CHE - Inorganic: Organometallic/Bioinorganic
DMR - SOLID-STATE CHEMISTRY
CHE - CHE - Analytical and Surface Chemistry: Electrochemistry and Surface Chem

SECTION A: PROJECT SUMMARY

This RUI-CRIF Department Multi-User Instrumentation proposal seeks funding for the purchase of research grade equipment for handling air sensitive inorganic and organometallic materials under an inert atmosphere. The three systems requested are a dedicated research grade glove box system optimized for synthetic studies, a dedicated research grade glove box system optimized for analytical studies, and a lab set of 10 vacuum lines. Each of the glove boxes will have a high capacity dry train, water and oxygen sensors, and the accessories required for carrying out the designated synthetic or analytical studies. As with the other research grade instrumentation at YSU, these items will be made available at no charge for undergraduate research and educational purposes to YSU's two dozen collaborating PUI partners. It is expected that at least two dozen undergraduate and masters students and high school science teachers will routinely use it in their materials research projects while our seniors and those in adjacent disciplines will use the vacuum lines as part of their inorganic chemistry and polymer science labs. Specific research projects from the YSU Inorganic/Organometallic Materials Group expected to benefit the most directly from routine access to this instrumentation include the study of: NS heterocyclic materials, organometallic crystal engineered materials, alkanethiol monolayers, monolayer organometallic films, metallocenophanes, organometallic nanoscale rigid-rod and star shaped materials (Organometallic NanoWires and Organometallic NanoStars), and solid state nitride/fluoride compounds.

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B	Table of Contents (NSF Form 1359)	1	
C	Project Description (plus Results from Prior NSF Support) (not to exceed 15 pages) **(Exceed only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)**	15	
D	References Cited	3	
E	Biographical Sketches (Not to exceed 2 pages each)	6	
F	Budget (NSF Form 1030, plus up to 3 pages of budget justification)	5	
G	Current and Pending Support (NSF Form 1239)	6	
H	Facilities, Equipment and Other Resources (NSF Form 1363)	4	
I	Special Information/Supplementary Documentation	10	
J	Appendix (List below.) **(Include only if allowed by a specific program announcement/ solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)**		
	Appendix Items:		

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

SECTION C: PROJECT DESCRIPTION

C1. RESULTS FROM PRIOR NSF SUPPORT

The project participants have had several recent NSF, state, foundation, and institutionally funded research and educational projects, including: "research" type grants aimed at funding *disciplinary research*, "instrumentation" type grants aimed at *enabling* undergraduate research and curricular revision, "educational materials" type grants aimed at the *production* of specific new curricular materials, and "course development/enrichment" grants for *specific audiences*. **The central goal of our program at YSU is to *use appropriate technology to facilitate student learning via both formal class and lab work and via research* and thus to provide *better educated and trained scientists, professionals in allied disciplines, teachers, and citizens*.**

C1a. Research Grants:

To date, most disciplinary research in the PI's, Co-PIs', and other senior personnel's research groups has been funded by a combination of internal funds and smaller external grants. The latter have included both American Chemical Society Petroleum Research Fund and Research Corporation Cottrell Research grants. These individuals are now moving to the next stage of their careers and are starting to apply for and receive major NSF RUI, NIH AREA, DOD, DOE, etc., research grants.

C1a(i) NSF CHEM-REU "REU - Research Experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities." This new NSF Research Experiences for Undergraduates grant ($180,000 NSF, 2001-2003, D. Mincey PI, S. Lovelace-Cameron, J. Jackson, A. Hunter, and T. Wagner Co-PIs) will fund the integration of 10 undergraduates from regional Predominantly Undergraduate Institutions, PUIs, into the YSU Chemistry Department's research program each summer. Approximately one third of these NSF funded undergraduate researchers along with a similar proportion of other undergraduates and high school students funded out of individual grants and by the department will use the proposed equipment each year.

C1a(ii) NSF INT 0086313: "Structural Investigations of Main Group Heterocyclic Rings and Cages." This *RUI - International Division - Cooperative Activities* grant ($13,200 NSF, $84,000 YSU and St. Andrews match) is partially funding the PI's 2000/2001 academic year sabbatical at St. Andrews University in Scotland (which concludes on June 27th, 2001) with professors Derek Woollins and Alex Slawin as hosts. Typical of most of the PI's work, it has both chemical education and chemical disciplinary research components with the educational component focused on writing a "hands on" text and supporting electronic materials for undergraduates on routine single crystal diffraction studies. The disciplinary component involves the synthesis and charge density diffraction and theoretical analysis of a series of nitrogen-sulfur heterocyclic rings and chains to explain observed differences in the aromaticity of the heterocyclic rings. The advanced diffraction work is in collaboration with Simon Coles and Michael Hursthouse of the UK EPSRC facility at Southampton and with Claude Lecomte and Niels Hansen at the University Henri Poincaré and with Christian Van Alsenoy's theoretical group at the University of Antwerp.

C1a(iii) NSF CHEM/DMR 0111511: "RUI - Organometallic NanoStars." This *RUI* grant from **A. D. Hunter**, PI, has been recommended for funding by the *NSF Divisions of Chemistry and Materials Research* ($350,000 NSF, 07/15/2001 - 07/14/2004). It involves the synthesis and chemical characterization of star shaped organometallic materials, NanoStars, $M\{[(\mu\text{-CN-Arene-NC})Mo(PR_3)_4]_n(\eta^1\text{-CN-Arene-X})\}_z^{x+}$ (where z = 3 to 7). Structure/property relationships will be developed to relate these properties to the molecular structures, particularly the numbers of arms, the arm length, the degree of conjugation down the backbones of the arms, and the metal vertex. The potential of these materials for applications related to their backbone conjugation and molecular affinities will be evaluated. In particular, their use as electroactive surface modifiers will be emphasized as will the differences between their properties and those of dendrimers. [Note: This grant

is the lead external funding in a major international collaboration on nanoscale organometallic materials which also involves Curtin and Lovelace-Cameron of YSU Organometallic Materials Group and leading materials research groups in Europe and Australia (i.e., see Section G).]

C1b. Instrumentation Infrastructure Grants:

The PI on the current proposal is the Director of the Youngstown State University Structure & Chemical Instrumentation Center, YSU-S&CIC, which serves the advanced chemical and materials characterizations instrumentation needs of YSU students and faculty and those of our collaborators at over two dozen PUIs. The PI is also one of the principles of the related Center for Biomedical and Environmental Research, CBER, center which serves our biological materials characterization needs. He has written and served as PI on most of the external grant proposals used to fund these centers and was Co-PI on most all of the rest. It is in this role of Director of the YSU-S&CIC that he is the author and PI on the current grant proposal. It is noteworthy that every YSU chemistry instrumentation grant funded over the last 8 years has had at least one, and often several, of the PI and Co-PIs on the current CRIF proposal as its PI or Co-PI.

C1b(i) NSF-DUE-ILI #9851107**: **"Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment." These funds ($44,600 NSF, $50,000 YSU match, 1998-2001, **A. Hunter** PI and S. Brower, T. Kim, D. Mincey, and **T. Wagner** Co-PIs) have been used to purchase: (a) a TA Instruments 2910 DSC and a 2050 TGA, (b) a Cannon CT-518 constant temperature bath, (c) a GBC Instruments/Polymer Labs GPC-SEC-HPLC system (i.e., autosampler, column oven, and RI and diode array UV-Vis detectors), (d) a Jasco 410 FT-IR (0.9 cm^{-1} resolution), and (e) a used (and very basic) Vacuum Atmospheres HE-43-2 inert atmosphere glove box described in more detail elsewhere in this proposal.[1]

C1b(ii) NSF-DUE-ILI #9551683**: **"Integration of GC-MS into the Undergraduate Curriculum." This grant ($34,450 NSF, $50,000 YSU match, 1995-96, J. Jackson PI and **A. Hunter**, S. Schildcrout, R. Falconer, and **T. Wagner** Co-PIs) was used to purchase a Finnigan GCQ Gas Chromatograph - Ion Trap Mass Spectrometer which has subsequently (Dec. 1999) been upgraded with a new system controller, data system, and software. This instrument is now fully integrated into student research, senior level Organic, Physical, and Inorganic Lab courses (i.e., 50 students a year), and into the Sophomore Organic sequence (i.e., ≈ 200 students a quarter).[2,3] Based in large part on our success with this instrument, we have subsequently received an Ohio Board of Regents, OBoR, grant of $88,900 towards our LC-MS system (again Hunter was a Co-PI on this OBoR proposal).

C1b(iii) NSF DUE-CCLI-A&I 0087210: "WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions" *(and Ohio Board of Reagents)* This grant ($200,000 NSF, $75,000 OBoR, $125,182 YSU match, 01/15/2001-01/14/2004, **A. Hunter**, PI, L. M. Hoistad, A. J. Jircitano, **T. R. Wagner**, and E. P. Zovinka, Co-PI's) is funding a new Bruker APEX CCD single crystal diffractometer, low temperature system, and other accessories. This instrument will form the core of the **YSU-PUI Undergraduate Diffraction Consortium** and will be housed in a newly remodeled, 1,200 square foot diffraction facility at YSU. The diffraction facility will be equipped so that anyone in the world with WEB access will be able to watch lab and instrument operations via fixed and pan/tilt/zoom WEB cameras. If they have a WEB camera on their own computer, they will also be able to video-conference with the operators or faculty and students in this lab. A new stereo polarizing microscope to be placed in this lab will be equipped with a color WEB camera, so that students at remote sites will be able to view the crystal selection and mounting operations. The grant also provides funds to upgrade the two current P4 diffractometers with new computer hardware and software so that they can be remotely controlled over the WEB as will be the CCD system. YSU is the Hub of a consortium of 27 other Predominantly Undergraduate Institutions, PUIs, (see Section I2) desiring to integrate diffraction methods into their undergraduate teaching and research programs. The installation date is July 2nd, 2001.

C1c: Educational Materials Grants:

C1c(i) NSF-DUE-CCLI-EMD-POC #9980921: "X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding." This grant ($74,707 NSF, $75,000 match, 05/01/2000 - 04/30/2002, **A. Hunter** PI) is funding the development of new documentation (texts and WEB documents), software, and other teaching materials to enhance the integration of single crystal diffraction methods into the undergraduate curriculum. Hunter's major coworkers on this project are a group of six high school science teachers, especially S. DiMuzio.[4-6] This grant is closely related to two of those discussed above (i.e., NSF RUI-INT 0086313 and NSF DUE-CCLI-A&I 0087210) and demonstrate the synergy that advanced instrumentation brings to our teaching and research programs.

C1d: Specific Course Grants:

C1d(i) NSF-DUE-CCLI-A&I #9981040: "Integration of Computer Technology into the General Chemistry Curriculum." This grant ($94,945 NSF, $104,000 match, **T. Wagner** PI and J. Mike co-PI) had a July 1st, 2000 starting date. Thirty LabWorks II workstations were purchased to introduce computer data acquisition capability into the freshman chemistry laboratory. The workstations were used for the first time during the Fall, 2000 semester in the General Chemistry I Laboratory course and were integrated into the General Chemistry II Laboratory course during the Spring semester. These lab courses have been almost completely revised to incorporate the new technology. The second semester course will culminate in discovery-based, independent projects where students used the workstations for data collection, storage, analysis, and tabulation/reporting of data. Students use the workstations to collect and analyze temperature, pH, conductivity, colorimetric, and titration data. Following each semester, students filled out customized questionnaire forms on-line at the NSF-supported site: *Student Assessment of Learning Gains*, centered at the University of Wisconsin–Madison. The assessment results indicated an overall positive impact of the equipment in their laboratory experiences.

C1d(ii) NSF DUE #9850079: "Investigative Approaches in the Natural Sciences." This *DUE* grant ($183,579 NSF, $200,000 YSU match, 1998-2001, J. Usis PI, **A. Hunter** and C. Singler co-PIs, **S. Lovelace-Cameron** Senior Personnel) is supporting the development of a new multidisciplinary lab course, Arts & Sciences 2600, having collaborative research-like projects. It is designed to teach students what science is by having them do actual science. It is a required as part of the new General Education program for all non-science/technology majors at YSU. Its approach to teaching lab science to students in the humanities is now being discussed as a model course for other Ohio Universities.[7]

C1d(iii) Department of Education Title II Grant: "Tri-County Partnership for Excellence in Teacher Education." This Department of Education grant (**S. Lovelace-Cameron** Senior Personnel) for ≈$2,500,000 over 5 years to the YSU Colleges of Arts & Sciences and Education is designed to assist YSU faculty in their continuing efforts to improve Science and Mathematics education in our regional area, primarily via teacher training in content areas and outreach to individual schools.

C1e. Research and Educational Outcomes of These and Related Grants:

These grants have helped YSU to build an excellent instrumentation facility dedicated to undergraduate teaching and research.[8] At YSU and at other Predominantly Undergraduate Institutions, PUI's, these and similar educationally related projects have been assessed[9,10] and shown to have positive student outcomes. Indeed, such changes to undergraduate instruction have been widely recommended at the national level.[11-14] They have also strongly influenced a change towards a more scholarly atmosphere on our campus.[15] Indeed, they have been a keystone in YSU's institutional transformation. For example, YSU has increased its external funding by 50-100% over each of the last 8 years to in excess of $3,000,000 annually and has increased its external publication rate and national reputation at a rapid rate as well. Indeed, applying for and receiving educationally related and instrumentation infrastructure grants is a key step for PUIs to make the transition from internally focused institutions to those who have joined the national research enterprise and have substantial externally funded scholarly agendas (see the RUI Impact Statement more details on the YSU

Chemistry plan in this area).[16] In **Teaching**, they have enabled the conversion of many lab courses away from the skills oriented/verification model to discovery research like experiences. The revised labs were designed based on current knowledge of how students learn and are consistent with recent recommendations for changes in how science is taught.[11-14] We Chemists also work closely with our colleagues in the Biology, Geology, Physics and Astronomy, and Chemical Engineering Departments, in programs such as Environmental Studies and Science Teacher education, and with other groups interested in teaching/learning on campus (e.g., the Arts & Science Master Teachers, the Project Kaleidoscope F21 Fellows, and the Carnegie Teaching Circles at YSU). As an extension of this effort, we have just instituted new research based masters in chemistry and masters in biology programs optimized for in-service science teachers (i.e., all required classes are available during evenings and/or summers and research takes place over ≈4 sequential summers). In **Disciplinary Research** terms, these education changes have substantially boosted the attitudes of our students towards our program and chemistry and both the number (by 5 fold so far) and quality of preparation of students participating in research. The equipment oriented grants have enabled our students to begin carrying out competitive research by providing the necessary instrumentation infrastructure.[8] The internal and external research grants have funded the student salaries, faculty summer salaries, and consumables and small equipment needed to carry out such research. ***In summary, these grant have been effectively used by YSU faculty to transform our learning environment in chemistry, to raise our national profiles, and to follow a sharply upwards trending research trajectory. See the RUI Impact Statement, Section I1, for more details.***

C2. Research Programs of Major Users

C2a. Project Overview:

C2a(i). Project Goals:

The central goal of this RUI-CRIF project is to provide access to equipment for handling air sensitive materials for the enrichment of materials related research at YSU and for the advanced inorganic chemistry and polymer science labs (for which the PI and Co-PIs are the instructors). Several representative examples of research projects to benefit from these instruments are described below. The more general research/teaching utilities of each of these instrumentation systems are described in Section C3.

C2a(ii). The YSU-PUI Diffraction Consortium:

YSU, an open enrollment publicly supported MS level institution, hosts this consortium whose other members are a very diverse group of over two dozen PUIs (i.e., see Section I2), including: highly selective through open enrollment institutions; public and private institutions; historically black universities; two year community colleges, liberal arts institutions, and MS level institutions; and institutions that have strong scholarly traditions as well as those just establishing a commitment to the scholarship of teaching and research. ***Representatives from these institutions will regularly visit YSU for faculty training programs and to carry out advanced characterization studies on our current and ordered X-ray diffraction, X-ray fluorescence, and LC-MS facilities at which point many will use the proposed glove box systems for sample preparation and/or crystal growth.***

C2b. The YSU Materials Research Group:

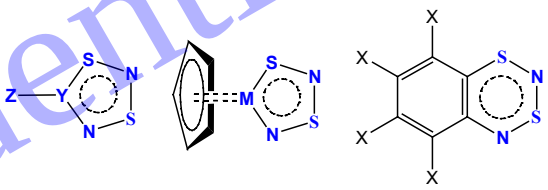
All of the groups listed below will use the requested research grade glove box systems and vacuum lines on a daily basis. The YSU Materials Group (i.e., Hunter, Lovelace-Cameron, Curtin, and Wagner) will account for ≈90% of the expected research use of these glove box and vacuum line systems. The three organometallic chemists each have individual research projects (i.e., see Section C2b(i) to C2b(iii), below) and there is considerable synergy between them, each having aspects of fundamental organometallic and electrochemistry and applications to materials chemistry/science, including: electronic/photonic materials and electrode/sensor materials. Due to this synergy, and the close cooperation that has been forged in our department, they have also developed joint research

interests in nanoscale organometallic materials, namely: Organometallic NanoWires and Organometallic NanoStars (i.e., see Section C2b(iv), below). Until recently, this collaborative Organometallic Materials project was largely funded internally (see the RUI Impact Statement, Section I1, for the rationale for this conscious choice), but it has recently been recommended for $350,000 in NSF and $30,000 of ACS-PRF funding on the NanoStars and a series of other proposals to NSF and other agencies are pending (i.e., see Section G). All of these projects which would use the proposed inert atmosphere systems, typically on a daily basis. Wagner's research on air sensitive nitride-fluoride solid state materials is described in section C2b(v), is currently funded by Research Corporation, and would also make heavy use of the glove box systems.

