COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 99-2

NSF 99-53 **06/07/99**

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

CCLI-EDUCATIONAL MATERIALS DEV

FOR NSF USE ONLY

NSF PROPOSAL NUMBER

9980921

DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION
				000000000	

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

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

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

NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE

Youngstown State University

AWARDEE ORGANIZATION CODE (IF KNOWN)

0031450000

ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE

Youngstown State University
410 Wick Avenue
Youngstown, OH. 445550001

NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE

PERFORMING ORGANIZATION CODE (IF KNOWN)

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

IS AWARDEE ORGANIZATION (Check All That Apply)
(See GPG II.D.1 For Definitions) ☐ FOR-PROFIT ORGANIZATION ☐ SMALL BUSINESS ☐ MINORITY BUSINESS ☐ WOMAN-OWNED BUSINESS

TITLE OF PROPOSED PROJECT **X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE
$ **74,707**	**24** months	**05/01/00**	

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

☐ BEGINNING INVESTIGATOR (GPG 1.A.3)
☐ DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.D.1)
☐ PROPRIETARY & PRIVILEGED INFORMATION (GPG II.D.10)
☐ NATIONAL ENVIRONMENTAL POLICY ACT (GPG II.D.10)
☐ HISTORIC PLACES (GPG II.D.10)
☐ SMALL GRANT FOR EXPLOR. RESEARCH (SGER) (GPG II.D.12)
☐ GROUP PROPOSAL (GPG II.D.12)
☐ VERTEBRATE ANIMALS (GPG II.D.12) IACUC App. Date _____
☐ HUMAN SUBJECTS (GPG II.D.12)
Exemption Subsection _____ or IRB App. Date _____
☐ INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES _____
☐ FACILITATION FOR SCIENTISTS/ENGINEERS WITH DISABILITIES (GPG V.G.)
☐ RESEARCH OPPORTUNITY AWARD (GPG V.H)

PI/PD DEPARTMENT
Department of Chemistry

PI/PD FAX NUMBER
330-742-1579

PI/PD POSTAL ADDRESS
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NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address
PI/PD NAME **Allen D Hunter**	**Ph.D.**	**1985**	**330-742-7176**	**adhunter@cc.ysu.edu**
CO-PI/PD				
CO-PI/PD				
CO-PI/PD				
CO-PI/PD				

CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

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

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

Name (Typed)	Signature	Social Security No.*	Date
PI/PD **Allen D Hunter**			
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			

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

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt status, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 99-2. 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

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

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	SIGNATURE	DATE
NAME/TITLE (TYPED) **Peter J. Kasvinsky/Graduate Dean**		**06/07/99**

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

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

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-Educational Materials Development**
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:

Project Data:

A. Major Discipline Code: **12**
B. Academic Focus Level of Project: **AL**
C. Highest Degree Code: **M**
D. Category Code: **X**
E. Business/Industry Participation Code: **PS**
F. Audience Code: **H T I S F**
G. Institution Code: **PUBL**
H. Strategic Area Code:
I. Project Features: **1 2 3 5 6**

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

J. Undergraduate Students: **500**
K. Pre-college Students: **150**
L. College Faculty: **10**
M. Pre-college Teachers: **10**

4. Project Summary

Recent advances in hardware, theory, and software coupled with the rapidly improving price and performance of personal computers have combined to make single crystal diffraction methods simultaneously more powerful and easier to perform. This is rapidly increasing their importance in fields as diverse as synthetic chemistry, materials science, and structural biology in both industry and academia. For these reasons, we are interested in integrating diffraction methods throughout the curriculum. This CCLI-EMD proof of concept project will assist this process via the development of instructor and student documentation, laboratory resources, software, and annotated data bases. At the introductory level, these materials will focus on the relationship between experimentally derived structural data and bonding theory. At the more advanced level, these materials will include a more comprehensive treatment of this structure/bonding relationship, modules on single crystal diffraction suitable for insertion into upper division courses of several types, and materials to support more extended treatments of these topics in dedicated courses and undergraduate research projects. The introductory materials will serve a broad student base, including all science and technology majors, health and human service majors, and pre-service science teachers. They will also be prepared in a form suitable for use with non-science and non-technology majors and high school chemistry students. The advanced materials will serve the needs of undergraduate students majoring in chemistry and allied disciplines (e.g., biology, geology, physics, materials science and engineering). All of the new materials produced will be comprehensively assessed by peer reviewers and by formal pre- and post-exposure student outcomes studies. This project strongly emphasizes the DUE theme of the integration of technology into education and has smaller teacher preparation and faculty development components.

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For font size and page formatting specifications, see GPG section II.C.

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A	Project Summary (not to exceed 1 page)	1	
B	Table of Contents (NSF Form 1359)	1	
C	Project Description (including 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)**	25	
D	References Cited	3	
E	Biographical Sketches (Not to exceed 2 pages each)	4	
F	Budget (NSF Form 1030, including up to 3 pages of budget justification)	7	
G	Current and Pending Support (NSF Form 1239)	2	
H	Facilities, Equipment and Other Resources (NSF Form 1363)	1	
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:		

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

6. Project Description

Results from Prior NSF Support:

i. NSF DMR 9403889: "Acquisition of a Single Crystal X-Ray Diffractometer"

This *research equipment* grant ($71,199, ≈ $200,000 match, 1994-96) was used to purchase 2 new Siemens P4 X-ray diffractometers, a low temperature attachment, a multi-wire area detector, and a number of SGI and PC workstations for data processing. These acquisitions have allowed integration of advanced diffraction methods into the junior/senior level chemistry curriculum at YSU.[1-6] A new 3 quarter hour course, "Chemistry 832: Solid State Structural Methods," that fully integrates this equipment is offered each year. It has directly led to several papers with undergraduate co-authors,[1] a laboratory manual,[2] and presentations at national crystallographic education meetings.[4-6] Powder and single crystal diffraction methods have also been integrated into five other upper level chemistry courses.[3]

ii. NSF DUE 9551683: "Integration of GC-MS into the Undergraduate Curriculum"

This *ILI* grant ($34,450, ≈ $40,000 match, 1995-96) was used to purchase a Finnigan 1020 Gas Chromatograph-Mass Spectrometer. This is now fully integrated into student research,[7a] senior level Organic Synthesis, Organic Analysis, and Inorganic Lab courses (i.e., 50 students a year), and into the Sophomore Organic sequence (i.e., ≈ 200 students a quarter, primarily from the natural sciences, engineering, and pre-medicine). In each case, it has facilitated a new collaborative learning/discovery-oriented approach.

iii. NSF DUE 9850079: "Investigative Approaches in the Natural Sciences"

This *DUE* grant ($183,579, ≈ $200,400 match, 1998-2001) is being used by a multidisciplinary team to develop a new lab course having collaborative "research like" projects. It is designed to teach students what science is by having them do science. It will be the normal path for non-science and non-technology majors to satisfy the natural science lab requirement in

the new general education program which starts in the fall of 2000. This course has just been piloted for the first time, three sections will be piloted next year, and multiple sections will be offered each semester during the 2000/2001 school year and beyond.

iv. NSF DUE 9851107: "Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment"

These *ILI* grant funds ($44,600, over $44,600 match, 1998-2000) have been stretched to purchase more capable instrumentation then originally proposed, including: (a) a TA Instruments 2910 DSC , a 2050 TGA, a Data System, and an upgrade of our older Dupont DSC/data system, (b) a Cannon CT-518 constant temperature bath, and (c) a GBC Instruments/Polymer Labs GPC-HPLC system (i.e., autosampler, isocratic/gradient pump, column oven, RI and diode array UV-visible detectors, and data system) as well as additional equipment (authorized by Susan Hixson, DUE, January 1999) including: (d) a Jasco 410 FT-IR (0.9 cm^{-1}) and (e) a Vacuum Atmospheres HE-43-2 inert atmosphere glove box with the residual funds. These have all been installed over the last three months and will be fully integrated into our courses by the Spring of 2000.

a) Project Overview:

Recent advances in X-ray diffraction hardware, theory, and software and in computer technology have simultaneously increased the power and ease of use of diffraction methods. These changes are rapidly increasing the importance of single crystal diffraction methods in solving both advanced and more routine problems in fields as diverse as synthetic chemistry, materials science and engineering, and structural biology. Despite this trend, the coverage of diffraction methods in the undergraduate curriculum is both thin and weak.[6,8]

It is therefore an opportune moment to develop the teaching resources required to integrate diffraction methods into undergraduate education. Indeed, this is the core idea of the

current proposal. These new materials will include: background reading materials for instructors and students at several levels of sophistication, tested curricular/lesson plans, laboratory handouts/exercises, software and appropriate documentation, and an annotated database of single crystal diffraction data sets. These materials will be developed from related materials the PI now uses in several upper level courses and from commercial diffraction analysis software. Over the two years of the project, draft versions of these materials will be: (i) prepared and evaluated, (ii) piloted on a small scale, (iii) reevaluated, revised, and expanded, (iv) piloted on a larger scale, and (v) given final evaluations before wider dissemination.

