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 99-5 **01/11/99**

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DIVISION OF CHEMISTRY

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Youngstown State University

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TITLE OF PROPOSED PROJECT **Advanced Diffraction Studies Consortium (ADSC): An Exciting Opportunity For Integrating Predominantly Undergraduate Institutions Into The National Research Enterprise**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE
$ **2,000,000**	**60** months	**06/01/99**	

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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**		**SSN's are confidential and are not displayed *ON FASTLANE SUBMISSIONS***	
Co-PI/PD **Bryan M Craven**			
Co-PI/PD **Mark D Foster**			
Co-PI/PD **A. Alan Pinkerton**			
Co-PI/PD **Menachem Shoham**			

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.

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Is the organization delinquent on any Federal debt? Yes ☐ No ☒

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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.

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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) **Robin W. Trail**		**01/11/99**

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A. Project Summary

The Advanced Diffraction Studies Consortium, ADSC, is a group of institutions centered in northern Ohio and western Pennsylvania with a strong intellectual focus on diffraction methods and crystallography. Youngstown State University is the lead institution in this group which includes 6 PhD and 4 MS granting universities and three federal research labs that are involved in strong collaborative interactions with over 20 two and four year colleges and a range of existing research consortia and industrial companies. In this RSEC proposal, we are seeking funding to deepen and broaden this collaborative web with the central goal of integrating these institutions and their faculty and students into the national research enterprise in a fashion that can serve as a national model.

There are main objectives of our project are: (1) to encourage and support the development of research collaborations between member institutions and individuals, (2) to help the participating undergraduate institutions and faculty develop sustainable research programs using diffraction methods, (3) to establish a series of accessible regional crystallographic/diffraction facilities suitable for both high volume conventional and more advanced studies, (4) to provide professional development opportunities to undergraduate faculty and other participants, (5) to broaden, deepen, and diversify the educational pipeline from the pre-college to the post employment stages, and (6) to maintain a strong focus on undergraduate students and individuals from groups that have been historically under-represented in science and engineering.

Key components of our operating plan include: (1) funding upgrades to the diffraction facilities at three MS level institutions which will serve as access points for conventional diffraction experiments and more modest contributions to several key advanced diffraction facilities, (2) providing support for an open diffraction lab which can be either used on site or to which samples can be submitted remotely, (3) providing funding to establish new collaborative relationships between nationally prominent researchers and undergraduate faculty and students, (4) providing support for both collaborative and independent research projects addressing important scientific problems, (5) providing quality student research experiences at both host and undergraduate institutions, (6) providing a series of structured professional development opportunities including "hands on" summer schools for faculty and students, (7) providing support for new curriculum development initiatives related to crystallographic education, and (8) providing a structured series of activities to make the ADSC and newly established collaborative and independent research programs self supporting after the termination of this RSEC grant.

This project is expected to have a major impact both regionally and nationally: (1) the completion of this project will see crystallographic/diffraction methods more fully integrated into the curriculum of all member institutions, (2) will see an increased emphasis on undergraduate research and its integration with teaching at all institutions, (3) will see faculty at undergraduate institutions fully integrated into the national research enterprise through independent and collaborative research, publications, and grant seeking, and (4) will see strenuous efforts to assess our programs and disseminate their results to the national research community.

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*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.

C. Project Description

C1. Educational and Intellectual Focus and Rationale

C1a. Overview of the Educational and Intellectual Focus for the ADSC Proposal to the NSF RSEC Program. The Research Sites for Educators in Chemistry, RSEC, proposal from the Advanced Diffraction Studies Consortium, ADSC, is designed to promote collaborations between predominantly undergraduate institutions, major research universities, and other federal and corporate organizations and between renowned researchers and undergraduate faculty and students. This collaboration is centered in northern Ohio and western Pennsylvania. It is focused on the use of both routine and advanced diffraction methods to solve important scientific problems and to enrich the education at the high school, undergraduate, graduate, and postgraduate levels. It will become self sustaining through a coherent development effort and will serve as a national model for collaborations between heterogeneous educational and research consortia. The central goal is to integrate undergraduate faculty and student participants into the national research enterprise.