C2b(i). Hunter's Individual Research Program:

Overview: Hunter's current research activities include a new interest in main group heterocyclic ring compounds having SNSN linkages, a long standing interest in organometallic model complexes, oligomers, and polymers having conjugation down their backbones, and an NSF funded program of Chemical Education Research (i.e., see Section G). His organometallic polymer interests include materials having arylene and fluoroarylene bridges (see below), (η^6-Arene)$Cr(CO)_3$ groups, and *trans*-$Mo(PR_3)_4(Isonitrile)_2$ centers. These new materials are characterized by a combination of analytical, physical, spectroscopic, electrochemical, and structural methods most of which would be facilitated or enabled by routine access to the proposed equipment: (1) the synthetic glove box for the synthesis, purification, and some characterization studies on his compounds, all of which are at least somewhat air sensitive and some of which are extremely air sensitive, (2) the analytical glove box for electrochemical and conductivity studies which form much of the scientific core of his materials work, and (3) the vacuum lines for his Polymer Science courses and for the December/January intersession and summer "overflow" students from his core lab.

Organic and Organometallic Complexes Having -SNSN- Rings: The heterocycle project was initiated during Hunter's current sabbatical at St. Andrews University in Scotland, and has received NSF-INT support. A series of organic and organometallic heterocyclic species having 5 and 6 membered SNSN rings have been prepared and characterized (e.g., 1,2-C_6X_4(SNSN), Y-X(SNSN), Z=X(SNSN), and L_nM(SNSN)). The bonding in these materials has been analyzed by high level molecular orbital calculations for the gas and solid phases. These results have been compared to those from spectroscopic measurement and conventional and high resolution (charge density) diffraction studies. Elucidating the factors influencing the bonding in the heterocyclic rings, especially the degree of their localization/delocalization as a function of the organic or organometallic fragment structures, is the core of this project. These compounds have delocalized π-systems and related systems exhibit interesting electrochemical behaviors.

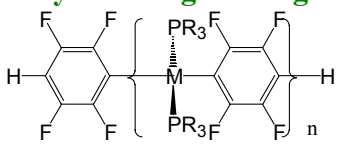


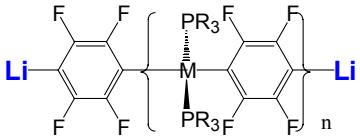
These NSNS heterocyclic materials will be characterized by cyclic voltammetry (high scan rates and microelectrodes will be required for many systems) to give redox potentials and/or decomposition/reaction kinetics that can be correlated with their structures, reactivities, and calculated molecular orbital energies. This will be done in the analytical glove box using the dedicated electrochemical system funded by NSF 0111511. The synthetic glove box will be used to grow crystals and store some of these products and to carry out their solid state - solute intercalation/redox reactions (i.e., where the insoluble heterocycles are reacted with soluble redox reagents). Solid-solid redox reactions (typically involving volatile redox agents such as I_2 or Cp_2Co) will be carried out in the analytical or solvent free boxes as will 4 probe conductivity studies on the neutral and redox products. The PI's continued participation in this project (which was funded by NSF 0086313) will require access to a research grade glove box for these studies.

This broad range of electrochemical, conductivity, crystal growth, and solid/solute or solid redox reactions are typical of the studies Hunter's students will carry out with each of his classes of

organometallic materials described in C2b(i).

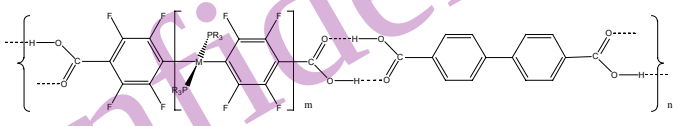
Arylene Bridged Organometallic Materials and Organometallic Crystal Engineering: Hunter's work to date has shown that arylene-bridged oligomers and polymers of μ-1,4-C_6F_4 and μ-4,4'-$(C_6F_4)_2$ and Ni, Pd, and Pt (e.g., Br-[-*trans*-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-$M(PR_3)_2$-Br and Z-(μ-fluoroarylene)-[-*trans*-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-Z, where n = 0 to 5 and Z = Li, Br, and H) can be prepared in good yields, that their steric and electronic properties can be varied independently of one another, and that the relative distances and angles between the arene substituents could be rationally designed.





While these final arylene bridged rigid-rod products are quite air stable, they are prepared from very air sensitive intermediates. Thus, if they are not kept strictly away the smallest traces of oxygen and moisture then pure samples of the higher oligomers and high molecular weight polymers are not obtained, complex mixtures of oligomers and lower molecular polymers being obtained instead. The absence of a modern research grade glove box has essentially prevented the synthesis of these higher molecular weight materials at YSU (i.e., by the PI's predominantly undergraduate research team). His experience shows that these high oligomer and polymer syntheses can be done on a good vacuum line by an experienced chemist but that BS students do not reach the requisite level of proficiency unless they work on the project for several terms and even many MS students only do so only near the end of their projects. However, his work at the University of Alberta showed that when carried out in a high quality glove box these reactions can be readily done even by BS students. For his research on both high molecular weight crystal engineering building blocks and the chemistry of the "pure" arylene bridged materials to proceed in YSU's PUI environment will require in house access to at least one well equipped research grade glove box. The synthetic reactions employing these air sensitive reactions are typically done at -120 to 0°C and experience shows that temperature control of these reactions is critical to obtaining the desired oligomers in adequate purity. The cold well requested for the synthetic glove box will be primarily used in these low temperature reactions.

Work in Hunter's labs on these organometallic systems and in other research labs on the analogous organic fluoroarylenes, indicates that these metal-halide and/or fluoroarylene-H, fluoroarylene-Br, and/or fluoroarylene-Li end groups should be readily convertible into a full range of oxygen and nitrogen based organic functional groups (e.g. $C(O)OH$, $C(CH_3)_2OH$, $C(CF_3)_2OH$, OH, NH_2, NR_2, C_5F_4N, and C_5H_4N) that are capable of a range of hydrogen bonding interactions as either H-bond donors and/or acceptors. In addition, the aromatic fluorine substituents and the metal centers may be able to act as H-bond acceptors in their own rights while the aromatic rings on the phosphines and fluoroarylene bridges will be involved in aromatic stacking interactions. The use of hydrogen bonds between rigid organic building blocks having aromatic cores is one of the most widely used ways to generate self assembled materials with relatively predictable and tunable geometries. In the proposed project, these will be used to prepare **zero-, one-, two-, and three-dimensional materials** for use as organometallic crystal engineering lattice rods. The new organometallic building blocks will have a range of steric and electronic properties at the metal centers and distances and angles between the hydrogen bonding substituents. The specific building blocks to be targeted include:



- X-(μ-fluoroarylene)-[-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-X,
- X-(μ-arylene)-[-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-$M(PR_3)_2$-(μ-arylene)-X,
- (NC_5F_4)-[-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-$M(PR_3)_2$-(C_5F_4N),
- (NC_5H_4)-[-$M(PR_3)_2$-(μ-fluoroarylene)-]$_n$-$M(PR_3)_2$-(C_5H_4N), and

- where fluoroarylene = C_6F_4, C_6F_3, and $(C_6F_4)_2$, arylene = C_6H_4 and $(C_6H_4)_2$, , M = Ni, Pd, and Pt, the metal geometries are *trans*, n = 0 to 5, C_5F_4N = tetrafluoropyridyl and C_5H_4N = pyridyl, X = C(O)OH, $C(CH_3)_2OH$, $C(CF_3)_2OH$, OH, NH_2, NR_2, C_5F_4N, and C_5H_4N

Crystallization of these building blocks with one another and co-crystallization with complementary organic building blocks, both in the presence of suitable guests, will result in the self assembly of new hydrogen bonded materials. They will be characterized by chemical, analytical, spectroscopic, electrochemical, thermal, and X-ray crystallographic means (***the electrochemical analyses will be done and many of the single crystal samples will be grown in the glove boxes***). These results will be correlated with the monomer and oligomer properties in solution and the solid state and with the framework structure and guest identity to derive new structure/property relationships. By varying the solubility characteristics of the organometallic building blocks along with their steric and electronic features, we expect to be able to prepare a wide range of self assembled materials having tunable properties including guest selectivities.

Electrochemical methods will be used both to determine the redox behaviors of the building blocks and also to detect the presence of guest molecules in the new crystal engineered host/guest lattices. Some of these analytical tests will be done in the analytical glove box while the synthesis of the lattices, which typically involves protic solvents, will be done in one of the current HE-43 systems which will be dedicated to such protic solvent studies over the summers.

Hunter and Wagner are in charge of YSU's diffraction facilities, and they and their group crystallographically characterize samples both that they make for themselves and, on a collaborative basis, are supplied to them by their YSU colleagues and from other US Predominantly Undergraduate Institutions. The growth, selection, and mounting of air sensitive samples from all of these sources will be facilitated by the improved glove box facilities.

C2b(ii). Curtin's Individual Research Program:

Overview: Dr. Curtin and his group have a variety of research interests including synthetic inorganic chemistry, self-assembled monolayers, conducting polymers and charge transfer salts, buckminsterfullerene, and electrochemistry. Each student who works with Dr. Curtin receives extensive training in synthetic methodology, spectroscopy, and cyclic voltammetry.

As above, many of the intermediates involved in Curtin's work are very air sensitive and students, particularly undergraduates, make much more progress in their synthetic projects when these key steps can be carried out in a glove box. A central core of Curtin's work is the electrochemical characterization of surface bound and soluble organometallic species. Having access to a glove box largely dedicated to electrochemistry and related analytical techniques will speed up the electrochemical studies. Carrying out these studies in the box will also reduce cost and high breakage rate of high performance electrochemical cells for air sensitive organometallics on the bench. A dedicated analytical box will also prevent contamination from the volatile solvents and other organics which is inevitable in a glove box being used regularly for synthesis.

Of the YSU faculty, Curtin has the greatest involvement with the electrochemistry of adsorbed and surface bound species, and other films. Because of their very low volume concentrations, these thin film species are particularly prone to damage/alteration by traces of oxygen, water, and adventitious solvents and volatile reagents. This is one of the key reasons why we would prefer to have a dedicated analytical glove box as any glove box used for synthesis is likely to have too "dirty" of an atmosphere for these purposes.

Alkanethiol Monolayers: One project involves the synthesis and electrochemical characterization of self-assembled alkanethiol monolayers containing ferrocene dimers which are separated via alkane chains of varying lengths. The study is designed to provide fundamental insight into electron and charge transfer rates in alkanethiol monolayers containing multiple redox centers. In order to produce useable devices based on monolayer chemistry, it is imperative to determine what factors affect the stability and electron transfer kinetics in these unusual systems. Ferrocene-containing dimers are

outstanding candidates for this purpose because of their extremely rapid and reversible electron transfer properties.

C_{60} Containing Polymers: Another project involves the spectroelectrochemical characterization of conducting polymers in which C_{60} has been covalently attached to the polymeric backbone. Upon the successful synthesis of C_{60} substituted tetraazaannulene or pyrrole monomers, cyclic voltammetry will be used to produce the conducting polymeric films. Spectroelectrochemistry will be used to study the extent of interaction between the C_{60} and the polymer when the polymer is in the conducting state (oxidized form) *and* the insulating state (reduced form). It is hoped that by incorporating C_{60} into a polymer matrix that new materials can be produced which have novel electronic and catalytic properties.

Monolayer Organometallic Films: The last project combines the advantages of self-assembled monolayer chemistry with those of conducting polymeric films. We have recently demonstrated that cobalt phthalocyanine and cobalt octafluorophthalocyanine can be axially ligated to self-assembled monolayers which terminate in a pyridine group. Multiple layers of metallocyanines can be constructed via repetitive exposure to solutions of pyrazine and phthalocyanine. Cobalt tetraazaannulene will be bound to the surface of a gold electrode via ligation to a pyridyl group which is exposed at the monolayer/solution interface. The bound monomer will then be polymerized via cyclic voltammetry. The overall goal of this research is to produce conducting polymeric films of a single molecular thickness. Such films should have enhanced performance in catalysis and molecular electronic devices because diffusion of counter-ions into/out of the film upon oxidation and reduction is eliminated.

Curtin will also be a primary user of the analytical glove box for the conductivity and other analysis of his organometallic thin films. As with their organic analogues such as polyacetylene, these materials are notoriously prone to oxidative and hydrolytic modification in their properties, even at low oxygen and moisture levels, (as well as to reactions/modifications by adventitious solvent or organic molecules). This is especially true in the partially oxidized and reduced states. All redox/analytical thin film studies will be done in the analytical glove box (i.e., to avoid these confounding effects of compounds that will inevitably be present at potentially damaging levels in a glove box that is also being used for synthesis) or in the rebuilt solvent free glove box (i.e., when the lowest possible volatile levels are needed), as appropriate.

C2b(iii). Lovelace-Cameron's Individual Research Program:

Overview: The aim of Dr. Lovelace-Cameron's projects are to answer fundamental questions about the electrochemical and chemical oxidation and reduction reactions of Cr, Mo, W, and Mn π-coordinated organometallic compounds. Various analytical instrumentation and glove box and vacuum line facilities are used in her investigations. Her overall research goals are to study the effects of electron transfer reactions on the reactivity and bonding modes of π-coordinated ligands and to study the synthesis of organometallic monomers which can serve as precursors for organometallic polymers.

Lovelace-Cameron's research products are often the most air sensitive of those produced by the organometallic group, many of the most scientifically interesting of these complexes are very challenging for any but the most skilled undergraduates to routinely handle on a vacuum line. The availability of a synthetic glove box will allow her to integrate undergraduates into the synthesis of these on a routine basis. As with the other synthetic chemists, the availability of a research grade system will speed many of the routine aspects of her synthetic and characterization studies of air sensitive organometallics and with therefore increase her students' research productivity. In addition, Lovelace-Cameron directs our ACS-SEED and related projects aimed at under-represented minority high school students. Each summer, she typically has two of these 11th or 12th grade students working in her group for 6 weeks (and the other faculty participants are likely to have several more). If this equipment is funded, these students high school students will do almost

all of their synthetic or electrochemical work in the glove box since such short project make it difficult for them both to learn vacuum line techniques and complete a significant research project.

Metallocenophanes: One class of compounds which the Lovelace-Cameron group is studying is the metallocenophanes. To relieve ring strain metallocenophanes may undergo ring opening polymerization. Appropriate metallocenophanes may lead to polymeric products with intriguing electrical, magnetic or mechanical properties. In addition, these materials may promote catalytic function in the stereoselective polymerization of olefins.

Organometallic Electrochemistry: The Lovelace-Cameron group utilizes electrochemistry and spectroelectrochemistry to probe the following questions about organometallic compounds: What insight does the electrochemistry data provide to explain chemical redox reactions? Is there electrochemical evidence of communication between metal centers in multi-metal centered complexes? How does temperature effect the electrochemistry? How do solvents effect electrochemical behavior? How many electrons are transferred and is the transfer reversible?

Lovelace-Cameron and her group generally carry out the most sophisticated solution phase electrochemical studies at YSU. She has obtained a used ESR which will be installed later this summer at which point she will also lead the ESR characterization efforts. The provision of a dedicated analytical glove box will greatly facilitate these electrochemical studies as well as the preparation of samples of her oxidized, native, and reduced products by bulk electrolysis and chemical redox reactions. Again, the most experienced PhD and postdoctoral fellows can handle many of these very/extremely air sensitive redox products on a vacuum line but this is generally beyond the capability of the novices that dominate the research teams at a PUI such as YSU.

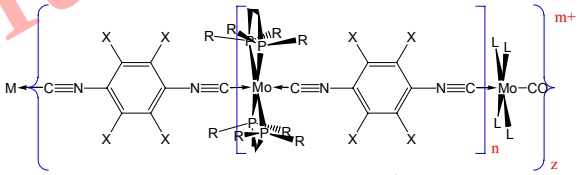
C2b(iv). Collaborative Research Program on Organometallic NanoWires and NanoStars, A. Hunter, S. Lovelace-Cameron, & L. Curtin:

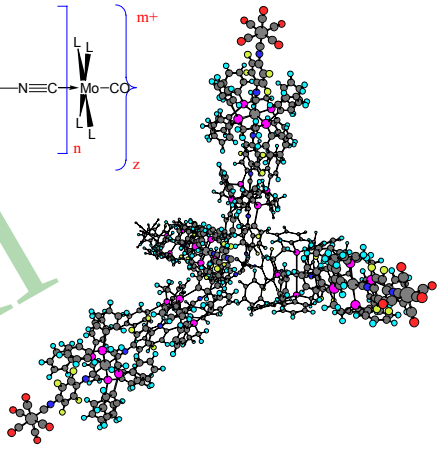
Overview of Collaborative Organometallic NanoWires and NanoStars Project: These species were designed to have rigid and thermally and chemically stable organometallic repeating units such as [*trans*-Mo($Ph_2PCH_2CH_2PPh_2$)$_2$(μ-CN-1,4-C_6H_4-NC)]. Two particularly valuable features of such isonitrile bridged species is that there is substantial conjugation down the oligomer backbones and that having phosphine ancillary ligands means that their steric and electronic properties can be varied largely independently of one another. In addition, the relative distances and angles between the arene substituents can be precisely controlled. In his project, there is an emphasis on the synthesis and characterization of linear and star shaped nanoscale materials having such organometallic arms and their potential utilities for materials science applications will be evaluated.

The availability of dedicated glove boxes is particularly valuable for the most demanding experiments to be done by the team members and their groups as is described above and below for such projects. However, most of the more "routine" synthesis and characterization studies can be done "on the bench" using vacuum line techniques. Indeed, for less air sensitive materials these are often more conveniently and quickly done using such Schlenk techniques. As the YSU materials groups have grown by recruiting increasing numbers of undergraduates and MS students, minority high school students, and high school science teachers (Hunter and Lovelace-Cameron play the lead roles in these areas) to their research, our per capita access to vacuum lines has decreased dramatically from almost one to one six years ago to as many as three or four students sharing a vacuum line now. Further, the current vacuum lines were bought out of the teaching budget and research access to them is very problematic when the inorganic and polymer labs are running since these must be given priority. To meet this expanded demand for vacuum lines in both teaching and research, we request funds to outfit the Advanced Synthesis Laboratory with 10 vacuum line (i.e., one for each 3 fume hood, two student work station). These will supplement the three currently in this lab which will be moved to the high capacity fume hoods at the lab corners for dedicated reactions using atypically smelly and/or toxic reagent). They will outfit a well equipped common lab for air sensitive chemistry during the research bulges at the December/January intersession and the

summer and will allow an increased emphasis on modern air sensitive techniques during the inorganic chemistry and polymer science lab courses.