For this project, the PI will provide crystallographic expertise, oversight, and will have primary responsibility for the junior/senior level materials. An experienced high school chemistry teacher with a MS in chemistry and a chemistry graduate student having an interest in chemical education will concentrate on the freshman/sophomore level materials. During this project, a range of resource materials for integrating diffraction methods into the undergraduate curriculum will be prepared and will go through two rounds of pilot studies. These materials and consequent student outcomes will be assessed using both peer evaluators and formal student assessment instruments. Finally, software vendor contracts and detailed plans for the national dissemination of the products of the project will be completed.

b) Goals and Objectives:

This project is designed to address several national *problems* and take advantage of several local and national *opportunities*, including:

Problem 1: While the use of diffraction methods in both academia and industry is rapidly growing, its integration into our undergraduate curriculum is both spotty and weak.[6,8] Science and technology graduates are typically not exposed to the requisite/appropriate content related to diffraction methods that they increasingly will need after they graduate.

Problem 2: It has become increasingly apparent that the "cook book" style labs which are all too common in our laboratory courses "turn students off" (especially non-traditional students such as women and under-represented minorities), have limited pedagogical value, and should be replaced with collaborative and more "research like" laboratory experiences.[9]

Problem 3: Students exiting general chemistry classes have many misperceptions about the relationship of molecular structure to bonding theory and about the relationship of experimental data to theory (e.g., typically failing to appreciate the importance and central nature of the experimental structural data).

Problem 4: Software is now available which is suitable for integrating diffraction methods into many classrooms. However, it is designed for use by crystallographic experts, appropriate written documentation and diffraction data sets are not available, and this software is too costly for use in large enrollment classes.

Opportunity 1: Because YSU will implement a new general education system and will convert from quarters to semesters during the fall term of 2000, all courses on campus are being revised. Therefore, a window of opportunity now exists locally for major curricular innovations.

Opportunity 2: Recent advances are making single crystal X-ray structure determinations much more accessible to non-experts. Indeed, we are now at the point where, for *screened/routine* data sets, this technique may be employed by students and other non-experts.

Opportunity 3: Essentially all colleges and high schools now have computer labs (all too often underutilized) whose PCs are capable of running modern diffraction analysis packages.

Opportunity 4: The "video game" generation of students we are now getting are very familiar with computers and actively enjoy activities that provide graphically rich experiences. This is something common to all modern diffraction analysis packages.

Opportunity 5: Students have high innate levels of interest in crystals and related topics.

To address these problems and take advantage of these opportunities, we have developed the following specific *goals* and *objectives* for this proof of concept EMD project:

Goal 1: To facilitate the full integration of diffraction methods across the curriculum and thus to involve our students in the use of an increasingly accessible characterization technique that is of growing academic and industrial importance.

Goal 2: To give all of our student a better understanding of the experimental nature of structural data and how this data relates to bonding theories.

Objective 1: To prepare *tested* background reading materials for instructors on single crystal diffraction methods at several levels of sophistication.

Objective 2: To prepare *tested* background reading materials for students on single crystal diffraction methods at several levels of sophistication.

Objective 3: To prepare *tested* curricular/lesson plans for diffraction methods modules that integrate both lecture and laboratory content for courses at the freshman/sophomore (and as a byproduct, high school) and junior/senior levels.

Objective 4: To prepare *tested* laboratory materials (i.e., printed lab experiments) for both instructors and students suitable for both levels.

Objective 5: With the assistance of the software vendors, to develop *"student"* versions of diffraction analysis software and *tested* documentation that is "user friendly" for non-experts. As important, this software must be sufficiently inexpensive that it can be purchased for use in large enrollment chemistry classes and/or by institutions with limited budgets.

Objective 6: To develop a *tested* and annotated database of single crystal diffraction data sets suitable for use in these labs at all levels and containing a variety of structure types.

Objective 7: To write and integrate these lecture/lab modules in such a way that they can be used by instructors who are non-experts in crystallography.

Objective 8: To negotiate signed contracts for the publication/dissemination of the modified "student" software and for the database and printed instructor/student materials.

Objective 9: To fully assess the materials prepared using both *peer evaluations* and *formal* student *outcomes assessment* instruments.

Objective 10: To disseminate the draft instructional materials and the outcomes assessments to the national chemical education and crystallographic communities.

Objective 11: To prepare a detailed plan for the development of the final instructional materials and the national dissemination of the curriculum innovations.

c) Detailed Project Plan:

i. Levels at Which Diffraction Methods will be Treated

As described in the previous section, the materials to be developed will be aimed at either the "advanced" (i.e., junior/senior) or the "entry" (i.e., the freshman/sophomore) levels. All materials will assume only a minimal computer background but will require access to a modern computer lab equipped with PCs using the Windows NT/2000 or 95/98 operating systems. [There are no plans to port the *software* to the Apple OS during this proof of concept stage.]

Advanced level materials are those designed principally for use by students majoring in chemistry/allied disciplines (e.g., materials science and engineering, biology, geology, physics, and environmental science) and for courses at the junior/senior levels. They will presume a solid background in mathematics and substantial college level laboratory science credits. They will typically be inserted as modules on diffraction methods into courses such as Instrumental Methods, Organic Analysis, Inorganic Chemistry, Physical/Biophysical Chemistry, Materials Science, Mineralogy, and Biochemistry/Structural Biology. A full length laboratory manual for those having a dedicated course or undergraduate research students will also be prepared.

Entry level materials are those designed principally for use by either science and

technology majors at the freshman/sophomore level or by students whose only exposure to chemistry at the college level will be a terminal course (e.g. "Chemistry for Poets"). They will only assume proficiency with high school level math and a relatively modest background in high school/freshman level sciences. They will typically be used as modules in courses such as General Chemistry, Allied Heath Chemistry, and Organic Chemistry. There will be a strong emphasis on relating the experimental nature of the structures derived from diffraction data to common molecular structure motifs and to theories of molecular bonding.

Discussions with numerous college and high school chemistry instructors, personal experience, and the education litterature,[9g,h] all indicate that there is often as much or more variability between individual students in a single section of a course as there is between "average" students in courses at adjacent year levels. Thus, one finds that the best students taking high school chemistry have a better understanding than the average student taking General Chemistry and better even than some sophomore chemistry majors. This is true even before schools/institutions having differing selectivity's/exclusivity's are taken into account. For this reason, materials designed for both the entry and advanced levels will prepared at several levels of sophistication (i.e., "tracks"), a *basic track*, a *typical track*, and an *accelerated track* (i.e., for those with the weakest, average, and strongest preparation/abilities, respectively). As a point of reference, the *typical track* materials will be paced for the typical YSU (an open admission public institution) General Chemistry student at the entry level and YSU chemistry junior at the advanced level. This will enable instructors to chose the "track" of coverage most suitable for their students. Since most of the actual laboratory work will be self paced in computer labs or even on home computers this approach will allow students having extra difficulty or seeking more of a challenge to adjust their approach. Students having an especially wide range of abilities and preparation take entry level General Chemistry classes. Materials at the *entry level*

will therefore be produced suitable for all three tracks. An added benefit of this is that the accelerated track materials will be highly suitable for typical sophomore students while the basic track materials will be suitable for inclusion in many high school chemistry courses.

ii. Specific Types of Materials which will be Prepared

By the end of this proof of concept project, the proposed materials will be in a sufficiently completed form and assessed thoroughly enough to move directly to commercial/electronic distribution channels (especially for the upper level materials) and/or to move beyond the proof of concept to the full proposal stage. These materials can be divided into several types:

Product 1, *Instructor and Student Background Materials:* The *tested* instructor materials will be prepared at several levels of sophistication and will be sufficiently detailed to assist instructors getting "up to speed" so that non-experts in crystallography will feel comfortable in introducing these student exercises into their classes. These will be conceptual/graphics intensive documents and they will include an annotated bibliography of further readings and a list of related Web based resources. The *tested* student materials, which will be prepared at several levels of sophistication, are designed to supplement the coverage given in the student's texts (which are generally inadequate for this purpose), and will be designed to help the students understand the new lecture content and laboratory exercises. These documents will concentrate on teaching the central concepts, they will be graphics intensive, and they will include a list of further appropriate readings and of Web based resources (see Appendix III).

Product 2, *Module Plans and Laboratory Exercises.* Plans for diffraction methods modules (i.e., suggested lecture content and laboratory exercises) that have been pilot *tested* and are ready to be introduced into specific courses will be prepared. A series of specific laboratory exercises that have been pilot *tested* will be prepared, including: instructor guides, student

handouts, a PowerPoint presentation and transparencies, and recommended data sets for use either in computer labs or on home computers (see Appendix IV).

