

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

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Edward P Zovin	ka	PhD	199		817-472-3573	5			
NSF Form 1207 (10/99)				F	Page 1 of 2				

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		SS an *ON	
Allen D Hunter		SSN and ON F	
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Timothy R Wagner		ntia 1. ye	
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Edward P Zovinka		NS*	

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 Federal debt status, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant
Proposal Guide (GPG), NSF 00-2. 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.

Debt and Debarment Certifications

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Is the organization delinquent on any Federal debt?		Yes 📙	No 🛛
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		SIGNATUR	E				DATE
NAME/TITLE (TYPED)							
Dr. Peter J. Kasvinsky/Gra	duate Dean						05/25/00
TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS					FAX N	UMBER
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NATIONAL SCIENCE FOUNDATION Division of Undergraduate Education

NSF FORM 1295: PROJECT DATA FORM

The instructions and codes to be used in completing this form are provided in Appendix II.

- 1. Program-track to which the Proposal is submitted: CCLI-Adaptation and Implementation
- 2. Name of **Principal Investigator/Project Director** (as shown on the Cover Sheet): Hunter, Allen
- 3. Name of submitting Institution (as shown on Cover Sheet):
 - Youngstown State University
- 4. Other Institutions involved in the project's operation:

Penn State University - the Behrend College

Saint Francis College

University of Northern Iowa

Central State University

Holy Cross

Indiana University of PA

Project Data:

- A. Major Discipline Code: 12
- B. Academic Focus Level of Project: UP
- C. Highest Degree Code: M
- D. Category Code: Y
- E. Business/Industry Participation Code: NA
- F. Audience Code: WMD H T I F
- G. Institution Code: CONS
- H. Strategic Area Code: KDI
- I. Project Features: <u>1</u> <u>2</u> <u>3</u> <u>5</u>

Estimated number in each of the following categories to be directly affected by the activities of the project during its operation:

- J. Undergraduate Students: 1000
- K. Pre-college Students: 0
- L. College Faculty: <u>60</u>
- M. Pre-college Teachers: 100

NSF Form 1295 (10/98)

NATIONAL SCIENCE FOUNDATION Division of Undergraduate Education

NSF FORM 1295: PROJECT DATA FORM

(cont'd) Other Institutions involved in the project's operation: John Carroll University Lorain County Community College Millersville University Morgan State University Norfolk State University North Carolina State University Seton Hill College Shawnee State University The College of New Jersey University of Dayton University of Michigan - Dearborn University of Minnesota - Duluth University of Pacific

Williams College, Wright State University

Section A. Project Summary

Recent improvements in diffraction hardware, theory, and software, and in computers have made diffraction methods increasingly routine for scientists, engineers, and professionals in It has also made them increasingly accessible to novices such as many disciplines. undergraduates. Experience at a variety of institutions has shown that these methods can be effectively integrated into the undergraduate curriculum in a wide variety of disciplines, including: biochemistry, biology, chemistry, geology, physics, materials science, engineering, and science teacher education. Excellent curricular and lab materials are now becoming available and positive student outcomes have been demonstrated. One of the biggest impediments to integrating diffraction more widely into undergraduate coursework is the lack of hands on access to appropriate diffractometers. This CCLI proposal aims to adapt and implement several existing collaborative models from regional Predominantly Undergraduate Institutions, PUIs, and research instrumentation networks. We will establish a WEB accessible diffraction facility that will emphasize single crystal methods but with some powder capabilities. It will be dedicated to undergraduate instruction in both formal courses and undergraduate research. A CCD equipped X-ray diffractometer and accessories will be purchased and other diffraction equipment will be upgraded. This facility will be made fully accessible over the WEB so that participating PUI faculty and their students will be able to both observe and control these diffraction instruments remotely as well as access databases located at YSU. Structure solution software for use at each home site will be provided as will faculty training and curriculum implementation help for the twenty two participating PUIs. Because of the operation over a distance model proposed for instrument access, this facility will be particularly useful to faculty and students in geographically remote regions, to those from less well funded institutions, or to those whose disabilities make travel problematic.

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Sectio	on	Total No. of Pages in Section	Page No.* (Optional)*
Cover	Sheet (NSF Form 1207) (Submit Page 2 with original proposal onl	ly)	
А	Project Summary (not to exceed 1 page)	1	
В	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	9	
Е	Biographical Sketches (Not to exceed 2 pages each)	14	
F	Budget (NSF Form 1030, plus up to 3 pages of budget justification)	9	
G	Current and Pending Support (NSF Form 1239)	9	
Н	Facilities, Equipment and Other Resources (NSF Form 1363)	3	
I	Special Information/Supplementary Documentation		
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:		
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*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 including Results from Prior NSF Support

<u>C1. Results From Prior NSF Support</u>

The project participants have had several recent NSF, state, foundation, and institutionally funded educational projects, including: "instrumentation" type grants aimed at *enabling* curricular revision in multiple courses, "educational materials" type grants aimed at the *production* of specific new curricular materials, and "course development/enrichment" grants for *specific audiences*. The central goal has been to *use appropriate technology to facilitate student learning* and thus to provide *better educated and trained scientists, professionals in allied disciplines, teachers, and citizens*. Some recent accomplishments in these areas, include:¹⁻⁶

C1a. Instrumentation Grants:

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, ~\$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 Vacuum Atmospheres HE-43-2 inert atmosphere glove box.^{1a}

NSF-DUE-ILI #9551683: "Integration of GC-MS into the Undergraduate Curriculum." This grant (34,450, \approx 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 1020 Gas Chromatograph-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).^{1b,4,6}

C1b. Educational Materials Grants:

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, >\$75,000 YSU match, 2000-02, **A. Hunter** PI and **S. Lowery Bretz** Senior Personnel) officially started on May 1st, 2000. It 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.^{1c,2,3} Hunter's major coworkers on this project are a group of six high school science teachers, especially S. DiMuzio.

C1c. Course Grants:

NSF-DUE-CCLI-A&I #9981040: "Integration of Computer Technology into the General Chemistry Curriculum." This grant (\$94,945, ≈\$104,000 projected match, **T. Wagner** PI and J. Mike co-PI) will fund the purchase of 28 LabWorks II workstations for YSU's General Chemistry lab.^{1d} This project officially starts July 1st, 2000.

NSF DUE #9850079: "Investigative Approaches in the Natural Sciences." This *DUE* grant (\$183,579, ≈\$200,000 YSU match, 1998-2001, J. Usis PI, A. Hunter and C. Singler co-PIs, S. Lovelace-Cameron and S. Lowery Bretz 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. This Fall, it will be required as part of the new General Education program for all non-science/technology majors at YSU. Its approach to teaching is now influencing our main sequence courses and it is being discussed as a model course for other Ohio Universities.^{1e,3d}

C1d. Educational Outcomes of These and Related Grants:

At YSU and at our collaborating Predominantly Undergraduate Institutions, PUI's, these and

similar projects have been assessed^{7,8} and shown to have positive student outcomes. They have enabled the conversion of many lab courses away from the conventional skills oriented/verification model to discovery 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.⁹ New approaches to teaching are typically first introduced into lower enrollment labs (e.g., at the upper level and in honors and summer sections) to gain experience and be debugged. Once a new approach has demonstrated that it meets education goals, it is translated to our large enrollment courses such Quantitative Analysis, Organic Chemistry, and General/Allied Health Chemistry. 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),

C2. Project Description

C2a. Goals and Objectives:

Curriculum Innovations: Convince \Rightarrow **Adapt** \Rightarrow **Implement**: 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 have a strong commitment to undergraduate education and have typically been early adopters of curriculum innovations such as research-like laboratory experiences,^{4,6b,10} collaborative learning strategies,^{4,11} and writing across the curriculum.^{5,12} However, approaches that require specialized instrumentation have been implemented more slowly at PUIs. While PUIs may be able to obtain the required capital funding, their limited operating budgets and technical support make instrument maintenance challenging.¹³

Instrument Access and Educational Effectiveness: 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.¹⁴ 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.^{3,14} 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.^{3,15} However, the impact of these instrumental methods on the curriculum and student learning can be substantially improved if these activities are coupled with *convenient and inexpensive real time remote access to the desired instrumentation over the WEB*.

Why Include Diffraction Methods in the Undergraduate Curriculum: Recent advances in diffraction hardware, theory, and software, and in computers have made diffraction methods simultaneously more powerful tools for answering scientific questions and much easier to use. For this reason, a rapidly increasing percentage of scientists, engineers, and technologists are using them as part of their repertoire of structural tools. Diffraction methods can be readily taught to undergraduates and they have been successfully integrated into the junior/senior level Biochemistry, Biology, Chemistry, Environmental Studies, Engineering, Geology, and Physics Curricula.^{2,3,15-19} They have also been used as tools to enrich courses aimed at more general audiences, including pre- and in-service teachers.^{3-6,15} Unfortunately, like superconducting NMRs, diffractometers are beyond the financial means of most PUIs to purchase and/or

maintain. Thus, most diffraction/crystallography experiments reported in the *Journal of Chemical Education*¹⁶⁻¹⁸ concentrate on theory, symmetry, dry labs, analogies, demonstrations, crystal growing exercises, and powder methods (whose instrumentation is more common²¹⁻²³ at PUIs) and relatively few involve actual student single crystal studies.^{2,3,15,16aaa,16lll} Where they are found, they typically use older instruments that are more difficult to operate and which collect data much more slowly than do newer models. They have therefore not been as widely integrated into the curricula at PUIs as they should be, especially at smaller institutions.

The central goal of this proposal is to provide access to X-ray diffraction instrumentation for the enrichment of the undergraduate curricula at participating Predominantly Undergraduate Institutions. This will be done by modernizing and expanding the PUI Diffraction Facility at the Youngstown State University host site to make it available for access over the WEB. This access will include the ability: (1) to observe everything happening in the diffraction lab via WEB cameras, (2) to video conference with those present in the lab or with other members of the consortium, and (3) and, most importantly, to control and monitor each instrument from remote sites as it *collects data on their samples*. This will enable students at remote sites to experience all aspects of the diffraction experiment, except for physically mounting the sample on the instrument, from their home institutions. There will also be workshops for the faculty users and assistance with implementing the new curricular materials:

C2b. Detailed Project Plan:

PUI Diffraction Consortia: The YSU Diffraction Consortium is based on similar regional PUI X-ray single crystal diffraction networks run by Katherine Kantardjieff^{23a} at California State Fullerton and Marcus Bond^{23b} at Southeast Missouri. It will have a central facility housing the instrumentation at YSU and local and remote access to the instruments will be provided. The governing structure, operational procedures, and outreach activities will also be directly modeled

on these two WEB accessible sites. It is also based on other remote instrumentation access groups run by the Department of Energy National Labs for electron microscopy, powder diffraction, and neutron diffraction, and synchrotron access (Dr. Camden Hubbard of the Oakridge High Temperature Materials Lab is our advisor on this).^{24,25}

Needs of the Collaborating Partners

As was noted above, to optimally integrate diffraction materials into the undergraduate curriculum, faculty at PUIs need convenient and low cost access to the appropriate instrumentation. They also need appropriate training and collaborative opportunities.

ii) PUI Diffraction Consortium

History of the Consortium: This consortium has grown out of several preexisting groups, including: the Pittsburgh Diffraction Society, the ACA Summer School Alumni, and the Ohio Diffraction Consortium. Many faculty from PUIs have been talking for the last several years about how to best integrate diffraction methods into the undergraduate curriculum^{2,3,15,19} and how to gain sufficient and timely access to the required instrumentation. This discussion led to the formation of the two current regional PUI diffraction consortia centered at California State Fullerton and at Southeast Missouri.²³ YSU was assisted in setting up the first stage of its diffraction facility by a NSF-DMR-IMR research instrumentation grant (#9403889).²⁰ This facility includes two Bruker-AXS P4 single crystal diffractometers. One is currently equipped with a Cu sealed tube source and an X-1000 multiwire area detector for powder studies and the other is equipped with a Mo sealed tube source, a serial detector, and LT-2 low temperature system for small molecule single crystal studies. These instruments have had a dramatic impact on student learning^{2,3} and undergraduate student research²⁶ at YSU. Like other research grade instrumentation at YSU (see section H), these instruments have been made accessible at no charge to visiting faculty and students from several regional PUIs when they are not in use by

YSU students and faculty. Currently, these instruments are used to essentially 100% capacity during Spring and Summer quarters and to about 50% capacity during the Fall and Winter quarters to meet the needs of YSU students and faculty for research and teaching. Much of the rest of the time is used by those from regional PUIs who commute here to use the systems. To increase the available instrument time and to provide new diffraction capabilities, this group applied unsuccessfully to last year's NSF-Chemistry Division RSEC program.²⁷ The current PUI Collaboration is a direct descendant of the education component of this RSEC grant.

Members of the Consortium: The host institution of this PUI Consortium is Youngstown State University, an open enrollment publicly supported MS level institution located in Ohio, about half way between Pittsburgh and Cleveland. The other consortium members are a very diverse group of almost two dozen PUIs, 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. This group is centered in Northeast Ohio but includes members from many states. Participating institutions include: Central State University,* College of the Holy Cross, Hiram College, Edinboro University of PA, Indiana University of Pennsylvania, John Carroll University, Lorain County Community College, Marshall University, Millersville University, Morgan State University,* Norfolk State University,* North Carolina State University, Penn State University - The Behrend College, Rollins College, Saint Francis College, Seton Hill College, Shawnee State University, The College of New Jersey, University of Dayton, University of Michigan - Dearborn, University of Minnesota - Duluth, University of Northern Iowa, University of the Pacific, Williams College, Wright State University, and Youngstown State University (* historically black Universities). Participating faculty include about four

dozen individuals at these institutions and range from people with substantial crystallographic expertise to those for whom crystallography is a new technique. To save space, the Biographical Sketches of only the PI, the co-PIs, and the Assessment and Minority Outreach Directors are appended in Section E. The names of individual faculty participants are given in Section I.

Structure of the Consortium: Dr. Hunter, the PI on this proposal and the Director of the YSU Structure Center, will be responsible for the daily operation of the consortium instrumentation. He, the co-PIs on the proposal, the Assessment Director, and the Minority Outreach Director will serve as the consortium's governing board. This group will meet at least once a year to review the annual operations, assessment, and outreach reports (prepared by Drs. Hunter, Lowery Bretz, and Lovelace-Cameron, respectively) and to set consortium policies.

iii) The Proposed YSU Diffraction Facility

Diffraction Lab: The current diffraction facility is rather cramped and, if this proposal is funded, will be moved to a remodeled 1,200 square foot facility in YSU's Ward Beecher Science Hall. This room will have space for small group interactions and video conferences, for crystal evaluation and mounting, and for the three diffractometers. It will be equipped with WEB-video conferencing facilities for long distance interaction, fixed WEB-cameras within each diffractometer safety enclosure, WEB-cameras on the crystal mounting microscope and crystal centering scopes, and pan/tilt/zoom WEB-cameras in the lab to allow complete visual access to the lab by remote users (using the same hardware and software used by the DOE for remote access to its facilities, Cam Hubbard and Cyrus Smith, advisors).²⁵ Items D1 (partial) and D4 in the Budget.

P4 Instruments: As noted above, YSU currently has two diffractometers, a Bruker P4/X-1000 multi-wire system used primarily for powder studies using Cu radiation and a Bruker P4 equipped with a serial detector and Mo radiation for small molecule work.²⁰ These instruments

are currently limited to local control. One element of this proposal is to upgrade the diffractometer control computers and software on these two systems to allow remote control from computers at other PUIs (this has been done successfully at other institutions using a variety of means, including "PC Anywhere" and similar programs along with some customized diffractometer control software). *Items D3 and parts of D1 and D4 in the Budget*.

We have considered trading one or both of these P4 systems in when we buy the CCD diffractometer. However, because of the popularity of CCD and Imaging Plate systems at research institutions and in industry, there is a glut of used point detector systems on the market (often available as gifts or selling for a few thousand dollars). We therefore feel that the pedagogical and scheduling advantages of having several different instruments on site, *one of which will be largely dedicated to meeting powder diffraction needs*, more than compensates for their minimal trade-in value.