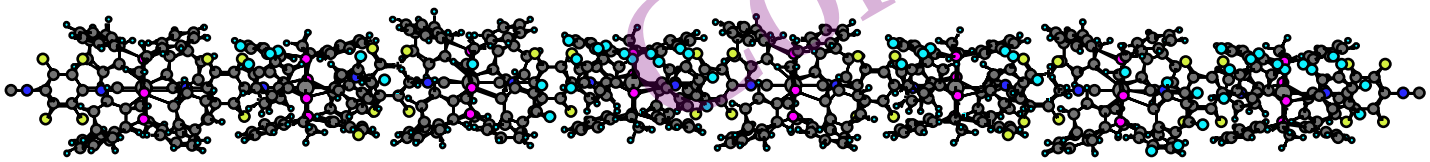
Organometallic NanoStars: The first step in this designed materials project will be the synthesis and characterization of a series of new rigid rod organometallic building blocks having [*trans*-$Mo(PR_3)_4(\mu\text{-CN-Arene-NC})]_n$ repeating units based on our successful pilot studies of the Mo and Fe systems. The monomers and oligomers will be prepared by condensation reactions between uncomplexed bifunctional isonitriles, and/or $Mo(PR_3)_4(N_2)$, and/or shorter monomers and oligomers. After they have reached the desired length, they will be capped on one end with the other end having an uncomplexed isonitrile group. By varying the side chains on the phosphine ancillary ligands and, to a lesser extent, the side chains on the aromatic rings in the isonitriles, the electronic, steric, and solubility properties of these building blocks should be readily tuned. Similarly, varying the number of aromatic rings in the isonitriles and the number of repeating units in the oligomer, the lengths of the building blocks should be readily tuned. This will give monofunctional rigid rod building blocks up to several tens of nanometers in length and having tunable solvent compatibilities. The capped organometallic building blocks will then be reacted with a range of substitutionly labile metal centers known to form homoleptic isonitrile complexes. This will produce novel star shaped organometallic materials having between three and seven rigid arms, Organometallic NanoStars, $M\{[(\mu\text{-CN-Arene-NC})Mo(PR_3)_4]_n(\eta^1\text{-CN-Arene-X})\}_z^{x+}$ (where z = 3 to 7). Each of these new materials will be characterized by analytical, spectroscopic, electrochemical, thermal, and X-ray crystallographic means at YSU and by surface methods at regional PhD institutions. Structure/property relationships will be developed to relate these properties to the molecular structures, particularly the numbers of arms, the arm length, the degree of conjugation down the backbones of the arms, and the metal vertex. The potential of these materials for applications related to their backbone conjugation and molecular affinities will be evaluated. In particular, their use as electroactive surface modifiers will be emphasized as will the differences between their properties and those of dendrimers.



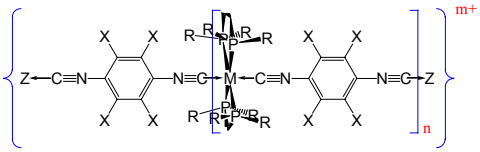


The final isonitrile bridged organometallic materials are quite air stable but some of the reagents used in their preparation, especially the dinitrogen and related starting materials, are very air sensitive. The synthesis of the NanoStars, like that of the NanoWires, will be done on vacuum lines for the less strongly electron rich phosphine ancillary and isonitrile bridging groups. For the more electron rich phosphines and isonitriles, the intermediates and even some of the products are very air sensitive and will therefore be prepared in the synthetic glove box. Single crystal growth will often take place in the freezers in the glove boxes. The strongest arguments for the glove box access for this project is for the electrochemical and conductivity studies which will be carried out in the analytical and solvent free boxes. The synthesis of the partially oxidized and reduced NanoStar and NanoWire species, many of which may have well over a dozen accessible redox states, will typically take place in the synthetic glove box.

Organometallic NanoWires: This collaborative materials research proposal also builds upon the PI's previous work on covalently bonded organometallic oligomers and main chain polymers



containing fluoroarylene and isonitrile bridges between adjacent metal phosphine centers, upon the Co-PI's work in organometallic electrochemistry, and upon their ongoing collaborations with a team of leading European and Australian scientists. The synthesis and characterization of a series of new symmetric and asymmetric model complexes, oligomers, and polymers having bridging isonitrile ligands and delocalized π-systems is proposed with a primary goal of evaluating the influence of molecular electron density gradients on the properties of these NanoWires. The intermetallic conjugation in these nanoscale materials will be rationally modified by varying the identity, geometry, electron density, and electron density gradients of the ligands, the repeating units, the capping groups, and the whole rigid-rods. Such tuning will be done by systematically changing:



(a) the electron donor/acceptor and steric properties of the chelating phosphine ligands, including those with chiral phosphorous centers,
(b) the electron acceptor and geometric properties of the bifunctional isonitrile bridges,
(c) the identity of the metal centers,
(d) the order of the specific repeating units,
(e) the identity of the capping groups, and
(f) the redox state of the polymetallic materials.

The redox derivatives of these materials will also be prepared using bulk electrolysis and chemical redox agents. The molecular structures and bonding of each new material will be evaluated using physical, spectroscopic, electrochemical, ESR, X-ray diffraction (conventional and high resolution charge density), and theoretical methods. The *materials-processability characteristics* will be evaluated using thermal, viscosity, and molecular weight determination methods. Finally, their *electrical and optical properties* will be evaluated by bulk and molecular conductivity and 2nd and 3rd order NLO measurements and a representative selection of materials will be *evaluated as solid state device components*. From this data, *structure-property relationships* will be developed with an emphasis on how rationally designed structural changes to the electron densities of the rigid-rod building blocks and electron density gradients of the rigid-rod backbones will influence the properties most closely related to practical materials applications.

Three of the core goals of these NanoWire and NanoStars projects are to evaluate and iteratively improve their electrical conductivity and non-linear optical properties, to evaluate their interactions with surfaces (especially electrode surfaces), and to evaluate the electrical and optical changes in their solids due to trace organics/inorganics (i.e., for sensor applications). Evaluating each of these applications requires access to a very clean inert atmosphere and will be carried out either in the analytical glove box or the solvent free system, as appropriate.

C2b(v). Wagner's Research Program:

Overview: Dr. Wagner's general research interests involve the syntheses and structural characterizations of inorganic extended solids. Related to this proposal, his major areas of interest involves studies of inorganic nitride-fluoride analogs of oxides. ***This project would benefit significantly from the proposed inert atmosphere equipment as many of these materials are remarkably sensitive to oxygen in its elemental form or from water or other protic solvents.***

Nitride-Fluoride Analogues: The proposed research project focuses on the synthesis and structural characterizations of a series of nitride-fluoride compounds formally derived from well-known oxides, mainly in the rocksalt and perovskite systems. Here, the composition of the nitride-fluoride analog is obtained by replacing two O^{2-} ions of the metal oxide with a $(NF)^{4-}$ group. This is an area of inorganic solid state chemistry which has been largely neglected, as evidenced by the fact that fewer than forty such nitride-fluoride compounds have been reported in the literature, as compared to several thousands of inorganic oxides and hundreds of inorganic nitrides and fluorides. One reason for this is probably related to the extreme air-sensitivity of many of the nitride-fluorides already known,

making them relatively difficult to prepare and characterize. Although progress has been made in recent years towards computing the likely structure of a given inorganic crystalline composition, it is still not possible at present to routinely predict from first principles whether or not a proposed composition will be the one prepared under given conditions. Thus, this project is exploratory in nature, and is motivated by both the possibility of preparing new compounds with potentially useful properties, as well as expanding knowledge in the inorganic nitride-fluoride system. Such an exploratory approach to synthesis of inorganic oxides has in the past led to many materials with significant optical, magnetic, and electrical properties.

Previous Work: The previously reported nitride-fluoride compounds all contain only one metal atom, and several of these were originally prepared as analogs of rocksalt-type binary oxides. For example, nitride-fluoride compounds with compositions Ca_2NF, Sr_2NF and Ba_2NF have been reported as analogs of CaO, SrO and BaO. Based on qualitative powder X-ray diffraction data, all three of these compounds were reported as having the rocksalt structures of their oxide analogs. Recently, however, we successfully prepared single crystalline samples of Ca_2NF and completed the structural characterization using single crystal X-ray diffraction. The results indicated that Ca_2NF does not have the rocksalt structure, but rather has a tetragonal structure with Ca atoms in square pyramidal coordination, similar to the structure proposed for Mg_2NF by Anderson. Qualitative analysis of powder samples of Sr_2NF synthesized in Wagner's lab suggests that Sr_2NF also has a Mg_2NF-type structure. Besides the nitride-fluorides containing Mg, Ca, Sr and Ba, the only other metals used to make inorganic nitride-fluoride compounds are apparently Ti, Zn, Zr, Tc, Th, and U. Of the approximately 40 nitride-fluoride compounds reported in these systems, less than 20 were structurally characterized, mostly by qualitative powder X-ray diffraction and our results on this system to date indicate that some of these qualitative characterizations may well be inaccurate/incomplete.

Proposed Research: The proposed research involves first synthesizing nitride-fluoride analogs of binary oxides, and then progressing to analogs of more complex oxides. Thus, the first part of the project (already in progress), is focusing on the preparation of the following nitride-fluoride compounds: Ba_2NF, Cu_2NF, TiNF, and $Y_2(NF)_{1.5}$. These are analogs of the binary oxides BaO, CuO, TiO_2 and Y_2O_3, respectively. The main reason these particular binary analog compositions were chosen is because they will be used as precursors in the preparation of the more complicated analogs in the next part of the project. Of these compounds, it is expected that Ba_2NF (and possibly Cu_2NF) can be characterized in single crystalline form, similarly to the Ca_2NF study recently completed. For these materials, single crystals can be made by slow cooling a mixture of the metal, M, and MF_2 from the melt under N_2 flow. The other two binary-analog compounds must be prepared in the solid state via an ammonolysis reaction, and so will be prepared as powders. The proposed nitride-fluoride analogs of the more complex oxides, discussed below, will also be necessarily prepared as powders. Thus, structural characterization of these materials will require high quality powder diffraction data that will enable structure solution and/or refinement of the powder samples.

In the next phase of the project, preparation of a nitride-fluoride analog to a ternary oxide is proposed. The ternary oxide chosen as a model for study in the nitride-fluoride system is perovskite, as there is currently a great deal of interest in perovskite-type compounds due to their structural relationship to the high temperature superconductors. Perovskite itself has composition $CaTiO_3$, and its nitride-fluoride analog would have composition $CaTi(NF)_{1.5}$. The primary synthesis route proposed for preparation of this compound involves using nitride-fluoride analogs for the entire reaction, and not just the final product. For example, $CaTiO_3$ can be synthesized by mixing stoichiometric amounts of CaO and TiO_2, i.e.,

$$CaO + TiO_2 \rightarrow CaTiO_3$$

and it is proposed that $CaTi(NF)_{1.5}$ be prepared analogously, i.e.

$$\tfrac{1}{2}\, Ca_2NF + TiNF \rightarrow CaTi(NF)_{1.5}$$

This reaction scenario is preferred over a direct synthesis approach, in which the precursors are simple compounds or elements that do not need to be pre-synthesized (i.e. they are easily purchased). For example, one could try reacting Ca metal with TiF_4 in N_2 gas. As our pilot studies have shown however, the problem with this approach is that often undesired intermediate compositions (such as CaF_2 in this case) are preferentially formed. Using a stoichiometric mixture of nitride-fluorides as proposed above should greatly increase the likelihood of obtaining a single-phase product with the desired composition. Undergraduate research students working in my lab have already successfully prepared Ca_2NF powder, and one student is currently working on preparation of TiNF using an ammonolysis route reported in the literature. Thus, it is expected that the first trials of the proposed reaction will be completed by Fall, 2001. Successful synthesis of the proposed $CaTi(NF)_{1.5}$ compound would be significant, since no nitride-fluoride analogs of ternary oxides have been previously reported.

A long-term goal of the proposed research involves synthesis of a nitride-fluoride analog to the well-known 1-2-3 high temperature superconductor, $YBa_2Cu_3O_{7-x}$. The overall reaction typically used for synthesis of the oxide material and the corresponding proposed nitride-fluoride reaction are: and its analogues, e.g.

oxide model reaction: $1/2\ Y_2O_3 + 2\ BaO + 3\ CuO \rightarrow YBa_2Cu_3O_{6.5}$

N—F analog reaction: $1/2\ Y_2(NF)_{1.5} + Ba_2NF + 3/2\ Cu_2NF \rightarrow YBa_2Cu_3(NF)_{3.25}$

Successful preparation of this phase would be highly significant in terms of comparison of conductivity properties with the analogous oxide material. Whether or not the new material is superconducting (which also cannot be predicted), valuable insight could be gained as to the role oxygen plays in the superconducting properties of the 1-2-3 oxide phase.

In terms of its relevance to the current proposal, the most notable observation from Wagner's studies to date relates to the extreme hydrophilicity of many of the nitride-fluoride products. Indeed, some even seem able to abstract surface bound waters on silica and quartz glass, from silicone grease, etc. The handling of these materials therefore needs to take place in an extremely air and water (and perhaps solvent) free environment. Thus, these materials will be routinely handled in the analytical glovebox and/or the solvent free glove box, as appropriate.

C3. DESCRIPTION AND CAPABILITIES OF THE PROPOSED SYSTEMS

C3a. Glove Box Systems:

To meet the varied needs the four participating materials research groups who will regularly use them we are requesting a two glove boxes, one optimized for synthetic purposes and the other for analytical experiments. Both will be equipped with oxygen and moisture meters to continuously monitor the quality of its atmosphere and a gas cooler and solvent trap to keep its internal temperature low and relatively solvent free. The -35 °C refrigerator is critical for growing single crystals and for storing air sensitive product while the built in cold well will be used to carry out reactions at sub-ambient temperatures. To maintain compatibility with our current glove boxes and because of our experience with these systems, we are requesting a Vacuum Atmospheres system. We will routinely carry out electrochemistry, especially cyclic voltammetry and electrochemical quart microbalance, studies in the glove box. In addition, we will install a video microscope (to be purchased with other funds) in the box for the selection and mounting of air sensitive single crystals. Samples of air sensitive solids will be prepared for spectroscopic and DSC analysis in the box as will samples for high temperature solid state synthesis. ***As discussed in the Budget Justification, no research grade glove box system exists on our campus and the proposed system will fill a critical need for our materials group which includes Hunter, Curtin, Lovelace-Cameron, and Wagner and their collaborators. With the funding of the two proposed systems, we will be able to dedicate individual glove boxes to functions which are each critical to our research but which are mutually incompatible with one another.***

C3b. Vacuum Line Systems:

In a research institution, each research group that handles air sensitive chemicals has a range of inert atmosphere vacuum line systems, ideally one for each active research student, and these are very distinct from those in the teaching labs. At YSU, typically for a Predominantly Undergraduate Institution, there is not a sharp dividing line between advanced instruction and research and for both cost and space reasons most major and even minor equipment and instrumentation is shared for both teaching and research and between research groups. Thus, the advanced synthesis lab at YSU is used both for our senior level inorganic, organic, and polymer labs during the academic year and for student research (for half a dozen different faculty) during the other academic year days and during the December/January intersession and the summer. Further, our research groups share this lab space for some of their "core" students when their individual groups are larger (they typically change in relative size in a cyclical fashion) and for the "bulge" in participant numbers that occurs at certain times, especially the summer. It therefore makes substantially more sense in our collaborative environment to hold instrumentation like vacuum lines in a common space where they can be used both for teaching and for research. ***Therefore, in this proposal PI and Co-PI's are seeking funds to purchase 10 inert atmosphere vacuum line systems which will be placed in the advanced synthesis lab to support our common research and teaching agendas as multi-user instrumentation.***

C4. EDUCATIONAL IMPACT OF THE PROPOSED INSTRUMENTATION

For a new lab experience to be widely *implemented*, it must first be developed at one or more test sites; then the educational outcomes must be assessed and disseminated so that faculty at new institutions can be convinced of its value. Once they are *convinced*, they must obtain copies of the new instructional materials and be trained in their use. Finally, they must *adapt* these curriculum materials to their own institution, curriculum, course structure, and students. Predominantly Undergraduate Institutions such as YSU have a strong commitment to undergraduate education and have typically been early adopters of curriculum innovations such as research-like laboratory experiences, collaborative learning strategies, and writing across the curriculum. However, approaches that require specialized instrumentation have been implemented more slowly at PUIs. For the above reasons, PUI faculty and students often either forego such hands-on instrumentation experiences or get occasional access to the appropriate instrumentation through collaborations with other PUIs or with regional research institutions. In too many cases, this access is either too expensive/inconvenient for routine use and/or it is difficult to get sufficient/timely instrument access due to the busy instrumentation schedules at research institutions. These conventional collaborative access arrangements can be effective when the theory taught in class is combined with occasional field trips to the remote sites (i.e., for tours and hands-on activities) along with dry/simulated labs. However, the impact of these instrumental methods on the curriculum and student learning can be substantially improved if these activities are available for routine hands on use.

It is now widely acknowledged that meaningful participation in nationally competitive research is one of the most, if not the most, important component of an undergraduate degree experience. This is true with respect to the amount and quality of knowledge that the students build from their coursework, their attitudes towards science, and their interest in potential research careers. For students interested in the areas of materials chemistry/science being investigated at YSU, such projects involve exposure to and an intense use of inert atmosphere equipment such as glove boxes and vacuum lines. The acquisition of the requested equipment will facilitate student research projects in materials science/chemistry at YSU by our high school, BA/BS, and MS students and our high school teacher-researchers and the implementation of new research like laboratory experiences in the inorganic chemistry and polymer sciences courses taught by the PI and Co-PIs.