The current proposal for the ADSC arose out of existing long term research and educational interactions focused on structural methods between institutions and individuals in our region. These have included several types, most importantly: the Pittsburgh Diffraction Society, the American Crystallographic Association Summer School, several consortia funded by the Ohio Board of Regents (i.e., the Ohio Computing, Materials, MS, NMR, and, especially, Crystallography Consortia), and other shared resources such as the OhioLink library exchange system and the Ohio Supercomputer Center. These helped nourish ongoing collaborations between individuals and institutions and have created one of the richest webs of collaborations involving structural methods (especially crystallographic/diffraction methods) in the United States. It therefore seemed natural to expand upon the current crystallographic strengths of our region and form the ADSC which was formally constituted on December 12th of 1998. The ADSC is committed to the enrichment of diffraction research and education, especially that involving undergraduate faculty and students, and to the enhancement of our national prominence in these areas.

Crystallography is arguably the single most important method for determining the structures of materials in the solid state and certainly gives the most detailed structural information we have available. It includes a range of X-ray and neutron diffraction techniques that are used on single crystal and powdered (polycrystalline and amorphous) samples. The relative importance of diffraction methods in structural studies is rapidly growing due to recent and ongoing advances in the theory of diffraction, in computer technology, in crystallographic software, and in diffractometer hardware (including sources, optics, sample stages, detectors, and controls). These advances have simultaneously reduced the cost and increased the speed and sensitivity of individual data collections. This has substantially increased the pace at which diffraction data is collected and *potentially* increases the quality of this data. The relative difficulty in using this new diffractometer hardware and crystallographic software has also rapidly decreased. This increased pace of data collection and decreasing difficulty of usage has meant that a *large and growing proportion* of diffraction data is no longer collected and analyzed by crystallographic professionals. Rather, this data is more commonly being collected and analyzed by *crystallographic novices* (e.g., synthetic chemists, biologists, materials scientists) far too many of whom have had little and/or only weak training in diffraction methods and therefore approach crystallography as a "black box" tool. On the other hand, the speed and ease with which modern diffraction methods can answer structural questions in biology, chemistry, engineering, geology, materials science, physics, etc., means that its use and importance will continue to grow.

The traditional method of training crystallographers has most commonly consisted of some coursework and an "apprenticeship at the hands of a master" to train new "master crystallographers". These individuals update their crystallographic skills through their knowledge of the literature, at professional conferences, and at short courses designed for those who already have high skill levels. At most schools, especially those that are predominantly undergraduate in nature, crystallographic education for "the masses" is usually much more limited, especially at the undergraduate level. It too commonly consists only of a discussion of Bragg's law in several undergraduate courses along with, perhaps, the odd powder diffraction laboratory, a discussion of where most bond length and angle information comes from at the start of synthetic chemistry classes, and/or a discussion of diffraction equipment in the instruments course. At some universities, this may be supplemented by specialized crystallography courses. While this method is still able to produce new "masters" (although arguably in too low of numbers), it has not kept up with the educational needs of the much larger numbers of occasional diffraction users. This is also true for the substantial number of novices who want to progress past this stage to some degree of expertise in one or more crystallographic areas. Most current advanced crystallography short courses (e.g., those given at ACA national meetings) are designed more for experts, are too abbreviated in time to be of maximum use to novices, and do not provide the important function of allowing the new students to practice their newly learned skills under expert supervision, i.e., they are not sufficiently "hands on." [Note: this is not true of the excellent ACA summer school in

crystallography, previously offered at The University of Pittsburgh. However, cost and other considerations mean that this single course does not nearly fill all needs.] These problems are particularly severe for faculty and students at predominantly undergraduate institutions who typically have limited resources of time and money, no routine affordable access to diffraction facilities, and limited access to appropriate professional development opportunities in crystallography. This problem is exacerbated by the fact that undergraduate faculty often have insufficient training/experience in crystallography and diffraction methods to fully integrate these important methods into their teaching. As a consequence, many schools produce students who proceed to jobs or graduate school with inadequate crystallographic/diffraction training.

These problems in crystallographic training for undergraduate faculty and students parallel probl ems that they have in effectively and fully integrating crystallographic methods into their research programs. Again, problems of time, money, and access limit their utilization of both routine/conventional and cutting edge diffraction methods. This, and their practical isolation from our major research universities, means that they are seldom fully integrated into the "national research enterprise" and too often do not reach their full potential for carrying out competitive research projects and getting these published and externally funded . This is particularly unfortunate because of the nature of crystallographic research which typically involves relatively short periods of time actually at the diffractometer with most of the research time being done at the crystallographer's computer. This makes *crystallographically intensive research ideally suited to undergraduate faculty and students* who can quickly collect their data at host institutions and then return to their home institution for the more scientifically interesting and demanding task of solving the structure and interpreting its meaning. Of major importance, this can be done on the personal computer(s) and/or departmental/college workstation(s) (which even the smallest and poorest colleges already have in place) *if the correct skills, software, and access to facilities is in place*.