CCD Diffractometer: We are requesting a CCD diffractometer because experience at both $PUI^{2,3,15,23}$ and research institutions^{15,28} has shown that these instruments have several advantages over serial diffractometers when large numbers of "teaching" samples need to be run. These advantages largely stem from the much higher rate at which area detector systems collect diffraction data. On good quality crystals, one can routinely collect data sets suitable for teaching purposes within 1 hour or less. One can also collect data of very high quality or data from crystals that are too small or weakly diffracting for conventional diffractometers using longer (i.e., 6 - 18 hour) data collections. This data collection speed can be especially important with samples that students prepare in a lab course, since many of these crystals are not of sufficiently high quality for routine data collection on a serial diffractometer, but are suitable for use with a CCD system.

This high data collection speed enables real data collections to be completed during a single

laboratory period. Thus, students can make the compound and grow the crystals at their PUI, evaluate crystal quality by optical microscopy, and then mount them on brass pins and mail/courier them to YSU for data collection *during the subsequent lab period*! This also permits *each student or group of students in a class to collect data on their own sample*! Finally, this will give the diffraction facility the capacity to handle the teaching and undergraduate research needs of the almost two dozen PUI partner institutions. *Item D1 in the Budget*.

Accessories: For these facilities to have the maximum pedagogical impact, the consortium will provide one of the most powerful and user friendly diffraction analysis packages, SHELXTL/XSHELL, as a site license to each of the PUI sites. It will also purchase a range of goniometer heads so that one good quality head can be assigned to the needs of each collaborating institution. *Item D1 in the Budget*. Finally, the lab will have several WEB accessible data bases including those for single crystals, macromolecules, and powders (e.g., the CCDB, Brookhaven, and ICDD data bases, respectively).

New and Improved Capabilities: With the proposed upgrades and new purchases, the YSU Diffraction Center will be able to meet the needs of its PUI consortium partners for WEB based access to single crystal diffractometers (and some powder diffraction needs) for undergraduate instruction and undergraduate student research.

iv) PUI User Access

Access: Collaborating faculty and students will be able to use all of the diffraction facilities at YSU if/when they visit in person. They can also mail/courier samples that have been grown, selected, and mounted at their home institutions. At a scheduled time, an undergraduate and/or MS student assistant at YSU will physically mount the crystal(s) on the appropriate diffractometer(s), center the crystal(s) in the X-ray beam, and then enable remote control of the diffractometer from the designated PUI IP address. The students and faculty at the remote site will then be able to remotely control the diffractometer(s) while viewing it (them) over the various WEB cameras. They will perform the diffraction experiments they desire before transferring the resulting data to their home institution over the WEB for subsequent structural analysis using the provided SHELXTL/XSHELL software. This WEB access will be provided using the software and hardware packages previously demonstrated by other shared instrumentation centers.^{14,23-25} The first priority for instrument access will be for undergraduate instruction followed by undergraduate research and then faculty research. We expect that the collaborating PUIs will use approximately 50% of the available time on each of the three diffractometers with approximately 35% of the time being used by YSU users and 15% for maintenance/new experiment development.

v) PUI Faculty Training

Training Materials: Over the first summer, the PI and co-PIs will adapt and implement diffraction experiments chosen from the literature^{2,3,15-19} suitable for meeting the range of educational needs represented in the consortium. They will then test these materials with their own students and assess the educational results (i.e., under the direction of Dr. Bretz). These materials and the assessment results will then be disseminated to other participating faculty. The **Short Course/Workshop** at YSU during the second summer of the grant period, will teach both hands-on and remote instrument operation. It will involve 6 days of intensive group and individual instruction and practice. Other training opportunities will be provided via one-on-one interactions, *WEB based tutorials*, and a biennial short course on diffraction methods. This YSU course for PUI faculty and students is modeled on the successful ACA and BCA short courses²⁹ (many of the participants in this ACA course are advising us on ours) but will have a greater emphasis on the use of diffraction methods in undergraduate instruction and research.

vi) Expected Project Outcomes

Educational Outcomes: At the completion of this project, each participating institution will have enriched the contribution that diffraction methods make to its curriculum, by offering: (1) *WEB adapted diffraction courses* emphasizing the hands-on use of diffraction methods at most schools,^{2,3,15,19,23} (2) *WEB adapted* 1 to 3 week *diffraction lab modules* that can be introduced to upper division courses such as condensed matter physics, inorganic chemistry, instrumental methods, materials science, mineralogy, organic analysis, physical chemistry, structural biology/biochemistry, etc.,^{2,3,15,18} and (3) *WEB adapted diffraction content* in lower division courses such as general chemistry and science methods for teachers.^{2,3} This change will be facilitated by integrating the new hands-on diffractometer access over the WEB and by participant's new familiarity with these techniques. These courses are taken by science, engineering/technology, and allied health majors, and by pre-and in-service teachers. A group of six in-service high school science teachers are currently helping Drs. Hunter and Bretz with this curriculum integration.

Student Research, Publications, Grants: Single crystal diffraction methods are one of the few ways an undergraduate can complete a full research project and see the results submitted for publication in a single term. In addition, the information that these methods provide can accelerate other research projects in areas as diverse as organic synthesis, materials science, and mineralogy. It is expected that this facility will be used in about four dozen formal student research projects at PUIs each year as well as in additional research-like experiences embedded within formal courses. The results will be published in peer reviewed journals and will facilitate the writing of new grant proposals. In addition, as more people become familiar with WEB access to instrumentation, it is likely to spur additional WEB based instrumentation consortia.

vii) Timetable for the Project

In Year One, the CCD instrument will be selected and installed and the senior project

participants will adapt and implement appropriate curriculum materials for testing the following winter. In **Year Two**, a summer short course on running the instruments and on using them in one's own curricula will be offered to one faculty member from each participating PUI. The assessment and minority outreach activities will be accelerated. In **Year Three**, the assessment phase of this project will be completed and the diffraction instruments will be integrated into a wider range of courses and structural research projects at participating PUIs.

viii) Facilities and Resources

Diffraction Facilities: At the completion of this project, the YSU Diffraction Center will be equipped with three WEB accessible diffractometers. One of the current P4s will be left with Cu radiation and the current multi-wire area detector, primarily to help meet powder diffraction needs (i.e., since the facility does not currently have a dedicated powder diffractometer). The second P4 will be left on Mo radiation and will be used with strongly diffracting single crystal samples or where the relative simplicity of serial diffraction data collection, despite the much longer data collection times, makes more pedagogical sense. The new CCD diffractometer will be used for real time data collection and for smaller, more weakly diffracting samples.

Support Services: In addition to the training described above, the YSU Center and other consortium members will serve as a resource base for PUI faculty and students with questions about diffraction methods in teaching and research.

C2c. Experience and Capability of the Principal Investigators:

The senior people on this proposal are all very well qualified for their proposed roles (see their Biographical Sketches) as are the dozens of users cited in the supplementary documents. The PI-PD, founded and directs the YSU Structure Center and is a founding member of three regional instrumentation networks (i.e., as the PUI representative on the Ohio MS, NMR, and X-Ray Research Instrumentation Consortia). Hunter is also very involved in the scholarship of teaching, especially via diffraction methods. The co-PIs, Laura Hoistad, Alan Jircitano, Tim Wagner, and Ed Zovinka, are all experienced crystallographers who have successfully integrated diffraction methods in their teaching and undergraduate research. The Assessment Director, Stacey Lowery Bretz, is a nationally known expert in the scholarship of teaching, especially in the area of assessment of curriculum innovations. The Minority Outreach Director, Sherri Lovelace-Cameron, has a strong track record of recruiting members of under-represented populations into the sciences. The two Project Consultants, Katherine Kantardjieff and Marcus Bond, are the directors of two established PUI Diffraction Consortia. Two advisors, Camden Hubbard and Cyrus Smith, from DOE-Oakridge, have helped to set up remote access to several DOE instrumentation facilities while the others listed in the supplementary materials are all experienced with using diffraction methods for undergraduate teaching and research.

C2d. Evaluation Plan:

Stacey Lowery Bretz will be the Director of Assessment for this project.⁷ Through both formative and summative measures, Dr. Bretz will evaluate the central goal of this project as stated on page C5 (i.e., assess both access to and enrichment of the undergraduate curriculum). Through both qualitative and quantitative measures, Dr. Bretz will assess the degree of success with respect to the expected project outcomes identified above (e.g., the impacts of this project on faculty teaching styles and content, changes in students' attitudes and goals, changes in the content and structure of student learning, and in faculty grant activity and student research output).⁸ This information will be collected from both embedded and single purpose assessment instruments, including: structured faculty and student interviews and surveys, student work products and exams, and student learning instruments. The quantitative measures will measure the magnitude of this project's success while the qualitative pieces will document the all-important context (i.e., "the hows and whys" so critical to successful dissemination and further

adaptation of the WEB diffraction consortium model). The two Project Consultants, Katherine Kantardjieff and Marcus Bond, along with Arnie Rheingold (University of Delaware), Bernie Santarsiero (Scripts Institute), Bob McDonald (University of Alberta), Cam Hubbard (HTML-Oakridge), Derek Woollins and Alex Slawin (Saint Andrews University, Scotland), John Hughes (Geology, Miami University), Simon Bott (University of Houston), Vic Young (University of Minnesota), and Mike Zaworotko (University of South Florida) have helped with developing this proposal, have broad experience with teaching crystallography, and will also contribute to the assessment phase. Dr. Lovelace-Cameron will lead the assessment of our minority outreach efforts, especially to historically black institutions, faculty, and students.

C2e. Dissemination Plan:

The outcomes of this project will be disseminated in several ways, including:

- the training of faculty from over twenty different PUI institutions in the use of this diffraction facility in undergraduate education.
- the WEB site and WEB-video broadcasting from this site to any PUI on the net.
- poster and oral presentations at regional and national American Crystallographic Association, American Chemical Society, Biennial Conference on Chemical Education, Council on Undergraduate Research, National Science Teachers Association, and Project Kaleidoscope meetings (i.e. several at each venue by 2003).
- > peer reviewed educational papers in the Journal of Chemical Education, the Chemical Educator, the Journal of College Science Teaching, the CUR Quarterly, etc., as well as research papers in ACS and other research journals.
- specialized symposia the PI is organizing/has proposed at the 2001 ACA national meeting,^{30a} the 2002 Fall ACS national meeting,^{30b} and the 2002 Pittsburgh Conference^{30c} and as a topic in the Chautauqua series.^{30d}

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C. H. L.: "A Novell X-ray Powder Diffraction Experiment," J. Chem. Educ., 1974, 51, 265. (y) Howald, J. C.; Smith, G. D.: "Crystallography - A January Term on the Properties of Crystals," J. Chem. Educ., 1976, 53, 224. (z) March, R. E.; Nordman, C. E.: "Interpretation of a Patterson Map - A Dry-Lab Experiment in X-ray Crystallography (IE)," J. Chem. Educ., 1977, 54, 318. (aa) Huebner, J. S.; Allen T. J.: "Diffraction X-rays with Photographic Film," J. Chem. Educ., 1977, 54, 751. (bb) Schenk, J.: "solving the Phase Problem in Crystal Structure Determination: A Simple Introduction to Direct Methods," J. Chem. Educ., 1979, 56, 383. (cc) Speakman, J. C.: "The Discovery of X-ray Diffraction by Crystals (SBS)," J. Chem. Educ., 1980, 57, 489. (dd) Julian, M. M.: "Crystals and X-rays: A Demonstration," J. Chem. Educ., 1980, 57, 737. (ee) Brady, K. T.: "Models as an aid to courses in crystallography and mineralogy," J. Chem. Educ., 1983, 60, 36. (ff) Enemark, J. H.: "Introducing Chemists to X-ray Diffraction Structure Determination (SYMP)," J. Chem. Educ., 1988, 65, 491. (gg) Glusker, J. P.: "Teaching Crystallography to Non-Crystallographers (SYMP)," J. Chem. Educ., 1988, 65, 474. (hh) Loehlin, J. H.; Norton, A. P.: "Crystallographic Determination of Molecular Parameters for K2SiF6: A Physical Chemistry Laboratory Experiment (SYMP), J. Chem. Educ., 1988, 65, 486. (ii) Wuenseh, B. J.: "The Teaching of Crystallography to materials Scientists and Engineers (SYMP)," J. Chem. Educ., 1988, 65, 494. (jj) Duax, W. L.: "teaching Biochemists and Pharmacologists How to Use Crystallographic Data (SYMP)," J. Chem. Educ., 1988, 65, 502. (kk) Goldstein, B. M.: "Introduction to the Crystallographic Literature: A Course for the Nonspecialist (SYMP)," J. Chem. Educ., 1988, 65, 508. (11) Glasser, L.: "Diffraction at Your Finger Tips," J. Chem. Educ., 1988, 65, 707. (mm) Chesick, J. P.: "Fourier Analysis and Structure Determination. Part III. X-ray Crystal Structure Analysis," J. Chem. Educ., 1989, 66, 413. (nn) Rodriguez, G.: Rodriguez, S.: "An X-ray Diffraction Pattern Simulator (CS)," J. Chem. Educ., 1989, 66, 648. (oo) Cooper, J. N.; Smith, D. A.; Kastner, M. E.: "The Space Group of cis-bis(ethylenediamine)bis(azido)cobalt(III) Nitrate: An Undergraduate Physical Inorganic Experiment," J. Chem. Educ., 1989, 66, 968. (pp) Kastner, M. E.: "Instructional Videotape Introduction to the Precession Camera," J. Chem. Educ., 1989, 66, 969. (qq) Segschneider, C.; Versmold, H.: "A Simple Bragg Diffraction Experiment with harmless Visible Light," J. Chem. Educ., 1990, 67, 967. (rr) Lisensky, G. C.; Kelly, T. F.; Neu, D. R.; Ellis, A. B.: "The Optical Transform: Simulating Diffraction Experiments in Introductory Courses," J. Chem. Educ., 1991, 68, 91. (ss) Spencer, B. H.; Zare, R. N.: "Direct Visualization of Bragg Diffraction with a He-Ne Laser and an Ordered Suspension of Charged Microspheres," J. Chem. Educ., 1991, 68, 97. (tt) Rosenthal, J.: "Spreadsheet Calculation for X-ray Powder Diffraction Patterns (BULLETIN)," J. Chem. Educ., 1991, 68, A285. (uu) Rodriguez, S.: "On an X-ray Diffraction Pattern Simulator (LTE)," J. Chem. Educ., 1991, 68, 969. (vv) Goldberg, S. Z.: "On an X-ray Diffraction Pattern Simulator (LTE)," J. Chem. Educ., 1991, 68, 969. (ww) Pu, Q.: "Simulation of Xray Powder Diffraction (CS)," J. Chem. Educ., 1992, 69, 815. (xx) Drake, S. R.: "Crystals in Capillary Tubes for X-ray Structural Analysis: Anaerobic Low-Temperature Handling and Sealing," J. Chem. Educ., 1993, 70, 499. (vy) D'Agostino, A. T.: "A Multitechnique Approach for Materials Characterization: Using X-Ray Diffractometry, Visible Spectroscopy, and Atomic Absorption Analysis to Determine Thin Metal Film Thickness," J. Chem. Educ., 1994, 71, 892. (zz) Potillo, L. A.; Kantardjieff, K. A.: "A Self-Paced Tutorial on the Concepts of Symmetry (CS)," J. Chem. Educ., 1995, 72, 399. (aaa) Bond, M. R.; Carrano C. J.: "Introductory Crystallography in the Advanced Inorganic Chemistry Laboratory," J. Chem. Educ., 1995, 72, 451. (bbb) Lipkowitz, K. B.; Pearl, G. M.; Robertson, D. H.; Schultz, F. A.: J. Chem. Educ., 1996, 73, 105. (ccc) Masson, B. L.: "X-

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- 20) Funded: "Acquisition of a Single Crystal X-Ray Diffractometer," T. R. Wagner, A. D. Hunter, J. A. Jackson, and R. E. Beiersdorfer, the National Science Foundation Division of Materials Research: Research at Undergraduate Institutions Program and the Ohio Board of Regents Action Fund (NSF DMR RUI 9403889 and CAP-098), \$71,199 and \$60,000, respectively, with >\$140,000 in internal match, 1994-96. http://www.as.ysu.edu/~adhunter/YSUSC/9403889.IMR.Diffractometer.pdf
- 21) Powder Diffraction Grants: NSF-DUE: #9151040, #9151089, #9151146, #9151164, #9151286, #9151549, #9152749, #9153022, #9350939, #9352151, #9451509, #9452316, #9550888, #9551926, #9552162, #9552209, #9650840, #9651022, #9751355, #9851090, #9950700, #9950729, #9952296, and #9952345. NSF-DMR-IMR #9802781
- 22) Single Crystal Diffractometer Grant: Carrano, C. J.; "X-ray Crystallography in the Undergraduate Curriculum," NSF-DUE-ILI #9151286.
- (a) Katherine Kantardjieff, Cal. State Fullerton, Department of Chemistry and Biochemistry, W. M. Keck Foundation Center for Molecular Structure (CMolS), W. M. Keck Foundation, <u>http://www-structure.llnl.gov/scaurcon99/cmols2.html</u>
 (b) Marcus Bond, Southeast Missouri State University, Department of Chemistry, NSF-DUE-CCLI-A&I 9951348 "Establishment of a WEB Accessible X-ray Diffraction Facility."
- 24) "Remote Access to Analytical Facilities via the Internet (Workshop, Dave Matty Organizer)," the Council for Undergraduate Research National Meeting, Jun 21st 25th, 2000.