Product 3, *Comprehensive Single Crystal Diffraction Methods Lab Manual:* This *tested* manual will include exercises on: crystal growth, crystal selection and mounting, data collection, data analysis, the crystallographic literature and the Cambridge and ICDD data bases, and analyzing and preparing crystallographic publications. This manual will be based on the PI's current lab manual[2] and Chemistry 832 lab exercises (see Appendices I, II, and V).

Product 4, *Student Diffraction Analysis Software and Software Documentation:* The PI has verbal commitments from the vendors of the two most user friendly X-ray diffraction analysis programs (SHELXTL/XSHELL from Bruker AXS, Sue Byram, and teXsan from Molecular Structure Corporation, Bev Vincent) to provide "student" versions of their software (i.e., ones that have had their advanced features removed to eliminate competition with their "research grade" products) for this proof of concept study. During this grant, these two products will be evaluated and modified, where required, to assess and improve their "student friendliness" and formal contracts will be signed with one or both vendors to set the conditions and costs for their national educational release. Both manufacturers have stated that upon completion of this work they will be willing to release these "student" versions at reduced or even no cost. The PI will prepare "non-expert friendly" documentation on these products for use by instructors and students (see Appendix VI).

Product 5, *Annotated Diffraction Data Sets:* This project will include the collection (largely from current contacts) of a pilot scale database of single crystal diffraction data sets (i.e., from 25 to 50 sets for each category of structure, including: simple organic compounds, medicinal compounds, inorganic/organometallic compounds, extended solids/minerals, and biomolecules (i.e., peptides, carbohydrates, and lipids)). In addition to all diffraction data

required to solve each of these structures (i.e., properly formatted for the diffraction packages) there will be instructor and student files for each. The instructor files will describe the typical problems students have with solving and understanding each structure and the PI's solutions to these problems while the student files will give background information on each compound and hints on the solving the structure (see Appendix VII).

Product 6, Web Site: All of these proof of concept materials, with the possible exception of the software, will be posted on a YSU Web site as .html and .pdf files with access for students and instructors (the latter password protected).

Product 7, Assessment Information and Dissemination: All materials prepared for this proof of concept grant will be formally assessed and will be disseminated as described below.

iii. Roles of the Project Participants

These individuals (see section 6d) will work together closely as members of a team, however, each team member will have specific areas of primary responsibility, specifically:

Dr. Allen D. Hunter, PI: Allen will be responsible for overall planning, budgeting, and integration of team activities and for the assessment and dissemination efforts. He will have primary responsibility for preparing, piloting, and assessing all of the advanced level materials. He will also be responsible for interactions with the software suppliers/publishers and will have the lead role in annotating the diffraction data sets.

Mr. Steven J. DiMuzio: Steve will be primarily responsible for modifying the advanced into entry level materials and for piloting and assessing the materials at the high school level.

The Graduate Student: The graduate student will be primarily responsible for testing each entry in the database (i.e., that each data set runs as described in the diffraction analysis documentation and lab handouts). This student will also run the actual pilot studies in the General Chemistry labs and will collect the assessment data for these.

The Advisory Panel: The Advisory Panel will be composed of individuals with varying levels of experience in crystallography/crystallographic education, including: Margaret Kastner, Bucknell University; Vivien Yee, Case Western Reserve University; John Woolcock, Indiana University of Pennsylvania; Mike Serra, YSU; Tim Wagner, YSU; and Neil Walsh, Ohio Dominican College. It will be responsible for part of the peer-review of the educational materials prepared and for oversight of the project assessment and dissemination efforts.

iv. Time Table for Project

Work to Date: All of these materials have been developed and/or piloted to a limited extent either with small groups of students and/or in upper level chemistry classes. For example, this approach to integrating diffraction methods with structure and bonding was piloted several years ago with a group of nine high school chemistry teachers. The basic laboratory materials for the advanced level have also been tested for several years.[2-6] However, in their present format these materials require the instructor to have substantial expertise in diffraction methods and in the specific diffraction program used. This project is designed to minimize these needs, to prepare more polished products, and to conduct carefully controlled evaluations of the pilot studies. [Note: the timing of the assessment and dissemination activities is described separately in sections 6e and 6f, below.]

Summer of 2000: During the first summer, the team will prepare first drafts of the written materials described above and will post ≈ 50 annotated data sets to the Web site.

Fall/Winter of 2000/2001: During this time, the team will pilot test these materials in a selection of representative high school chemistry, General Chemistry, and junior/senior level chemistry classes (approximately 5 classes in total) at the home institutions/departments of the team members. The "student" versions of the software will be completed and formal contracts will be negotiated with the software vendors listing the costs, distribution pathways, and any

restrictions on the "student" versions of their software.

Summer of 2001: During this time, the assessment results will be used to revise the written materials, these and the Web site will be updated and expanded for a greater range of courses, and the rest of the annotated data sets will be prepared. Faculty development activities for the new instructors who will pilot these materials the following fall/winter will be given.

Fall/Winter of 2001/2001: During this time, the pilot studies will be extended to a larger number of sections (i.e., ≈ 15), with the first outside instructors, courses, and institutions (including: Margaret Kastner at Bucknell University), a final report will be prepared, and funding for the national distribution of these materials will be sought.

v. Facilities and Resources for Accomplishing the Project

The YSU Chemistry Department already has all the major facilities and equipment needed to accomplish this project including: two X-ray diffractometers, two computer labs (i.e., one with 16 Windows NT computers and one with 24 Windows 96 computers), and a functioning computer network with both hardware and software service personnel. The PI has also obtained licenses and commitments from the two vendors to provide versions of both commercial diffraction packages suitable for the pilot studies. We also have extremely strong ongoing relationships with other science departments and colleges on campus, with regional universities and colleges (including those in the Ohio X-Ray Consortium and the Advanced Diffraction Studies Consortium), and with high schools where these materials will be tested and from whom we can borrow any requisite expertise. As discussed in the Budget Justification section, several small items including a CD writer, an additional hard drive, and a two year license for the Cambridge data based will be purchased partly out of grant funds.

d) Experience and Capability of the Principle Investigators/Project Personnel:

The PI, Dr. Allen D. Hunter, is the founder and director of the Advanced Diffraction

Studies Consortium, a group of several dozen PhD and predominantly undergraduate institutions, federal research labs, and companies (predominantly in northern Ohio and western Pennsylvania, http://www.as.ysu.edu/~adhunter/ADSC/index.html). He is also a founding member and is on the governing board of the Ohio X-Ray Consortium (i.e., http://www.icenter.utoledo.edu/icenter/occ.htmlx). Finally, he is on the educational sub-committee of the International Center for Diffraction Data and he serves on the advisory board of the W. M. Keck Foundation Center for Molecular Structure at Cal State Fullerton. His research interests include synthetic organometallic, supramolecular, and polymer chemistry, the application of diffraction methods to solving chemical problems, and chemical education.[2-7] Many excellent text books exist for full lecture courses on diffraction methods[10] and various aspects of X-ray diffraction have been discussed in the *Journal of Chemical Education*.[11] However, few materials suitable for use in short lecture/lab modules on single crystal methods are available. In addition, no suitable lab text is available to teach novices how to solve diffraction data for molecular structures. This stimulated the PI's interest in developing curricular materials related to diffraction methods.[2-6] He has published a paper in the *Journal of Chemical Education* on the use of diffraction methods in non-traditional courses[3] and has released (as two .pdf files) a 275 page manual for novices on solving crystal structures (see Appendices I and II).[2] He has also given talks/posters at several regional and national crystallography meetings on more general aspects of teaching crystallography to non-experts.[4-6] Over the last 5 years, the PI has been involved in extensive efforts to extend the integration of diffraction methods throughout the curriculum, including: teaching a "hands on" course on structural methods for high school chemistry teachers, teaching modules on diffraction methods in courses as diverse as Biophysical Chemistry and Organic Analysis, and investigating the use of diffraction methods with pre-college students.

Steven DiMuzio, is the second member of the team. He has BS and MS degrees in chemistry from YSU where he took an extensive range of undergraduate and graduate courses including our X-ray diffraction course. He has taught high school chemistry and science for three years at both inner city and suburban schools. His relatively moderate background in diffraction methods will be an advantage in converting the PI's advanced level instructional materials to entry level instructional materials.