The theme around which everything in this proposal revolves is an attempt to address these interrelated issues in a systematic way. The idea being that if we can sufficiently increase the quality, diversity, and diameter of the crystallographic education pipeline at all levels and if we can provide sufficient opportunities to undergraduate faculty and students to get involved in collaborative research involving diffraction methods with nationally recognized leaders in this area, then we can create a critical and self sustaining mass of undergraduate faculty and students and develop a positive feedback cycle in crystallography. This will both reinvigorate crystallographic/diffraction training at their home institutions and lead to their developing competitive individual and collaborative research programs effectively utilizing diffraction methods. In turn, this should have a broader impact on research activities at their universities.

C1b. Overall project goals of the ADSC proposal. The central goals that we have articulated include:

C1b(i). Collaborative Research Programs: This project will help develop new long term research collaborations between member faculty and institutions. These collaborations will include those between undergraduate faculty and established researchers at the PhD institutions, between researchers at universities and those at federal labs, between faculty and local industry, and between researchers and students. This will accelerate the integration of faculty from predominantly undergraduate institutions into the national research enterprise.

C1b(ii). Sustainable Research Programs: This project will help develop sustainable research programs at undergraduate research institutions involving both routine and advanced diffraction methods and will be supported by the new collaborations, training opportunities, access to facilities, and peer network. These new and reinvigorated research programs will result in an increased stream of publications and external grants and contracts.

C1b(iii). Regional Research Facilities: This project will establish a series of accessible regional crystallographic/diffraction research facilities suitable for routine single crystal and powder studies for research and teaching that are available to undergraduate faculty and students at costs consistent with their resources. This network of upgraded facilities for conventional diffraction experiments will complement those for the most advanced diffraction studies which are already in place at the participating research institutions. Thus, facilities suitable for conventional to advanced experiments will be put in place within a short drive of all participating institutions while access will be provided to the most advanced experimental tools at nationally prominent diffraction facilities and federal labs. In addition, Youngstown State University, YSU, will provide a "full function" diffraction facility to which both routine and more challenging samples can be sent for remote data collection at no direct cost to undergraduate faculty and student participants.

C1b(iv). Professional Development Opportunities: The ADSC will organize and offer a series of student and professional development training opportunities. These will include intensive "hands on" summer short courses ranging from introductory single crystal and powder methods to the most advanced diffraction methods courses taught by experts in the field. In addition, the participating faculty will have available a network of facilities on which their new skills can be used and more experienced crystallographic/diffraction methods experts they can consult with. The collaborative research initiatives will also provide more extended training opportunities (i.e., akin

to apprenticeships). The consortium will also provide assistance with the development of new research programs and teaching activities and with grant proposal writing to support these goals.

C1b(v). Strengthening the Educational Pipeline: As part of its efforts, the ADSC will develop new tools for crystallographic/diffraction methods education. These, along with the summer short courses and research experiences, will reinvigorate the teaching of diffraction topics throughout our region. In addition, there will be additional research opportunities for these students on diffraction related topics. These factors, in turn, will provide an increased stream of more highly motivated, educated, and experienced undergraduate students to proceed into our regional PhD programs and into local industry. A central component of all of these efforts will be attempts to diversify the student populations moving towards research and industrial careers. A special effort will be placed upon recruiting from populations traditionally under-represented and under-served in science and engineering.

C1b(vi). Target Groups. The two key target groups for the consortium's activities are: faculty and students from predominantly undergraduate institutions and/or individuals drawn from groups which have historically been under-represented in science and engineering. We will emphasize ways to encourage more of these students to move through the educational pipeline towards research careers with a particular emphasis on crystallography/diffraction and to help them and their faculty mentors to more fully join the mainstream of the "national research enterprise". As the consortium matures, we will open it up to a broader definition of our region and eventually open it up nationally to these target groups consistent with available space, facilities, and funding and how they would fit our consortium goals. It is expected that for the first three years, almost all participants in consortium funded activities will come from our region. After this point, it is expected that the consortium will be in a position to start broadening the reach of its activities. If the consortium receives additional funds to support its activities, the rate of this expansion will be increased.