- 25) (a) DOE Micromaterials Characterization Collaboratory: http://tpm.amc.anl.gov/mmc/#ANL (e.g.: http://tpm.amc.anl.gov/TPMSelect.html) (b) The Oakridge DOE High Temperature Materials Lab: http://www.ornl.gov/doe2k/tech/index.html & http://www.ornl.gov/doe2k/mmc cameras/index.html, (c) The DOE High Flux Isotope Reactor & National Synchrotron Light Source: http://www.ornl.gov/doe2k/hfir/index.html (d) The Stanford Synchrotron Research Lab, SSRL, http://wwwproject.slac.stanford.edu/hepix/Nick Sauter HEPiX talk files/v3 document.htm
- 26) See, for example: (a) Smith, C. C.; Jacyno, J. M.; Zeiter, K. K.; Parkanzky, P. D.; Paxson, C. E.; Pekelnicky, P.; Harwood, J. S.; Hunter, A. D.; Lucarelli, V. G.; Lufaso, M. W.; Cutler, H. G.: "Nitration of Cyclopentenecarboxaldehyde: Studies Toward 1-Amino-2-Nitrocyclopentanecarboxylic Acid,' *Tetrahedron Letters*, **1998**, *39*, 6617-6620. (b) Cashman, J. R.; Berkman, C. E.; Underliner, G.; Kolly, C. A.; Hunter, A. D.: "Cocaine Benzoyl Thioester: Synthesis, Kinetics of Base Hydrolysis, and Application to the Assay of Cocaine Esterases," *Chem. Res. Toxicol.*, **1998**, *11*, 895-901. (c) Landis, K. G.; Hunter, A. D.; Wagner, T. R.; Curtin, L. S.; Filler, F. L.; Jansen-Varnum, S. A: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt (Ph₂PCH₂CH₂PPh₂)M(Maleonitriledithiolate) Congeners," *Inorganica Chimica Acta*, **1998**, *282*, 155-162. (d) Wagner, T., and Styranec, T.: "Preparation and Crystal Structure Analysis of Ba2BiGa11020," *J. Solid State Chem.*, **1998**, *138*, 313-320.
- 27) Not Funded: "Advanced Diffraction Studies Consortium (ADSC): An Exciting Opportunity For Integrating Predominantly Undergraduate Institutions Into The National Research Enterprise," <u>A. D. Hunter</u>, B. M. Craven, M. D. Foster, A. A. Pinkerton, and M. Shoham, the National Science Foundation, Division of Chemistry, Research Sites for Educators in Chemistry (NSF 9974858, submitted January 11th, 1999), \$2,000,000, 1999-2004: <u>http://www.as.ysu.edu/~adhunter/YSUSC/9974858.RSEC.ADSC.pdf</u>
- 28) (a) Rheingold, A. L., University of Delaware, Department of Chemistry. (b) Zaworotko, M., University of South Florida, Department of Chemistry. (c) Young, V., University of Minnesota, Department of Crystallography. (d) Bott, S. G., University of Houston, Chemistry.
- 29) (a) The American Crystallographic Association, ACA, Crystallography Summer Course, July 7th 19th, 2000. Athens Georgia. <u>http://bcl15.bmb.uga.edu/Aca00/ACA00/page1.html</u>
 (b) The British Crystallographic Association, BCA, Intensive Course in X-Ray Structural Analysis, March 30 April 6, 2001. <u>http://crystsun1.unige.ch/iucr-top/index.html</u>
- 30) (a) Hunter, A. D. (Organizer of Symposium): "Diffraction Methods in Undergraduate and Graduate Education," American Crystallographic National Meeting, July 21st-26th, 2001, Los Angles, CA. (b) Hunter, A. D. (Organizer of Symposium): "Diffraction and Other Structural Methods in Undergraduate Education," American Chemical Society Fall National Meeting, August 18th-22nd, 2002, Boston, MA. (c) Hunter, A. D. (Organizer of Proposed Short Course): "Teaching Diffraction Methods to Novices," March 18th-22nd, 2002, New Orleans, LA. (d) Hunter, A. D. (Organizer of Proposed Short Course): "Single Crystal Diffraction Methods in the Undergraduate Curriculum," the Chautauqua Program, 2002.

Biographical Sketch for Allen D. Hunter

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a. **Professional Preparation:**

University of British Columbia, Chemistry	Honors Chemistry	BS	1981
University of British Columbia, Chemistry	Inorganic Chemistry	PhD	1985
Australian National University, RSC	Organometallic Chemistry	Post. Doc.	1986
University of Alberta, Chemistry	Crystallography	Post. Doc.	1987
b. Appointments:			
Youngstown State University, Chemistry	Full Professor	1998-I	Present
University of Pittsburgh, Crystallography	Visiting Associate Professor	199:	5-1996
Youngstown State University, Chemistry	Associate Professor	1992	2-1998
University of Alberta, Chemistry	Adjunct Professor	1992	2-1995
University of Alberta, Chemistry	Assistant Professor	198′	7-1992

c. Publications: Allen has a total of 40 peer reviewed publications (22 since 1992) and has also given 36 oral/poster presentations.

(i) Most Closely Related Publications:

- 1. Smith, C. C.; Jacyno, J. M.; Zeiter, K. K.; Parkanzky, P. D.; Paxson, C. E.; Pekelnicky, P.; Harwood, J. S.; Hunter, A. D.; Lucarelli, V. G.; Lufaso, M. W.; Cutler, H. G.: "Nitration of Cyclopentenecarboxaldehyde: Studies Toward 1-Amino-2-Nitrocyclopentanecarboxylic Acid," Tetrahedron Letters, 1998, 39, 6617-6620.
- 2. Cashman, J. R.; Berkman, C. E.; Underliner, G.; Kolly, C. A.; Hunter, A. D.: "Cocaine Benzoyl Thioester: Synthesis, Kinetics of Base Hydrolysis, and Application to the Assav of Cocaine Esterases," Chem. Res. Toxicol., 1998, 11, 895-901.
- 3. Landis, K. G.; Hunter, A. D.; Wagner, T. R.; Curtin, L. S.; Filler, F. L.; Jansen-Varnum, S. A: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: Structures Isomorphous X-Rav Crystal of the Ni. Pd. and Pt (Ph₂PCH₂CH₂PPh₂)M(Maleonitriledithiolate) Congeners," *Inorganica Chimica Acta*, **1998**, 282, 155-162.
- 4. Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," Journal of Chemical Education, 1998, 75, 1297-1299.
- 5. 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 Journal of Chemical Education, 1999, 76, 163 Newsletters, and in the ACA and IUCr see: http://www.as.ysu.edu/~adhunter/YSUSC/index.html

(ii) Other Significant Publications:

- 6. Hunter, A. D.: "A Capstone Writing Experience in Polymer Chemistry: Writing a Proposal to Management for the Purchase of New Polymer Characterization Instrumentation," Journal of Chemical Education, 1998, 75, 1424.
- 7. 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," *Journal of Chemical Education*, **1998**, 75, 891-893.

d. Synergistic Activities:

Allen's interests in the scholarship of teaching has been recognized at YSU by his being designated a Master Teacher in the College of Arts & 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, 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 is the representative for Ohio's Predominantly Undergraduate Institutions on the Ohio NMR, MS, and X-Ray Crystallography Research 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 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 with whom he collaborates on his projects.

e. Collaborators & Other Affiliations:

(i) Collaborators:

Alex Slawin, St. Andrews University (co-host for Dr. Hunter's 2000-2001 Sabbatical) Bernard Santarsiero, Scripts Institute Bryan Craven, Indiana University of Pennsylvania and the University of Pittsburgh Chase Smith, Holly Cross Derrick Woollins, St. Andrews University (co-host for Dr. Hunter's 2000-2001 Sabbatical) George Richter-Addo, University of Oklahoma Jim Adrian, Union College John Cashman, Seattle Biomedical Institute Mike Zaworotko, University of South Florida Philip Coppens, University of Buffalo Simon Bott, University of Houston Steven DiMuzio, LaBrae High School

(ii) Graduate and Post Doctoral Advisors:

Elliot Burnell (BS), University of British Columbia Peter Legzdins (PhD), University of British Columbia Martin Bennett (Post. Doc.), Australian National University Martin Cowie (Post. Doc.), University of Alberta Dietmar Seyferth (Collaborator while a Post. Doc.), M.I.T.

(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.

Biographical Sketch for Laura M. Hoistad

Department of Chemistry, University of Northern Iowa, Cedar Falls, Iowa, 50614 319-273-6139, <u>laura.hoistad@uni.edu</u>

a. Professional Preparation:				
Saint Olaf College, Chemistry	Chemistry	BA	1988	
University of Michigan, Ann Arbor, Chemistr	у	Chemistry	MS	
University of Michigan, Ann Arbor, Chemistr	у	Solid	State	
Chemistry	PhD	1993		
CNRS, Nantes, Institut de Materiaux	Solid State Chemistry	Post. Doc.	1994	
Iowa State University, Chemistry	Solid State Chemistry	Post. Doc	1996	
b. Appointments:				
University of Northern Iowa, Chemistry	Assistant Professor	1998-P	resent	
Lander University, Chemistry	Assistant Professor	1997	7-1998	
University of Northern Iowa, Chemistry	Visiting Assistant Professor	1996	5-1997	
Iowa State University - Ames, Chemistry	Adjunct Instructor		1996	

c. Publications: Laura has a total of 12 peer reviewed publications (5 since 1996) and has also given 7 oral/poster presentations.

(i) Most Closely Related Publications:

Professional Proparation.

- 1. Hong, S-T.; Hoistad, L. M.; Corbett, J. D.: "La₄₈Br₈₁Os₈: Isolated Clusters in an Unusual Superstructure with Significantly Greater Intercluster Bonding," *Inorg. Chem.*, **2000**, *39*, 98.
- Jensen, E.; Hoistad, L. M.; Corbett, J. D.: "Lanthanum and Praseodymium Bromide Pnictides. A Convergence of Interstitial Chemistry in Cluster Halides and Intermetallic Pnictides," *J. Solid State*, **1999**, *144*, 175.
- Lulei, M.; Martin, J. D.; Hoistad, L. M.; Corbett J. D.: "Two Closely Related Structures Types with Unprecedented Bioctahedral Rare-Earth Metal Clusters Centered by Transition Metals: A₂R₁₀I₁₇Z₂ (A = Rb, Cs; R = La, Ce, Pr; Z = Co, Ni, Ru, Os) and La₁₀I₁₅Os₂," *J. Am Chem. Soc.*, **1997**, *119*, 513.
- 4. Van der Lee, A.; Hoistad, L. M.; Evain, M.; Foran, B.; Lee, S.: "Resolution of the 66-Fold Superstructure of Dy₁₁Se₂₀ by X-Ray Diffraction and Second-Moment Scaled Hückel Calculations," *Chem. Mater.*, **1997**, *9*, 218.
- 5. Lee, S.; Hoistad, L. M.: "Second Moment Scaling, Metallic and Covalent Structure Rationalization and Electron Counting Rules," *J. Alloys Compd.*, **1996**, *229*, 66.

(ii) Other Significant Publications:

- 6. Hoistad, L. M.: "Structure Maps for Intermetallic Phases Using Second Moment Scaling Theory," *Inorg. Chem.*, **1995**, *34*, 2711.
- Hoistad, L. M.; Meerschaut, A.; Bonneau, P.; Rouxel, J.: "Structure Determination of the Misfit Compound (Gd_εSn_{1-ε}S)_{1.16}(NdS₂)₃," J. Solid State Chem., **1995**, 114, 435.
- 8. Meerschaut, A.; Lafond, A.; Hoistad, L. M.; Rouxel, J.: "Structure Determination and Magnetic Susceptibility of Gd_{2/3}Cr₂S₄" *J. Solid State Chem.*, **1994**, *111*, 276.
- 9. Lee, S.; Hoistad L. M.; Kampf, J.: "The Statistical Distortion in Ta_{1-x}Ti_xTe₂ and Band Calculations on Ditellurides," *New J. Chem.*, **1992**, *16*, 657.
- 10. Hoistad, L. M.; Pasternak, J.; Lee, S.: "Geometry Optimization through Second Moment Scaling," J. Am. Chem. Soc., 1992, 114, 4790.

1990

d. Synergistic Activities:

Laura's research interests lie in both the synthetic and computational aspects of solid-state chemistry. In order to pursue her scholarly activity with students, she has been granted 3 undergraduate summer stipends (1 for the summer of 1999 and 2 for the summer of 2000). The students who receive these stipends give two oral presentations and participate in a poster session at the end of the 10 week summer program. Since Laura's arrival at UNI, she has been instrumental in the development of a sophomore level descriptive inorganic chemistry course. Her work on the curriculum committee to revise the course requirements for the various bachelor degrees offered by the department placed the descriptive inorganic chemistry course as a core course requirement for all chemistry majors. Laura has also received a UNI Provost Mini-grant to develop new experiments using computer based data acquisition probes for the descriptive inorganic course.

Collaborators & Other Affiliations:

(i) Collaborators:

e.

Ken DeNault, University of Northern Iowa John D. Corbett, Iowa State University

(ii) Graduate and Post Doctoral Advisors:

Stephen Lee (PhD), Cornell University Alain Meerschaut (Post. Doc.), Institut des Materiaux de Nantes John D. Corbett (Post. Doc.), Iowa State University

(iii) Thesis and Postgraduate Scholar Sponsor:

None at the Graduate (doctoral or master's level)

Laura has directed research for 8 undergraduate students, 4 of them in the past 6 years.

Biographical Sketch for Alan J. Jircitano

Department of Chemistry, Penn. State University - The Behrend College, Erie, PA, 16563 814-898-6400, a0j@psu.edu, http://onsager.bd.psu.edu/~jircitano/index.html

a. Professional Preparation:

a. I foressional i reparation.			
Niagara University, Chemistry	Chemistry	BS	1977
University of Kansas, Chemistry	Inorganic Chemistry	PhD	1982
Ohio State University, Chemistry	Chemistry	Post. Doc.	1984
b. Appointments:			
PSU - The Behrend College, Chemistry	Associate Professor	1999-F	Present
PSU - The Behrend College, Chemistry	Assistant Professor	1984	4-1999

c. Publications: Alan has a total of 28 peer reviewed publications (19 since 1984) and has also given 32 oral/poster presentations.