C5. IMPACT ON EXISTING INFRASTRUCTURE:

As indicated in Section H, the YSU chemistry department has a well equipped pair of instrumentation facilities for a Predominantly Undergraduate Institution and these facilities support the strong emphasis on hands-on undergraduate research as well meeting as most of the research instrumentation needs of the faculty and their graduate students. The most significant impact of the proposed inert atmosphere equipment on the department/university infrastructure, then, are that they add new capabilities that do not presently exist on campus. In particular, support our developing ***inorganic/organometallic materials emphasis***. This will make YSU a more comprehensive learning, research, and teaching center for students and faculty across disciplines and institutions, especially for those carrying out research at the boundary of inorganic chemistry and materials science. More detailed information on the infrastructure impact of this instrumentation is provided in Sections H and I1.

It is worth emphasizing again that while the YSU Chemistry Department does have two older and very basic Vacuum Atmospheres HE-43 glove box systems, they do not have the advanced research grade capabilities required for much of the research described above, no such research grade glove box exists on campus, and the proposed new systems will lead to both quantitative, and more importantly, qualitative improvements in the scope and type of materials research projects that we can successfully undertake. The vacuum line systems will be particularly valuable for improvements in our inorganic and polymer labs but would also play an important role in student research, especially during the intersession and summer bulge periods.

C6. MAINTENANCE AND OPERATION:

The general operation plan for this new research grade instrumentation is modeled on those we currently use for our other research grade instrumentation. Dr. Hunter, the PI on this proposal and the Director of the YSU Structure & Chemical Instrumentation Center, will be responsible for the instrumentation selection and purchase and, in consultation with the Co-PIs and Departmental Chair, in setting policy. See the discussion above and Sections F and H for more details on this and on instrument maintenance. ***In the context of the current proposal, it is worth noting that our "in service" rate of even instrumentation as complex as our 400 MHz NMR is as good as that at research universities and that the administration has consistently expanded its support for maintenance to meet new equipment purchases.***

SECTION D: REFERENCES

Leading references to each of the individual research projects can be found on the Biographical Sketches of the individual research group directors. Some more general leading references emphasizing the educational and infrastructure impacts are found below.

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2. Hunter, A. D.; Bianconi, L. J.; DiMuzio, S. J.; Braho, D. L.: "Synthesis and Structure/Property Relationships in (η^6-Arene)$Cr(CO)_3$ Chemistry: from Guided Experiments to Discovery Research. Physical Properties, IR, MS, and Multinuclear NMR Spectra, and Cyclic Voltammetry," *J. Chem. Educ.*, **1998**, *75*, 891-893.

3. (a) Schildcrout, S. M.: "No, the Molecular Mass of Bromobenzene Is Not 157 AMU. An Exercise in Mass Spectrometry and Isotopes for Early General Chemistry," *J. Chem. Educ.*, in press (accepted Dec. **1999**). (b) Schildcrout, S. M.: "Gaseous-Ion Fragmentation Mechanisms in Chlorobenzenes by GC/MS and GC/MS/MS: A Physical Chemical Approach for Undergraduates," *J. Chem. Educ.*, **2000**, *77*, 501-502. (c) Norris, P.; Freeze, S.; Gabriel, C. J.: "Synthesis of a Partially Protected Azidodeoxy Sugar: A Project Suitable for the Advanced Undergraduate Organic Chemistry Laboratory," J. *Chem. Ed.*, **2001**, *78*, 75-76.

4. (a) Hunter, A. D.: "New Approaches to Teaching Crystallography to Undergraduates: One Day Experiments and a Step by Step Lab Manual," Pittsburgh Diffraction Society Annual Meeting, November 5th, **1998**. (b) Hunter, A. D.: "New Approaches to Teaching Crystallography to Undergraduates: One Day Experiments, a Step by Step Lab Manual, and the Integration of Single Crystal and Powder Methods," International Center for Diffraction Data Annual Meeting, March 18th, **1999**. (c) Hunter, A. D.: "Broadening the Pipeline: Integrating Diffraction Methods into the Undergraduate Curriculum," American Crystallographic Annual Meeting, May 25th, **1999**. (d) Hunter, A. D.: "Integrating Diffraction Methods into the Curriculum: from K - 16+, Challenges and Opportunities," The Ohio Project for Science Education, OSU, Columbus Ohio, January 28th, **2000**. (e) Hunter, A. D.: "Undergraduates and Research: Should We Send Them Away," Panelist at the Council for Undergraduate Research, CUR, round table on the RUI program at the CUR annual meeting, Wooster, Ohio, June 21st, **2000**. (f) Hunter, A. D. and DiMuzio, S. J.: "X-Ray Diffraction Analysis For High School and College Freshman Students: A Powerful Tool for Understanding Molecular Structure and Bonding," Biennial Conference on Chemical Education, University of Michigan at Ann Arbor, American Chemical Society Division of Chemical Education, July 30th - August 3rd, **2000**. (g) Hunter, A. D. and DiMuzio, S. J.: "X-Ray Diffraction Analysis For High School and College Freshman Students: A Powerful Tool for Understanding Molecular Structure and Bonding," European Crystallographic Meeting, Nancy, France, August 24th - 31st, **2000**.

5. (a) Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *J. Chem. Educ.*, **1998**, *75*, 1297-1299. (b) Hunter, A. D.: *Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction*, Fall 1998 Version F98D1 © 1997, 1998, 275 pages. Has been released electronically as .pdf files to well over 200 individuals at over 150 Universities around the world. Described in the *J. Chem. Educ.*, **1999**, *76*, 163 and in the ACA and IUCr Newsletters, see: http://www.as.ysu.edu/~adhunter/YSUSC/index.html (c) Hunter, A. D.: Allen

Hunter's Guide to Growing Single Crystals, see: http://www.as.ysu.edu/~adhunter/Teaching/Chem832/ADHChXIV.pdf (d) Hunter, A. D.: "Single Crystal X-Ray Diffraction Analysis: A Routine Structural Tool for Chemists," a text under contract for inclusion in the Royal Society of Chemistry's "*Tutorials in Chemistry*" series, Woollins, D. Ed., manuscript in preparation.

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7. Hunter, A. D.: "Integrating Diffraction Methods into the Curriculum: from K - 16+, Challenges and Opportunities," The Ohio Project for Science Education, OSU, Columbus Ohio, January 28th, **2000**.

8. Hunter, A. D., Hoff, R., Levison, B., and Team YSU: "The Youngstown State University PUI Instrumentation Center," the CUR annual meeting, Wooster, Ohio, June 21st, **2000**.

9. (a) Bretz, S. L.: "Evaluation: An Introduction to Why and How," *CHED Newsletter*, American Chemical Society Division of Chemical Education, Spring **1997**, 8-11. (b) Bretz, S. L.: "Concept Maps: A Metacognitive Tool for Teaching Students to Learn How to Learn," Chemistry in Context Instructor's Resource Guide, W. C. Brown, **1997**. (c) Bretz, S. L.: "CiC and Concept Webs," *Chemunity News*, **1997**, *7*, 18-19. (d) Bretz, S. L.: "Human Constructivism and Meaningful Learning," *J. Chem. Educ.*, in press. (e) Bretz, S. L.; Meinwald, J. "The Language of Chemistry," Submitted for publication *to J. Coll. Sci. Teaching*. (f) Bretz, S. L.: "What is Teaching? What is Learning? Using Fox's Hierarchy to Demonstrate an Educational Philosophy," Submitted for publication to *J. Chem. Educ.*

10. (a) Adamchik, C. F. Jr.: "The Design and Assessment of Chemistry Portfolios," *J. Chem. Educ.*, **1995**, *72*, 909. (b) Frechtling, J.; Sharp, L.: "User - Friendly Handbook for Mixed Method Evaluations," NSF-Division of Research, Evaluation, and Communication, August **1997**. (c) Coppola, B. P.; Ege, S. N.; Lawton, R. G.: "The University of Michigan Undergraduate Chemistry Curriculum 2. Instructional Strategies and Assessment," *J. Chem. Educ.*, **1997**, *74*, 84. (d) Moore, J. W.: "Assessment, Achievement, and Understanding," *J. Chem. Educ.*, **1997**, *74*, 477. (e) Arnaiz, F. J.: "Assessment of Knowledge," *J. Chem. Educ.*, **1997**, *74*, 1384. (f) Dreisbach, J. H.; Hogan, T. P.; Stamford, A. M.; Greggo, J. W.: "Focus Groups and Exit Interviews are Components of Chemistry Department Program Assessment," *J. Chem. Educ.*, **1998**, *75*, 1330. (g) Robinson, W. R.: "A View from the Science Education Research Literature: Concept Map Assessment of Classroom Learning," *J. Chem. Educ.*, **1999**, *76*, 1179.

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12. "Academic Excellence: The Role of Research in the Physical Sciences at Undergraduate Institutions," Doyle, M. P., Ed., Research Corporation, Tucson, **2000**.

13. "Bringing the Excitement of Science to the Classroom," Research Corporation, Tucson, **2000**.

14. Tobias, S.: " Rethinking Science as a Career: Perceptions and Realities in the Physical Sciences," Research Corporation, Tucson, **1995**.

15. Hunter, A. D.: "Undergraduates and Research: Should We Send Them Away," Panelist at the Council for Undergraduate Research, CUR, round table on the RUI program at the CUR annual meeting, Wooster, Ohio, June 21st, **2000**.

16. Hunter, A. D.; Brothers, B.; Kasvinsky, P.; Mincey, D. W.: "Six DUE Grants as Catalysts for the Transformation of a PUI Chemistry Department," *J. Chem. Educ*., manuscript in preparation

SECTION E: BIOGRAPHICAL SKETCHES:

Biographical Sketch for Allen D. Hunter, PI

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555-3663,
330-742-7176, adhunter@cc.ysu.edu

a. Professional Preparation:

University of British Columbia, Chemistry	Honors Chemistry	B.Sc.	1981
University of British Columbia, Chemistry	Inorganic Chemistry	Ph.D.	1985
Australian National University, RSC	Organometallic Chemistry	Post. Doc.	1986
University of Alberta, Chemistry	Crystallography	Post. Doc.	1987

b. Appointments:

St. Andrews University, Scotland	Visiting Professor	2000-2001
Youngstown State University, Chemistry	Full Professor	1998-Present
University of Pittsburgh, Crystallography	Visiting Associate Professor	1995-1996
Youngstown State University, Chemistry	Associate Professor	1992-1998
University of Alberta, Chemistry	Adjunct Professor	1992-1995
University of Alberta, Chemistry	Assistant Professor	1987-1992

c. Publications:

Allen has a total of 49 peer reviewed publications (31 since 1992 and 18 since 1996).

(i) 5 Most Closely Related Publications:

1. Chukwu, R.; Hunter, A. D.; Santarsiero, B. D.; Bott, S. G.; Atwood, J. L. *Journal of Organometallic Chemistry,* **1996,** *526*, 1-14.
2. Hunter, A. D.; Guo, X. A. *The Polymeric Materials Encyclopedia, Volume 6*, CRC Press, **1996,** 4813-4822.
3. Guo, X. A.; Hunter, A. D.; Chen, J. *J. Polymer Science, Part A*, **1994**, *32*, 2859-2866.
4. Guo, X. A.; Sturge, K. C.; Hunter, A. D.; Williams, M. C. *Macromolecules*, **1994**, 27, 7825-7829.
5. Hunter, A. D.; Mozol, V.; Tsai, S. D. *Organometallics*, **1992**, *11*, 2251-2262.

d. Synergistic Activities:

Allen is very involved in the scholarship of teaching. This has been recognized at YSU by his being designated a Master Teacher in the College of Arts and Sciences, by his receiving substantial Faculty Development Funding for new curriculum innovations, and by his being appointed the Science representative on the General Education Committee during the development of the new Gen. Ed. program last year, at the state level by his being invited to be a founding member of The Ohio Project for Science Education, and at the national level by several NSF Teaching Instrumentation, Education Materials Development, and Curriculum Innovation grants. He has also published 3 papers in the *Journal of Chemical Education* over the last three year and has released a 275 page student text on diffraction methods via the WEB. He is a founding member and the representative for Ohio's Predominantly Undergraduate Institutions on the Ohio NMR, MS, and X-Ray Crystallography Consortia. He is on the Advisory Board of the W. M. Keck Foundation Center for Molecular Structure (Cal. State. Fullerton). He is also active in the International Center for Diffraction Data, including its Crystallographic Education subcommittee, in the International Union of Crystallography: Committee on Crystallographic Education, and in the Council of Undergraduate Research, and he is the organizer of sessions on crystallographic education at upcoming ACA and ACS national meetings. Finally, Allen is very involved with professional development opportunities for regional science teachers. Indeed, he has spearheaded our efforts to launch a YSU MS program optimized for this group.

e. Collaborators & Other Affiliations:

(i) Collaborators: (in last 4 years and in addition to YSU colleagues and collaborators named in this grant).

Chase Smith, Holly Cross. Cliff Berkman, San Francisco State University. George Richter-Addo, University of Oklahoma. Jim Adrian, Union College. John Cashman, Seattle Biomedical Institute. Viktor Zhdankin, University of Minnesota - Duluth. Vyacheslav (Slava) Samoshin, University of the Pacific.

(ii) Graduate and Post Doctoral Advisors:

- Elliot Burnell (B.Sc.), University of British Columbia.
- Peter Legzdins (Ph.D.), University of British Columbia.
- Martin Bennett (Post. Doc.), Australian National University.
- Martin Cowie (Post. Doc.), University of Alberta.

(iii) Thesis and Postgraduate Scholar Sponsor:

X. Andrew Guo, PhD 1994 (University of Alberta), Stan Tsai, PhD 1995 (University of Alberta) Xiaochung Wang, MS 1994 (YSU), Larry J. Bianconi, MS 1994 (YSU), Stanislaus Tsai, PhD 1995 (University of Alberta), Dianne Braho, MS 1995 (YSU), Steven DiMuzio, MS 1996 (YSU), and Bev Smith-Papa, MS 1997 (YSU). ADH has served as the principle advisor for 2 PhD students, 6 MS students, 3 postdoctoral fellows, 3 research associates, and over a dozen undergraduate researchers. He is also involved in chemical education and disciplinary research, that will eventually lead them to MS degrees, with several regional high school science teachers.

Biographical Sketch for Larry S. Curtin, Co-PI

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555
330-742-7101, lscurtin@cc.ysu.edu

a. Professional Preparation:

Northern Illinois University, Chemistry	Chemistry	BS	1985
University of Wisconsin-Madison, Chemistry	Inorganic Chemistry	MS	1986
University of Wisconsin-Madison, Chemistry	Inorganic Chemistry	PhD	1990
University of North Carolina-Chapel Hill	Electrochemistry	Post. Doc.	1990

b. Appointments:

Youngstown State University, Chemistry	Associate Professor	2000-present
Youngstown State University, Chemistry	Assistant Professor	1995-2000
Temple University	Assistant Professor	1992-1995

c. Publications:

(i) 5 most Closely Related Publications:

1. McCarley, T. D.; Lufaso, M. W.; Curtin, L. S. and McCarley, R. L. "Multiply Charged Redox-Active Oligomers in the Gas Phase: Electrolytic Electrospray Ionization Mass Spectrometry of Metallocenes," *J. Phys. Chem. B*, **1998**, *Vol 102, No. 49*, 10078.
2. Landis, K. G.; Hunter, A. D.; Wagner, T. R.; Filler, F. L.; Jansen-Varnum, S. A. and Curtin, L. S. "The Synthesis and Characterization of Ni, Pd and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd and Pt ($Ph_2PCH_2CH_2PPh_2$)M(Maleonitriledithiolate) Congeners," *Inorg. Chim.* Acta, **1998**, *Vol. 282*, 155.
3. Richardson, J. N.; Rowe, G. K.; Tender, L. M.; Curtin, L. S.; Peck, S. R.; Murray, R. W. "Electron Transfer Kinetics of Self-Assembled Ferrocene(C12)alkanethiol Monolayers on Gold Electrodes from 125 K to 175 K," *Electrochim. Acta*, **1995**, *40(10)*, 1331-1338.

4. Peck, S. R.; Curtin, L. S.; Tender, L. M.; Terrill, R. H.; Murray, R. W.; Collman, J. P.; Little, W. A.; Duan, H. M.; Dong, C.; Hermann, A. M.; Rowe, G. K.; Creager, S. E. "Electrochemistry of Self-Assembled Ferroceneoctanethiol Monolayers on Metal-Coated High Temperature Superconductor Electrodes at Sub-T_c Temperatures," *J. Am. Chem. Soc.* **1995**, *117(3)*, 1121-1126.
5. Richardson, J. N.; Peck, S. R.; Curtin, L. S.; Tender, L. M.; Terrill, R. H.; Carter, M. T.; Murray, R. W.; Rowe, G. K.; Creager, S. E. "Electron Transfer Kinetics of Self-Assembled Ferroceneoctanethiol Monolayers on Silver Electrodes at 115 K to 170 K," *J. Phys. Chem.* **1995**, *99(2)*, 766-772.

(ii) Other Significant Publications:

1. Curtin, L. S.; Pietro, W. J. "Student Solutions Manual to accompany Chemistry: Science of Change," Saunders College Publishing, Philadelphia, 1990.

d. Synergistic Activities:

Larry typically has a large research group including graduate and undergraduate students. His research crosses many of the traditional boundaries in chemistry, involving organic, analytical and physical chemistry. Thus, his students are extremely well versed in such diverse areas as synthesis and synthetic methodology, spectroscopy, electrochemistry and X-ray diffraction. His research program is designed so that undergraduate and graduate students enjoy a great deal of success, as indicated by the many poster and oral presentations at local and national scientific meetings. Several honors students have done research related projects with Larry to fulfill their additional requirements. Larry has had extensive collaboration with Drs. Timothy Wagner and Allen Hunter on his X-ray crystallographic studies of transition metal compounds. He also has an on-going collaboration with Dr. Robin L. McCarley at Louisiana State University which has already resulted in a publication in *The Journal of Physical Chemistry, B*. Larry has also had extensive interaction with the local grade and high schools through the many chemical demonstration shows which he does every year. His emphasis in these shows is upon staying in school and that chemistry can be fun and a good career choice. These shows also help to educate the teachers on new and interesting ways to present chemistry, as well as acting as a recruiting tool to convince students on the benefits of an education at YSU.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Robin L. McCarley, Louisiana State University
Allen D. Hunter, Youngstown State University
Timothy R. Wagner, Youngstown State University

(ii)Graduate and Post Doctoral Advisors:

William J. Pietro (PhD)
Royce W. Murray, (Post. Doc.)