The *graduate student* will be a student with a BS degree in chemistry who plans on obtaining a MS degree in chemistry with an emphasis on chemical education. They will be either a current high school chemistry teacher returning to get their MS or a chemistry BS student planning on teaching high school chemistry after graduation. [We typically have one or two such students each year and due to recent changes in teacher certification in Ohio (i.e., typically requiring MS degrees in content areas) we expect this number to increase rapidly.]

e) Evaluation Plan for this Proof of Concept Proposal:

In the *first stage* of the evaluation process, the PI will *formally* survey experts in chemical education and crystallography on the current state of crystallographic education and educational materials (the *informal* phase of this was completed at the recent American Crystallographic Association meeting).[6,8] To provide *baseline data* and guide the writing of the project materials, the project team will also survey representative instructors, high school and general chemistry students, science and technology majors (i.e., taking sophomore level chemistry, biology, physics, and geology classes), and majors in chemistry and allied disciplines (i.e., taking junior and senior level chemistry courses) on their attitudes towards, and interest in, crystallography/diffraction methods and the relationship of structural data to bonding theories. [Note: All assessment instruments will be prepared and evaluated with the assistance of the YSU Office of Institutional Research and Assessment (Becky Geltz, director) and the established

YSU Faculty of Arts and Sciences project assessment team (Jennifer L. Hampston, Psychology, team leader).]

In the *second stage*, the project team will distribute the draft materials prepared during the first summer of this grant to the Advisory Panel for commentary and subsequent revision before pilot testing over the 2000/2001 school year. These students will be given pre- and post-tests on their attitudes towards and knowledge of the material covered. The results of this preliminary testing will be presented to the Advisory Committee, at the national American Chemical Society (Chemical Education Division) and American Crystallographic Association meetings, and the regional Science Teachers Association meeting for comment and feedback.

In the *third stage*, this feedback will be used to revise these materials and pilot them with a wider selection of classes. Again pre- and post-tests will be used and the results evaluated by the Advisory Committee and will be presented for commentary and feedback at national meetings. The results will also be distributed electronically to the relevant communities for commentary and will be published as papers and as a manual to provide formal peer review.

f) Dissemination of Results:

As described above, there will be extensive dissemination of the results of this work at science teacher, chemical education, and crystallography conferences. In addition, the formal evaluations of the project outcomes will be published in educational journals, the new lecture and lab materials prepared will be published in peer reviewed print and electronic journals (i.e., the Journal of Chemical Education and the Chemical Educator, respectively), and the advanced lab manual and diffraction software will be under contract. Finally, all of the actual "proof of concept" teaching materials will be made available through a combination of commercial publishers and/or distribution over the web as the PI currently does for his draft manual.

11. Appendices

Appendix I: Current User List for "Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction" (i.e., Reference 2)

Below is the authorized user list, as of May 31st, 1999, for the .pdf version of this manual:

#	User Name	University	Department
1.	A. J. Blake	University of Nottingham	Chemistry
2.	Alan J. Jircitano	Penn State Erie-Behrend College	Chemistry
3.	Alexandr V. Belushkin	Joint Inst. for Nuclear Research, Dubna	Neutron Physics
4.	Anders Palmqvist	UC Santa Barbara	Chemistry
5.	Andreas Decken	University of New Brunswick	Chemistry
6.	Andy McDonald	Laurentian University	Earth Sciences
7.	Angelo Mugnoli	University of Genova, Italy	Chemistry
8.	Angus P. Wilkinson	Georgia Tech	
9.	Anne C. Bloomer	Cambridge	MRC Molecular Biology
10.	Arkady Ellern	Ben-Gurion University of the Negev	
11.	Armin Ruf	BASF-AG	
12.	Armin Wagner	Freie Universitaet Berlin	Inst. fuer Kristallographie
13.	Arnold L. Rheingold	University of Delaware	Chemistry
14.	Arthur Mar	University of Alberta	Chemistry
15.	Ashwani Vij	University of Idaho	Chemistry
16.	B. C. Wang	University of Georgia	Biochemistry
17.	Barry Hicks	US Air Force Academy	Biochemistry
18.	Beatrix Wagner	University of Virginia	Pharmacology
19.	Bernhard Spingler	MIT	Chemistry
20.	Bernie Santarsiero	University of California at Berkeley	Structural Biology
21.	Bob McDonald	University of Alberta	Chemistry
22.	Bob Sparks	Bruker AXS	Crystallography
23.	Bobby Barnett	Procter & Gamble	Health Care Research
24.	Branton Campbell	UC Santa Barbara	Materials Research Lab.
25.	Bruker AXS	Bruker AXS	Vendor
26.	Camden Hubbard	ORNL	HTML
27.	Casey Raymond	Kent State	Chemistry
28.	Chaveng Pakawatchai	Prince of Songkla University, Thailand	Chemistry
29.	Chong Zheng	Northern Illinois University	Chemistry
30.	Christopher L. Cahill	SUNY - Stony Brook	Chemistry
31.	Chuck Campana	Bruker AXS	Vendor
32.	Claude Lecomte	University of Nancy	
33.	Dane A. Boysen	Cal Tech	
34.	Daren J. Leblanc	Dalhousie University	Chemistry
35.	David Grossie	Wright State University	Chemistry
36.	Donald L. Ward	Michigan State University	Chemistry
37.	Doug Powell	University of Wisconsin at Madison	Chemistry
38.	Elizabeth Maclean	CLRC Daresbury	
39.	Ewa Skrzypczak-Jankun	University of Toledo	Chemistry
40.	Fred (Flieg) Hollander	UC Berkeley	Chemistry
41.	Gabriella Bombieri	Milano University	Medicinal Chemistry
42.	Ged Parkin	Columbia University	Chemistry
43.	George Richter Addo	University of Oklahoma	Chemistry
44.	George M. Sheldrick	(author of SHELX)	

45.	Georgina Rosair	Heriot-Watt University, UK	Chemistry
46.	Gervais Chapuis	University of Lausanne	Inst. of Crystallography
47.	Glenn P. A. Yap	University of Ottawa	Chemistry
48.	Gregory A. Stephenson	Lilly	
49.	Guido Kickelbick	Vienna	Inst. Fuer. Anorg. Chemie
50.	Guy Crundwell	Central Connecticut State University	Chemistry
51.	Hans Preut	Universitaet Dortmund	Fachbereich Chemie
52.	Hilary Jenkins	St. Mary's University	Chemistry
53.	Hong-Kun Fun	Universiti Sains Malaysia	Physics
54.	J. Vitali	University of Texas	
55.	J. Derek Woolins	Loughborough University, UK	Chemistry
56.	Jagadese J. Vittal	National University of Singapore	Chemistry
57.	James C. Fettinger	University of Maryland	Chemistry
58.	Jane E. A. Wibley	Leicester, UK	
59.	Janeen Vanhooke	University of Wisconsin at Madison	Biochemistry
60.	Janet Moloney	University of Durham	Chemistry
61.	Jeanette Krause Bauer	University of Cincinnati	Chemistry
62.	Jeff W. Kampf	University of Michigan	
63.	Jens-Boie Suck	CHEMNITZ, Germany	Physics
64.	Jim Kaduk	BP Amoco	Naperville
65.	Jim Gano	University of Toledo	Chemistry
66.	Jim Golen	University of Massachusetts Dartmouth	Chemistry
67.	John C. Bollinger	Indiana University	Molecular Structure Center
68.	John D. Protasiewicz	CWRU	Chemistry
69.	John Gnabre	Johns Hopkins University	Biology
70.	John Hughes	Miami University	Geology
71.	John J. Rupp	St. Lawrence University	Chemistry
72.	John Malone	Queens University - Belfast	
73.	John Parise	SUNY Stony Brook	Geosciences
74.	John Ricci	University of South Maine	Chemistry
75.	John Rose	University of Georgia	Biochemistry
76.	John Woolcock	Indiana University of PA	Chemistry
77.	Karin Ruhlandt-Senge	Syracuse University	Chemistry
78.	Kate Crennell	Crystallography News	Editor
79.	Katherine Kantardjieff	Cal. State Fullerton	Chemistry
80.	Kenneth I. Hardcastle	Cal. State Northridge	Chemistry
81.	Kenny Stahl	Technical University of Denmark	Chemistry
82.	Klaus Eichhorn	Universitaet Karlsruhe	Inst. fur Kristallographie
83.	Kyung Hyun Kim	Korea University	Biotechnology
84.	Kurt D. Berndt	Karolinska Institute, Sweden	Biosciences
85.	Larry S. Curtin	YSU	Chemistry
86.	Lee Brammer	University of Missouri - St. Louis	Chemistry
87.	Lee M. Daniels	Texas A & M University	Chemistry
88.	Linda H. Doerrer	Oxford University	Inorganic Chemistry
89.	Lothar Stahl	University of North Dakota	Chemistry
90.	Margaret Kastner	Bucknell University	Chemistry
91.	Martha Teeter	Boston College	Chemistry
92.	Masood Parvez	University of Calgary	Chemistry
93.	Massimo Di Vaira	Florence	Chemistry
94.	Massy Shoja		
95.	Menachem Shoham	CWRU	Biochemistry
96.	Michael A. Serra	YSU	Chemistry
97.	Michael Carducci	University of Arizona	Chemistry
98.	Michael D. Hopkins	University of Pittsburgh	Chemistry
99.	Michael Lufaso	OSU	Chemistry
100.	Michael O. Eatough	Sandia National Labs	
101.	Miquel A. Seco	Barcelona	Inorganic Chemistry