(i) Most Closely Related Publications:

- Sommerer, S. O.; Friebe, T. L.; Jircitano, A. J.; MacBeth, C. E.; Abboud, K. A.: "trans-Diaquabis(2-thienyl 2-pyridyl ketone-O,N)copper(II) Tetrafluoroborate," Acta Cryst. Sec. C., 1998, C54, 178-179
- Jircitano, A. J.; Sommerer, S. O.; Abboud, K. A.: "trans-Bis[4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole-N1,N']copper(II) Bis(tetrafluoroborate)," Acta Cryst. Sec. C., 1997, C53, 434-436.
- Szczepura, L. F.; Giambra, J.; See, R. F.; Lawson, J.; Janik, R. S.; Jircitano, A. J.; Churchill, M. R.; Takeuchi, K. J.: "Crystal Structures of *trans*-[Ru(dppe)₂(CO)(Cl)](BF₄).toluene and *trans*-[Ru(dppm)₂ (CO)(Cl)](BF₄).CH₂Cl₂: A Study of the Steric and Electronic Ligand Effects of *trans*-Positioned Diphosphine Ligands," *Inorg. Chim. Acta*, 1995, 239, 77-85.
- 4. Sommerer, S. O.; Westcott, B. L.; Jircitano, A. J.; Abboud, K. A.: "The Synthesis and Structure of Two Metal-Di-2-Pyridyl Ketone Oxime Dimers," *Inorg. Chim. Acta*, **1995**, *238*, 149-153.
- 5. Jircitano, A. J.; Sommerer, S. O.; Shelley, J. J.; Westcott, B. L.; Suh, I.-H.: "The Self-Condensation of a Derivative of *o*-Aminobenzaldehyde: The Structure of the Polycyclic, Bisanhydro-Trimer," *Acta Cryst., Sec. C.*, **1994**, 50, 445-447.

d. Synergistic Activities:

Alan's research interests occur at the intersection of inorganic chemistry, crystallography, and chemical education. He feels that an undergraduate research experience is just as important a learning opportunity as any other aspect of an undergraduate's career. A research component has been part of the chemistry major at Behrend since 1989. Thirteen of Alan's students have received semester and summer support through a local grants program. The chemistry department at Behrend College has been involved with the National Conference on Undergraduate Research (NCUR) since its inception in 1987. Twenty of Alan's students have presented their work at NCUR, in addition to Behrend College's own local research conference. The chemistry department has also been involved in community outreach programs particularly as part of National Chemistry Week (NCW). The students and faculty of Behrend College have given a number of demonstrations and workshop in conjunction with NCW. For a number of years, he has offered an upper level X-ray crystallography/molecular modeling course (Chmbd 435) at Behrend College since he feels that these tools are an increasingly important aspect of chemistry and undergraduates should

get some exposure to the field. Since they do not have a diffractometer at Behrend College, there is not a laboratory component to the course. We can take field trips to view diffractometers (as we did last year to YSU), but the students miss the full impact that handson experience would give them. Having remote access to a diffractometer opens up the possibilities of allowing each student to solve a structure, including samples of their own making. Alan has been very active in the national chemical education community, including: his ACS local section, BCCE, Chautauqua, NCUR, and pKal meetings. In addition to developing new chemistry and crystallography courses, he also developed a new astronomy course.

e. Collaborators & Other Affiliations:

(i) Recent Collaborators:

Ken Takeuchi, SUNY Buffalo Khalil H. Abboud, University of Florida Lisa Szczepura, Illinois State Shaun O. Sommerer, formerly of Barry University, Florida

(ii) Graduate and Post Doctoral Advisors:

Kristin Bowman-James (PhD, formerly Kristin B, Mertes), University of Kansas Daryl H. Busch (Post. Doc.), University of Kansas (formerly at Ohio State University)

(iii) Thesis and Postgraduate Scholar Sponsor:

Alan has supervised over two dozen undergraduate student research projects.

Biographical Sketch for Sherri R. Lovelace Cameron

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:**

a. I foressional i reparation.				
Drexel University, Chemistry	Chemistry	BS		1986
University of Pittsburgh, Chemistry	Organometallic Chemistry	PhD)	1992
University of Vermont, Chemistry	Electrochemistry	Post	t. Doc.	1995
b. Appointments:			1005 0	

Youngstown State University, Chemistry

Assistant Professor

1995-Present

c. Publications: Sherri has a total of 6 peer reviewed publications and has also given 4 oral/poster presentations.

(i) Most Closely Related Publications:

- 1. Connelly, N. G.; Geiger, W. E.; Lovelace, S. R.; Metz, B; Paget, P; Winter, R.: "Reduction of $[ML(alkyne)_2(\eta-C_5R'_5)]^+$ (M=Mo or W, L=MeCN or CO, R'=H or Me, C₅R'₅=C₅HPh₄): 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(Ph₂PCH₂CH₂PPh₂)," 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 $[Mn(\eta^6-C_6H_6)(CO)_3]^+$: 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 $[Mn(\eta^{5}-C_{9}H_{7})(CO)_{3}]$ Complex and Reversible Indenyl Counterion-Controlled Comproportionation of $[Mn(\eta^5-C_9H_7)(CO)_3]$ and $[Mn(\eta^3-C_9H_7)(CO)_3]^{2-}$ To Give $[Mn(\eta^5-C_9H_7)(CO)_3]^{2-}$ C₉H₇)(CO)₃]," Organometallics, **1995**, 14, 19741982.

(ii) Other Significant Publications:

6. Chin, T. C.; Lovelace, S. R.; Geiger, W. E.; Davis, C. M.; Grimes, R. N.: "Infrared Spectroelectrochemistry of Boron-Hydrogen Stretches: A Tool for Diagnosis of Delocalization in Mixed-Valent Metallacarborane Complexes," J. Am. Chem. Soc., 1994, 116, 9359-9360.

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 combine 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.

Collaborators & Other Affiliations: (i) Collaborators:

Fola Ladipo, University of Kentucky

e.

(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 Stacey Lowery Bretz

Before July 15th, 2000:

Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI, 48128

313-593-5157, <u>slbretz@umich.edu</u>

After July 15th, 2000:

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

a. Professional Preparation:

Cornell University	Chemistry	BA	1989
Pennsylvania State University	Inorganic Chemistry	MS	1991
Cornell University	Chemical Education	PhD	1994
University of California, Berkeley	Chemical Education	Post-Doc	1995
b. Appointments:			

Youngstown State University, ChemistryAssociate ProfessorStarts: July 15th, 2000University of Michigan-Dearborn, ChemistryAssistant Professor1995-2000

c. Publications: Stacey has a total of 9 peer reviewed publications (6 since 1995 when she joined U. Michigan) and has also given 27 oral/poster presentations.

(i) Most Closely Related Publications:

- 1. Bretz, S. L. "Evaluation: An Introduction to Why and How," *CHED Newsletter*, American Chemical Society Division of Chemical Education, Spring **1997**, pp. 8-11.
- 2. Bretz, S. L. "Human Constructivism and Meaningful Learning," J. Chem. Educ., in press
- 3. Bretz, S. L.; Meinwald, J. "The Language of Chemistry," Submitted for publication *to J. Coll. Sci. Teaching.*
- 4. 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.
- Bretz, S. L. "Concept Maps: A Metacognitive Tool for Teaching Students to Learn How to Learn," <u>Chemistry in Context Instructor's Resource Guide</u>, W. C. Brown, 1997.

(ii) Other Significant Publications:

- 6. Bretz, S. L. "CiC and Concept Webs," *Chemunity News*, **1997**, 7(2), 18-19.
- Bommarito, S. L.; Lowery Bretz, S. P.; Abruña, H. D. "Homogeneous and Heterogeneous Synthesis of Redox Polymers and Copolymers of [M(4-vinyl-4'-methyl-2,2'bipyridine)3](PF6)2 (M=Ru,Os)," Synlett, 1993, 6, 375.
- Bommarito, S. L.; Lowery Bretz, S. P.; Abruña, H. D. "Synthesis and Characterization of Redox Polymers of [M(4-vinyl-4'-methyl-2,2'-bipyridine)3](PF6)2 (M=Ru,Os)," *Inorganic Chemistry*, 1992, 31, 495.
- Bommarito, S. L.; Lowery Bretz, S. P.; Abruña, H. D. "Synthesis and Characterization of Redox Copolymers of [Ru(4-vinyl-4'-methyl-2,2'-bipyridine)3]²⁺ and [Os(4-vinyl-4'-methyl-2,2'-bipyridine)3]²⁺: Unusual Energy Transfer Dynamics," *Inorganic Chemistry*, 1992, 31, 502.

d. Synergistic Activities:

Stacey's research looks broadly at the roles of assessment, evaluation, metacognition, and reflection in improving both the teaching and the learning of chemistry. Her research has included both quantitative and qualitative papers addressing meaningful learning, science literacy, curriculum design and analysis, pedagogy, and assessment, and the pertinence of these to challenges facing both the teachers and the students of college chemistry. Her participation in the NSF Systemic Initiatives for College Chemistry with both the ChemLinks

and the ModularChem Consortia has spanned the range from evaluation design to classroom testing of the modular approach to teaching chemistry in the context of real-world problems or applications. A symposium organized on theories of learning (and currently in press) has received wide acclaim in the chemical education research community. Her leadership in the scholarship of chemical education includes recognition as a Project Kaleidoscope F21 Scholar, and invitations to serve as a member of both the ACS DivCHED Committee on Chemical Education Research and the Examinations Institute Committee. Stacey is also deeply committed to improving the teaching of chemistry, from designing courses consonant with the National Science Education Standards for pre-service elementary teachers to organizing a conference funded by the Dreyfus Foundation focusing on teaching assistant training in graduate chemistry departments.

e. Collaborators & Other Affiliations:(i) Collaborators:

Angelica Stacy, University of California, Berkeley Brock Spencer, Beloit College Conrad Stanitski, University of Central Arkansas Elaine Seymour, University of Colorado Jerrold Meinwald, Cornell University Loretta Jones, University of Northern Colorado Mary Nakhleh, Purdue University Peter Atkins, Oxford University Rick Moog, Franklin & Marshall College Truman Schwartz, Macalester College William Robinson, Purdue University

(ii) Graduate and Post Doctoral Advisors:

Angelica Stacy (Post-Doctoral Advisor), University of California, Berkeley Joseph Novak (PhD Advisor), Cornell University Roald Hoffmann (PhD Co-Advisor), Cornell University Ayusman Sen (MS Advisor), Pennsylvania State University

(iii) Thesis and Postgraduate Scholar Sponsor:

None at the graduate or post-doctoral level. S. L. Bretz has mentored nine undergraduate student researchers during her tenure at the University of Michigan-Dearborn.

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 Arizona State University, Chemistry Hughes Aircraft Company Northwestern University, Materials

b. Ar

D. 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

Chemistry

Solid State Chemistry

Electron Microscopy

Radar Software

BS

PhD

Post. Doc.

1981

1986

1988

1990

Publications: Tim has a total of 8 peer reviewed publications (4 since 1992) and has also given 4 oral/poster presentations.

(i) Most Closely Related Publications:

- 1. Norris, P. and Wagner, T.: "Solution and Solid State Structure of the D-talo-2,6-anhydro-1,1bis(ethylsulfonyl)-3,4,5-trihydroxyhexane," Carbohydrate Research, 1999, 322(1-2), 147-150.
- 2. 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.
- 3. Wagner, T.; Styranec, T.: "Preparation and Crystal Structure Analysis of Ba₂BiGa₁₁O₂₀," J. Solid State Chem., 1998, 138, 313–320.
- 4. Wagner, "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type Barium Hexagallate," J. Solid State Chem., 1998, 136, 120-124.
- 5. Wagner, T.: "HREM of Electron-Beam-Induced Damage in L-Ta₂O₅," J Solid State Chem., **1991**, *91*, 189-203.

(ii) Other Significant Publications:

- 6. Wagner T.; O'Keeffe, M.: "Bond Lengths and Valences in Aluminates with the Magnetoplumbite and β-Alumina Structures," J. Solid State Chem., 1988, 73, 211-216.
- 7. Wagner T.; O'Keeffe, M.: "A Structural Model for Barium Hexagallate," J. Solid State Chem., 1988, 73, 19-26.
- 8. Wagner, T.; O'Keeffe, M.: "Electron Microscopy of Defects and Disorder in Barium Hexagallate," Acta Cryst., 1985, B41, 108-112.

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 research facility (as the PI on the DMR-IMR grant). 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 handson 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-DUE-CCLI-A&I 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, expected graduation: Summer, 2000. Tim has also served as research advisor for 15 undergraduate students.

Biographical Sketch for Edward P. Zovinka

Department of Chemistry, Saint Francis College (PA)

814-472-3373, ezovinka@sfcpa.edu, http://faculty.sfcpa.edu/ezovinka

a. Professional Preparation:

Roanoke College, Chemistry	Chemistry	BS	1987
University of California - Davis, Chemistry	Chemistry	PhD	1992
North Carolina State, Chemistry	Chemistry	Post. Doc.	1994
b. Appointments:			
Saint Francis College, Chemistry	Associate Professor	1998-I	Present
Saint Francis College, Chemistry	Assistant Professor	19	994-98
Davidson College, Chemistry	Visiting Assistant Professor		1994

c. Publications: Ed has a total of 14 peer reviewed publications (7 since 1994) and has also given 20 oral/poster presentations.

(i) Most Closely Related Publications:

- 1. Cornman, C. R.; Zovinka, E. P.; Boyajian, Y. D.; Olmstead, M. M.; Noll, B.C.: "Synthesis and Structure of a Vanadium (IV)-amide metallacyclic complex," *Inorganica Chimica Acta*, **1999**, *285*, 134-137.
- Howard, R. J.; Ropp, J. A.; Wasil, C.; Zovinka, E. P.: Rural Outreach Chemistry for Kids (R.O.C.K.) A Service Project to Involve More than Chemistry Majors in a Chemistry Club," *The Chemical Educator* http://journals.springer-ny.com/chedr 1997, 2.
- Balch, A. L.; Koerner, R.; Latos-Grazynski, L.; Lewis, J. E.; St. Claire, T. N.; Zovinka, E. P.: "Coupled Oxidation of Heme without Pyridine. Formation of Cyano Complexes of Iron Oxophlorin and 5-Oxaporphyrin (Verdoheme) from Octaethylheme," *Inorg. Chem.*, 1997, 36, 3892-3897.
- Crowder, M.; Wang, Z.; Franklin, S. L.; Zovinka, E. P.; Benkovic, S. J.: "Characterization of the Metal-binding Site of β-Lactamase from *Bacteroides fragilis*," *Biochemistry*, **1996**, *35*, 12126-12132.
- Cornman, C. R.; Zovinka, E. P., Meixner, M. H.: "Vanadium Complexes of the Active-Site Peptide of Protein Tyrosine Phosphatase 1B: V^{IV}O(VHCSAG-NH₂)_n," *Inorg. Chem.*, 1995, 34, 5099-5100.

(ii) Other Significant Publications:

- Cornman, C. R.; Zovinka, E. P.: Chapter 14 "Mechanistic Aspects of the Chemistry of N-Alkyl Porphyrins" in <u>Mechanistic Bioinorganic Chemistry</u> ACS Advances in Chemistry Series #246, Thorp, H. H. and Pecoraro, V. L.(eds.) 1995, 373-403.
- Cornman, C. R.; Zovinka, E. P.; Boyajian, Y. D.; Geiser-Bush, K. M.; Boyle, P.; Singh, P.: "Structural and EPR Studies of Vanadium Complexes of Deprotonated Amide Ligands: Effects on the ⁵¹V Nuclear Coupling Constant," *Inorg. Chem.*, **1995**, *34*, 4213-4219.

d. Synergistic Activities:

Ed has been recognized by Saint Francis College for his efforts to inculcate a more scholarly culture on the Saint Francis College campus by the awarding of the Swatsworth award after his third year on campus. The award is given to the professor that exemplifies teaching, research, and service. In addition, the Council for the Advancement and Support of Education (CASE) named Ed the 1997 Pennsylvania Professor of the Year. He has taken a leadership role on campus undergraduate research by organizing the Undergraduate Research

Discussion Group (URDG) that for the past two years has awarded \$2500 in grants to assist undergraduate research projects. He has served continuously on the faculty senate since 1996 as well as serving on the General Education committee. He is also involved in science education issues through Project Kaleidoscope (pKal) and the Council of Undergraduate Research. He was the 1998 pKal Scientist in Residence and presided over the 1998 National Assembly and Steering Committee. He has received numerous equipment grants to modernize the Saint Francis College facilities as well as the organizer of Rural Outreach Chemistry for Kids (R.O.C.K.). The ROCK program is designed to demonstrate the science can be fun and interesting through the use of hands on activities with students. The program began modestly in 1995 but has grown to average 59 events reaching over 1400 K-12 students each academic year. In addition, he has collaborated with a local high school teacher (Nancy Gobert) to initiate Little ROCK, a program where high school students are trained to visit elementary classrooms to present hands-on activities.

Collaborators & Other Affiliations:

(i) Collaborators:

e.