(iii)Thesis and Postgraduate Scholar Sponsor:

William J. Filler, MS 1992, Francesca L. Filler, MS 1992, Katy Landis, MS 1998, Charles van Kirk, MS 1999. LSC has also served as the principle advisor of 14 undergraduate research associates.

Biographical Sketch for Sherri R. Lovelace Cameron, Co-PI

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555
330-742-1997, srlovela@cc.ysu.edu, http://cc.ysu.edu/~srlovela/index.html

a. Professional Preparation:

Drexel University, Chemistry	Chemistry	BS	1986

University of Pittsburgh, Chemistry	Organometallic Chemistry	PhD 1992
University of Vermont, Chemistry	Electrochemistry	Post. Doc. 1992-1995

b. Appointments:

Youngstown State University, Chemistry	Assistant Professor	1995-Present

c. Publications:

(i) 5 most Closely Related Publications:

1. Connelly, N. G.; Geiger, W. E.; Lovelace, S. R.; Metz, B; Paget, P; Winter, R.: "Reduction of $[ML(alkyne)_2(\eta\text{-}C_5R'_5)]^+$ (M = Mo or W, L = MeCN or CO, R' = H or Me, $C_5R'_5 = C_5HPh_4$): Characterization of Radical Intermediates in the Reductive Coupling of Coordinated Alkynes." *Organometallics,* **1999**, 18, 3201-3207.
2. Rulkens, R.; Lough, A. J.; Manners, I.; Lovelace, S. R.; Grant, C.; Geiger, W. E.: "Linear Oligo (ferrocenyldimethylsilanes) with between Two and Nine Ferrocene Units: Electrochemical and Structural Models for Poly (ferrocenylsilane) High Polymers," *J. Am. Chem. Soc.,* **1996**, *118*, 12683-12695.
3. Koeslag, M. A.; Baird, M. C.; Lovelace, S. R.; Geiger, W. E.: "Synthesis and Properties of the 17-Electron, Tantalum-Centered Radical $Ta(CO)_4(Ph_2PCH_2CH_2PPh_2)$," *Organometallics*, **1996**, *15*, 32893302.
4. Lee, S.; Lovelace, S. R.; Arford, D. J.; Geib, S. J.; Weber, S. G.; Cooper, N. J.: "Reductively Induced Dimerization of the Ligated Benzene in $[Mn(\eta^6\text{-}C_6H_6)(CO)_3]^+$: Formation of the Initial C-C Bond by Anion/Cation Addition," *J. Am. Chem. Soc.,* **1996**, *118*, 4190-4191.
5. Lee, S.; Lovelace, S. R.; Cooper, N. J.: "Two-Electron and One-Electron Reduction of the Indenyl Complex $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]$ and Reversible Counterion-Controlled Comproportionation of $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]$ and $[Mn(\eta^3\text{-}C_9H_7)(CO)_3]^{2-}$ To Give $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]$," *Organometallics*, **1995**, *14*, 19741982.

d. Synergistic Activities:

Sherri actively participates in, and coordinates much of, YSU's outreach activities to members of communities traditionally under-represented in science. Indeed, she has been involved in such efforts since graduate school. She has extensive experience working with Youngstown's majority minority Public School system. She is the creator and coordinator of the YSU Summer Science Academy program for 7th and 8th graders. The goal of this summer program is to encourage students of color to excel, and to continue their interest in the sciences. At the Science Academy students perform hands on activities that require the integration of math and science skills. The activity modules utilize computer technology and combined both physical and life sciences. She is also currently serving as the coordinator for the Delta Leadership Academy. The academy is an after school program for at risk girls, between the ages of 11 to 14. The academy encourages the consideration of careers that utilize science, math, and technology. She has been the Director of the YSU Chemistry Department's ACS SEED Project for four years. As an African American scientist, she is a role model and mentor for YSU's African American students, many of whom she has influenced into switching into science and technology degree programs. She has also worked closely with other members of our African American Studies program to institute a new General Education Course, Chemistry 2602: African and African American Contributions to Science. For her work in science education, she has been selected as a Master Teacher by the College of Arts & Sciences and been designated a Project Kaleidoscope F21 Scholar.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Fola Ladipo, University of Kentucky

Allen Hunter, Youngstown State University

(ii) Graduate and Post Doctoral Advisors:

N. John Cooper (PhD), University of Pittsburgh.

William E. Geiger (Post. Doc.), University of Vermont

(iii)Thesis and Postgraduate Scholar Sponsor:

Gretchen Metz, MS 1997. Sherri has also mentored 4 pre-college students, and 7 undergraduate students (including 4 thesis students and 2 minority work program students) in her group over the last 5 years and currently has several students in her group.

Biographical Sketch for Timothy R. Wagner

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555
330-742-1960, trwagner@cc.ysu.edu, http://www.as.ysu.edu/~trwagner/index.html

a. Professional Preparation:

University of Wisconsin - River Falls	Chemistry	BS	1981
Arizona State University, Chemistry	Solid State Chemistry	PhD	1986
Hughes Aircraft Company	Radar Software		1988
Northwestern University, Materials	Electron Microscopy	Post Doc.	1990

b. Appointments:

Youngstown State University, Chemistry	Associate Professor	1998-Present
Youngstown State University, Chemistry	Assistant Professor	1992-1998
Illinois Institute of Technology, Chemistry	Visiting Assistant Professor	1990-1992

c. Publications:

i. Five Most Closely Related Publications:

1. Nicklow, R; Wagner, T.; and Raymond, C.: "Preparation and Crystal Structure Analysis of Ca_2NF," *J. Solid State Chemistry*, **in press**.
2. Wagner, "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type Barium Hexagallate," *J. Solid State Chemistry*, **1998**, *136*, 120-124.
3. Wagner T.; O'Keeffe, M.: "Bond Lengths and Valences in Aluminates with the Magnetoplumbite and β-Alumina Structures," *J. Solid State Chemistry.*, **1988,** *73*, 211-216.
4. Wagner T.; O'Keeffe, M.: "A Structural Model for Barium Hexagallate," *J. Solid State Chemistry*, **1988,** *73*, 19-26.
5. Wagner, T.; O'Keeffe, M.: "Electron Microscopy of Defects and Disorder in Barium Hexagallate," *Acta Cryst.*, **1985**, *B41*, 108-112.

ii. Five Other Significant Publications:

6. Freeze, S; Norris, P.; and Wagner, T.; "Formation of D-Galactose-derived Ethylene Diamine Ligand and its Complex with Pd(II)," *Carbohydrate Research*, **in press**.
7. Norris, P. and Wagner, T.: "Solution and Solid State Structure of the 2,6-anhydro-1,1-bis(ethylsulfonyl)-1-deoxy-D-talitol," *Carbohydrate Research*, **1999**, *322(1-2)*, 147-150.
8. Landis, K.; Hunter, A.; Wagner, T.; Curtin, L.; Filler, F.; Jansen-Varnum, S.: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt Congeners", *Inorganica Chimica Acta*, **1998**, *138*, 155–162.
9. Wagner, T. and Styranec, T.: "Preparation and Crystal Structure Analysis of $Ba_2BiGa_{11}O_{20}$," *J. Solid State Chem.*, **1998**, *138*, 313–320.

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

d. Synergistic Activities:

Since joining the chemistry department at YSU, Tim has focused much effort on establishing a departmental infrastructure for solid state structural analysis. He played the lead role in establishing the department's existing X-ray facility, as the PI on the NSF DMR-IMR grant which provided major funding for the facility. He also set-up the department's transmission electron microscope laboratory by locating two donor instruments and combining them into one functional instrument. He is a major proponent of the department's policy regarding hands-on access to research-grade instrumentation by any undergraduate student who desires training. Tim has worked on X-ray (both powder & single crystal) diffraction projects with high school students completing projects for science fairs; with general chemistry students doing hands-on experimental honors projects, and with both undergraduate and graduate research students. He has incorporated hands-on X-ray diffraction analysis as a mandatory part of his inorganic laboratory course (10 to 20 students annually), and has also worked with students in other courses (e.g. Physical Chemistry Laboratory) doing independent studies in X-ray analysis. Tim has also served as a consultant with industrial scientists and other external users needing X-ray diffraction data. More recently, Tim has focused his efforts on the general chemistry curriculum, and is the PI on a successful NSF-CCLI grant which will be used to incorporate computer technology into the general chemistry laboratory.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Casey Raymond, Kent State University

(ii) Graduate and Post Doctoral Advisors:

Michael O'Keeffe (PhD), Arizona State University

Lawrence Marks (Post. Doc.), Northwestern University

(iii)Thesis and Postgraduate Scholar Sponsor:

Ma'en Amad, MS, 1994; Joseph Potkinicky, MS, 1997; Rhea Nicklow, MS, 2000. Tim has also served as research advisor for 15 undergraduate students.

It is worth re-emphasizing that each of the PI and Co-PIs have used inert atmosphere glove box systems throughout their careers and have instructed others in its use in both formal teaching and research settings. Based on this experience, they have chosen the requested research grade equipment and accessories which is currently not available on campus. It is simply not feasible to go to other universities to use their glove box facilities on a daily basis!

SUMMARY PROPOSAL BUDGET

YEAR 1

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Youngstown State University**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Allen D Hunter**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - PI&PD**	0.00	0.00	0.00	$ 0	$
2. **Larry S Curtin - Co-PI**	0.00	0.00	0.00	0	
3. **Sherri R Lovelace-Cameron - Co-PI**	0.00	0.00	0.00	0	
4. **Timothy R Wagner - Co-PI**	0.00	0.00	0.00	0	
5.					
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0	
7. (4) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00	0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0	
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	0	
3. (0) GRADUATE STUDENTS				0	
4. (0) UNDERGRADUATE STUDENTS				0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0	
6. (0) OTHER				0	
TOTAL SALARIES AND WAGES (A + B)				0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
D1. Glove Box System for Synthetic Studies $ 63,220					
D2. Glove Box System for Analytical Studies 51,368					
D3. Vacuum Line Systems 68,970					
D4. Less YSU Capital Match -51,779					
TOTAL EQUIPMENT				131,779	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				0	
2. FOREIGN				0	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ 0					
2. TRAVEL 0					
3. SUBSISTENCE 0					
4. OTHER 0					
TOTAL NUMBER OF PARTICIPANTS (0) TOTAL PARTICIPANT COSTS				0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0	
3. CONSULTANT SERVICES				0	
4. COMPUTER SERVICES				0	
5. SUBAWARDS				0	
6. OTHER				0	
TOTAL OTHER DIRECT COSTS				0	
H. TOTAL DIRECT COSTS (A THROUGH G)				131,779	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **(Rate: , Base:)**					
TOTAL INDIRECT COSTS (F&A)				0	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				131,779	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 131,779	$

M. COST SHARING PROPOSED LEVEL $ **51,779** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*: **Allen D Hunter** DATE

ORG. REP. TYPED NAME & SIGNATURE*: **Kasvinsky, Peter** DATE

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET

Cumulative

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION
Youngstown State University

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR
Allen D Hunter

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - PI&PD**	0.00	0.00	0.00	$ 0	$
2. **Larry S Curtin - Co-PI**	0.00	0.00	0.00	0	
3. **Sherri R Lovelace-Cameron - Co-PI**	0.00	0.00	0.00	0	
4. **Timothy R Wagner - Co-PI**	0.00	0.00	0.00	0	
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00	0	
7. (**4**) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00	0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00	0	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00	0	
3. (**0**) GRADUATE STUDENTS				0	
4. (**0**) UNDERGRADUATE STUDENTS				0	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				0	
6. (**0**) OTHER				0	
TOTAL SALARIES AND WAGES (A + B)				0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) $ 131,779					
TOTAL EQUIPMENT				131,779	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				0	
2. FOREIGN				0	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ 0					
2. TRAVEL 0					
3. SUBSISTENCE 0					
4. OTHER 0					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				0	
3. CONSULTANT SERVICES				0	
4. COMPUTER SERVICES				0	
5. SUBAWARDS				0	
6. OTHER				0	
TOTAL OTHER DIRECT COSTS				0	
H. TOTAL DIRECT COSTS (A THROUGH G)				131,779	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				0	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				131,779	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 131,779	$

M. COST SHARING PROPOSED LEVEL $ **51,779** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*
Allen D Hunter
DATE

ORG. REP. TYPED NAME & SIGNATURE*
Kasvinsky, Peter
DATE

FOR NSF USE ONLY		
INDIRECT COST RATE VERIFICATION		
Date Checked	Date Of Rate Sheet	Initials - ORG

NSF Form 1030 (10/99) Supersedes all previous editions

C***SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)**

SECTION F: BUDGET JUSTIFICATION

Operation and Maintenance: As described in more detail in Section H, the Youngstown State University Structure & Chemical Instrumentation Center, YSU-S&CIC, and the Youngstown State University Center for Biomedical and Environmental Research, YSU-CBER, serve the scientific instrumentation needs of YSU. This CRIF's PI is the Director of the YSU-S&CIC and plays a lead role in YSU-CBER. He and other relevant faculty set policy for these centers. Their day to day operations are managed by two full time staff members: Mr. Ray Hoff, out electronic instrumentation specialist, with a BS in Physics and over a decade's experience at maintaining advanced research equipment (i.e., at Tulane University before he came to YSU 2 years ago) and Bruce Levison with PhD in Analytical Chemistry and over a dozen years experience at analytical lab management, who is in charge of user support function. We have also recently received approval for three additional instrumentation technician budget lines (at the MS level) to support Ray and Bruce with their maintenance and user support duties. multiple students are employed each semester as instrument operators (i.e., typically those wishing a career as industrial analytical chemists upon graduation) on a part time basis (i.e., the undergraduates) or *in lieu* of teaching assignments (i.e., the MS students). This skilled staff keep all instrumentation in excellent operating condition. Our core departmental budget for instrument maintenance is sufficient for routine costs, major users provide contributions to maintenance costs (e.g., the PI's NSF 0111511 grant will fund $3,000/year), and major expenses are covered out of the Dean's account (e.g., a quench to the 400 MHz NMR two years ago required a single phone call to get a "blank check" for its repair which was completed in 2 weeks). Since their inception 8 years ago, the YSU administration has provided very strong support for these centers, including: an *automatic* matching funds policy (i.e., providing all required matching funds based on the RFP requirements), providing over 1.5 million dollars for capital equipment purchase, and providing new budget lines for its maintenance and operation.

D. Equipment: The PI and Co-PIs on this proposal all require access to excellent facilities for handling air sensitive molecular and/or solid state materials on a daily basis. Each of the items of equipment whose purchase is described in this proposal (please see attached quote in Section I4) will be used for a range of student and faculty research projects here at Youngstown State University. To this end, the models chosen typically had to have more flexibility than they might if used only by a single research group. Thus, the core inert atmosphere glove boxes will be used to meet the research needs of 4 faculty members and their groups and the teaching needs of several courses. However, some of the individual accessories will be initially used by only one or two research groups. Such a glove box system or systems would typically be found within an individual research group at a PhD school. However, at a PUI such as YSU they are best purchased and used jointly and thus will be used by the 4 materials research groups. The glove box system will also have significant utilization by the two dozen collaborating partner PUIs in the YSU-PUI Undergraduate Diffraction Consortium (Section I2). The Department currently has two old and very basic Vacuum Atmospheres HE-43 glove boxes (i.e., each is equipped with the basic dry train and Peditrol but no oxygen or water meters, freezer, solvent trap, etc.) which have positively influenced our choice of preferred vendors.

Current Older Glove Box Dedicated to Instructional & Protic Solvent Applications: One of the current HE-43's is over 20 years old and the other was purchased used (its age is uncertain but it is certainly not one of the newer models) two years ago from a NSF-DUE-ILI-IP grant. This glove boxes is located in the advanced synthesis teaching lab where and is designated for the teaching of glove box techniques and for several experiments in the senior inorganic and polymer lab sequences. Because of class room role, its moisture and oxygen quality will vary over a substantial range, being particularly low at the beginning of each semester when the rate of "learner" mistakes is relatively frequent. This DUE funded **instructional glove box** is ideal for its

instructional purpose and we plan on keeping it dedicated to teaching during the academic year when these labs run. During the summer, it will be used for handling **protic solvents** (e.g., ROH) for Hunter's organometallic crystal engineering project (i.e., Section C2b(i)) which makes it unsuitable for the other purposes described herein.

Current Older Glove Box to be Dedicated to Solvent Free Applications: The second HE-43 glove box is currently in Lovelace-Cameron's lab and is the sole glove box for research on campus. Thus, we and our students use it to handle air sensitive solids and to carry out synthesis and characterization studies. However, it is definitely showing its age and, from a research perspective, the biggest problems are with the atmosphere quality due to cracks in its from panel, its limited dry train, and its lack of solvent removal capabilities (which is not always optimum and for which there are no sensors) and the conflict between its multiple roles. Namely, we use solvents in this box for several purposes and these react with many of the solid state samples we would like to handle in it. In addition, the presence of several solvents at any one time and any volatile reagents gives it a "dirty" atmosphere which substantially interfere with analytical studies (e.g., electrochemistry). Finally, it is too small for both the number of current users and their varied equipment and does not have a freezer, cold well, etc., required for our work. With the installation of the proposed research grade glove boxes, this older system would be stripped down, thoroughly cleaned, and the seals changed (i.e., at YSU expense and this was last done 2-3 years ago) and it would then become **a dedicated *solvent free* glove box** used only for the handling of air sensitive solids and for solid state measurement (e.g., some electrical conductivity tests) that are incompatible with solvents.

To meet the varied needs of the four inorganic/organometallic research groups outlined in Section C, we **are requesting funds to purchase two modern research grade glove boxes**. One is to be used for the synthesis, purification, crystallization, and some characterization studies of air sensitive materials. The other is to be used for analytical studies on air sensitive materials (particularly electrochemical studies). While we could employ a single glove box for both purposes, the experience of the PI and Co-PIs, that of our colleagues at other schools, and even that of reviewers on last winter's unsuccessful MRI application is that the two uses are not compatible. In particular, in a "synthetic" glove box one uses a wide range of solvents and volatile reagents in substantial volumes and these cause interference problems with the sensitive analytical applications. While the funding of a single research grade glove box would certainly be a big improvement over our current situation, we are requesting funds for two new research grade systems, to give us greater experimental and scheduling flexibility and to avoid this analytical contamination problem.