C1c. Overall Project Outline of the ADSC Proposal. Major components in this project include:

C1c(i). *Building Accessible Diffraction Facilities for Routine and Advanced Studies*. Funds will be used to upgrade the X-ray diffraction facilities at four MS level host institutions in the consortium. Of particular note are the facilities at YSU which will be used for both onsite and remote data collection (i.e., with the assistance of the new laboratory director), improvements to the single crystal capabilities at Bucknell and Wright State Universities, access to a new ultra high intensity X-ray line on the Advanced Photon Source (i.e., the MB-CAT), and access to a complete range of crystallographic data bases at YSU.

C1c(ii). Support for Undergraduate Faculty Research. Most of the proposed budget will fund 50 competitively awarded Undergraduate Faculty Research Participants. These faculty from predominantly undergraduate schools will receive summer support of $7,500 to engage in collaborative research at the host institution and will receive about $7,000 towards their research costs. [Note: All Faculty Fellows from predominantly undergraduate schools will be assisted in preparing external grant proposals. Submission of these will be one condition of their participant support awards.] This component will be central in integrating these faculty into the national research enterprise.

C1c(iii). Support for Student Research. The proposed budget will also fund approximately 30 Student Research Participants (i.e., for undergraduate and MS students and high school teachers) at a rate of $2,500 per student for students engaged in collaborative research projects. This will serve to help get these students at the non-PhD schools involved in nationally prominent research at earlier stages in their careers. There will also be support via research funds and access to facilities for additional student researchers.

C1c(iv). Support for Intensive Summer Short Courses in Diffraction Methods. The proposed budget will fund intensive "hands on" graduate level courses ranging from basic single crystal and powder methods to the most advanced diffraction methods. The consortium will also develop teaching materials and provide software purchased from grant funds that can be used to invigorate teaching at participating institutions.

C1c(v). Support for Minority Enhancement Programs. The proposed budget will provide seed funding for a series of minority recruitment, enhancement, and retention efforts.

C1c(vi). Support for Evaluation and Dissemination. The proposed budget will fund efforts to evaluate the strengths and weakness of the consortium's activities and to disseminate the research and educational results.

C1d. Expected Impact of the ADSC Proposal. At the conclusion of this grant, it is expected that the undergraduate faculty participants will be actively involved in externally funded research (especially that related to crystallography), that many new long term research collaborations initiated during its term will have developed, that crystallography and diffraction methods will be integrated in a more extensive and fundamental way into teaching at member institutions, that new teaching tools related to diffraction methods will have been disseminated nationally, and that the ongoing activities of the ADSC will be fully supported by conventional channels.

C2. Scientific Activities of the Project

C2a. Participants in the ADSC and their Roles. The Advanced Diffraction Studies Consortium, ADSC, is centered on a group of institutions running along the south shore of Lake Erie from Toledo to Pittsburgh, namely those in northern Ohio and western Pennsylvania. This group is regionally concentrated to retain our intellectual focus and to keep our resources concentrated into a critical density. These boundaries have been expanded somewhat for the sake of including predominantly undergraduate institutions where these and/or their faculty have a history of collaborations with the host institutions and for several historically black colleges from outside our immediate area that have strong reputations for graduating chemistry majors and that have expressed an interest in participating. The consortium will have institutional members that fit into two main categories. The first is "host institutions" at which the bulk of the consortial research and faculty development activities will take place. The second is "participating institutions/home institutions" from which the bulk of the undergraduate faculty and students will come. There will be some overlap in these two categories, especially for institutions whose highest chemistry degree is the MS. To complicate this overly neat division, some faculty and students from PhD schools will participate as "users" in consortium funded activities (e.g., the summer courses) while some undergraduate faculty will act as course instructors and research mentors.