Lynn Maelia, Mount Saint Mary College

(ii) Graduate and Post Doctoral Advisors:

Alan Balch, (PhD) University of California, Davis

Charles R. Cornman, (Post. Doc.) North Carolina State University

Steven Benkovic, (summer of research after 1st year at Saint Francis College) Pennsylvania State University

(iii) Thesis and Postgraduate Scholar Sponsor:

Project SEED mentor to Dawn Cox

Honors Thesis Mentor to Rebecca Espenlaub

Undergraduate research advisor for 6 Saint Francis College students, all graduate or are attending or accepted into graduate school in chemistry

Page E14-Biographical Sketches

	T 1E	AR			USE ONL	v
ORGANIZATION	- •	PRO	POSAL		1	DN (months)
Youngstown State University			FUSAL	NO.	Proposed	, <u> </u>
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		۵۱۸	/ARD N		1 1000300	
Allen D Hunter				ю.		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates	N	SF Funde	d	F	l Funds	Funds
(List each separately with title, A.7. show number in brackets)		ACAD		Real	uested By oposer	granted by NSF (if different)
1. Allen D Hunter - PI & Project Director		0.00			2,970	, ,
2. Laura M Hoistad - co-PI		0.00				
					2,300	
3. Alan J Jircitano - co-PI		0.00			2,800	
4. Timothy R Wagner - co-PI		0.00			2,730	
5. Edward P Zovinka - co-PI		0.00			2,500	
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)		0.00			0	
7. (5) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	2.50		13,300	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)	0.00	0.00	0.00			
1. (0) POST DOCTORAL ASSOCIATES		0.00			0	
2. (2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	
3. (3) GRADUATE STUDENTS					0	
4. (3) UNDERGRADUATE STUDENTS					0	
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. (0) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					13,300	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					1,995	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					15,295	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEED)						
D1. SMART APEX CCD Diffractometer System	\$		0,339			
D2. Crystal Mounting Microscope			4,840			
D3. WEB Upgrade to P4 Systems			3,946			
D4. WEB Video and Control		:	5,005			
TOTAL EQUIPMENT			-	1	44,130	
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NSF Form 1030 (10/99) Supersedes all previous editions

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

SUMMARY PROPOSAL BUDGE	T YE	AR				~	
ORGANIZATION	•	PPO	POSAL			ON (months)	
Youngstown State University		FRO	USAL	NO.	Proposed	· · · · · · · · · · · · · · · · · · ·	
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		010	ARD N	0	Fioposed	Granieu	
Allen D Hunter		AN	AND N	0.			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates	N	SF Funde erson-mos	d	F	unds	Funds	
(List each separately with title, A.7. show number in brackets)		ACAD		Requ	lested By oposer	granted by NSF (if different)	
1. Allen D Hunter - PI & Project Director		0.00			1,570	,	
2. Laura M Hoistad - co-PI		0.00		φ	1,200	Φ	
3. Alan J Jircitano - co-PI		0.00			1,200 1,440		
4. Sherri Lovelace Cameron - Minority Outreach		0.00			$\frac{1,440}{2,450}$		
5. Stacey Lowery Bretz - Assessment Director		0.00			<u>2,430</u> 3,860		
6. (2) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)		0.00			2,700		
7. (7) TOTAL SENIOR PERSONNEL (1 - 6)		0.00			13,220		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)	0.00	0.00	2.30		13,220		
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00		0		
2. (2) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)		0.00			<u> </u>		
3. (3) GRADUATE STUDENTS	0.00	0.00	0.00		0		
4. (3) UNDERGRADUATE STUDENTS					0		
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					<u> </u>		
6. (0) OTHER					<u> </u>		
TOTAL SALARIES AND WAGES (A + B)					13,220		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					1,983		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					15,203		
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING	G \$5 000))			15,205		
TOTAL EQUIPMENT E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESS 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4,800		5			0 2,000 0		
3. SUBSISTENCE							
4. OTHER TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTIC		0.0010			4,800		
G. OTHER DIRECT COSTS		00010			-,000		
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1. MATERIALS AND SUPPLIES					1,000		
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NSF Form 1030 (10/99) Supersedes all previous editions

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

SUMMARY PROPOSAL BUDGET COMMENTS - Year 2

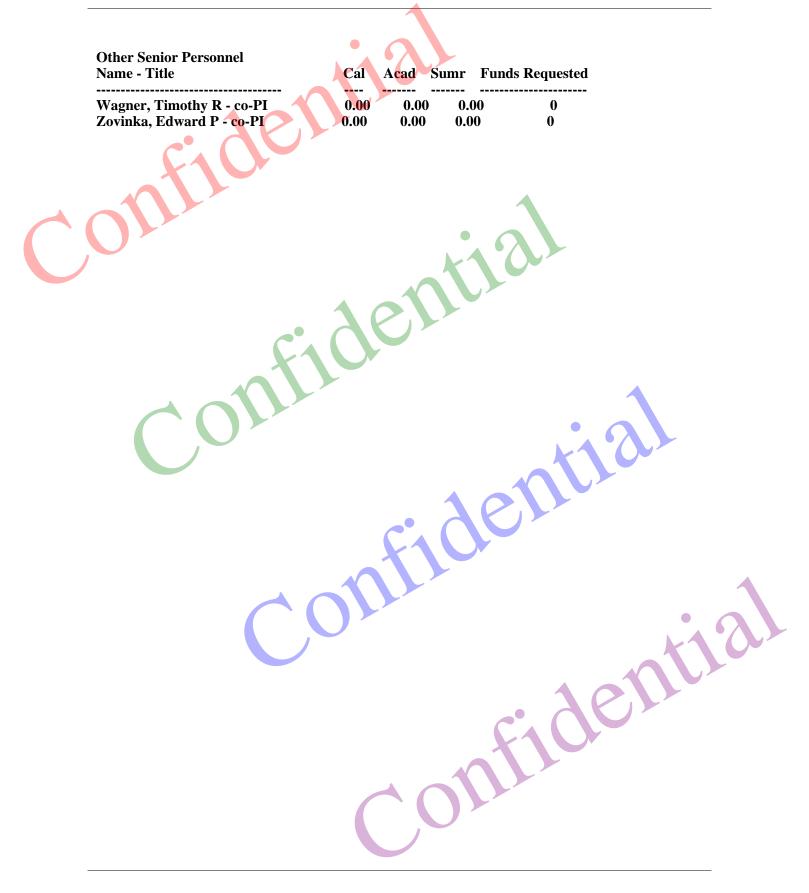
Other Senior Personnel Name - Title		nds Requested
Wagner, Timothy R - co-PI Zovinka, Edward P - co-PI	0.00 0.00 0.25 0.00 0.00 0.25	1430 1270
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Youngstown State University	-					Proposed	d Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTO	DR		AM	ARD N	Э.		
Allen D Hunter		N	SE Eurodo	d		<u> </u>	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty (List each separately with title, A.7. show num	and Other Senior Associates		SF Funde erson-mos		Requ	Funds Jested By	Funds granted by NSF
			ACAD			oposer	(if different)
<u>1. Allen D Hunter - PI &amp; Project Di</u>	rector		0.00		\$		\$
<u>2. Laura M Hoistad - co-PI</u>			0.00			0	-
<u>3. Alan J Jircitano - co-PI</u>			0.00			0	
4. Sherri Lovelace Cameron - Minor			0.00			1,300	
5. Stacey Lowery Bretz - Assessmen			0.00			2,680	
6. (2) OTHERS (LIST INDIVIDUALLY ON BUD	GET JUSTIFICATION PAGE)		0.00			2 000	
7. ( <b>7</b> ) TOTAL SENIOR PERSONNEL (1 - 6)		0.00	0.00	0.75		3,980	
B. OTHER PERSONNEL (SHOW NUMBERS IN BE	RACKETS)	0.00	0.00	0.00			
1. ( 0) POST DOCTORAL ASSOCIATES			0.00			0	
2. (2) OTHER PROFESSIONALS (TECHNICIA	N, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	-
3. (3) GRADUATE STUDENTS		-				0	
3) UNDERGRADUATE STUDENTS						0	
5. ( 0) SECRETARIAL - CLERICAL (IF CHARG						0	
6. ( <b>0</b> ) OTHER						<u> </u>	
TOTAL SALARIES AND WAGES (A + B)	00070					3,980	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT TOTAL SALARIES, WAGES AND FRINGE BEN						<u>592</u>	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT						4,572	
TOTAL EQUIPMENT E. TRAVEL 1. DOMESTIC (INCL. CANAE	DA, MEXICO AND U.S. POSSE	SSIONS)				0 4,000	
	DA, MEXICO AND U.S. POSSE	SSIONS)				0 4,000 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAD	DA, MEXICO AND U.S. POSSE	SSIONS)					
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN	DA, MEXICO AND U.S. POSSE	SSIONS)		X			
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS	-	SSIONS)					
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$	0	SSIONS)					
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$	-	ssions)	5				
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$	0	ssions)	5				
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER		Je			3	0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS (		Je	COSTS		3		
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS		Je				0	
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E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0 0 0 1,000	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0 0 1,000 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0 0 1,000 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0 0 1,000 0 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER	0 0 0 0 0 0) TOTAL PAR	Je	COSTS			0 0 1,000 0 0 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS	0 0 0 0) TOTAL PART SSEMINATION	Je	COSTS			0 0 1,000 0 0 0 1,000	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G)	0 0 0 0) TOTAL PART SSEMINATION	Je	COSTS			0 0 1,000 0 0 0 1,000	
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E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. RESIDUAL FUNDS (IF FOR FURTHER SUPPO	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0					0 0 0 1,000 0 0 0 0 0 0 0 0 9,572 0	
E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. RESIDUAL FUNDS (IF FOR FURTHER SUPPO L. AMOUNT OF THIS REQUEST (J) OR (J MINUS	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		3 II.D.7.j	)	\$	0 0 1,000 0 0 1,000 9,572 0 9,572	
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E. TRAVEL 1. DOMESTIC (INCL. CANAE 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 2. TRAVEL 3. SUBSISTENCE 4. OTHER TOTAL NUMBER OF PARTICIPANTS ( G. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DIS 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A)(SPECIFY RATE AND E <b>(Rate: , Base: )</b> TOTAL INDIRECT COSTS (F&A) J. TOTAL DIRECT AND INDIRECT COSTS (H + I) K. RESIDUAL FUNDS (IF FOR FURTHER SUPPO L. AMOUNT OF THIS REQUEST (J) OR (J MINUS M. COST SHARING PROPOSED LEVEL \$ <b>15</b>	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		S II.D.7.j	.) FOR N CT COS	ISF US	0 0 1,000 0 0 0 0 0 0 0 0 9,572 0 9,572 0 9,572 0 9,572 0 9,572	\$

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

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

## SUMMARY PROPOSAL BUDGET COMMENTS - Year 3



	т	mulat		110-		v
PROPOSAL BUDGE	.1				USE ONL	
ORGANIZATION		PRO	POSAL	NO.		ON (months)
Youngstown State University					Proposed	d Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		AW	/ARD N	0.		
Allen D Hunter	N	SE Eundo	d		 Firm da	- Eurote
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)		SF Funde		Req	Funds uested By	Funds granted by NS (if different)
		ACAD				
1 Allen D Hunter - PI & Project Director		0.00			4,540	
2. Laura M Hoistad - co-PI		0.00			3,500	
3. Alan J Jircitano - co-PI		0.00			4,240	-
4. Sherri Lovelace Cameron - Minority Outreach		0.00			3,750	
5. Stacey Lowery Bretz - Assessment Director		0.00			6,540	
6. ( 2) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)		0.00			7,930	
7. ( <b>7</b> ) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	5.75		30,500	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( 0) POST DOCTORAL ASSOCIATES		0.00			0	
2. ( 6) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0	
3. ( 9) GRADUATE STUDENTS					0	
4. (9) UNDERGRADUATE STUDENTS					0	
5. ( 0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					Ō	
6. ( <b>0</b> ) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					30,500	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					4,570	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					35,070	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDIN	IG \$5.00	))				
				1	14 120	
TOTAL EQUIPMENT E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES)	SIONS)			1	144,130 8,000	
	SIONS)			]		
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES	SIONS)				8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN	SIONS)				8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN F. PARTICIPANT SUPPORT COSTS	SIONS)				8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0					8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 4 800	SIONS)	5			8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS \$ 0 2. TRAVEL 3. SUBSISTENCE 4,800 0		5			8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0	e	5			8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES) 2. FOREIGN F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTIC	e	COSTS			8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24)	e	COSTS			8,000 0 4,800	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES	e	COSTS			8,000 0 4,800 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION	e	COSTS			8,000 0 4,800 0 3,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4. OTHER 0 C. OTHER 0 C. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES	e	COSTS			8,000 0 4,800 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION	e	COSTS			8,000 0 4,800 0 3,000 5,000 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4. OTHER 0 C. OTHER 0 C. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES	e	COSTS			8,000 0 4,800 0 3,000 5,000 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4,800 3. SUBSISTENCE 4,90 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER	e	COSTS			8,000 0 4,800 0 3,000 5,000 0 0 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4. 00 3. SUBSISTENCE 4. 00 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS	e	COSTS			8,000 0 4,800 0 3,000 5,000 0 0 8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 4,800 3. SUBSISTENCE 4,90 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER	e	COSTS			8,000 0 4,800 0 3,000 5,000 0 0 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESS 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS  C. TRAVEL C. TRAVEL C. TOTAL C.	e				8,000 0 4,800 0 3,000 5,000 0 0 8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESS 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0  TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G)	e				8,000 0 4,800 0 3,000 5,000 0 0 8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESS 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. OTHER 0  TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G)	e				8,000 0 4,800 0 3,000 5,000 0 0 8,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESS 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. 00 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS (24) TOTAL PARTICIPANTS 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL OTHER DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)	e				8,000 0 4,800 0 3,000 5,000 0 0 0 8,000 200,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN 2. FOREIGN 5. SUBAVARDS 6. OTHER DIRECT COSTS 1. MATERIALS AND SUPPLIES 2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION 3. CONSULTANT SERVICES 4. COMPUTER SERVICES 5. SUBAWARDS 6. OTHER TOTAL DIRECT COSTS H. TOTAL DIRECT COSTS (A THROUGH G) 1. INDIRECT COSTS (F&A)	CIPANT		Ċ		8,000 0 0 4,800 0 3,000 5,000 0 0 8,000 200,000	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 3. SUBSISTENCE 4. 0  4. OTHER 0  TOTAL NUMBER OF PARTICIPANTS (24) TOTAL P	CIPANT		Ċ		8,000 0 4,800 0 3,000 5,000 0 0 8,000 200,000 0 0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSES: 2. FOREIGN  F. PARTICIPANT SUPPORT COSTS 1. STIPENDS 2. TRAVEL 0 2. TRAVEL 0 3. SUBSISTENCE 4,800 4. OTHER 0 TOTAL NUMBER OF PARTICIPANTS (24) TOTAL PARTICIPANT (24) TOTAL PARTICIPAN		3 II.D.7.j	.)		8,000 0 4,800 0 3,000 5,000 0 0 8,000 200,000 0 200,000	
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NSF Form 1030 (10/99) Supersedes all previous editions

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

## F. Budget Justification

<u>A.</u> Senior Personnel: The 2.5 months salary support requested for the PI and 4 Co-PIs in the first year are to develop the facility operating procedures at YSU and at representative remote sites. The 1.25 months of summer support requested for the PI and Co-PIs in the  $2^{nd}$  year are to run the on-site training program. The 1.25 months of summer support requested for Dr. Bretz in the final two years are to support the project assessment activities (including training participating faculty to assess the impacts of this proposal on their own students). The 0.75 months of summer support requested for Dr Lovelace are to assist her in her outreach efforts. For each individual, academic year reassigned time for this project will be provided as shown.

*A1.* Dr. Allen D. Hunter, PI and Project Director: 0.5+0.25+0 months NSF SUMR \$4,540; 3+3+3 months YSU ACAD \$56,350; Total \$60,890.

*A2. Laura M. Hoistad, Co-PI*: 0.5+0.25+0 months NSF SUMR \$3,500; 2+1+1 months UNI ACAD \$24,000; Total \$27,500.

*A3. Alan J. Jircitano, Co-PI*: 0.5+0.25+0 months NSF SUMR **\$4,240**; 2+1+1 months PSU ACAD <u>\$24,000</u>; Total <u>\$28,240</u>.

*A4. Sherri Lovelace Cameron, Minority Outreach Director*: 0+0.5+0.25 months NSF SUMR **\$3,750**; 1+1+1 months YSU ACAD **\$18,000**; Total **\$21,750**.

A5. Stacey Lowery Bretz, Assessment Director: 0+0.75+0.5 months NSF SUMR **\$6,540**; 1+2+3 months YSU ACAD **<u>\$36,000</u>**; Total **<u>\$42,540</u>**.