D1. Glove Box System Dedicated to Synthetic Studies: This modern research grade Vacuum Atmospheres system (i.e., see Section I4) has a package cost of **$49,850**. It will be equipped with oxygen and moisture meters to continuously monitor the quality of its atmosphere and a high capacity dry train. To deal with the heat generated in a "synthetic" box and the longer times a user typically spends in it, a gas cooler is requested to keep its internal temperature from building up as it would otherwise. There will also be a solvent trap system to keep atmospheric solvent levels as low as possible. The -35°C refrigerator is critical for growing single crystals and for storing air sensitive products while the built in cold well will be used to carry out reactions at sub-ambient temperatures. Reagents for syntheses and solid samples that are to solvent sensitive, will be weighed inside the glove box using the requested analytical balance (Aldrich Catalogue #Z40,886-7, **$4,018**). [Note: Samples of air and solvent sensitive solids will be prepared for spectroscopic and DSC analysis in the solvent free box as will samples for high temperature solid state synthesis using the requested pellet press (Aldrich Catalogue #Z28,588-9, **$2,065**).] This new glove box will be used extensively for the synthesis and purification of air sensitive materials. To facilitate this, it will contain two compact stirring hot plates (Aldrich Catalogue #Z26,210-2, **$315**), a solid block heater (Aldrich Catalogue #Z42,061-1, **$1033**, #Z2,019-31, **$86**, and Z21,019-9, **$86**), and a Teflon vacuum pump

with vacuum controller (Aldrich Catalogue #Z28,820-9, **$2,832** and #Z28,823-3, **$2,860**). In several cases, these items will be modified by our staff to place their controls outside of the glove box. The total cost for the **synthetic glove box system is $63,220**.

D2. Glove Box System Dedicated to Analytical (Especially Electrochemical) Studies: This analytical glove box system will have the same Vacuum Atmospheres components as the "synthetic" glove box with the exception that there will be no cold well (i.e., having a total cost of $49,850 less $2,500 for the cold well, **$47,350**) and there will be additional integrated electronic leads. The -35°C refrigerator is required for storing air and thermally sensitive products and for some single crystal growth operations and the solvent traps to keep the ambient gas phase solvent levels as low as possible. We will routinely carry out analytical experiments such as electrochemistry, (i.e., especially cyclic voltammetry and bulk electrolysis using the new electrochemical system the PI had funded in 0111511), electrochemical quart microbalance, and electrical conductivity studies in the glove box. In addition, we will install a video microscope in the box for the selection and mounting of air sensitive single crystals to serve the needs of the YSU-PUI Undergraduate Diffraction Consortium. [Note: All of this characterization equipment is in hand, is funded, or is to be purchased with other funds except for an analytical balance (Aldrich Catalogue #Z40,886-7, **$4,018**)]. This gives a total cost for the **analytical glove box system is $51,368**.

D1. Vacuum Line Systems: The number of student researchers participating in student research at YSU (i.e., at the BA, BS, and MS levels and including high school students and teachers) has increased by a factor of approximately 5 over the last 5 years and this number is still rapidly growing. Because of this, our smaller instrumentation such as vacuum lines is tremendously over subscribed and additional vacuum line systems are therefore required for both teaching and research purposes. This is especially true during the December/January intersession and the summer months when the number of undergraduate researchers, minority high school students, and/or high school science teachers doing research swells enormously and the MS students are not involved in teaching and coursework. We request the funds to purchase complete vacuum line assemblies with the components being selected from different vendors to minimize the total cost of packages, including: (a) explosion proof direct drive pump will include a oil mist eliminator, hose adapter, and hosing (i.e., Fisher Model M8C pump system, $2,856 each, Catalogue numbers 01-257-8CX, 01-257-7B, 01-257-12, and 14-175H), (b) Vacuum manifolds (to be supplied by ACE Glass since YSU does not have a glass shop, catalogue number 7818-10), and (c) the requisite nitrogen regulators, Dewar flasks, and associate minor components (i.e., VWR part numbers 55850-424 (1 at $193 each/line), 33920-236 (2 at $268 each/line), and 60142-546 (2 at $126 each/line) and Aldrich part number Z21,713-1 (2 at $234 each/line) totaling $1,453 for each vacuum line system) at a total cost of **$6,897 each**. These inert atmosphere systems will be placed in the advanced synthesis lab which is a dual use facility that serves our polymer science, organic synthesis, and inorganic lab courses and also houses most of our undergraduate research students, especially in the summer. The **10 new vacuum line systems requested for $68,970** will allow the students taking the lab courses to have at least one per pair of students during the lab periods (this lab is scheduled for up to 20 students) on lab days and for the research students of the PI and Co-PIs to each have there own vacuum line during non-lab days in the academic year and during the December/January intersession and the summer. *While it may seem unusual at first site to request such vacuum line systems from the CRIF program, at YSU they will certainly be "multi-user instrumentation" as defined by the RFP with their users changing day to day during the academic year as well as semester to semester as individual research groups grow and shrink. In addition, since YSU has no glass shop they have to be purchased from external suppliers.*

M. Cost Sharing Proposed Level: On this basis CRIF RFP (00-81), YSU will meet its cost sharing requirement (i.e., ($183,558 - $80,000)/2 = $103,558) with a **$51,779** capital match.

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Allen D. Hunter, PI & PD**

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

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

Project/Proposal Title: X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding

Source of Support: NSF-DUE-CCLI-EMD-POC # 9980921

Total Award Amount: $74,707 Total Award Period Covered: 05/01/2000 – 04/30/2002

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 3 Sumr: 1.0, 1.0

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

Project/Proposal Title: REU - Research Experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities

{Note: Two Supplementary Funding requests for this REU Grant (NSF 0128153 and 0128154) have been submitted for consideration. One involves Lovelace-Cameron as a Co-PI and is to fund two undergraduates for a collaborative NLO study of models of Organometallic NanoWires with researchers at Australian National University. The other involves Curtin as a Co-PI and requests and RET supplement for two teachers to work with the principles on a collaborative NanoWires project with faculty and students from St. Andrews University in Scotland.}

Source of Support: NSF-CHEM-REU #0097682

Total Award Amount: $180,000 Total Award Period Covered: 06/01/2001 - 05/31/2004

Location of Project: YSU

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

Project/Proposal Title: WEB Accessible Single Crystal X-Ray Diffractometer for a Consortium of Predominantly Undergraduate Institutions

Source of Support: NSF-DUE-CCLI-A&I and the Ohio Board of Regents Investment Fund

Total Award Amount: $200,000 + $75,000 Total Award Period Covered: 01/15/2001 - 12/31/2003

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.50, 0.25, & 0

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

Project/Proposal Title: Structural Investigations of Main Group Heterocyclic Rings and Cages

Source of Support: NSF: Int Div (Western Europe), Collaborative Projects #0086313

Total Award Amount: $13,200 Total Award Period Covered: 02/01/2001 - 08/31/2001

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: 5 Sumr:

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

Project/Proposal Title: RUI - Organometallic NanoStars

{Note: This Proposal has been recommended for joint funding by the CHEM & DMR divisions and await approval by the Division of grants.}

Source of Support: NSF-DMR/CHEM-RUI

Total Award Amount: $ 350,000 Total Award Period Covered: 07/15/2001 - 07/14/2004

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

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

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Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Allen D. Hunter, PI & PD** (continued)

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

Support: ■ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Electroactive Organometallic NanoStars
Source of Support: American Chemical Society-Petroleum Research Fund, Type B
Total Award Amount: $30,000 Total Award Period Covered: 08/01/2001 - 08/31/2003
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: 0.25 Acad: Sumr:

Support: ☐ Current ■ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: RUI - Crystal Engineering Using Organometallic FluoroArylene Bridged Building Blocks of Ni, Pd, and Pt
Source of Support: NSF-CHEM/DMR-RUI
Total Award Amount: $367,466 Total Award Period Covered: 08/15/2001 - 08/14/2004
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

Support: ☐ Current ■ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: RUI-MRI: -Acquisition of a Powder X-Ray Diffractometer System
Source of Support: NSF-MRI
Total Award Amount: $170,310 Total Award Period Covered: 08/01/2001 - 07/31/2003
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

Support: ☐ Current ■ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Chiral Organometallic NanoWires: the synthesis and characterization of isonitrile bridged materials with potentials as components of molecular electronic devices.
Source of Support: Dreyfus Foundation: Scholar/Fellow Program for Undergraduate Institutions
Total Award Amount: $105,000 Total Award Period Covered: 08/15/2002 - 08/14/2004
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

Support: ☐ Current ■ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: RUI - Polarized NanoScale Organometallic Rigid-Rods for Electronics/Photonics Applications: Collaborative Materials Research Project Between the European Union and YSU Scientists.
Source of Support: NSF US-EU Materials Science Collaborations (NSF 01-105)
Total Award Amount: $1,151,856 Total Award Period Covered: 01/01/2002 - 12/31/2005
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

Support: ☐ Current ■ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: AWARE - RUI - Collaborative Investigation of NLO Active Organometallic NanoWires by Youngstown State University and Australian National University Teams
Source of Support: NSF
Total Award Amount: $909,985 Total Award Period Covered: 3/01/2002 - 2/31/2005
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Allen D. Hunter, PI & PD** (continued)

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

Grant Proposals to European Funding Agencies.

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

Project/Proposal Title: Organometallic NanoWires: New Nanoscale Components for Molecular Electronic & Organometallic Optical Applications.

Source of Support: **European Union - Research Training Networks program**

Total Award Amount: 1,200,000 ECUs Total Award Period Covered: 01/01/2002 - 12/31/2005

Location of Project: UK, Italy, France, Germany, and Belgium (collaborative work at YSU)

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

Project/Proposal Title: BEONS: Bonding and Electronic/Optical Studies of NS and Related Heterocyclic Ring Compounds: Potentials for Materials Applications.

Source of Support: **European Union - Research Training Networks program**

Total Award Amount: 1,200,000 ECUs Total Award Period Covered: 01/01/2002 - 12/31/2005

Location of Project: UK, Italy, France, Germany, and Belgium

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

Project/Proposal Title: Structure-Property Relationships of NSNS Heterocyclic Rings: Potential Electronic/Optical Materials

Source of Support: the **UK Engineering and Physical Sciences Research Council, EPSRC**

Total Award Amount: £323,661 Total Award Period Covered: 09/01/2001 - 08/31/2004

Location of Project: St. Andrews University, Scotland

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

General Note: Hunter was the lead author on these proposals to European funding agencies during his 2000-2001 sabbatical in Scotland during which time he also played the key role in founding the European Organometallic NanoWires network described in the proposal. This European funding is in addition to the national funding already in place for our Belgian, French, German, Italian, and UK collaborators. If funded, these grants would provide additional support for the European component of the described NanoWires projects, none of this funding would be available to support the PI's work in the US.

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Larry S. Curtin, Co-PI**

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

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

Project/Proposal Title: REU - Research Experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities

{Note: Two Supplementary Funding requests for this REU Grant (NSF 0128153 and 0128154) have been submitted for consideration. One involves Lovelace-Cameron as a Co-PI and is to fund two undergraduates for a collaborative NLO study of models of Organometallic NanoWires with researchers at Australian National University. The other involves Curtin as a Co-PI and requests and RET supplement for two teachers to work with the principles on a collaborative NanoWires project with faculty and students from St. Andrews University in Scotland.}

Source of Support: NSF-CHEM-REU #0097682

Total Award Amount: $180,008 Total Award Period Covered: 06/01/2001 - 05/31/2004

Location of Project: YSU

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Sherri R. Lovelace-Cameron, Co-PI**

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

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

Project/Proposal Title: Investigative Approaches in the Natural Sciences

Source of Support: NSF-DUE-IWR #9850079

Total Award Amount: $183,579 Total Award Period Covered: 06/01/1998 – 05/31/2001

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 2.0 Sumr:

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

Project/Proposal Title: REU - Research Experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities

{Note: Two Supplementary Funding requests for this REU Grant (NSF 0128153 and 0128154) have been submitted for consideration. One involves Lovelace-Cameron as a Co-PI and is to fund two undergraduates for a collaborative NLO study of models of Organometallic NanoWires with researchers at Australian National University. The other involves Curtin as a Co-PI and requests and RET supplement for two teachers to work with the principles on a collaborative NanoWires project with faculty and students from St. Andrews University in Scotland.}

Source of Support: NSF-CHEM-REU #0097682

Total Award Amount: $180,00 Total Award Period Covered: 06/01/2001 - 05/31/2004

Location of Project: YSU

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

Project/Proposal Title: WEB Accessible Single Crystal X-Ray Diffractometer for a Consortium of Predominantly Undergraduate Institutions

Source of Support: NSF-DUE-CCLI-A&I and the Ohio Board of Regents Investment Fund

Total Award Amount: $200,000 + $75,000 Total Award Period Covered: 01/15/2001 - 12/31/2003

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: 0.25, 0.25, & 0.25

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Sherri R. Lovelace-Cameron, Co-PI** (continued)

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

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

Project/Proposal Title: AWARE - RUI - Collaborative Investigation of NLO Active Organometallic NanoWires by Youngstown State University and Australian National University Teams

Source of Support: NSF

Total Award Amount: $909,985 Total Award Period Covered: 3/01/2002 - 2/31/2005

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

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

Project/Proposal Title: RUI - Polarized NanoScale Organometallic Rigid-Rods for Electronics/Photonics Applications: Collaborative Materials Research Project Between the European Union and YSU Scientists.

Source of Support: NSF US-EU Materials Science Collaborations (NSF 01-105)

Total Award Amount: $1,151,856 Total Award Period Covered: 01/01/2002 - 12/31/2005

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 1 Sumr: 1

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this

Investigator: **Timothy R. Wagner, Co-PI**

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

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

Project/Proposal Title: Integration of Computer Technology into the General Chemistry Curriculum

Source of Support: NSF-DUE-CCLI-A&I

Total Award Amount: $94,945 Total Award Period Covered: 07/01/2000 - 06/30/2002

Location of Project: Youngstown State University

Person-Months Per Year Committed to the proj. Cal: Acad: 1.5 Sumr:

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

Project/Proposal Title: Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment

Source of Support: NSF-DUE-ILI #9851107

Total Award Amount: $44,600 Total Award Period Covered: 06/01/1998 – 05/31/2001

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: Acad: 0.5 Sumr:

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

Project/Proposal Title: Synthesis and X-Ray Structure Characterizations of Nitride-Fluoride Analogs to Metal Oxides

Source of Support: Research Corporation Cottrell Grant

Total Award Amount: $39,719 Total Award Period Covered: 05/15/1999 - 12/31/2001

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Cal: Acad: 3 Sumr: 2

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this

Investigator: **Timothy R. Wagner** (continued) | Other agencies (including NSF) to which this proposal has been/will

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

Project/Proposal Title: REU-Research experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities

Source of Support: NSF-CHEM-REU #0097682

Total Award Amount: $180,000 Total Award Period Covered: 06/01/2001 – 05/31/2004

Location of Project: Youngstown State University

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

Project/Proposal Title: WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions

Source of Support: NSF-DUE-CCLI-A&I and Ohio Board of Regents

Total Award Amount: $200,000 + $75,000 Total Award Period Covered: 01/01/2000 - 12/31/2003

Location of Project: Youngstown State University and a Consortium of 22 other Predominantly Undergraduate Institutions

Person-Months Per Year Committed to the Cal: 2.0 Acad: Sumr:

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

Current and Pending Support

See GPG Section II.D.8 for guidance on information to include on this form.)

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

Investigator: **Hunter, Curtin, and Lovelace-Cameron** | Other agencies (including NSF) to which this proposal has been/will be submitted.

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

Project/Proposal Title: RUI - Purchase of Light Scattering Instrumentation for NanoScale Materials Characterization

{Note: This system will be used to determine the absolute molecular weights, molecular geometries in solution, degrees of aggregation, etc. It will support the research projects of Hunter, Curtin, and Lovelace-Cameron as well as well over a half dozen other faculty and students from YSU whose research interests span the range of organic and analytical/environmental chemistry and molecular biology. ***Because of the differences in the breadth of the target audiences to be served as well as space constraints, this was written as a separate CRIF application.****}*

Source of Support: NSF-CHEM-CRIF

Total Award Amount: $94,970 Total Award Period Covered: 01/01/2002 - 12/31/2004

Location of Project: YSU

Person-Months Per Year Committed to the Project. Cal: 0.1 Acad: Sumr:

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

NSF Form 1239 (7/95) USE ADDITIONAL SHEETS AS NECESSARY

SECTION H: Facilities, Equipment, and Other Resources

H1. Laboratory Facilities: The Youngstown State University Chemistry, Biology, and Physics Departments are located in the Ward Beecher Hall (i.e., on the top, middle, and bottom two floors, respectively) which is directly adjacent to the Engineering Science building. Ward Beecher Hall was originally built in the mid-1960s, was extensively upgraded in the mid-1980s, and plans are currently in place and partial funding identified for the building of a substantial extension and/or new building emphasizing research facilities in 2005. The labs and instrumentation rooms to be used by PI's, Co-PI's, and major users' students on this project are all located adjacent to one another on the south end of this building. Each student has their own desk and keyed access to science computer labs housing forty workstations in Chemistry with a similar number in Biology an in other departments. These computers have an exceptional range of software {including: NMR prediction software, PC Spartan Pro, SHELX-TL software for diffraction analysis, online access to the holdings of OhioLink which includes almost all chemistry journals, and software for remote control of the university's LC-MS and diffractometer instruments}. We have approximately 1.5 fume cupboards dedicated to research per "wet chemistry" research student and thus are well equipped in this regard. It is noteworthy that like the proposed multi-purpose teaching/research vacuum line systems requested for the advanced synthesis lab, these fume cupboards are also shared between teaching and student research and are shared by the inorganic/organometallic research group as well as by other areas of emphasis at YSU.