Youngstown State University has been designated the *Lead Institution* for the ADSC in this proposal. YSU and its Chemistry Department has volunteered for this role which is centrally related to their declared missions; which are to become a Premier Metropolitan University and a benchmark MS level Chemistry Department (i.e., "top ten"). YSU has long served as an intermediary between the PhD research institutions and predominantly undergraduate institutions in several major research consortia in Ohio (i.e., the Ohio MS, NMR, and Crystallography Consortia) and YSU faculty have close contact with participating institutions. To demonstrate its commitment to the importance of the ADSC, it has provided substantial internal resources to this project including faculty and staff time having a value of $792,283, including: $79,200 of new money to support the Diffraction Laboratory Scientist, $398,000 in cash funds for requested diffraction equipment, $95,000 for renovations and increased maintenance funds, and a $100,000 reduction in the housing fees for ADSC participants in activities at YSU. It has also allowed us to structure the budget so that only about 5% of the total budget is lost to overhead.

The formal *Managing Institution* for the ADSC proposal to the RSEC is Case Western Reserve University, CWRU, which has extensive experience in this role and a long history of collaborations with many ADSC participants, including YSU. We request that the award be made to CWRU which will subcontract the execution of this project to YSU. CWRU will maintain an oversight role on the Advanced Diffraction Studies Consortium's activities and, in particular, will assist YSU and other consortium members with budgetary questions.

Dr. Allen D. Hunter from YSU is the ADSC Director and PI of this proposal. Since 1987 he has been the PI or a major co-PI on external grants totaling 1.2 million dollars to support his personal research, scientific instrumentation purchases, and/or educational initiatives. While at the University of Alberta and Youngstown State University, he has mentored several dozen post doctoral fellows, research associates, and PhD, MS, BS, and high school research students. He is on the governing bodies of the Ohio MS, NMR, and Crystallography Consortia where he serves as the representative of predominantly undergraduate institutions and he founded the YSU Structure Center. He has active research collaborations with faculty at research universities, predominantly undergraduate schools, and in industry. He therefore has both the experience to carry out the duties of the ADSC Director and PI of this grant and the confidence of the participating institutions and individuals. To support his role, YSU has committed to a 100% reduction in his teaching duties for the first year of this grant (to ensure a smooth start), a 50% reduction for the other 4 years, and a 50% reduction during the following year when he will help "wind up" the grant, assess, report, and disseminate its results, and develop continuing activities for the consortium.

C2a(i). PhD Granting Host Institutions. Faculty from the following *PhD granting host institutions* have agreed to participate and these schools will provide the sites for most of the advanced diffraction methods collaborative research (providing research mentors and advanced diffraction facilities) and sites for some of the advanced diffraction methods courses: Carnegie Mellon University, Case Western Reserve University, Duquense University, The University of Akron, the University of Pittsburgh, and the University of Toledo.

C2a(ii). MS Granting Host Institutions. Faculty from the following *MS granting host institutions* have agreed to participate and these schools will provide the sites of the basic diffraction methods courses, some of the research sites/facilities (especially those available for remote data collection), and many of the course instructors: Bucknell University, Indiana University of Pennsylvania, Wright State University, and Youngstown State University.

C2a(iii). Non-University Host Institutions. We will also include the following *Non-University Host Institutions* at which some of the collaborative research projects will take place: the Advanced Photon Source MB-

CAT, the Cleveland Clinic Foundation, the Cleveland Center for Structural Biology, the NASA Lewis Research Center, and the Oak Ridge National Laboratory.

C2a(iv). Participating Institutions (i.e., the Predominantly Undergraduate "Home" Institutions). These include institutions from which individuals have already indicated that they would like to participate in the Consortium's activities in some fashion (e.g., as research mentors/collaborators, as course participants/instructors, and/or as applicants for consortial research support). The predominantly undergraduate institutions listed below are those in our region from which faculty members will be eligible to apply for consortium research support and those from outside our region whose faculty have expertise in crystallographic/diffraction methods education and have volunteered to act as summer school instructors. In addition, several historically black institutions outside our immediate region are also included. The following is a listing of the *participating (i.e., home) institutions* which have already committed themselves to the ADSC. MS/PhD granting participating institutions: Cleveland State University and Miami University. Predominantly Undergraduate Participating Institutions: (degree granting 4 year institutions) Allegheny College, Bowie State University, Clarion State University, Gannon University, Hiram College, John Carroll University, Kenyon College, Lincoln University of Pennsylvania, Mercyhurst College, Morgan State University, Mount Union College, Oberlin College, Ohio Northern University, Penn State Erie-The Behrend College, Saint Francis College, Slippery Rock University, Thiel College, Washington and Jefferson College, and Westminster College and (2 year community colleges) Kent State University-Stark Campus, Lorain County Community College, and Wayne College Community College of the University of Akron. Over a dozen others are in our immediate region and will be eligible to apply for ADSC funding.