*A7. Timothy R. Wagner, Co-PI*: 0.5+0.25+0 months NSF SUMR **\$4,160**; 3+2+2 months YSU ACAD **\$42,000**; Total **\$48,160**.

*A8. Edward P. Zovinka, Co-PI*: 0.5+0.25+0 months NSF SUMR **\$3,770**; 2+1+1 months SFC ACAD <u>\$24,000</u>; Total <u>\$27,770</u>.

Because of the CCLI budget cap, the NSF request for these individuals is for less summer support than we feel optimum.

## **B.** Other Personnel:

*B2i.* Other Professionals, Raymond Hoff, YSU Science Departments: Senior Electronic Instruments Maintenance Specialist: 3+2+2 months YSU CAL match: <u>\$29,850</u>. Total <u>\$29,850</u>. *B2ii.* Other Professionals, Bruce S. Levison, YSU Center for Biomedical and Environmental Research: Senior Instrumentation Operator: 1.5+1.5+1.5 months YSU CAL match: <u>\$19,300</u>.

# Total **\$19,300**.

*B2iii.* Other Professionals, Mike Graham, Multimedia Instructional Support: 2+0.5+0.5 months YSU CAL match: <u>\$11,400</u>. Total <u>\$11,400</u>.

*B3. (3) MS Student Assistants*: 1 years support for each; YSU match for Stipend (\$11,500/year) and Tuition (\$13,820/year): <u>\$75,960</u>. Total <u>\$75,960</u>.

*B4. (3) Undergraduate Student Assistants*: 20 hours per week, \$6.65/hour, 1040 hours/year, 3 years; YSU CAL match: <u>\$20,750</u>. Total <u>\$20,750</u>.

*B5. Dorothy Untch, Secretarial Support*: 0.5+0.5+0.5 months YSU CAL match: <u>\$3,700</u>. Total <u>\$3,700</u>.

Because of the budget cap, the NSF request is **\$0** for these individuals.

C. Fringe Benefits:

Fringe Benefits are charged at 34% for full time faculty during the academic year and full time staff year round, 15% in summer for faculty, and 1% for students. Institutional match is <u>\$56,470</u> and NSF request is \$4,570 on total Fringe Benefits costs of <u>\$61,040</u>.

**<u>D.</u>** Equipment: Please see attached quotes.

*D1. SMART APEX CCD Diffractometer*: Including all items shown on the attached Bruker quote, including a 3 kW sealed tube generator, PLATFORM goniometer, APEX CCD detector, diffractometer control software and data system, safety enclosure, refrigerated water to water heat exchanger, upgrade of low temperature system to fit PLATFORM goniometer, 24 xyz and 3

eucentric goniometer heads, and site license for SHELXTL/XSHELL structure solution software. Academic package price is \$295,860 minus \$35,000 discount for Bruker's distribution of Hunter's SHELXTL Manual:^{2b} YSU match is \$130,521 and NSF request is \$130,339 on a purchase cost of \$260,860.

*D2. Crystal Mounting Microscope:* Zeiss Binocular, Polarizing Microscope with Video Camera Attachment, Monitor, and WEB feed: YSU match is <u>\$4,840</u> and NSF request is **\$4,840** on a purchase cost of <u>\$9,680</u>.

D3. WEB Upgrade to P4 Systems: New Windows NT computers on each P4 and Upgrades to P4 Controllers and Software (from Bruker): YSU match is \$3,946 and NSF request is \$3,946 on a purchase cost of \$7,892. The upgrades to the diffractometer control software, including the GADDS powder package, are included as part of the APEX CCD quote, *D1* above.

D4. WEB Video and Control: Axis 2400 Video Sever, (2 @ \$1,399), Cannon Pan/Tilt/Zoom Camera and cabling (5 @ \$1,199 + 45), and Fixed Cameras (3 @ \$225 + \$79 + \$12 + \$15), for a Package Price of \$10,011: YSU match is \$5,006 and NSF request is \$5,005 on a purchase cost of \$10,011. This WEB video system will serve both the X-ray Diffraction facility described in detail in this proposal and our current LC-MS facility (i.e., to make it more WEB accessible).

Both Bruker-AXS (at the CMolS site at Cal. State Fullerton) and Nonius (at Southeast Missouri) have demonstrated remote access and control of their CCD instrumentation and Rigaku/MSC expects to do so by this fall. We prefer the Bruker system for this proposal because its hardware costs are comparable to the other two vendors for similar packages while its software license is both extremely open (i.e., it will allow us to add additional PUI sites at no cost) and very inexpensive (\$5,000 for the PUI site license). We also believe the Bruker hardware to be superior as evidenced by its much wider usage and longer term installed base. This base has displayed an excellent track record of very low maintenance in the field. The Bruker APEX system is substantially more sensitive (by perhaps 2 fold meaning 75% shorter data collection times) and less maintenance intensive that other CCD systems (largely because its 4K CCD chip does not require an optical taper). In addition, the Bruker system is more compatible with our current P4 systems using a common X-ray generator and control and data processing software. This will simplify maintenance requirements and student training. We believe that the Bruker instrumentation control software and its data analysis software are both more powerful and easier to use than those of the competing manufacturers. In addition, our faculty and students are already familiar with these packages from our own P4 systems and from the use of other Bruker instruments. Finally, the PI has developed the "standard" student training manual for the Bruker structure solution package, SHELXTL, which Bruker recommends. They are therefore willing to give us additional discounts on their systems. While on sabbatical for 2000-2001, the PI will be using Bruker, Nonius, and MSC/Rigaku instruments which will help in the final post funding (I hope) vendor selection. If one of the other vendors comes out with a superior instrument in that time, it will be considered for purchase.

Following current YSU instrumentation policy, PUI users of the diffraction facility will not be charged for instrument use in undergraduate teaching (unless large volumes of consumables such as liquid nitrogen are used). High volume research users will be asked to request a nominal amount ( $\approx$ \$50-100 per data set) from external granting agencies but these fees will be waved for occasional users and for those without external grant support. Undergraduate teaching will have highest overall priority on these instruments (specific times/dates will be schedulable up to one semester in advance). The remaining instrument time will be available on a first come first served basis with undergraduate research projects having the highest research priority (and will be schedulable up to several weeks in advance). All participating institutions, including YSU, will have the same priority for access.

## E. Travel:

The domestic travel budget is for the senior project personnel to visit the YSU host site and the remote home sites of the PUI participants as well as to present the results of this project to science education conferences. Institutional match is <u>\$8,000</u> and NSF request is <u>\$8,000</u> out of a travel budget of <u>\$16,000</u>.

#### F. Participant Support Costs:

F1. Travel: The domestic travel budget is for 24 Predominantly Undergraduate Institution faculty collaborators to visit the YSU host site for the summer short course and for individual training. Institutional match is \$7,200 and because of the budget cap *no funding is requested from NSF* out of \$7,200 (i.e.,  $\approx$ \$300 each).

F2. Subsistence: The subsistence budget is for 24 Predominantly Undergraduate Institution faculty collaborators to cover expenses for visits to the YSU host site for training on the diffraction instrumentation and diffraction teaching during the summer short course and other visits. Institutional match is <u>\$9,600</u> and NSF request is <u>\$4,800</u> out of a budget of <u>\$14,400</u> (i.e., a subsistence cost of  $\approx$ \$600 each for the 6 days of the short course and for one additional visit).

G. Other Direct Costs:

G1. Materials and Supplies: The materials and supplies budget is to cover operation and maintenance of the YSU diffraction facility and the home sites. The YSU institutional match is  $\underline{\$50,000}$  for instrument maintenance and room renovations for the 3 years of this project. Consumables (including liquid N₂ cryogen) for teaching at the YSU home and host participants are estimated to total an additional  $\underline{\$40,000}$  over three years. Note: YSU professional staff member Ray Hoff (B2i, above) will be sent to the two Bruker X-ray diffractometer technician maintenance course to ensure timely and skilled maintenance, total cost:  $\underline{\$15,000}$ . Because of the NSF CCLI budget cap, the NSF request is \$0. The department will also provide a Silicon Graphics INDY workstation for use as a WEB server for the CCDB, Brookhaven, and ICDD data bases and will purchase the CCDB and ICDD databases with multi-user licenses for the consortium (estimated costs for 5 years,  $\underline{\$,000}$  as a YSU cash match).

G2. Publication Costs/Documentation/Dissemination: To cover the paper, toner, printer, mailing, and phone costs of this project, estimated total cost: \$15,000. Because of the budget cap, the institutional match on these will be \$12,000 and the NSF request is \$3,000.

G3. Consultant Services: To ensure the timely and effective implementation of this WEB based diffraction facility, the PIs on the two current PUI diffraction centers that we are modeling ourselves after (i.e., Katherine Kantardjieff and Marcus Bond) will be hired as consultants. Each will visit YSU twice (once in each of the first two years), will give the PI a detailed tour of their facilities, will answer question by phone and the internet, and will participate in the assessment effort (consultant fees: 3,000 each plus 1,000 each for expenses and 2,000 in expenses for the PI's visits to the consultants' sites and to the Oakridge HTML site). Total cost: <u>\$10,000</u>, Institutional match: <u>\$5,000</u> and the NSF request is \$5,000.

M. Cost Sharing Proposed Level:

Because of the \$200,000 cap on NSF-DUE-CCLI-A&I proposals, the institutional cash matches are at or substantially above 50%. In sections A and B, the proposed institutional match for faculty academic year salaries, professional staff support, and students (wages and tuition) is **\$288,600**. In section C, the proposed institutional match for faculty, staff, and student benefits is **\$56,470**. In section D, the institutional capital cost cash match is **\$144,190**. In section E, the institutional travel match is **\$8,000**. In section F, the participant support match is **\$16,800**. In section G, the institutional match on materials and supplies, publication and dissemination costs, and consultant services is **\$130,000**. This represents a total institutional match of  $\approx$ **\$644,000**, **76%**, out of a total project budget of  $\approx$ **\$844,000** and an NSF request of **\$200,000**.

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
Investigator: Allen D. Hunter, PI & Project Director Other agencies (including NSF) to which this proposal has been/will be NSF-CHEM-CRIF-RUI (60% proposal overlap)
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: \$74,707Total 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
Support:       Image: Current       Pending       Submission Planned in Near Future       *Transfer of Support
Project/Proposal Title: The Ohio Project for Science Teaching
Source of Support: Ohio Board of Regents
Total Award Amount: \$4,000 to YSUTotal Award Period Covered: 07/01/1999 – 06/30/2000
Location of Project: Youngstown State University and other Ohio Universities
Person-Months Per Year Committed to the Project. Cal: 0.5 Acad: Sumr:
Support: © Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title: A Proposal to Establish a State-of-the-Art Ohio Mass Spectrometry Consortium
\$1,860,000 to a consortium of 8 Ohio Universities
Funding for a LC-MS at YSU + other shared instrumentation Source of Support: Ohio Board of Regents Investment Fund
Total Award Amount: \$88,900 to YSU Total Award Period Covered: 06/01/1999 – 05/31/2000
Location of Project: Youngstown State University and other 7 Ohio Universities
Person-Months Per Year Committed to the Project. Cal: 0.5 Acad: Sumr:
Support:   Image: 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: 0.1 Acad: 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: \$44,600Total Award Period Covered: 06/01/1998 - 05/31/2001
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. for 2000-01 Cal: 1 in 2000 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

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
Investigator: Allen D. Hunter, PI & PD (continued)
Support:  Current Pending Submission Planned in Near Future  Transfer of Support
Project/Proposal Title: A Proposal for Fulfilling the Goals of the Oho Mass Spectrometry Consortium
Funding for consortial MS instruments including a high resolution ICP-MS
Source of Support: Ohio Board of Regents Investment Fund
Total Award Amount: \$500,000 to Consortium Total Award Period Covered: 06/01/2000 – 05/31/2001
Location of Project: YSU and 7 other Ohio Universities
Person-Months Per Year Committed to the Project. no additional Cal: Acad: Sumr:
Support: Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title: RUI- Cooperative Research Project – Structural Investigations of Main
Group Heterocyclic Rings and Cages
Source of Support: NSF-International Division-Western Europe
Total Award Amount: \$15,460Total Award Period Covered: 12/01/2000 – 12/31/2000
Location of Project: St. Andrews University (Scotland) and Youngstown State University
Person-Months Per Year Committed to the Project. Cal: Acad: 7 Sumr:
Support:       Current       Pending       Submission Planned in Near Future       *Transfer of Support
Project/Proposal Title: Investigative Approaches in Advanced Synthesis Laboratories:
Inorganic, Organic, and Polymeric Materials
Source of Support: NSF-DUE-CCLI-A&I
Total Award Amount: \$ ≈70,000 Total Award Period Covered: 01/01/2001 – 12/31/2003
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: 1.5 Acad: Sumr:
Support: Current Pending Submission Planned in Near Future Transfer of Support
Project/Proposal Title: State Matching Funds for the WEB Accessible Diffraction Facility
(contingent on receiving this CCLI grant, ≈60% overlap with this CCLI grant)
Source of Support: Ohio Board of Regents Action Fund
Total Award Amount: \$75,000 Total Award Period Covered: 01/01/2001 - 12/31/2001
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. no extra Cal: Acad: Sumr:
Support:       Current       Pending       Submission Planned in Near Future       *Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility
for a Consortium of Predominantly Undergraduate Institutions
(≈60% overlap with this CCLI Proposal) Source of Support: NSF-CHEM-CRIF
Total Award Amount: $\$ \approx 260,000$ Total Award Period Covered: $04/01/2001 - 03/31/2004$
Location of Project: Youngstown State University and a Consortium of other Predominantly Undergraduate Institutions
Person-Months Per Year Committed to the Project. Cal: 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

NECESSARY

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
Other agencies (including NSF) to which this proposal has been/will Investigator: Allen D. Hunter, PI & PD (continued)
Support: Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title: Diffraction Methods in the Undergraduate Curriculum & in Research
Source of Support: Dreyfus Foundation: Scholar/Fellow Program for Undergraduate Institutions
Total Award Amount: \$65,000 Total Award Period Covered: 07/15/2001 – 07/14/2003
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:
Support: Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title:
Source of Support:
Total Award Amount: \$ Total Award Period Covered:
Location of Project:
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Project/Proposal Title:
Source of Support:
Total Award Amount: \$ Total Award Period Covered:
Location of Project:
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Total Award Amount: \$ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: 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

See GPG Section II.D.8 for guidance on information to include on this	
The following information should be provided for each investigator and other senior person	
Investigator: Laura M. Hoistad, Co-PI	ch this proposal has been/will
Support: Current Pending Submission Planned in Near Future	*Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility	1
for a Consortium of Predominantly Undergraduate Institutions	
(≈60% overlap with this CCLI Proposal)	
Source of Support: NSF-CHEM-CRIF	
Total Award Amount: $\ \approx 260,000$ Total Award Period Covered: $04/01/2001 - 03/31/2$	
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Project/Proposal Title:	1
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Person-Months Per Year Committed to the Cal: Acad:	Sumr:
*If this project has previously been funded by another agency, please list and furnish informati	on for immediately preceding
funding period.	-
NSF Form 1239 (7/95) USE	ADDITIONAL SHEETS AS