H2. YSU Instrumentation: Youngstown State University has two closely related instrumentation centers. The YSU Center for Biomedical and Environmental Research, YSU-CBER, is housed on the 4th floor of the Ward Beecher science hall and specializes in instrumentation for the characterization of biological and macromolecular materials. The YSU Structure & Chemical Instrumentation Center, YSU-S&CIC, is housed on the 5th floor of the Ward Beecher science hall and specializes in the characterization of non-biological materials. The two centers work closely together, sharing both staff, faculty participants, and instrumentation funding. Both centers were established to serve the teaching and research needs of faculty and students from YSU and other PUIs and to help meet the needs of users from local governmental organizations and industry (in that priority). They have a full time PhD Scientist, Bruce Levison (with a PhD in chemistry and nearly 15 years of post-graduate experience with analytical instrumentation), to assist with data collection and analysis, 0.75 of a full time Instrumentation Service Specialist, Ray Hoff (with a BS in Physics and a dozen years university instrumentation service experience), a new full time electronics technician (see below), trained undergraduate and MS student assistants to run the instruments and collect data for infrequent users, and faculty advisors to assist with instrumentation operation and experiment development (10 individuals).

The major instruments in these centers are all research grade and were purchased with a combination of NSF, Foundation, State, and internal funds with the PI or Co-PIs on the current proposal as the PI in each case. In addition to the smaller GC-MS (2 new instruments), chromatographic, spectroscopic, physical, and analytical instruments expected at any MS level institution, we are equipped with a particularly wide range of advanced instrumentation. *A general advantage of having all of these systems is that there is plentiful instrument time available. In turn, this means that the students can spend the amount of time on each instrument needed to get to know it well and to take it to its full capabilities. The students learn to use this instrumentation in their Junior and Senior labs which means that research time is spent primarily on honing skills and collecting research data.* We have a Bruker Daltonics Esquire LC-MS instrument with an autosampler and a Solid Phase Micro Extraction, SPME, interface

and both Electro-Spray, ESI, and Atmospheric Pressure Chemical Ionization, APCI, inlets. This instrument can be run from remote locations over the WEB. YSU was the first Bruker Esquire customer to accomplish the remote control of this LC-MS instrument (see Section I(e)). *This instrument is ideal for analyzing inorganic and organometallic materials and organic and biological macromolecules too involatile for a conventional direct insertion MS. In particular, they are excellent for high molecular weight species and oligomers and for materials ranging from relatively non-polar organic species to biological materials such as proteins and glycoproteins. Their $(MS)^n$ capabilities will be used to provide structural information on many of the systems described in Section C. The combination of this electrospray ion trap LC-MS with the proposed HPLC-Light Scattering System will provide a powerful and synergic combination of tools for the characterization molecular weights, molecular weight distributions, an compositions of macromolecular materials, whether they be of synthetic, environmental, or biologic origin.* We have a substantially upgraded Varian Gemini-2000 400 MHz multinuclear NMR with four probes (i.e., 5 m and 10 mm VT broadband probes, the Quadruply Tuned PFG probe, and the Inverse Detection probes), Variable Temperature, VT, Inverse Detection, and Pulsed Field Gradient, PFG, accessories, and several work stations. *This instrument is ideal for routine solution phase characterization studies for several reasons, including its high sensitivity and the solvent suppression capabilities provided by the inverse detection and Z-gradient PFG system. In addition, the students have plentiful NMR time available. Thus, having 24 hours of uninterrupted NMR time on our 400 MHz system allows a student to get results that they would never obtain in a 15 minute time slot on a triple channel 500 MHz system. The new $^{1}H/^{13}C/^{19}F/^{31}P$ Quadruply Tuned PFG probe allows our students to collect data on all of the nuclei of routine interest without having to retune the probe (unless they want to collect ^{29}Si, etc.). The Inverse probe allows them to collect the spectra of particularly insensitive nuclei such as nitrogen and metals (via ^{1}H or ^{19}F inverse detection where appropriate).* We have a TA Instrument model 2910 DSC (with quench cooling accessory for temperatures down to ≈ -160 °C) and a model 2050 TGA. *These thermal analysis instruments will be critical for monitoring the phase changes and decomposition reactions of our new materials.*

H3. YSU Diffraction Facility and the YSU-PUI Undergraduate Diffraction Consortium: The YSU Diffraction Facility has two 6 year old Bruker-AXS P4 single crystal diffractometers. One has a X-1000 multiwire area detector and a Cu tube and is used primarily for studies of organic molecules and for *qualitative* powder studies. The other has a serial detector, a LT2 low temperature system, and a Mo tube and is used for the large majority of single crystal samples. The NSF (i.e., DUE-CCLI-A&I 0087210) and the Ohio Board of Regents (i.e., OBoR-AF #491) have just funded our proposal "WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions") and these funds will be used to purchase a Bruker-AXS APEX CCD diffractometer (or equivalent for June 2001 installation). This will be used by faculty and students from the two dozen PUI institutions who are members of the **YSU-PUI Undergraduate Diffraction Consortium**. It is housed at YSU and external users will be able to use the instrument on site or mail in crystals mounted on brass pins or for selection at YSU (depending on their level of expertise). These will be mounted and centered on the diffractometer by YSU staff and the external users will then be able to fully control the instrument from their home institution for their classes or research. There will also be WEB cameras in the lab and in the diffractometer radiation enclosure to monitor its operation. *One of the primary purposes of the inert atmosphere glove box in the current proposal will be to facilitate the growth and mounting of the most air sensitive crystals by both YSU students and faculty and by those visiting from the YSU-PUI consortium.*

H4. Equipment Maintenance: A surprisingly common *perception* is that Predominantly

Undergraduate Institution's do not have the expertise and resources to adequately maintain advanced instrumentation and ensure its continued utilization after the initial grant period. While there may occasionally be some truth to this perception in specific cases, Youngstown State University has had an exemplary record with the maintenance of its advanced instrumentation with a level of "down time" as good as the PhD schools in our region. [Note: This topic is also briefly discussed in the Budget Justification Section.]

During the early 1990s, the instrumentation in the YSU Chemistry Department was maintained by faculty, by staff borrowed from the university electronics and mechanical shops, and by service calls from the instrument vendors and third party service companies (e.g., MR Resources). As the breadth and sophistication of the department's instrument holdings increased, so did the cash resources allocated to instrument support and maintenance. For example, a new College of Arts & Science computer staff of three individuals was added that provides resources for the networking and maintenance of our computer networks. In 1998, the instrumentation holdings of the YSU-S&CIC and CBER (see H2 and H3, above, and Section H) became sufficiently large that it made economic and professional sense to hire an experienced and dedicated instrumentation/electronics specialist. To this end, we hired Mr. Ray Hoff (see Section E), an individual with a BS in Physics and more than a decade of professional experience in this field, most recently, in the Tulane University Chemistry Department. Staff are seldom directly involved in maintenance any more. The following year, we hired a second full time senior staff member for our instrumentation centers, Bruce Levison, a PhD analytical chemist with over a decade's experience in academia and industry. Both of these individuals are on the university's professional/administrative track, which is parallel to the academic track, and which command salaries and benefits comparable to senior associate/junior full professors. Where they require it, these two professionals can borrow personnel and resources from other bodies on campus including our computer centers and electronics shop. When we purchase items of major equipment, one or both of these individuals are typically sent to the manufacturer's factory maintenance technician training program (e.g., most recently to the Finnegan GC-MS program and the Bruker-Daltonics LC-MS program and this coming Summer/Fall to the Bruker-AXS diffractometer training program). For major problems and/or when time is critical, we have a budget sufficiently large that it allows us to bring in vendors' maintenance staffs.

This technical training process has been so successful that YSU acts as a maintenance resource for regional PUIs (i.e., as part of our service mission) and Ray and Bruce have even been "lent" to Bruker-Daltonics to do LC-MS installation work at PhD schools in Northern Ohio. Indeed, we and Bruker have a formal understanding for their further employment when these do not conflict with their YSU duties!!! As a reflection of the confidence which Ohio's PhD granting universities hold in YSU's skills at instrument operation and maintenance, it is worth noting that we are the designated PUI representative on the Ohio MS, NMR, and X-Ray Diffraction consortia with the PI of this MRI proposal serving on their governing boards. It is also noteworthy that YSU was the first Bruker-Daltonics customer to make its Esquire LC-MS accessible over the internet. Further, Bruker-Daltonics and the Ohio MS Consortium chose to hold its Esquire training session for its Northern members, including Kent State University, the University of Akron, and University of Toledo, at YSU (see Section I(e)).

For minor maintenance tasks (especially on smaller equipment) we also make use of paid undergraduate and masters students from our analytical chemistry program. These students also carry out the routine "service" tasks running samples submitted by faculty and students who are only occasional users. These students are essentially involved in internal internships to prepare them for the varied roles they will face as professional analytical chemists in industry.

As the university's instrumentation holdings increase, so will the university's financial commitment to their maintenance and operation. Indeed, we currently have a proposal before the

YSU Foundation (the holder of the universities substantial endowment) for the hiring of several additional BS, MS, and PhD level maintenance and scientific staff for our instrumentation centers (i.e., via endowed positions). We expect that these new permanent staff positions will be funded this coming year and will give us an instrumentation support and operations staff equivalent to that of many PhD programs. Indeed, the department was just informed that we will be able to hire an additional full time electronics technician to help with increasing maintenance workload. On those rare occasions when outside service technicians are required, we have always been *immediately* authorized to bring them in. For example, the Dean of College of Arts and Sciences gave us an *open authorization* to cover *all* costs when the used magnet on our NMR quenched last year (this only took a single phone call)!

H5. Equipment Access: YSU has a policy of no-charge access to undergraduate students from YSU and other Predominantly Undergraduate Institutions to all of its instrumentation for both teaching and research. Indeed, over two dozen PUIs are actively involved in various YSU-PUI instrumentation consortia. For the instrumentation to be purchased from this current MRI grant, priority for access will be given to undergraduate and masters students for their research and coursework (in that order and with external PUI users having equal priority) followed by YSU and other PUI faculty. Our only direct user charge is that major instrumentation users are expected to request funding in major external grants for replacement parts (e.g., circuit boards and X-ray tubes) from the funding agency *in lieu* of hourly access charges. In all other cases, the YSU administration has made the decision to fund student access from internal sources so that our instruments will be used as widely as possible. We believe this to be an excellent way to raise our University's profile in the region and nationally, to justify a more complete range of instrumentation, and to attract bachelors and masters students to our programs (i.e., from 2 and 4 year colleges, respectively)! We also believe that this policy removes a tremendous paper work burden on faculty, staff, and students and also means that we don't have to officially distinguish between research and educational uses of the instruments.

H5. Inert Atmosphere Equipment: As described in detail in the Budget Justification Section F, YSU currently has two very basic Vacuum Atmospheres HE-43 Inert Atmosphere Glove Boxes. At least one is older than the typical student using it and the other was purchased two years ago as a used system of uncertain (but not recent) age. Although state of the art 25 years ago, neither of these systems would be considered "research grade" in a modern materials chemistry/science lab. One was recently purchased using DUE funds and thus is to be dedicated to instructional purposes in the teaching labs during the academic year (and for the handling of protic solvents during the summer when these labs are not in session). While heavily used, the other is no longer suitable for the many demands put upon it, especially the combined needs of 4 research groups for the handling of air sensitive solids in the absence of solvents, for synthetic studies, and for analytical studies. Neither has "modern/research grade" accessories such as a low temperature freezer, cold well, water and oxygen meters, atmosphere cooler and solvent removal system, etc. The Project Description and Budget Justification Sections describe our plans for upgrading our glove box capabilities. As for vacuum lines, both our inorganic and organometallic teaching and research students (whose numbers have grown 5 fold in the last 5 years) are massively underserved in this area, always being forced to share vacuum lines with multiple other individuals, especially during the December/January intersession and the summer, our most intensive research times. The provision of a well equipped (and shared!) advanced synthesis labs with 10 complete vacuum line sets will facilitate both our advanced lab courses and the student-researchers who use this space year round, especially during the bulge periods.

SECTION I1: RUI IMPACT STATEMENT

The Situation at Predominantly Undergraduate Institutions, PUIs: PUIs have significantly different emphases in their missions than do PhD granting research universities. In general, their mission is more heavily focused on undergraduate students and less on graduate research. In many cases, PUIs also have a greater level of support/encouragement for the scholarship of teaching. This difference in missions is reflected in many areas, including: teaching loads that are typically much higher than at larger universities, smaller class sizes with fewer advanced offerings, and an emphasis on undergraduates as the primary research personnel. In addition, the trend across the country at PUIs is get all undergraduates involved in research like laboratory experiences and in publishable research projects. This research involvement is extremely beneficial to the students but it is also very time consuming for the faculty. This combination of factors has been widely recognized to lower the productivity of undergraduate faculty *in terms of publication rate*. However, it does have a more positive side in that it does tend to allow/encourage: a greater degree of one on one interactions with undergraduates, more experimentation with novel approaches to teaching, more interest in the scholarship of teaching, and more emphasis on the integration of teaching and research.

Youngstown: Youngstown is a mid size urban center located in Northeast Ohio approximately half way between Cleveland and Pittsburgh. It has only recently begun to recover from the collapse of its heavy industry industrial base (especially steel making) in the 1970s. The five county area in Northeastern Ohio and Northwestern PA from which most of our students are drawn has the lowest average per capita income of any of Ohio's urban centers and YSU is the largest institution of higher education in this region. YSU is playing a central role in the economic renewal of our region and community service is one of YSU's three primary goals (i.e., it is synergic with education and research). We work closely with regional employers, governmental organizations, and school systems.

Youngstown State University: Youngstown State University is an urban PUI situated in the heart of downtown Youngstown that is in many ways typical of larger MS granting public Universities. It has approximately 12,000 undergraduates (51% female, 9% under-represented minority, and 26% non-traditional) enrolled in 1 and 2 year associate degrees (more commonly found at community colleges) and in 4 year bachelors degrees from our Colleges of Arts & Sciences, Business, Education, Engineering, Fine & Performing Arts, and Health & Human Services. YSU has approximately two dozen MS level programs (including those in Biology, Chemistry, and Math) enrolling approximately 1,200 students (primarily in the college of education) but offers no PhDs. YSU is an *open enrollment commuter institution* (more than 90% of our students live off campus). Reflecting our region's blue collar roots, the typical YSU student is in the first generation of their family to attend college and works an average of 30 hours per week to support their studies. Our students are a relatively hard working and motivated group, but this combination of factors significantly impacts our ability to get them involved in research.

Collaborating Colleges and Universities in the YSU-PUI Undergraduate Diffraction Consortium: Approximately two dozen PUIs collaborate with YSU for routine access to our instrumentation facilities, see Section I2 for a partial listing. They represent the range of such institutions in the US and include a community college, three historically black institutions, both small and larger public BS and MS granting institutions, and both relatively open enrollment and highly selective liberal arts colleges. Although they have different geographical locations, target populations, and histories they share a common mission which puts undergraduate education (in both formal classes and as research projects) as their top priority.

Encouraging Undergraduates to Participate in Research: Undergraduate research is a core component of this educational process. As with other PUIs, YSU is participating in the national trend to encourage greater research participation by all students. At YSU, the General Education program (on which committee the PI served until 06/01/2000) has been entirely restructured and it was first implemented in the Fall of 2000. One aspect of this change has been to very strongly encourage all lab

(and to the extent possible, lecture) courses to follow a *discovery oriented collaborative research model*. This is facilitated by the small size of our upper level labs and courses (i.e., 5 to 25 students). In addition, many (and eventually all) science labs even at the freshman/sophomore levels are being restructured to integrate research like (or even real research) projects with the more traditional skills oriented exercises. Finally, YSU now requires all bachelors students to complete a capstone course which integrates research, written and oral communication, and critical thinking components. In the sciences, this course will typically be a undergraduate research project coupled to a course that gives formal training in how to carry out and write up research projects in the discipline. Although each of the partner institutions is encouraging undergraduate research by its own combination of methods, the results are similar: an increasing proportion of all undergraduate science majors now complete at least one research project as an integral part of their undergraduate experience. For these projects to be of maximum benefit, the students need *routine* access to the appropriate instrumentation. We are currently doing this with our research grade MS, NMR, and X-ray diffraction, etc., facilities* and will do so with the proposed instrumentation as well.

The Research Situation in Chemistry Departments: As on most PUI campuses, the YSU Chemistry Department is considered one of the strongest on campus and the administration holds it up as the model of how to integrate scholarship, teaching, and service in a synergic fashion. With 15 full time faculty positions (divided between its Biochemistry, Analytical, Inorganic, Organic, and Physical Divisions and its new Chemical Education Division) and several affiliated scholars, it is large enough to support the operation and maintenance of the proposed instrumentation, see Section H. Chemistry research is very dependent on having access to appropriate instrumentation and, because of cost considerations, much of this needs to be shared between institutions. With its strong track record in this regard, YSU is an ideal home for the proposed instrumentation.

Recent Changes in the YSU Chemistry Department: 10 of the YSU Chemistry Department's 15 faculty have been at YSU for 9 years or less. This, coupled with the strong support of the senior and retired faculty and a total replacement of the administration, has enabled a dramatic change in our department's activities and profile. A decade ago, the scale of externally funded research in our department was limited (largely due to administrative impediments and excessive teaching loads) and was concentrated in the Analytical and Physical Divisions. With our rejuvenation, almost all faculty are now involved in research. Both our publication rates and our success at raising external funding to support this effort have increased dramatically (e.g., by more than an order of magnitude for external grants). The PI and the Department have been particularly successful in funding state of the art instrumentation for use in our courses and student research projects. Similar transitions are now occurring at many of the participating PUIs as the "bulge" of faculty hired in the late sixties and early seventies are replaced after their retirements. The PI, Co-PIs, and major users on this proposal have all applied for, and almost all received, external research grants (most commonly from Research Corporation and/or ACS-PRF Type B) over the last several years and are now beginning to apply for major grants from NSF, NIH, etc.† The requested equipment will increase our

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* Such access has the most student impact when obtained "hands on" and this is what YSU strives to give our students (a process that is facilitated by the relatively large size of our BS and MS programs and the very high priority the YSU administration gives this goal). When financial and/or other considerations prevent an institution from having the requisite instrumentation on site, the next best thing is a combination of site visits/field trips and remote access. The latter can be accomplished using mailed samples in two ways. In the more familiar, data collection is carried out by local staff and emailed back to the remote PUI for data processing there. More recently, it has become possible to run remote instruments over the WEB after the sample is physically mounted by local staff. YSU serves our PUI partners in each of these ways and is leading in the implementation of the remote access paradigm for PUI instrumentation access (e.g., for LC-MS and diffractometers, see Sections H and I(e)).