102. Mohammed Bakir	UWI Jamaica	Chemistry
103. Neil Walsh	Ohio Dominican University	Chemistry
104. Niels Thorup	Technical University of Denmark	Chemistry
105. Nigam P. Rath	University of Missouri - St. Louis	Chemistry
106. Omar Steward	Duquesne University	Chemistry
107. Partha Basu	Duquesne University	Chemistry
108. Paolo Lubini	Locarno, Switzerland	
109. Paul Williard	Brown University	Chemistry
110. Peter Burns	University of Illinois at Champaign/Urbana	Geology
111. Peter Turner	University of Sydney	Chemistry
112. Phil Fanwick	Purdue University	Chemistry
113. Rasika Dias	University of Texas at Arlington	Chemistry
114. Raul E. Cachau	National Cancer Institute	Adv. Biomed. Comp. Center
115. Raul Mariezcurrena	Montevideo, Uruguay	Chemistry
116. Ray J. Butcher	Howard University	Chemistry
117. Richard J. Staples	Harvard	Chemistry
118. Robert E. Bachman	Georgetown University	Chemistry
119. Robert P. Hammond	Syracuse University	Chemistry
120. Roland Boese	Universitaet Essen	Inst. fuer Anorg. Chemie
121. Rudy Luck	Michigan Technical University	Chemistry
122. Russell G. Baughman	Truman State University	Chemistry
123. Sarah L. Heath	University of Sheffield	Chemistry
124. Sarah Stoll	Oberlin College	Chemistry
125. Sax Mason	ILL	
126. Scott Thornburgh	Dow AgroSciences	Discovery Research
127. Sheldon G. Shore	OSU	Chemistry
128. Sherri Lovelace	YSU	Chemistry
129. Shih-Chi Chang	Duquesne University	Physics
130. Shu-Cheng Yu	National Cheng Kung University, Taiwan	Earth Sciences
131. Simon Bott	University of Houston	Chemistry
132. Simon J. Teat	CLRC Daresbury Laboratory, UK	
133. Songping D. Huang	Kent State University	Chemistry
134. Steve Geib	University of Pittsburgh	Chemistry
135. Steve Guggenheim	University of Illinois at Chicago	Geology
136. Steve Pilgrim	Alfred University	Ceramics
137. Steven Hardinger	UCLA	Chemistry
138. Steven Koch	SUNY Stony Brook	Chemistry
139. Subhadra Guha	Jadavpur University, Calcutta	Chemistry
140. Sue Byram	Bruker AXS	
141. Sue-Lein Wang	National Tsing Hua University, Taiwan	Chemistry
142. Susie Miller	Colorado State University	Chemistry
143. Timothy J. Hubin	University of Kansas	Chemistry
144. Timothy R. Wagner	YSU	Chemistry
145. Tom Emge	Rutgers University	Chemistry
146. Tom Richmond	University of Utah	Chemistry
147. Tony Linden	University of Zurich	Chemistry
148. Tony Willis	Australian National University	Chemistry
149. Urs Geiser	Argonne National Laboratory	Chemistry and Materials Science
150. Victor Young	University of Minnesota	Chemistry
151. Vimal Icharam	University of Witwaterand	Structural Chemistry
152. Vivien Yee	CWRU - CCF - CCSB	Pharmacology
153. Vratislav Langer	Gothenburg, Sweden	Env. Inorg. Chemistry
154. Wiley Youngs	University of Akron	Chemistry
155. W. Robert Scheidt	University of Notre Dame	Chemistry

Appendix II: Title Page and Abbreviated Contents for "Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction" (i.e., reference 2)

ALLEN HUNTER'S YOUNGSTOWN STATE UNIVERSITY

X-RAY STRUCTURE ANALYSIS LAB MANUAL:

A BEGINNER'S INTRODUCTION

OPTIMIZED FOR USE WITH SHELXTL AND DOS

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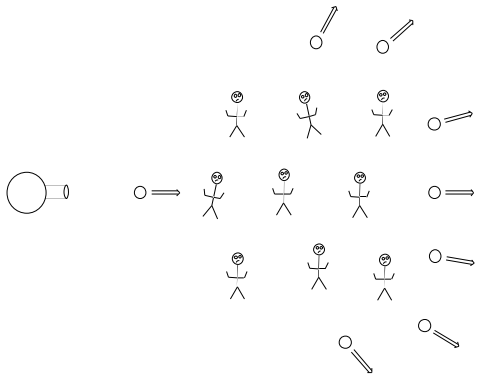
Winter 1999 Draft Release: Version W99D1

Detailed Comments On This Draft Manual Are Requested From All Users



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This 275 page manual is available as two .pdf files from the PI my emailing the PI at adhunter@cc.ysu.edu with your request. This manual will also for the basis for the expanded student lab manual described in the Project Description section and in Appendix V.

Appendix III: Proposed Product 1, Instructor and Student Background Materials

Instructor Background Materials for the Diffraction Lab, Entry Level: This package will include sections on: (1) crystals and unit cells, (2) diffraction of waves and by crystals, (3) diffractometer hardware, (4) diffraction data sets, (5) the diffraction analysis software packages, (6) solving routine data sets, (7) graphical and tabular presentations of structural data, (8) mining the data for structural information, (9) the relationship of this data to bonding theories, and (10) bibliography and Web references. Each of these sections will have three parts, a quick introduction, a qualitative/graphical treatment, a semiquantitative treatment. Based on the outlines already developed, it is expected that the total package will be 150 typed pages in length. The "quick introduction" materials will be extracted as a short ≈ 30 page pamphlet while these materials with the "qualitative/graphical" sections will be a 75-100 page booklet.

Instructor Background Materials for the Diffraction Lab, Advanced Level: This package will include all of the materials described above with each section being expanded to include a more quantitative/mathematical treatment of the topic. In addition, sections on: (11) solving the phase problem, (12) estimating the reliability of data, and (13) dealing with common problems observed in even "routine" data sets will be included. Based on the outlines already developed, it is expected that these materials will add an additional 150 typed pages.

Student Background Materials for the Diffraction Lab: These materials at both levels will be based on the instructor materials modified with a "need to know" filter. At the basic track these materials will be very short (i.e., 3-5 pages), for the typical track it will be 10-15 pages in length, while the advanced track will include all of the information in the instructor materials minus the commentary on dealing with common student questions/problems.

Appendix IV: Proposed Product 2, Module Plans and Laboratory Exercises

Outline of a Typical Entry Level Module: These will focus on solving basic structures, mining the resultant data to find common structural motifs, and then relating these to bonding theories. *Lecture Component:* This will typically include 2 to 4 hours of lecture content with recommendations on topics to be presented, audio-visual aids and in class activities (Microsoft PowerPoint presentations and transparencies from this project and from other sources), and ideas on taking advantage of "lectures" held in the computer lab or in a lecture hall having computer projection capabilities. *Laboratory Component:* This will typically include 2 to 6 lab hours. In the first 0.5-2 hours, the students all work through the same structure solution together with the instructor to learn the software "hands on". They will then break into groups of 2 or 3 to solve the structures of different molecules from the data base (each collaborative group solving one or more different structure(s)). Next, they mine their structure(s) to determine typical structural fragments and the bond angles and distances associated with them (e.g., bond angles around 2, 3, and 4 coordinate carbon and bond distances between pairs of carbons having different numbers of attached atoms). From this, they will then be asked to propose general rules to explain the data. Finally, they relate this in a final report to the predictions of theories (i.e., the Lewis, Valence Bond, and Molecular Orbital approaches).

Outline of a Typical Advanced Level Module: These will typically follow the same general structure as described above with the exceptions that the lecture and laboratory components will be tailored to the individual courses. Thus, the Physical/Biophysical, Inorganic, Biochemistry/Molecular Biology, and Instruments modules will emphasize the math and theory of the diffraction process, inorganic and organometallic examples, biomolecular examples, and diffraction instrumentation and optimizing data collection, respectively.