C2a(v). Associate Members. Individual schools and school districts will be eligible to participate in consortium activities. YSU and its faculty are already working closely with the Youngstown City Schools and various schools in Mahoning and Trumbull counties. Additional schools and school districts will be added over the next year as our outreach activities develop.

C2a(vi). Industrial Partners. The current academic members of the ADSC have a long history of collaborations with regional industrial companies and diffraction equipment suppliers that are now members of the ADSC, these include: Bruker AXS, Delphi Packard Electric, Dow Agrochemicals, Ferro Corp., Goodyear, Molecular Structure Corporation, and Zincoa.

C2a(vii). Individual Participants. The *senior project participants* (including the PI and co-PIs) will play the central role in the research (i.e., as research mentors) and/or educational (i.e., in instructional development and as course instructors) aspects of the proposal. Their names, affiliations, and major roles in this proposal follow:

- Alan Jircitano (Penn State Erie-The Behrend College, small molecule crystallography and crystallographic instruction)
- Alan Pinkerton (University of Toledo, co-PI, charge density studies)
- Allen Hunter (Youngstown State University, PI and Consortium Director, small molecule crystallography and crystallographic instruction)
- Bob Stewart (Carnegie Mellon University, theoretical basis charge density studies)
- Bryan Chakoumakos (Oak Ridge National Lab - HFIR, neutron diffraction)
- Bryan Craven (Indiana University of Pennsylvania, co-PI, charge density studies and crystallographic instruction)
- Cam Hubbard (Oak Ridge National Laboratory, materials crystallography under extreme conditions)
- David Grossie (Wright State University, small molecule crystallography and crystallographic instruction)
- Edward Zovinka (Saint Francis College, small molecule crystallography)
- Ewa Skrzypczak-Jankun (University of Toledo, protein crystallography and crystal growth)
- Gloria Borgstahl (University of Toledo, protein crystallography)
- Guy Crundwell (Central Connecticut State University, materials diffraction)
- Jeanette Krause-Bauer (University of Cincinnati, small molecule crystallography and crystallographic instruction)
- Jim Gano (University of Toledo, Ohio Crystallography Consortium Director and NLO materials)
- John Hughes (Miami University, diffraction analysis of minerals and crystallographic instruction)
- John Protasiewicz (Case Western Reserve University, small molecule crystallography)
- John Rosenberg (University of Pittsburgh, protein crystallography)
- Karen Magnus (Case Western Reserve University, protein diffraction studies and education)
- Katherine Kantardjieff (Cal. State Fullerton, protein crystallography and crystallographic instruction)
- Margaret Kastner (Bucknell University, small molecule crystallography and crystallographic instruction)
- Mark De Graef (Carnegie Mellon University, crystallographic instruction)

- Mark Foster (University of Akron, co-PI, polymer and materials diffraction)
- Menachem Shoham (Case Western Reserve University, co-PI, protein crystallography)
- Mike Hopkins (University of Pittsburgh, theoretical prediction of inorganic structures)
- Mike Nathal (NASA-Lewis, Chief of Advanced Metallic Division, materials diffraction)
- Mike Serra (Youngstown State University, free radical degradation of proteins and protein crystallography)
- Omar Steward (Duquesne University, small molecule crystallography)
- Partha Basu (Duquesne, small molecule crystallography)
- Sherri Lovelace Cameron (Youngstown State University, Coordinator of Minority Enhancement Programs)
- Shih-Chi Chang (Duquesne University, small molecule crystallography and crystallographic theory)
- Steven Geib (University of Pittsburgh, small molecule crystallography and crystallographic instruction)
- Tim Wagner (Youngstown State University, extended inorganic solids diffraction and crystallographic instruction)
- Vivien Yee (Case Western Reserve University and Cleveland Clinic Foundation, protein diffraction studies)
- Wiley Youngs (University of Akron, small molecule crystallography)
- Xiche Hu (University of Toledo, theoretical prediction of protein structures)

[Note: These individual all fit into the NSF categories "Other Senior Personnel, Auxiliary Personnel, and Other Personnel Having Exceptional Qualifications. However, in the interest of brevity of the overall proposal, we have only included Biographical Sketches and Current and Pending Support information on a *representative selection* of individuals, including several faculty from predominantly undergraduate institutions. This approach was verbally approved by Dr. Janet G. Osteryoung on November 17th, 1998.] In addition to these senior project participants, about a dozen other experienced researchers in our region will have a more limited involvement in this proposal and about three dozen other individuals, at predominantly undergraduate institutions in our region, have expressed their interest in participating in ADSC activities, as undergraduate faculty research participants and/or as participants in the 1st summer courses. In addition, a dozen other will be participating in consortium activities.