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: Alan J. Jircitano, Co-PI
Support:   Current   Pending   Submission Planned in Near Future   *Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility
for a Consortium of Predominantly Undergraduate Institutions
(≈60% overlap with this CCLI Proposal)
Source of Support: NSF-CHEM-CRIF
Total Award Amount: \$ ≈260,000         Total Award Period Covered: 04/01/2001 – 03/31/2004
Location of Project: Youngstown State University and a Consortium of other Predominantly Undergraduate Institutions
Person-Months Per Year Committed to the Project. Cal: 1 Acad: Sumr:
Support. Current Pending Submission Planned in Near Future *Transfer of Support
Project/Proposal Title:
Source of Support:
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Location of Project:
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Support: Current Pending Submission Planned in Near Future *Transfer of Support
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Location of Project:
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Location of Project:
Person-Months Per Year Committed to the Cal: 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
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Current and Pending Support See GPG Section II.D.8 for guidance on information to include on thi	s form.)
The following information should be provided for each investigator and other senior perso	· · · · · · · · · · · · · · · · · · ·
Investigator: Sherri Lovelace Cameron, Minority Other agencies (including NSF) to white	
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:\$183,579Total 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: 1.0
Support: Current Pending Submission Planned in Near Future	Transfer of Support
Project/Proposal Title: Investigative Approaches in Advanced Synthesis Laboratories:	
Inorganic, Organic, and Polymeric Materials	
Source of Support: NSE DUE CCULARI	
Source of Support: NSF-DUE-CCLI-A&I	2002
Total Award Amount: \$ ≈70,000 Leasting a Speciest Version of State United State U	2003
Location of Project: Youngstown State University	9
Person-Months Per Year Committed to the Project.Cal: 2.0Acad:Support:CurrentPendingSubmission Planned in Near Future	Sumr:
Support: Current Pending Submission Planned in Near Future Project/Proposal Title: What is a Scientist?	
Project/Proposal Title, what is a Scientist?	
Source of Support: NSF-EHR #0086332	
Total Award Amount: \$99,914 Total Award Period Covered: 10/01/2000 - 03/3	0/2002
Location of Project: Youngstown State University	
Person-Months Per Year Committed to the Cal:	Sumr: 0.5
Support: Current Pending Submission Planned in Near Future	*Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility	<u> </u>
for a Consortium of Predominantly Undergraduate Institutions	
(≈60% overlap with this CCLI Proposal)	
Source of Support: NSF-CHEM-CRIF	~
Total Award Amount: \$ ≈260,000 Total Award Period Covered: 04/01/2001 – 03/31/	2004
Location of Project: Youngstown State University and a Consortium of other Predominantly Underg	graduate Institutions
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Current and Pending Support	
See GPG Section II.D.8 for guidance on information to include	
The following information should be provided for each investigator and other senio	
Investigator: Stacey Lowery Bretz, Assessment	) to which this proposal has been/will
Support:  Current Pending Submission Planned in Near Futu	
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	04/20/2002
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:	1 Sumr: 0.5
	e Transfer of Support
Project/Proposal Title: Investigative Approaches in Advanced Synthesis Laboratories: Inorganic, Organic, and Polymeric Materials	
morganic, Organic, and Porymetric Materials	
Source of Support: NSF-DUE-CCLI-A&I	
Total Award Amount: \$ ≈70,000 Total Award Period Covered: 01/01/2001 -	- 12/31/2003
Location of Project: Youngstown State University	
Person-Months Per Year Committed to the Project. Cal: 1.0 Acad:	Sumr:
Support: Current Pending Submission Planned in Near Future	e Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility	
for a Consortium of Predominantly Undergraduate Institutions	
(≈60% overlap with this CCLI Proposal)	
Source of Support: NSF-CHEM-CRIF	
Total Award Amount: \$ ≈260,000 Total Award Period Covered: 04/01/2001 -	
Location of Project: Youngstown State University and a Consortium of other Predominantly	
Person-Months Per Year Committed to the Project. Cal: 1 Acad:	Sumr:
Support: Current Pending Submission Planned in Near Fu	ture Transfer of Support
Project/Proposal Title:	
Source of Support:	
Total Award Amount: \$ Total Award Period Covered:	
Location of Project:	
Person-Months Per Year Committed to the Cal: Acad:	Sumr:
Support: Current Pending Submission Planned in Near Fu	
Project/Proposal Title:	
Source of Support:	
Total Award Amount: \$ Total Award Period Covered:	
Location of Project:	
Person-Months Per Year Committed to the Cal: Acad:	
*If this project has previously been funded by another agency, please list and furnish in funding period.	nformation for immediately preceding
NSF Form 1239 (7/95)	USE ADDITIONAL SHEETS AS
	NECESSARY

Current	and	Pending	Support
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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
Project/Proposal Title: Integration of Computer Technology into the General Chemistry Curriculum
Source of Support: NSF-DUE-CCLI-A&I
Total Award Amount: \$94,945Total Award Period Covered: 07/01/2000 - 06/30/2002
Location of Project: Youngstown State University
Person-Months Per Year Committed to the year 1 only Cal: Acad: 1.5 Sumr: 1.5
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: \$39,719Total Award Period Covered: 05/15/1999 - 05/14/20001
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Cal: Acad: 3 Sumr: 2
Support:       Current       Pending       Submission Planned in Near Future       *Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility
for a Consortium of Predominantly Undergraduate Institutions
(≈60% overlap with this CCLI Proposal)
Source of Support: NSF-CHEM-CRIF
Total Award Amount: \$≈260,000 Total Award Period Covered: 04/01/2001 – 03/31/2004
Location of Project: Youngstown State University and a Consortium of other Predominantly Undergraduate Institutions
Person-Months Per Year Committed to the Project. Cal: 1 Acad: Sumr:
Support:       Current       Pending       Submission Planned in Near Future       *Transfer of Support
Project/Proposal Title: Investigative Approaches in Advanced Synthesis Laboratories:
Inorganic, Organic, and Polymeric Materials
Source of Support: NSF-DUE-CCLI-A&I
Total Award Amount: \$ ≈70,000         Total Award Period Covered: 01/01/2001 – 12/31/2003
Location of Project: Youngstown State University
Person-Months Per Year Committed to the Project. Cal: 1.0 Acad: Sumr:
*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.
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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: Edward Zovinka, Co-PI
Support: Current Pending Submission Planned in Near Future Transfer of Support
Project/Proposal Title: Investigation of Thiaporphyrins and Dithiaporphyrins as Photodynamic Therapy Agents
Source of Support: NIH - AREA
Total Award Amount: \$100,000Total Award Period Covered: 06/01/2001 - 01/31/2004
Location of Project: Saint Francis College
Person-Months Per Year Committed to the Cal: Acad: 1 Sumr: 2
Support:   Current   Pending   Submission Planned in Near Future   Transfer of Support
Project/Proposal Title: RUI-WEB Accessible Single Crystal X-Ray Diffraction Facility
for a Consortium of Predominantly Undergraduate Institutions
(≈60% overlap with this CCLI Proposal)
Source of Support: NSF-CHEM-CRIF Total Award Amount: \$≈260,000 Total Award Period Covered: 04/01/2001 – 03/31/2004
Total Award Amount: \$≈260,000       Total Award Period Covered: 04/01/2001 – 03/31/2004         Location of Project: Youngstown State University and a Consortium of other Predominantly Undergraduate Institutions
Person-Months Per Year Committed to the Project. Cal: 1 Acad: Sumr:
Support:     Current     Pending     Submission Planned in Near Future     *Transfer of Support
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Source of Support:
Total Award Amount: \$ Total Award Period Covered:
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Person-Months Per Year Committed to the Cal: Acad: Sumr:
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Project/Proposal Title:
Source of Support:
Total Award Amount: \$ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: Acad: Sum:
Support:     Current     Pending     Submission Planned in Near Future     *Transfer of Support
Project/Proposal Title:
Source of Support:
Source of Support: Total Award Amount: \$ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Cal: 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

## H. Facilities, Equipment and Other Resources

## H1. The Participating PUI Home Institutions:

The approximately two dozen participating PUI home institutions each has available:

- appropriate lab space to synthesize and/or isolate new materials from biological, environmental, geological, inorganic, organic, organometallic, solid state materials, etc., sources and to grow single crystals of the molecular materials.
- at least a basic range of analytical, chromatographic, and spectroscopic instrumentation to partially characterize the target materials (samples requiring more advanced characterization methods can be sent to YSU, see below).
- > at least one optical microscope that can be used to help evaluate crystal quality and mount the single crystals on fibers.
  - a computer (i.e., a password protected Windows NT computer) in a relatively secure location that is connected to the internet and that can be used to control the diffractometers at YSU.
- multiple computers connected to the internet to view the YSU diffraction lab, to transfer files from the YSU server and between home sites, and to search the diffraction databases at YSU.
- multiple computers (having either the DOS/Windows 95-98 or the Windows NT operating systems) upon which can be loaded the site licensed SHELXTL/XSHELL structure solution package.
- At least one faculty member who has crystallographic experience or who plans on gaining it through the consortium and, more importantly, an interest in integrating diffraction methods into their undergraduate curriculum.

## H2. The Youngstown State University Host Institution:

## H2a. The YSU Instrumentation Centers:

Youngstown State University has two closely related instrumentation centers. The YSU Center for Biomedical and Environmental Research is housed on the 4th floor of the Ward Beecher science hall and specializes in instrumentation for the characterization of biological materials. The YSU Structure Center is housed on the  $5^{th}$  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), trained undergraduate and MS student assistants to run the instruments and collect data, 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. In addition to the smaller chromatographic, spectroscopic, physical, and analytical instruments expected at any MS level institution, the centers are equipped with the following modern instrumentation:

a LC-MS instrument with an autosampler and an 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. Unfortunately, there are currently no cameras in the LC-MS lab for remote viewing which limits the utility of the remote access. YSU was the first Bruker Esquire customer to accomplish this remote control.

- an automated DNA sequencer.
- > a C/H/N/O/S combustion analyzer.
- several <u>Atomic Absorption</u>, AA, and <u>Inductively Coupled Plasma</u>, ICP, elemental analyzers.
- several electrochemical systems
- two inert atmosphere glove boxes
- > a 400 MHz multinuclear NMR with four probes, <u>Variable Temperature</u>, VT, and <u>Pulsed</u> <u>Field Gradient</u>, PFG, accessories, and several work stations.
  - two automated GC-MS systems (both with autosamplers and one with a solids probe and one with an SPME interface). One of these is optimized for synthetic samples and one for trace environmental samples.
- a materials characterization lab including: a <u>D</u>ifferential <u>S</u>canning <u>C</u>alorimeter, DSC, a <u>T</u>hermal <u>G</u>ravimetric <u>A</u>nalyzer, TGA, and a <u>G</u>el <u>P</u>ermeation <u>C</u>hromatograph, GPC.
- > older, but functioning, electron microscopy, TEM and SEM, instruments.

Each of these instruments is fully available to external users and we have had users from about a dozen PUIs over the last few years. While we charge conventional rates to industrial users (to subsidize undergraduate costs), we have a policy of not charging faculty and student users from PUIs (except for consumables for the largest scale users).

## H2c. The YSU Science Hall Computer Facilities:

The Ward Beecher science hall has five computer labs having from 12 to 24 workstations each. One lab is equipped with Macintosh computers while the others are equipped with Windows 95/98 computers or Windows NT workstations. We also have a half dozen Silicon Graphics and SUN engineering workstations in advanced computer labs for the most demanding applications. All are connected with T1 lines to the WEB and to other campus computing resources and labs and to the Ohio Super Computer Center. On the 5th floor of the Science Hall is a lab equipped with 12 Windows NT computers, video projection capabilities, fast printers, etc., and that was designed for teaching advanced instrumental methods, including remote instrument operation. The YSU facility will also have several diffraction data bases on a server that will be available to users over the WEB. We currently have such a CCDB "consortium" license, the Brookhaven macromolecular database is free on 3 CDs to education users, and have negotiated such a "consortium" license with the ICDD on a 5 year experimental basis to start when/if this proposal is funded.

#### H2c. The Current YSU Diffraction Facility:

The YSU Structure Center Diffraction Facility is currently located in a 400 square foot lab with adjacent dark room. This lab contains two 6 year old Bruker-AXS P4 diffractometers. One has a X-1000 multiwire area detector and a Cu tube and is used primarily for 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.

## H2d. The Proposed WEB Accessible Diffraction Facility:

If this grant is funded, the YSU Structure Center Diffraction Facility will be moved to a 1,200 square foot room to allow additional space for the new instrument and, especially, more instructional space near the instruments. With the grant and matching funds, this lab will be set

up 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. The new stereo microscope to be placed in this lab will be equipped with a color WEB camera so that students in the attached instructional space or at remote sites will be able to view the crystal selection and mounting operations.

With funds from this grant, the two current P4 diffractometers will be upgraded with new computer hardware and software so that they can be remotely controlled over the WEB. Similarly, the new CCD instrument will be made WEB accessible for both the diffractometer control software and the crystal centering scope. The current LT2 system will be upgraded to the LT3 standard to improve its low temperature performance (which is marginal below -80° in Ohio's summer humidity) and to make it compatible with the PLATFORM goniometer on the Bruker APEX CCD system.

When on site, all users will be able to mount and center their own crystals. They will also be able to use the local computers to control all aspects of diffractometer operation and for structure solution. When at remote sites, the users will select and mount their own crystals on brass pin mounts and mail/courier these to YSU. At the time prearranged for their class, an assistant in the YSU lab will mount these crystals on the diffractometer, optically center them, and ensure that the X-ray generator is set to the desired power output. All other aspects of data collection will be remotely controllable.

To maximize system safety and security while also maximizing the educational utility of this center, those activities that are not dangerous to the occupants of the lab and/or the instruments will be controllable from anyplace on the WEB (e.g., the tilt/pan/zoom cameras). To minimize operator, instrument, and computer safety problems, the following general procedures will be adopted (i.e., modeled after those at other remote sites): A mechanical switch will be added to the X-ray shutter wiring so that the shutter will not be operable unless the local users feel it is safe (this will minimize any chance of accident for the YSU assistants). The ability to control the diffractometers will be limited to certain approved IP addresses at participating schools to prevent unauthorized or malicious use. As a further precaution, each IP address will be able to take control of the scheduled instrument(s) only during its scheduled time slot(s) (this will also prevent one user from accidentally interfering with another user's experiment). However, all users will be able to monitor all diffractometers at all times. For maximum educational utility, users will be able to book time for specific classes/days up to a semester in advance.

#### H2e. Instrumentation Maintenance:

The YSU Structure Instrumentation Centers are well equipped to keep our instruments operating. In fact, the two X-ray diffractometer have had less than a months down time over the last six years, while the NMR has had less than two weeks down time in five years, in each case while waiting for parts. This in service rate is comparable to that of major research institutions which is quite remarkable since over 80% of instrument operation is by undergraduates, mostly in courses. Our Instrumentation Service Specialist, Ray Hoff, is exceptionally skilled at instrumentation maintenance and we routinely send him to the instrument vendors own service technician courses when we buy a new instrument. On those rare occasions when outside service has been required, we have always been immediately authorized to do so. At least one faculty member per instrument, and Bruce Levison for many instruments, are also trained in instrument maintenance, which is especially valuable when it is not clear if the problem is instrumental or with the sample chemistry.