† Discussions by the PI with program officers from NSF, NIH, PRF, and Research Corporation at the recent Council for Undergraduate Research meeting in Wooster (June 21st, 2000) indicated that YSU has one of the most rapidly rising rates

ability to carry out competitive materials and macromolecular research and to win such grants.

The Chemistry Program at YSU: Our department graduates approximately 30 – 40 BA and BS majors in Chemistry and 5 –10 MS students each year. YSU is in the top 5% of BS and MS institutions nationally in terms of the number of our students who go on to complete PhD degrees elsewhere.* Our students have developed an *extremely strong regional and growing national reputation* for the quality of their preparation for either graduate school or industry. As part of our new General Education program, and reflecting the simultaneous change from quarters to semesters, we have fundamentally revised our undergraduate and MS course sequences. For example, our BA and ACS approved BS students will now complete all of their required courses in their first three years. This will leave our Seniors free to focus on research like laboratory courses, undergraduate research projects, and (for many) internship experiences. This should significantly enhance the integration of their teaching and research experiences and the extent of their evolvement in research. We have decreased the formal course load which our MS students are required to take and rearranged our offerings so that the students will be able to complete them in their first year (rather than the 5 quarters typical now). We have also instituted more formal training in chemical safety, research, writing, and presentations. Again, this combination should significantly increase their research productivity. Finally, we have always had several less formal programs to support the professional development needs of regional teachers. We are now instituting more formal programs, including: a new College of Arts and Sciences/College of Education program for pre-service teachers and new masters level programs for in-service teachers. The masters programs will include a part time MS in Chemistry with a Chemical Education Emphasis. During 2000/2001, this pilot program started with 6 teachers and 14 more have indicated a desire to enroll during the coming year. This research based MS program is a part time degree offered only to in service teachers. It will require the same core "content" courses as our other MS programs but will also include three Chemical Education courses and their theses will have both Chem. Ed. and disciplinary research components. As described in Section H, YSU has an exceptional range of research instrumentation for a MS level institution that facilitates our students' involvement in advanced research and educational projects. The other YSU Science programs have undergone similar revitalizations. For example, the Biological Sciences program serves a similar number of MS but a much larger number of BS majors.

The Long Term Research Funding Strategy in the YSU Chemistry Department: As described elsewhere in this section and this proposal, the number and quality of students participating in research as well as the research emphasis of the faculty have increased dramatically in the last few years. In the first few years of this renewal effort, this research and the requisite equipment was almost entirely internally funded (not atypical for a PUI where internal funds to maintain a small group of undergraduates were readily obtained). However, for synthetic and especially materials chemists, the research equipment situation was quite poor. For example, the NMR we used to characterize our research products on campus was a 60 MHz ^{1}H CW system and little modern equipment other than a FT-IR and GC-MS was available. Most product characterization had to be done at adjacent schools

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of proposal pressure and external grants success in the US. This is particularly notable because proposal pressure from most PUIs has dropped substantially (by up to 50% for many programs) in the last decade.

* The NSF WebCaspar data base at http://caspar.nsf.gov/cgi-bin/WebIC.exe indicates that for the 1987-1996 decade there were about 450 institutions (out of the approximately 455 Carnegie Comprehensive I Universities, Public and Private) whose students went on to complete PhDs in Chemistry. Of these, YSU was in the top 20, sending 25 students on to complete PhD degrees in Chemistry compared to a maximum of 44 at the top ranked school and 430 institutions with 20 or fewer! Since that time, total enrolment in chemistry undergraduate and masters programs and the number of students going on to PhD degrees at YSU has grown significantly and we expect our national ranking to increase substantially for the current decade.. We believe that, in large part, this growth is due to substantially increased undergraduate participation in research and due to greater excitement about chemistry developed when our students *routinely* use research grade instrumentation for both research and teaching.

with the consequent disadvantages and disincentives this brings. In the mid 1990's, we went through and extended self analysis and planning effort that resulted in a new (and amazingly influential given the usual fate of such things) Departmental Mission and Goals Statement. It was realized that we needed to increase the scale and quality of our research efforts, move our department's research from an internally funded to an externally funded model, revamp our program to embody the best of current educational practices and to encourage much greater student research participation, and raise the national profile of the department. With the many changes that such an effort would require at the personal, departmental, and college levels, we realized that all of these things could not be done at once and had to be prioritized and scheduled. We looked at the opportunities and impediments on campus, at the experience of other PUIs that had made this transition, and at feedback from outside consultants. Based on these considerations, we decided that:

- Increasing the quality of our undergraduate and MS teaching practices, courses, programs, and student experiences had to take first priority. This was both because the mission of a PUI such as YSU puts such educational issues as the top priority and because new faculty are much more willing to invest the time and energy to radically restructure these since they have little invested in the traditional approaches and they would then have decades to reap the benefits. These efforts accelerated until the late 1990's but most of the requisite changes have now been put into place. Major benefits of this early effort was a rapid increase in the size and quality of our undergraduate and MS research population as well as a growing national profile as a leading PUI.
- To employ the best approaches to integrated undergraduate "lecture ↔ lab" instruction and to enable modern "cutting edge" research to be carried out would require access to advanced instrumentation typically associated with PhD granting rather than PUI schools. This would ideally be located on campus so that students could use it routinely and be "immersed" in it. This would require a large amount of capital funding as well as new budget lines for the operation and maintenance of this equipment. Further, much of this instrumentation would have to be in place before many of the faculty members research projects moved from the pilot to the full scale execution phase. Upon this realization, we and the administration made it a very high priority to assemble at YSU (under the YSU-S&CIC and YSU-CBER) a full range of research grade equipment more typical of that found at a small-moderate PhD granting department. To this end, the Chemistry Department traded in one faculty line and one stores clerk line to hire an experienced Electronic Instrumentation Specialist, Ray Hoff, on a permanent staff line (at a salary greater than half the chemistry faculty!) to oversee instrument maintenance and remove it from the faculty work loads. The Biology Department did something similar to hire Dr. Bruce Levison at a senior level to oversee user services such as training and service operation. Because of the measurable success of these individuals, the decision has been made by YSU to hire three further MS level instrumentation support. A similarly important decision was that internal instrumentation funding would be transformed into matching funding (i.e., external matching funds are now automatic) as this external peer process would sharpen our grant writing skills, stretch our dollars, and help spread knowledge of our department. This process has now passed its peak and is into the plateau phase. Thus, we are now no longer funding general equipment such as MS, NMR, and X-ray diffraction systems but those more directed to specific research foci of our faculty teams.
- The large majority of our faculty were new and did not have independent research and/or funding track records. At this early stage, it was decided that new faculty energies should be concentrated on their teaching duties with their research being funded internally (perhaps not fully correctly in retrospect). Thus, internal funds were made available sufficient for small research groups of several undergraduates and MS students/faculty member. All of the tenured faculty's programs have now reached the stage where they clearly merit external funding and most have obtained their first or second external grants from agencies like the ACS-PRF or Research Corporation (i.e., those that emphasize "starter" grants to new PUI faculty). The department has also received its first REU site

grant. Many of these projects have now shown enough results that they merit major external grants and the Faculty are now starting to apply for and get NIH and NSF grants for both conventional disciplinary and chemical education research.

- In the current CRIF proposal we are seeking NSF funding for specialized, but shared use, instrumentation to support the research programs of our new(ish) faculty with common interests and instrumentation needs in inorganic/organometallic materials chemistry/research. Besides the internal funding which supports many of the students on these projects, they also received the first or second round of ACS-PRF, Research Corporation, and NSF research grants in the last 2 years.

The Faculty's Scholarly Programs: Each of the participating faculty (see Sections C) has needs for the requested items of instrumentation. The core materials group at YSU (Hunter, Bretz, Curtin, Lovelace-Cameron, and Wagner along with their external Chemistry, Physics, and Materials and Internal Physics and Engineering collaborators) will each be heavy users of all three items of equipment for their teaching and research. Thus, they will use the **synthetic glove box** to synthesize, purify, crystallize, and/or characterize their air sensitive organometallic/inorganic materials. These new materials will be electrochemically characterized using cyclic voltammetry and bulk electrolysis and, in many cases, using more advanced techniques such as the rotating disk electrode and electrochemical quartz microbalance studies in the **analytical glove box**. Most of this electrochemical work (with the exception of those experiments using the dropping mercury electrode) will be carried out in the inert atmosphere glove box. The glove boxes will be used to a limited extent by our organic chemistry group and will be used heavily to grow and mount single crystals by YSU faculty and students and those from our consortium partners. Each of the faculty's students will also make heavy use of the requested lab set of **vacuum line systems**.

Why Not Use Similar Instrumentation at Other Universities?: The *routine* integration into student research and coursework and, indeed, their proposed materials chemistry/science research projects, requires access to the proposed systems on a daily basis. While these research groups might have sufficient demand to justify one of these glove boxes for their sole use it would not be optimum for the varied requirements within the group (i.e., for synthesis, for analytical applications, for solvent free applications, for protic solvent applications), their aggregate demand justifies having several glove boxes each optimized for a particular purpose and will keep these instruments heavily used.

Educational Impact: Each of requested pieces of instrumentation will be used mainly in undergraduate research projects (approximately 2 dozen students in chemistry each year) during the academic year (i.e., Chemistry 4850 and 4850L, Chemistry Research, our required capstone course) and during the December/January intersession and summers (i.e., as part of our new REU site or on projects funded through other grants). The next largest user group will be our masters students which include up to dozen students in the Materials Group. We also will have several minority high school students (often part of our YSU-ACS SEED program) doing research with us each year. The main YSU undergraduate laboratory courses that will be impacted by this instrumentation each year (where they will be employed during some periods of the day) are shown below.[☼] All of these courses are taught by the PI, the Co-PIs, and/or the major users and will use the glove box system.

- Chemistry 5831, Inorganic Chemistry Lab
- Chemistry/Chemical Engineering 5861, Polymer Science 1: Polymer Chemistry and Plastics
- Chemistry/Chemical Engineering 5862, Polymer Science 2: Polymer Rheology, Processing, and Composites
- Chemistry Undergraduate Research

[☼] Again, it would be more difficult to justify each of these instruments by any one course or research program, however, the aggregate rationale is clear. Thus, all Chemistry majors will use each of these instruments at least twice during their degrees and approximately a third of seniors will use them during their senior research projects.

LIST OF FACULTY PARTICIPATING IN THE YSU-PUI UNDERGRADUATE DIFFRACTION CONSORTIUM

Non-YSU Faculty Participating in the YSU-PUI Undergraduate Diffraction Consortium

Name	Department	University
Al Jircitano	Chemistry	Penn State University – The Behrend College
Ed Zovinka	Math and Physical Science	Saint Francis College
Laura Hoistad	Chemistry	University of Northern Iowa
Omokere Odje	Chemistry	Central State University*
John Polo	Physics and Technology	Edinboro University of PA
George Shields	Chemistry	Hamilton College
Chase Smith	Chemistry	Holy Cross
Charles Lake	Chemistry	Indiana University of PA
Jayne Giniewicz	Physics	Indiana University of PA
John Woolcock	Chemistry	Indiana University of PA
Ron See	Chemistry	Indiana University of PA
Mike Nichols	Chemistry	John Carroll University
Paul Challen	Chemistry	John Carroll University
Terry Green	Chemistry	Lorain County Community College†
Michael Castellani	Chemistry	Marshall University
Charles Scharnberger	Earth Sciences	Millersville University
Lynn Marquez	Earth Sciences	Millersville University
Santosh Mandal	Chemistry	Morgan State University*
Kenneth Hicks	Chemistry	Norfolk State University*
Tim Usher	Chemistry	North Carolina State University
Sarah Stoll	Chemistry	Oberlin College
Neil Walsh	Chemistry	Ohio Dominican College
Cliff Berkman	Chemistry & Biochemistry	San Francisco State University
Susan Yochum	Math, Science & Computer Tech.	Seton Hill College
Rob Mauldin	Chemistry	Shawnee State University
Steve Bennett	Chemistry	Shawnee State University
Snezana Dalafave	Physics	The College of New Jersey
Melinda Greer	Chemistry	University of Dayton
Charlotte Otto	Provost's Office	University of Michigan – Dearborn
Paul Zitzewitz	Natural Sciences	University of Michigan – Dearborn
Viktor Zhdankin	Chemistry	University of Minnesota - Duluth
Vyacheslav Samoshin	Chemistry	University of the Pacific
Lee Park	Chemistry	Williams College
Mark Schofield	Chemistry	Williams College
Tom Smith	Chemistry	Williams College
David Grossie	Chemistry	Wright State University

* Historically Black University
† 2 Year Community College

YSU Faculty Participating in the YSU-PUI Undergraduate Diffraction Consortium

Individual	Department	University
Allen Hunter ♠	Chemistry	Youngstown State University
Tim Wagner ♠	Chemistry	Youngstown State University
Sherri Lovelace Cameron ♠	Chemistry	Youngstown State University
Ray Hoff ⊗	Chemistry	Youngstown State University
Bruce Levison ⊗	Biology	Youngstown State University
Mike Graham	Instructional Technology Center	Youngstown State University
Carl Johnson	Biology	Youngstown State University
Daryl Mincey ♠	Chemistry	Youngstown State University
Diana Fagan	Biology	Youngstown State University
Eric Mintz	Biology	Youngstown State University
Ikram Khawaja	Geology	Youngstown State University
Jeanette Garr	Chem. Eng.	Youngstown State University
Jeff Carroll	Physics	Youngstown State University
Jeff Dick	Geology	Youngstown State University
Jeff Smiley ♠	Chemistry	Youngstown State University
John White	Anthropology	Youngstown State University
Larry Curtin	Chemistry	Youngstown State University
Michael Serra	Chemistry	Youngstown State University
Mike Moseley	Fine Art	Youngstown State University
Peter Norris	Chemistry	Youngstown State University
Ray Beiersdorfer	Geology	Youngstown State University
Scott Martin	Civil-Environ. Eng.	Youngstown State University

♠ This individual is PI and/or Co-PI on the current MRI grant proposal.

⊗ These individuals are primarily responsible for maintenance of the equipment to be purchased from the current MRI grant proposal.

VACUUM/ATMOSPHERES
11 Sylvan Street, Suite 1
Danvers, MA 01923
(978) 762-0085
Fax: (978) 762-0091

Quote Number: 32483

QUOTE

Page

Quote To:
ALLEN HUNTER
YOUNGSTOWN STATE UNIVERSITY
1 UNIVERSITY PLAZA
YOUNGSTOWN OH 44555-3663

Phone: 330/742-7176
Fax: 330/742-1579

Date: 1/23/01
Expires: 3/24/01

Reference:

Sales Representative: Vacuum Atmospheres

Quoted by: Kenneth J O'Brien

1-23-01: Revised for requested changes
Delivery: 60 - 90 Days, ARO
Terms: Net 30 Days
FOB: Hawthorne, CA

Line	Part Number	Description	Revision	UM	Drawing
1	VAC System 32483	Consisting Of * VAC 100039, Nexus Assy, Std, 4 Port, S, 110 VAC, 60Hz, Ref: Technical Bulletin #100039 * VAC 2682-2, qty 2 pr, Butyl Rubber Gloves, L&R, 0.030" * VAC 100618, qty 1, Vacuum Pump, 6.9 CFM * VAC 100401, qty 1, Analyzer Assy, Oxygen * VAC 100088, qty 1, Analyzer Assy, Moisture * VAC 100167, qty 1, Antechamber Control Assy, Auto, Pirani, with Inert Gas * VAC 100595, qty 1, Cold Storage Assy, Refrigerator * VAC 019333, qty 1, Cold Well * VAC 100170, qty 1, Cooler Assy, Inert Gas, Left Hand Flow, Internal * VAC 016974A, qty 1, Dual Pressure Relief Bubbler * VAC 100626, qty 2, Interface Assy, 20 amp, 5-way Binding Post * VAC 014599, qty 1, Regulator Kit, Bottle Gas		EA	

VACUUM/ATMOSPHERES
11 Sylvan Street, Suite 1
Danvers, MA 01923
(978) 762-0085
Fax: (978) 762-0091

Quote Number: 32483

QUOTE

Quote To:
ALLEN HUNTER
YOUNGSTOWN STATE UNIVERSITY
1 UNIVERSITY PLAZA
YOUNGSTOWN OH 44555-3663

Phone. 330/742-7176
Fax: 330/742-1579

Date: 1/23/01
Expires: 3/24/01

Reference:

Sales Representative: Vacuum Atmospheres

Quoted by: Kenneth J. O'Brien

Line	Part Number	Description	Revision	UM	Drawing
		* VAC 100630, qty 1, Static Eliminator, 40", Single Length * VAC 023915, qty 1, Trap Assy, External, Solvent System price reflects a 20% Educational Discount			

Part Number: VAC System 32483

Quantity	Unit Price
1.00	49,850.00

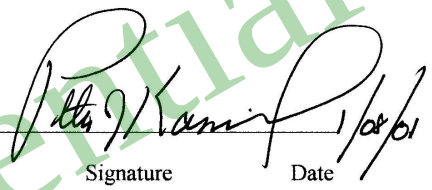
Quote Total : $49,850.00

----------Certification of RUI Eligibility----------

"By submission of this proposal, the institution hereby certifies that the originating and managing institution is an institution that offers courses leading to a bachelor's or master's degree, but has awarded an average of no more that 10 doctoral degrees per year in NSF-supported disciplines over the 2-to-5-year period preceding proposal submission."

Authorized Institutional Representative

Dr. Peter J. Kasvinsky
Dean of Graduate Studies and Research
Youngstown State University



Typed Name and Title | Signature | Date

Supplementary Documentation