Appendix V: Proposed Product 3, Comprehensive Single Crystal Diffraction Methods Lab Manual

This will be an evolutionary development of the PI's current manual on the solution of diffraction data sets to obtain structural information (i.e., *Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction*)[2] and of the materials used in the PI's current lab course at YSU (i.e., Chemistry 832: Solid State Structural Methods).[4-6] A primary differences will be their expansion to cover all of the topics below:

Section	Section Headings	»Pages
	Table of Contents	
1	General Introduction to This Manual and Single Crystal Diffraction Methods (i.e., based on Chapter I of current manual[2])	≈ 30
2	Conventional/Serial and Systematic/Parallel Approaches to Growing Single Crystals Suitable for Diffraction Analysis (i.e., based on Chapter XIV of current manual[2] and on other sources[8g])	≈ 30
3	Selecting and Mounting Crystals for Diffraction Studies (i.e., based on his current lab course[4-6])	≈ 30
4	Single Crystal Data Collection Strategies on Diffractometers Equipped with Serial and Area Detectors (i.e., the serial detector component based on the current lab course[4-6])	≈ 100
5	Analysis of Single Crystal Diffraction Data to Obtain Structural Information (i.e., based on Chapters II-VI of current manual[2])	≈ 150
6	The Crystallographic Literature and Evaluating and Extracting Data from Crystallographic Papers	≈ 30
7	Using Crystallographic Data Bases Including the Cambridge Single Crystal and ICDD Powder Data Bases	≈ 30
8	Preparing Single Crystal Diffraction Data for Publication (i.e., based on Chapters VII, VIII, and XII of current manual[2]) in Word and CIF Formats	≈ 60
9	Introduction to the YSU Database of Annotated Single Crystal Diffraction Data Sets	≈ 30
10	Appendices on Advanced Topics, Including: Disorder, Twining, and Problem Structures; Atomic Resolution Macromolecular Data Sets; Incommensurate Structures; Synchrotron, Data, and Multiple Wavelength Data Sets [Note: These topics will be treated, many with the assistance of other crystallographers, in an abbreviated fashion during this proof of concept project and in more detail during the later full proposal.]	≈ 5 each
	Complete Index	

Appendix VI: Proposed Product 4, "Student" Diffraction Analysis Software and Software Documentation

All "research grade" diffraction analysis packages contain many powerful features that are needed to deal with the complex problems found when dealing with "wild" data sets. These powerful features are only distractions to the undergraduate students this project is aimed at serving. In addition, our annotated database will be chosen so as not to include any data sets having the worst problems. Finally, these powerful features are a major component of what the vendors use to distinguish and "sell" their products. By stripping these "research grade" features off of the software one gets a package that is both more user friendly and will not compete with the commercial package. This will allow the vendors to make "student versions" available at either lower cost or even no cost (i.e., for the good will and advertising value). The documentation for these packages is designed for experts. Where required, we will ensure that documentation is prepared which is suitable for our student's needs.[2]

Appendix VII: Proposed Product 5, Annotated Diffraction Data Sets

These data sets will be chosen to be either entirely "well behaved" or to have only clearly defined "problem" features. The following classes of materials will be placed in the database:

Simple Organic Compounds: These compounds will be chosen to illustrate the most common structural and bonding features found in organic compounds. Included will be molecules with all of the common functional groups, including: alkanes, alkenes, alkynes, alcohols, ethers, aldehydes, ketones, carboxylic acids, esters, amines, amides, aromatics, and heteroatoms.

Medicinal Compounds: These will include data sets on some of the most common/important medicinal compounds including heterocyclic compounds.

Inorganic/Organometallic Compounds: These will include both main group and transition metal coordination and organometallic compounds.

Extended Solids/Minerals: These include extended solid state materials such as diamond and graphite, metal oxides and 123 superconductors, common salts and minerals, and metals.

Biomolecules: These will include examples of carbohydrates (e.g., simple sugars, sugar derivatives, and di-, tri-, and simple poly-saccharides including cyclodextrins), lipids (e.g., steroids, triglycerides, and similar materials), peptides (e.g., amino acids, di-, tri-, and simple poly-peptides), and simple RNA/DNA oligomers.

Additional compounds will be added to each of these classes as time permits. In addition, data sets from other structural classes and having more complex crystallographic problems will be added as time permits, including: disordered, twinned, problem space groups, atomic resolution macromolecular data sets, incommensurate structures, synchrotron data, neutron data, and multiple wavelength data sets.

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1. (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.

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2. *Allen Hunter' s Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner' s Introduction*, 2nd Edition, Spring 1999 Version S99D1 © 1997, 1998, 1999, 275 pages [While this manual has not been *formally* published it is recommended by the worlds leading diffractometer vendor and it has been requested by approximately 150 external organizations, Appendix I. It is available free of charge from the author as two .pdf files.] This manual contains many lead references on crystallography theory, practice, and teaching.

3. Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *Journal of Chemical Education*, **1998**, *75*, 1297-1299.

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5. Hunter, A. D.: "New Approaches to Teaching Crystallography to Undergraduates: One Day Experiments, a Step by Step Lab Manual, and the Integration of Single Crystal and Powder Methods," International Center for Diffraction Data Annual Meeting, March 18th, 1999.

6. Hunter, A. D.: "Broadening the Pipeline: Integrating Diffraction Methods into the Undergraduate Curriculum," American Crystallographic Annual Meeting, May 25th, 1999.

7. (a) Hunter, A. D.; Bianconi, L. J.; DiMuzio, S. J.; Braho, D. L.: "Synthesis and Structure/Property Relationships in $(\eta^6$-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.

   (b) 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 (supplementary materials at http://jchemed.chem.wisc.edu/Journal/issues/1998/Nov/abs1424.html).

8. The American Crystallographic Annual Meeting, 1999, had a Symposium featuring eight invited speakers. It was entitled "Teaching Crystallography to Non-Crystallographers" and included my paper (i.e., 6, above) as well as:

(a) Fanwick, P: "Botching the Basics--Crystallography in Introductory Chemistry," American Crystallographic Annual Meeting, May 25th, 1999.

(b) Glusker, J. P.: "Teaching Crystallography to Non-Crystallographers," American Crystallographic Annual Meeting, May 25th, 1999.

(c) McPherson, A.: "Wisdom Acquired from Teaching (or trying to) X-Ray Crystallography," American Crystallographic Annual Meeting, May 25th, 1999.

(d) Kantardjieff, K.; Campana, C.: "Crystallography for Chemistry - A Two Day Short-Course," American Crystallographic Annual Meeting, May 25th, 1999.

(e) Sparks, R. A.; Fait, J. F.; Christian, S.: "XSHELL-An Interactive Program for Solving X-ray Crystal Structures," American Crystallographic Annual Meeting, May 25th, 1999.

(f) Kastner, M., Nottis, K.: "Assessment of Crystallographic CourseWare," American Crystallographic Annual Meeting, May 25th, 1999.

(g) Ewing, F.; Pusey, M: "A Protein Crystal Growth Cookbook for Education," American Crystallographic Annual Meeting, May 25th, 1999.

9. (a) Chemistry and Engineering News, Committee on Professional Training 1995 Annual Report, January 20, 1997, p41.

(b) Hazen, M. and Trefil, J., *Science Matters: Achieving Scientific Literacy*, Doubleday, New York, 1991.

(c) Heller, P., Keith, R., and Anderson, S., "Teaching problem solving through cooperative grouping. Part 1: Group versus individual problem solving," *Am. J. Phys.* **60**, 627-636 (1992).

(d) Heller, P. and Hollabaugh, M., "Teaching problem solving through cooperative grouping. Part 2: Designing problems and structuring groups," *Am. J. Phys.* **60**, 637-644 (1992).

(e) Shaping the Future: New Expectations for Undergraduate Education in Science, Mathematics, Engineering and Technology; Executive Summary of its Review of Undergraduate Education by the Advisory Committee to the National Science Foundation (NSF 96-139, 1996).

(f) The Liberal Art of Science: Agenda for Action (The Report of the Project on Liberal Education and the Sciences); American Association for the Advancement of Science (1990), Wash. DC.

(g) Tobias, *They' re Not Dumb, They' re Different*, Research Corporation, Tucson, 1990.

(h) Tobias, Revitalizing Undergraduate Science: Why Some Things Work and Most Don' t, Research Corporation, Tucson, 1992.

10. (a) Glusker, J. P.; Lewis, M.; Rossi, M., *Crystal Structure Analysis for Chemists and Biologists*, VCH, New York, 1994.

(b) G. Rhodes, *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models,* Academic Press, San Diego, 1993.

11. (a) Bond, M. R.; Carrano C. J.: *J. Chem. Educ.* **1995**, *72*, 451.

(b) Masson, B. L.: *J. Chem. Educ.* **1996**, *73*, 918.

(c) Lipkowitz, K. B.; Pearl, G. M.; Robertson, D. H.; Schultz, F. A.: *J. Chem. Educ.* **1996**, *73*, 105.

(d) Butera, R. A.; Waldeck, D. H.: *J. Chem. Educ.* **1997**, *74*, 115.

(e) Pope, C. G.: *J. Chem. Educ.* **1997**, *74*, 129.

(f) Pu, Q.: *J. Chem. Educ.* **1992**, *69*, 815.

(g) Goldberg, S. Z.: *J. Chem. Educ.* **1991**, *68*, 969.

(h) Lisensky, G. C.; Kelly, T. F.; Neu, D. R.; Ellis, A. B.: *J. Chem. Educ.* **1991**, *68*, 91.

(i) Rodriguez, S.: *J. Chem. Educ.* **1991**, *68*, 969.

(j) Rosenthal, J.: *J. Chem. Educ.* **1991**, *68*, A285.