Section I. Supplementary Documentation

Index (1 page)

Participating Faculty Members from Outside of YSU (1 page)

Participating Faculty Members from Youngstown State University (1 page)

External Individuals Who Have Acted and/or Are Acting as Advisors to the Consortium (1 page)

Signed Cover Sheets (3 pages)

Bruker Quote (3 pages)

Crystal Mounting Microscope Quote (1 page)

Computers for WEB Upgrade of P4s Quote (2 pages)

WEB Video and Control Quote (1 page)

Letter from Bruker-Daltonics about the LC-MS Facility (1 page)

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	Department	University	User Typ
Al Jircitano	Chemistry	Penn State University – The Behrend College	Co-PI
Ed Zovinka	Math and Physical Science	Saint Francis College	Co-PI
Laura Hoistad	Chemistry	University of Northern Iowa	Co-PI
Omokere Odje 人	Chemistry	Central State University*	User
ohn Polo	Physics and Technology	Edinboro University of PA	
Chase Smith	Chemistry	Holy Cross	User
Charles Lake	Chemistry	Indiana University of PA	User
ayne Giniewicz	Physics	Indiana University of PA	User
ohn Woolcock	Chemistry	Indiana University of PA	User
Ron See	Chemistry	Indiana University of PA	User
Aike Nichols	Chemistry	John Carroll University	User
aul Challen	Chemistry	John Carroll University	User
Ferry Green	Chemistry	Lorain County Community College [†]	User
Aichael Castellani	Chemistry	Marshall University	User
Charles Scharnberger	Earth Sciences	Millersville University	User
Lynn Marquez	Earth Sciences	Millersville University	User
Santosh Mandal	Chemistry	Morgan State University*	User
Kenneth Hicks	Chemistry	Norfolk State University*	User
Tim Usher	Chemistry	North Carolina State University	User
Susan Yochum	Math, Science & Computer Tech.	Seton Hill College	User
Rob Mauldin	Chemistry	Shawnee State University	User
Steve Bennett	Chemistry	Shawnee State University	User
Snezana Dalafave	Physics	The College of New Jersey	User
Melinda Greer	Chemistry	University of Dayton	User
Charlotte Otto	Provost's Office	University of Michigan – Dearborn	User
Paul Zitzewitz	Natural Sciences	University of Michigan – Dearborn	User
/iktor Zhdankin	Chemistry	University of Minnesota - Duluth	User
/yacheslav Samoshin		University of the Pacific	User
Lee Park	Chemistry	Williams College	User
Mark Schofield	Chemistry	Williams College	User
Tom Smith	Chemistry	Williams College	User
David Grossie	Chemistry	Wright State University	User

# Participating Faculty Members from Outside of YSU

Individual	Department	University	Role
Allen Hunter	Chemistry	Youngstown State University	PI-PD
Tim Wagner	Chemistry	Youngstown State University	Co-PI
Stacey Lowery Bretz	Chemistry	Youngstown State University	Assessment
Sherri Lovelace	Chemistry	Youngstown State University	Minority
Cameron			Outreach
Ray Hoff	Chemistry	Youngstown State University	Tech. Service
Bruce Levison	Biology	Youngstown State University	Tech. Service
Mike Graham	Instructional	Youngstown State University	WEB Access
	Technology Center		
Ikram Khawaja	Geology	Youngstown State University	User
Jeanette Garr	Chem. Eng.	Youngstown State University	User
Jeff Carroll	Physics	Youngstown State University	User
Jeff Dick	Geology	Youngstown State University	User
John White	Anthropology	Youngstown State University	User
Larry Curtin	Chemistry	Youngstown State University	User
Michael Serra	Chemistry	Youngstown State University	User
Mike Moseley	Fine Art	Youngstown State University	User
Peter Norris	Chemistry	Youngstown State University	User
Ray Beiersdorfer	Geology	Youngstown State University	User
Scott Martin	Civil-Environ. Eng.	Youngstown State University	User
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## Participating Faculty Members from Youngstown State University

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# External Individuals Who Have Acted and/or Are Acting as Advisors to the Consortium

Individual	University	Role
Katherine Kantardjieff	Cal. State Fullerton	Current Director of PUI Diffraction Network (Using Bruker CCD Diffractometer) - Project Consultant
Marcus Bond	Southeast Missouri	Current Director of PUI Diffraction Network (Using
	Sourieust Missouri	Nonius CCD Diffractometer) - Project Consultant
Arnold Rheingold	University of	Bruker-AXS CCD Diffraction Methods in Research
	Delaware	and Teaching - Advisor
Bernard Santarsiero		Remote Access Instrumentation to CCD
	Advanced Light	Diffractometers Including Remote Crystal Mounting
	Source, ALS	Robot for the Advanced Light Source - Advisor
Camden Hubbard	Due - Oakridge	Director, High Temperature Materials Lab - Advisor on
	C	WEB Access and Control and Powder Diffraction
Cyrus Smith	DUE - Oakridge	Instrumentation and Controls Division - Advisor on
5	0	WEB Access and Control
Derek Woolins and	dSaint Andrews	Bruker-AXS and Rigaku-MSC CCD Diffraction
Alex Slawin		Methods in Research and Teaching - Advisors
John Hughes	Geology,	Diffraction Methods in Research and Teaching -
· · · · · · · · · · · · · · · · · · ·	Miami University	Advisor
Mike Zaworotko		CCD Diffraction Methods in Research and Teaching
	Florida	(Including Bruker-AXS APEX CCD) - Advisor
Robert McDonald	University of	Bruker-AXS CCD Diffraction Methods in Research
	Alberta, Canada	and Teaching - Advisor
Simon Bott	University of	CCD Diffraction Methods in Research and Teaching
	Houston	(Including WEB Based Diffraction Education) -
		Advisor
Victor Young	University of	Bruker-AXS CCD Diffraction Methods in Research
C	Minnesota	and Teaching - Advisor
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	Certification for Principa I certify to the best of my knowledge that						
	(1) the statements herein (excluding scie	The lowest cost and country on all	the electronic bac o of the land				
	(2) the text and graphics herein as well a signatories or individuals working inder t required progress reports if an award is n	s any accompanying publications or heir supervision. Fagree to accept n	other documents, unless otherwis	e indicated, are the original wor uct of the project and to provide	k of the the		
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	Co-PI/PD	1		confi ot dis NE SU			
	Alan J Jircitano						
	Co-PMPD Timothy R Wagner	Timothy R	Wagon	dentia played BMISSI	5/18/00		
	Co-PiPD Edward P Zovinka			ions.			
	Certification for Authori	zed Organizational Re	epresentative or Ind	ividual Applicant:			
	By signing and submitting his 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 reparcing Faderal debt status, debarment and suppression, drug free verification, and this supporting activities (see below), as set forth in Grant Proposal Grade (GPG), NSF 00-2. With provision of table information in this application and its supporting documents or in reports required under an ensuing award is a criminal referee (C). S. Coder, Tifle 8. 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 writen and enforced conflict of inflance 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 baticatority 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 assistancerily managed, reduced or eliminated must be disclosed to NSF.						
	Is the organization delinquent on any Feo Is the organization or its principals preser	Debt and Debarment Certifications       (If answer "yes" to sither, please provide explanation.)         Is the organization delinquent on any Federal dobt?       No IM         is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded       Yes I       No IM         Yes I       No IM       Yes I       No IM					
	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 \$100,000.						
	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 parson 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 goart, the making of any Federal floar, the ontaring into of any cooperative agreement, and the extension, confination, sneweal, a mendment, for modification of any Federal floar, the ontaring into of any cooperative agreement.						
	(2) If any tunds other than Foderal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of congress, or an employee of a Member of Congress in connection with this Federal contract, grant, kan, or cooperative agreement, the undersomed shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbyrg," in accordance with its instruction.						
	(3) The undersigned shall require that the language of this captification be included in the award documents for all subawards of all tiers including subcontracts, subgrants, and contracts under grants, loans, and occerative agreements and that all subrecipients shall cartify and disclose accordingly.						
	This certification is a material representat certification is a prerequisite for making or required cartification shall be subject to a AUTHORIZED ORGANIZATIONAL REPI	entering into this transaction imposi civil penalty of not less than \$10,000	ed by section 1352, title 31, U.S. (	Code. Any person who falls to 1	on of this le the DATE		
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	Dr. Peter J. Kasvinsky/Grad	luate Dean	171 - 1/5	ando	5/09/00		
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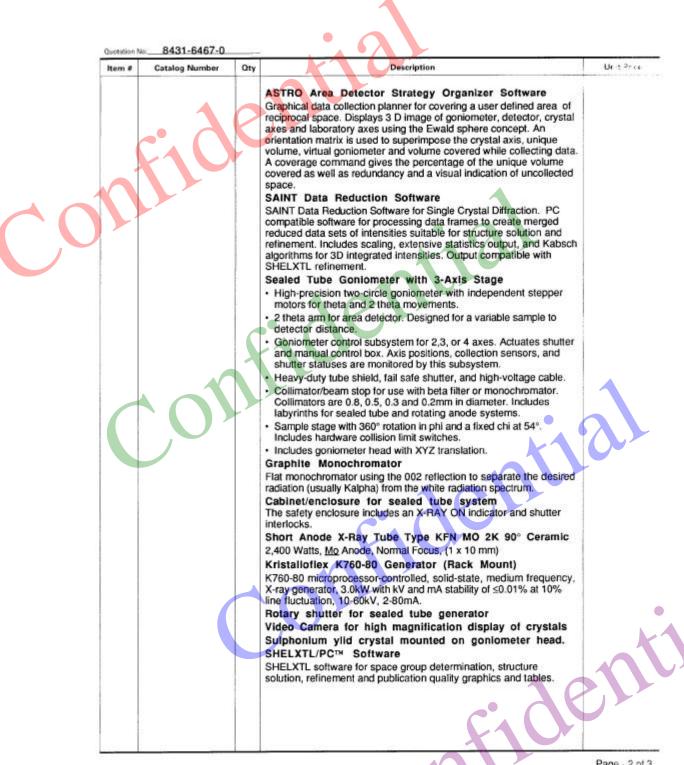


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Certification for Princip	oal Investigators and Co-Principal Inv	estigators:		
I certify to the best of my knowledge the	dt:			
(2) the text and graphics herein as well	antific hypotheses and scientific perions) are true and complete as any accompanying publications or other documents, unless or their supervision. Lagues to accept responsibility for the scient mode as a result of this proposal.	otherwise indicated, are the original work of th	le .	
Lunderstand that the withul provision of criminal offense (U.S.Code, Title 18, Se	talso information or concearing a material fact in this proposal or scion 1001).	r any other communication submitted to NSF	is a	
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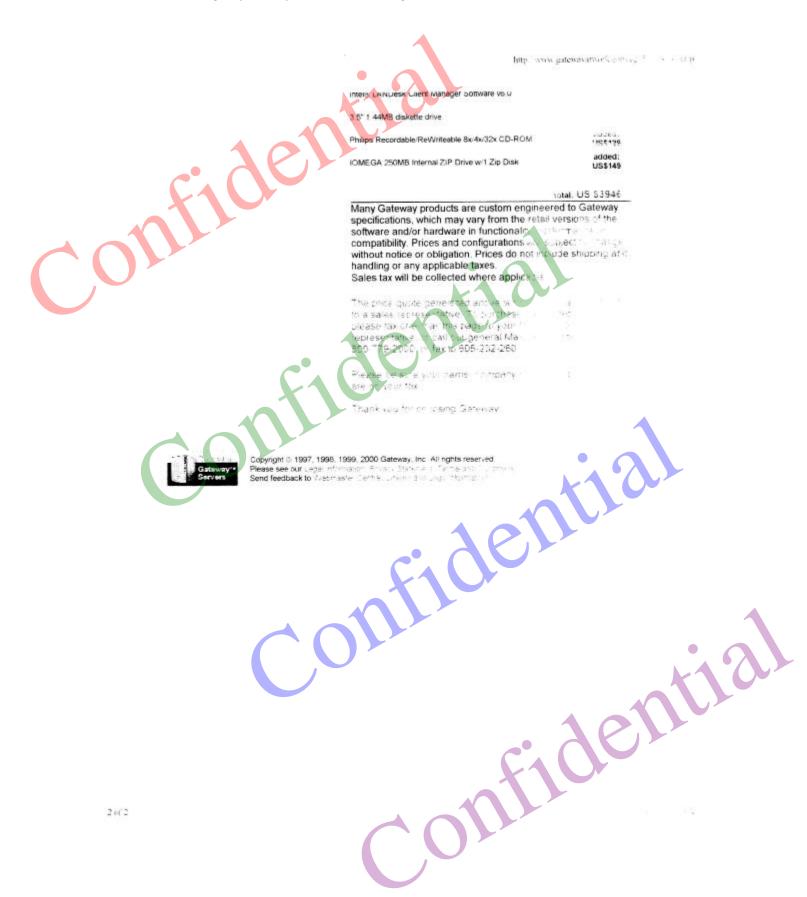


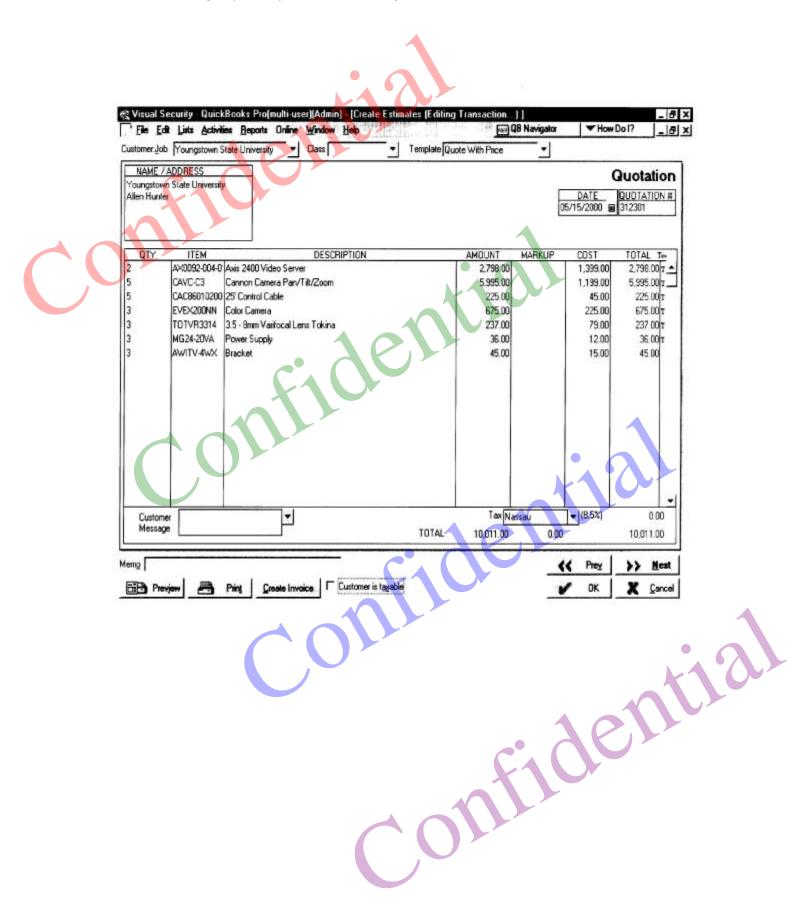
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Item #	Catalog Number	Qty	Description	Unit Erize
2	842-054600	1	Upgrade GADDS for DOS to GADDS NT This upgrades the GADDS software operating under DOS (must have a HI-STAR detector) to GADDS software operating under NT. Includes hardware modification to PDC which is done in Madison or Karlsruhe, new software, and manuals. Requires a computer upgrade (not included) to the NT operating system. Not for use with X-1000 detector system.	
3	842-058200	1	Upgrade from LT-2 to LT-3, PLATFORM Replaces glass links and LT-2 nozzle with all stainless steel delivery system and nozzle with warm stream surrounding cold stream. Requires source of dry compressed air.	
4	862-057300	1	Water to Water Refrigerated Heat Exchanger, Single Pump R100C <u>Mechanically refrigerated</u> heat exchanger uses low- pressure refrigerant. Heat removal capacity 3,850 Watts with 65° F cooling water, includes option ABCOB: flowmeter, high- temperature thermostat to shut off pump, water cooled condenser with water-saver feature, manual shut-off valves, and high-capacity pump. 325 lbs, 21°W x 29°D x 32°H. Single pump system. (208V, 60Hz, 1-phase)	
5	87-000-088	24	XYZ Gonlometer Head 49.mm with extension to 72 mm, lockable.	
	222-076101	3	Eucentric Goniometer Head	
6	222-0/6101	3	Eucentric goniometer head Eucentric goniometer head with dual sectors (±20° rotation) and X, Y, Z adjustment (±4 mm in X, Y).	
7	843-011400	24	SHELXTL/PC™ Version 5.1 Software License (per site) A multiple site license for the SHELXTL/PC™ software package is available for DOS. As a prerequisite, at least one SHELXTL/PC™ workstation must already be on-site, software may then be licensed for additional, user-supplied PC's at the incremental rate indicated. The license includes the right to copy SHELXTL/PC™ to one additional PC workstation and documentation. SHELXTL/PC™ Unlimited Users Site License Purchase a quantity of ten of part number 843-011400 to receive rights to unlimited users per site.	
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			Complete and installed including one (1) year labor and parts warranty.	SIL
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Allen D. Hunter Youngstown State University Department of Chemistry One University Plaza Youngstown, OH 44555

Monday, April 17, 2000

Dear Dr Hunter,

Thank you for offering to host the ESQUIRE-LC training course for our Northern Ohio users at Youngstown last week. We at Bruker Daltonics were exceptionally pleased with the facilities that we were able to use in the Chemistry Department, and also with the help and support of your computer and instrument specialists, Ray Hoff and Bruce Levison.

The use of your media lab with networked PCs enabled a large group of users to be simultaneously trained in the use of the acquisition and processing software for the ESQUIRE-LC. With PCAnywhere set up by Ray, we could even control the ESQUIRE-LC from a remote PC! At a later time this could also be done by users from a remote location, either by LAN or by modem. This would allow the ESQUIRE-LC to be used by a wide group of users in Ohio, either to run samples or as a teaching tool to show the capabilities of electrospray ion trap instruments.

Again, thank you for making the training course so productive, both for our Ohio customers and for Bruker Daltonics. If we need to do further advanced training for the users we will be very pleased to use your facilities at YSU again.

Best regards,

Catherine Stacey Ph.D. Ion Trap Product Manager Bruker Daltonics

19 Fortune Drive Biilerica, MA01821



Bruker Daltonics, Inc. Manning Park Billerica, MA 01821 USA Tel: (978) 667-9580 Fax: (978) 667-5993 ww.daltonics.bruker.com