C2b. Diffraction Methods and Research Opportunities. The large majority of diffraction studies that are done are "routine" powder and single crystal studies of small molecules and extended solids. These types of studies are still (and for the foreseeable future will still remain) the major interest of most non-crystallographers and novices and will represent the large majority of samples whose data they will want to collect and solve. Indeed, these routine diffraction methods are extremely valuable in solving scientific problems of interest to non-crystallographers. To meet this need, training in the best procedures for collecting data on routine single crystal and powder samples and the subsequent determination of their structures must remain the first stage of our educational and research programs. They will also need facilities for carrying out a substantial volume of such studies for teaching and research at a moderate cost. Once these faculty and students get familiar with conventional powder and single crystal diffraction methods, it is expected that many of them will be attracted to more "cutting edge" diffraction methods that "push the frontiers" of what is possible. Here the focus will be on the use of high resolution diffraction methods to solve important problems of fundamental and applied chemical interest. They will be introduced to such methods through participation in a series of advanced summer school courses to be held at several of the host institutions. This will facilitate their joining collaborative research projects with skilled crystallographers at the research institutions, initially funded by this grant and later through conventional granting channels. The specific types of diffraction facilities which these teaching and research efforts described in the following sections will require are outlined below:

C2b(i). Quality Conventional Single Crystal X-ray Diffraction Studies. These types of studies will represent a substantial majority of single crystal samples for which data will be collected and analyzed (but a much smaller portion of diffractometer time). Fortunately, these "routine" single crystal studies of small molecules, extended solids, and minerals can be done, with proper training and appropriate access, by relative novices using any modern single crystal diffractometer. Such diffractometers are available at each of the host sites, although access policies for instruments at each will differ. These types of studies can be done on conventional "laboratory" diffractometers equipped with serial detectors. Data collection times can be decreased, signal to noise ratios improved, and/or more weakly diffracting crystals used if these diffractometers are equipped with area detectors (most commonly CCD systems but also imaging plate systems) and/or higher intensity sources (e.g., sealed tube units with Gobel optics or rotating anode sources) are used. Consortium members will provide advice and consultation for dealing with problem structures. Youngstown State University, Bucknell University, Indiana University of PA, and Wright State University will fulfill most of this need for "on site" data collections while the YSU Diffraction Laboratory will be able to fulfill the requirement for "off site" data collections by participants.

C2b(ii). Quality Single Crystal Diffraction Studies on Weakly Diffracting Samples. The use of synchrotron sources are required where one has particularly small and/or otherwise weakly diffracting crystals for which quality data can't be collected with an area detector and/or rotating anode system. For accurate hydrogen atom positions (or other weakly diffracting elements in the presence of heavier elements) one must use neutron diffraction. Access to such high intensity and neutron sources will be facilitated by the consortium through access to the national labs.

C2b(iii). Quality Powder X-ray Diffraction Studies. These types of studies will represent a substantial majority of powder samples for which data will be collected and analyzed. Fortunately, these "routine" powder studies can be done, with proper training and appropriate access, by relative novices on any suitable powder diffractometer. Such powder diffractometers are available at many of the host sites and even at some of the smaller schools, although access policies for instruments at each will differ. With funding of the equipment purchases in the proposed budget, Youngstown State University will be able to fulfill a significant part of this requirement for offsite data collection by undergraduate faculty and students. Various consortium members will provide advice and consultation for dealing with problem structures. The use of more modern powder diffractometers with high intensity sources, area detectors, and/or automated sample changers can substantially increase data collection speed and data quality while decreasing the operator's workload.