(k) Spencer, B. H.; Zare, R. N.: *J. Chem. Educ.* **1991**, *68*, 97.

(l) Segschneider, C.; Versmold, H.: *J. Chem. Educ.* **1990**, *67*, 967.

(m) Cooper, J. N.; Smith, D. A.; Kastner, M. E.: **1989**, *66*, 968.

(n) Kastner, M. E.: **1989**, *66*, 969.

(o) Kantardjieff, K. A.; Hardinger, S. A.; Van Willis, W.: **1999**, *76*, 694.

Biographical Sketch for Allen D. Hunter

Department of Chemistry, Youngstown State University, Youngstown, OH, 44555
Ph: 330-742-7176, FAX: 330-742-1579, adhunter@cc.ysu.edu,
http://www.as.ysu.edu/~adhunter/index.html

A. Vitae. Allen Hunter received his Honors BSc and PhD degrees in Chemistry in 1981 and 1985 from the University of British Columbia under Dr. E.E. Burnell (i.e., A NMR Structural Determination of Azulene Oriented in a Nematic Liquid Crystal) and under Dr. P. Legzdins (i.e., Aspects of the Organometallic Nitrosyl Chemistry of Cr, Mo, and W), respectively. He worked as a postdoctoral fellow with Dr. M. Bennett of the Research School of Chemistry at the Australian National University in Canberra, Australia, doing phosphine and iron phosphine chemistry (1985-86) and with Dr. M. Cowie at the University of Alberta in Canada carrying out single crystal X-ray diffraction studies for Dr. D. Seyferth of M.I.T. (1987). From 1987 to 1992, Dr. Hunter was an Assistant Professor of Chemistry at the University of Alberta where he held an Adjunct appointment from 1992 until 1995.

On September 15th of 1992, Dr. Hunter joined Youngstown State University as an Associate Professor of Chemistry. For 1995/96 Dr. Hunter was a Visiting Associate Professor at the Department of Crystallography, University of Pittsburgh where he worked with Bryan Craven. On September 15th of 1998 he was promoted to full professor at YSU. He is a member of the American Chemical Society, the American Association for the Advancement of Science, the American Crystallographic Association, the Council of Undergraduate Research, the Pittsburgh Diffraction Society, the International Union of Crystallography, the International Center for Diffraction Data, and the American Physical Society. Dr. Hunter has extensive experience in synthetic chemistry of inorganic, organometallic, and polymeric materials and in their characterization by MS, NMR, IR, X-ray crystallography, etc. He is the founding Director of both the YSU Structure Center (housing our Bruker AXS P4 X-ray diffractometers, our Varian 400 MHz NMR, and a wide range of other polymer and small molecule characterization instrumentation) and the Advanced Diffraction Studies Consortium. Dr. Hunter plays a major role in the Ohio MS, NMR, and X-ray consortia where he represents both YSU and other predominantly undergraduate institutions, especially those in northeast Ohio.

Dr. Hunter's teaching has included lecture and laboratory courses at both the undergraduate and graduate levels on a wide range of topics, including: Chemistry for Non-Science Majors, Organic Chemistry, Inorganic Chemistry, Organometallic Chemistry, Polymer Chemistry, Structural Biochemistry, Instrumental Methods, NMR, X-Ray Crystallography, and Structural Methods for High School Science Teachers. He has been particularly active in new course development and the preparation of educational tools, see below.

Since 1994, he has developed a strong emphasis on X-ray diffraction studies of organic and organometallic molecules since such studies make great undergraduate research projects. More recently, he and Bryan Craven have begun a high resolution diffraction study of transition metal containing solid state materials and catalysts that is expected to be his central research project over the next 5 years. The goal of this collaborative project is to gain an understanding of these important materials via the application of charge density methods.

While at the University of Alberta, Dr. Hunter was PI on approximately $480,000 in external grants (excluding overhead and including 3/4 research and 1/4 equipment funds) from the Canadian federal science agency, NSERC, and US and Canadian Industry for his work on

organometallic polymers and biologically active organometallics. Since coming to YSU, he has been PI or co-PI on grants from the National Science Foundation and the Ohio Board of Regents totaling approximately $730,000. These grants have supported the YSU Chemistry Department's innovative program which emphasizes the integration of teaching and research at the undergraduate and MS levels.

B. Refereed Journal Publications. Dr. Hunter has had 40 refereed journal publications, half since 1992. His 4 chemical education publications are below while some crystallography research papers with undergraduate co-authors are listed in the reference section of this proposal as reference 1.

1. Hunter, A. D.: "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *Journal of Chemical Education,* **1998**, *75*, 1297-1299.

2. *Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction*, 2nd Edition, Spring 1999 Version S99D1 © 1997, 1998, 1999, 275 pages [While this manual has not been *formally* published it is recommended by the worlds leading diffractometer vendor and it has been requested by approximately 150 external organizations, Appendix I. It is available free of charge from the author as two .pdf files.]

3. 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.

4. 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.

C. Other Collaborators.

Dr. S. G. Bott, University of Houston.
Dr. Mike Burnett, Oakridge National Labs.
Dr. John Cashman, Seattle Biomedical Research Institute.
Dr. Bryan Craven, Indiana University of Pennsylvania.
Dr. Bernard Santarsiero, University of California at Berkeley.
Dr. Chase Smith, Ohio Northern University
Dr. M. J. Zaworotko, University of Manitoba.
Drs. Ray Beiersdorfer, Shane Brower, Larry Curtin, John Jackson, Jim Mike, and Tim Wagner at YSU.

D. Graduate Students. 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), Dianne Braho, MS 1995 (YSU), Steven DiMuzio, MS 1996 (YSU), and Bev Smith-Papa, MS 1997 (YSU). I have served as the principle advisor for 2 PhD students, 6 MS students, 3 postdoctoral fellows, 3 research associates, and over a dozen undergraduate researchers.

E. Advisors. Detailed in Section A, above, namely: Elliot Burnell and Peter Legzdins at the University of British Columbia, Martin Bennett at the Australian National University, and Marty Cowie at the University of Alberta.

Steven J. DiMuzio
263 Mill Creek Drive
Boardman, Ohio 44512
(330)788-7718
sdimucio@raex.com

EDUCATION

Youngstown State University, Youngstown Ohio

*Certification in Comprehensive Science — June 1997
Cumulative GPA- 3.42

*Master of Science in Chemistry — August 1996
Cumulative GPA-3.87

*Bachelor of Science in Chemistry — June 1994
Cumulative GPA-3.39

EDUCATIONAL EXPERIENCE

Student Teaching: Winter, 1997; Woodrow Wilson High School
Secondary School: Youngstown, Ohio: Grades 9-12.

* Taught Chemistry I, Biology I, and Biology II.
* Responsible for preparing lesson plans for six classes daily.
* Evaluated and assigned grades for each student.
* Replaced retiring teacher for the second semester of the 1996-97 school year.

Secondary Education Lab: Fall, 1996; Liberty High School
Secondary School: Liberty, Ohio: Grades 10-12.

* Developed lesson plans for Chemistry I and Physics I.
* Taught lessons and labs to students.

Graduate Assistant: September 1994-95; Department of Chemistry, YSU

* Prepared lessons and chemicals for 100 students weekly.
* Evaluated and assigned grades for each student.

HIGHLIGHTS OF QUALIFICATIONS

* Completed masters thesis.
* I have been published in *J. Chem. Ed.*
* Proficient in computer applications.
* Instructed Biology I/II, Chemistry, and General Science.
* Maintaining discipline in an urban school.
* Faculty advisor for peer mediation at Wilson High School.
* Involvement in proficiency remediation.
* Successful Classroom management.
* Mastery of content material.
* Training for chemical safety
* Over 1000 hours of lab experience.
* Skilled in computers/software including internet applications.
* Secretary of American Chemical Society at YSU
* Golden Key National Honor Society.
* Kappa Delta Pi Honor Society.
* Coached youth baseball for five years.

WORK EXPERIENCE	LaBrae High School (Science Teacher)	1998-Present
	Woodrow Wilson High School (Science Teacher)	Jan. 1997-June 1998
	YSU Chemistry (Lab Assistant)	December 1991-1996
	Youngstown City Schools (Sub. Teacher)	April-December 1996
	YSU Chemistry (Graduate Assistant)	Sept. 1994-1995

SUMMARY PROPOSAL BUDGET YEAR 1

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

ORGANIZATION: **Youngstown State University**

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

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - Project Director**	**0.00**	**0.00**	**2.00**	$ **12,250**	$
2.					
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**1**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**2.00**	**12,250**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**1**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**2.00**	**5,000**	
3. (**1**) GRADUATE STUDENTS				**3,000**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**20,250**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**1,868**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**22,118**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**2,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
(**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**3,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**500**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**3,500**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**27,618**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 20250)**					
TOTAL INDIRECT COSTS (F&A)				**8,505**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**36,123**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **36,123**	$

M. COST SHARING PROPOSED LEVEL $ **37,055** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE* DATE

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Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET COMMENTS - Year 1

**** B-2 Other Professionals**
Steven J. DiMuzio is a current high school chemistry teacher with a recent MS in Chemistry from YSU.
**** B-3 Graduate Students**
This individual will be a MS student in Chemistry with an interest in chemical education.
**** C- Fringe Benefits**
For this and the following year fringe benefits are 15% for ADH and 1% for the graduate student.
**** E- Travel**
Travel funds for both years will be used to attend national and regional chemistry, crystallography, and science education meetings to present the results, obtain evaluations, and disseminate new materials.
**** G-1 Materials and Supplies**
For both years these funds will be used to purchase required software and computer supplies
**** G-2 Publication Costs/Documentation/Dissemination**
For both years these funds will be used to prepare and distribute the new educational materials including costs of writable CDs, printing, and postage.

SUMMARY PROPOSAL BUDGET YEAR 2

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

ORGANIZATION: **Youngstown State University**

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

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - Project Director**	**0.00**	**0.00**	**2.00**	$ **12,863**	$
2.					
3.					
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**1**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**2.00**	**12,863**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**1**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**2.00**	**5,000**	
3. (**1**) GRADUATE STUDENTS				**3,000**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**20,863**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**1,959**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**22,822**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**2,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
(**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**2,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**3,000**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**5,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**29,822**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 20863)**					
TOTAL INDIRECT COSTS (F&A)				**8,762**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**38,584**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **38,584**	$

M. COST SHARING PROPOSED LEVEL $ **37,933** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY
Allen D Hunter		INDIRECT COST RATE VERIFICATION
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked / Date Of Rate Sheet / Initials - ORG

SUMMARY PROPOSAL BUDGET

Cumulative

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PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **Youngstown State University**

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

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - Project Director**	**0.00**	**0.00**	**4.00**	$ **25,113**	$
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**1**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**4.00**	**25,113**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**2**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**4.00**	**10,000**	
3. (**2**) GRADUATE STUDENTS				**6,000**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**41,113**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**3,827**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**44,940**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**4,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
(**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**5,000**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**3,500**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**8,500**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**57,440**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**17,267**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**74,707**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **74,707**	$

M. COST SHARING PROPOSED LEVEL $ **74,988** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE* DATE

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INDIRECT COST RATE VERIFICATION

Date Checked	Date Of Rate Sheet	Initials - ORG

NSF Form 1030 (10/98) Supersedes all previous editions

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

9. Budget Justification

General Issues: The funds requested from NSF, $74,707, are to be matched by at least $74,988, from Youngstown State University. Approximately half of these funds will be spent in each year of the project.

A. D. Hunter's Support: In each budget year, NSF funds are requested in this grant for two months of summer support for the PI at 2/9 of his academic year salary (i.e., $25,113 in salary and $3,767 in benefits in total). This will be matched by Youngstown State University by a 1/3 reduction in his normal teaching load each academic year of the project (this has a match value of $37,670 for salaries plus $12,054 in benefits). With this NSF and YSU funded time, the PI will be able to carry out his duties towards this project as delineated in the Project Description.

S. J. DiMuzio's Support: In each budget year, Mr. DiMuzio will receive $5,000 from this grant to fund two months of full time work on this project over the summer (this is substantially less that 2/9 his academic year salary). In addition, Mr. DiMuzio will continue to work on this project over the academic year (i.e., pilot testing the high school course modules and working on the curricular materials) at no charge to this grant and will assist in writing teacher development/dissemination proposals (e.g., and Eisenhower Grant).

MS Student's Support: In each budget year, this NSF grant will provide $3,000 of summer support for the MS student working on this project. As a match, YSU will fund this student over the academic year (i.e., $8,300 and $9,000 in stipend over the first and second years, respectively, and approximately $3,500 per year for their tuition remission). This support will fund this student's MS research on this project.

Fringe Benefits: Fringe benefits for the summer salaries are charged at the rate of 15% for the PI and 1% for the graduate student. To calculate matching funds, the benefit rate for the PI during the academic year is 32%.

Travel Funds: The $4,000 budgeted in this grant for domestic travel will be used to support the evaluation and dissemination of the curricular materials to be developed at the regional and national science education, chemistry, and crystallography conferences specified in the Project Description. This will be supplemented by YSU travel funds where necessary.

Materials and Supplies: The $5,000 requested from NSF for materials and supplies, to be matched by $1,000 from YSU, will be used to fund the direct incremental costs of this project. Specific items to be purchased under this category include: (1) A CD writer and additional hard drives on the PI's computer and a server to back up our materials/data base and support distribution of all grant products via CD-ROMs and the Web page. (2) A two year license to the Cambridge Structural Data Base, from which structures for our project will be identified and on which an upper level laboratory exercise will be developed. (3) Paper, toner cartridges, and printing charges for the printed materials to be used in the pilot sections.

Publication/Documentation/Dissemination Costs: The $3,500 requested from NSF will fund the costs of publishing, assessing, and disseminating the new curricular materials, including printing, page, phone, and mailing charges.

Total Direct Costs: The total direct costs of this project, $57,440, represent approximately 77% of the NSF request.

Total Indirect Costs: The total indirect costs of this project, $17,267, represent approximately 23% of the NSF request and were calculated as 42% of all salaries and wages.

Total YSU Match: Youngstown State University is committed to matching the NSF request for this project at a rate of at least 100%. In the sections above, the individual match components are specified totaling $74,988. In addition to this direct YSU match, YSU is providing at no charge the use of our departmental computer labs, computer network and server, and electronics and computer personnel to assist in implementing this project, and time from other faculty (especially: Drs. Tim Wagner and Mike Serra) and students who will assist in developing materials and pilot testing individual modules in their courses. In addition, the two single crystal diffraction software vendors, Bruker AXS and Molecular Structure Corporation, are providing copies of their "research grade" software for use in the early pilot studies and/or will modify this software to produce the more basic "student" versions, and will provide this for use in the later pilot studies. This represents a substantial, although not specified, commitment of matching funds.

Current and Pending Support

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

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

Investigator: **Allen Hunter**

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

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

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

Source of Support: **NSF DUE ILI 9851107**

Total Award Amount: $ **44,600** Total Award Period Covered: **07/01/98 - 06/30/00**

Location of Project: **Youngstown State University**

Person-Months Per Year Committed to the Project. Cal: Acad: **2.00** Sumr: **0.00**

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**

Source of Support: **Ohio Board of Reagents**

Total Award Amount: $ **2,980,000** Total Award Period Covered: **06/15/99 - 06/14/01**

Location of Project: **YSU and 6 other Universities**

Person-Months Per Year Committed to the Project. Cal: **0.50** Acad: Sumr:

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 9850079**

Total Award Amount: $ **183,579** Total Award Period Covered: **07/01/98 - 06/30/01**

Location of Project: **Youngstown State University**

Person-Months Per Year Committed to the Project. Cal: Acad: **0.50** Sumr: **0.00**

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:

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:

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

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

Current and Pending Support

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

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

Investigator: **Steven DiMuzio**

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

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

Project/Proposal Title: **none**

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: **0.01** 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:
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:
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:
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:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

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

Facilities, Equipment, and Other Resources for the Project

Youngstown State University is a moderately sized (i.e., ≈ 12,000 students, ≈ 10% at the MS level), open enrollment, urban institution, and has strong BS and MS chemistry programs. Our Chemistry Department has 16 full time faculty and graduates approximately 10-20 ACS certified and 30-40 non-certified BS chemistry and 10 MS chemistry students a year. We have an unusually complete array of chemical instrumentation, including a 400 MHz NMR spectrometer, two GC-MS systems, and a range of chromatographs and spectrometers. The YSU Structure Center is currently equipped with two five year old Bruker AXS P4 diffractometers having Mo and Cu sealed tube sources and serial and X-1000 multiwire area detectors for both single crystal and powder studies. The X-ray lab is maintained by the Chemistry Department's electronic instrumentation specialist, Ray Hoff, with support from the campus electronics shop and college and campus computer centers. [If required, we have a 12% share in the CCD and Imaging Plate equipped diffractometers of the Ohio Crystallography Consortium, we recently joined the MB-CAT consortium, via our partnership with CWRU, bidding for a new X-ray synchrotron line on the Advanced Photon Source in Chicago, and we have access to the HTML facilities at Oak Ridge.] We already have a site license for the Bruker AXS single crystal structure solution package SHELXTL-XSHELL and at the recent ACA meeting were offered access to the Molecular Structure Corporation teXsan package for this project. These instruments are used for "hands on" instruction of students and for faculty and student research by individuals from YSU and nearby institutions. The YSU Chemistry Department is also equipped with two new computer labs, one having 12 Windows NT and the other 24 Windows 95 machines, four lecture halls equipped with computer facilities and projection equipment, and access to college and university Web servers.