C2b(iv). Very High Resolution Single Crystal Diffraction and Charge Density Studies. One needs superior diffraction facilities, longer data collection times, and greater skill levels to collect data suitable for high resolution structural studies. The skill level needed to correctly analyze this high resolution data for applications such as charge density studies is also much higher, the software is substantially more sophisticated, and such studies should only be attempted with the assistance of an expert. Access to these methods will therefore typically be limited to individuals who have passed beyond the novice stage through advanced summer courses and/or collaborative research. This data is most commonly collected on the most modern "laboratory" diffractometers. These are typically fitted with some combination of a high intensity X-ray source (e.g., a sealed tube X-ray source using mirror optics or a rotating anode X-ray generator) and an area detectors for the multiplex advantage (most commonly a CCD detector). Low temperature data collection will also have to be used for all but the highest melting solids to reduce the displacement parameters. For many studies, one will also have to collect neutron diffraction data (especially if the light atoms are important) and/or data from ultra intense and tunable synchrotron radiation sources. Such sources are only available at the national labs such as the Advanced Photon Source in Chicago. Undergraduate faculty in the consortium will have access to this and other national facilities through our participation in the MB-CAT X-ray line at the APS, through the provision of funding for travel and lodging to collect such data, and the participation of Oak Ridge National Laboratory, ORNL.

C2b(v). Advanced Powder Diffraction Studies. As with single crystal methods, one can collect high resolution powder diffraction data. This data must be carefully collected with particular attention to accurately measuring base line and peak intensities and profiles since these contain the atomic position information. High resolution powder data, when analyzed by the Rietveld method, allows one to get quality information on the structures of extended solids or structurally simple molecular materials. However, this analysis is very non-trivial and should only be attempted where one has a good starting model and/or the advice of an expert.

C2b(vi). In Situ Diffraction Studies Under Extreme Conditions. For many materials studies, one desires structural data measured under extreme conditions, most commonly high temperatures and/or pressures. Such facilities are relatively specialized and will be available to consortium members through the participation of the High Temperature Materials Laboratory at ORNL and other national facilities. It also requires skill with using specialized software and analytical tools.

C2b(vii). Line Shape Analysis of Diffraction Peaks. The analysis of diffraction data line shapes is a technique which provides substantial information on topics of great interest to materials scientists, structural engineers, and catalyst developers including: crystallite sizes and size distributions, defect structures and distributions, crystal strain patterns, mosaicity, etc. Such studies on both powders and single crystals require diffraction data that have been carefully collected to be optimized to reduce the natural line width and also requires skill using specialized software and analytical tools.

C2b(viii). Protein Diffraction Studies. Proteins and related macromolecules have tremendous significance to both scientific and biomedical research, and we have a rapidly growing number of experts in their study in our region. They will form a cornerstone of our proposal and these studies will be principally carried out at the University of Toledo, the Cleveland Clinic Foundation/Case Western Reserve University/Cleveland Center for Structural Biology (i.e., CCF/CWRU/CCSB), and the University of Pittsburgh.

C2b(ix). Materials Diffraction Studies. Advanced materials such as solid state oxides and polymers are characterized by a wide variety of diffraction methods including those discussed above. In addition, a wide range of

other diffraction methods are also used to determine their morphologies, orientations, defect structures, etc., including diffraction methods that characterize both the bulk and the surface properties of these materials.

C2c. Examples of Specific Research Projects to be Pursued by ADSC Participants. In addition to "routine/conventional" powder and single crystal studies of molecular and extended solids, participants will be involved in advanced research areas including high resolution crystallography of small molecules, materials diffraction, and protein crystallography. Under this proposal, participating undergraduate faculty and their students will choose the topics of most interest to them. They will then usually join a collaborative research program, funded initially by this grant, with one or more of the established research groups. During this time, they will contribute scientifically to their host's project and develop their own skills in crystallography which will benefit both the teaching and research at their home institution. Once they have developed their skills in one or more of these areas, they can then either continue as part of the project team for a longer term or use these skills to study other classes of molecules with which they, or their non-crystallographic collaborators, have worked previously. For more experienced undergraduate faculty, the role of the PhD hosts will typically be more focused (i.e., providing instrument access and mentoring) although collaborative arrangements will still be encouraged. In the following sections, a representative sample of specific research projects involving diffraction methods are given as an idea of the range of research projects to be pursued by ADSC undergraduate faculty and student research participants.

C2c(i). Conventional Single Crystal and Powder Studies. For synthetic chemists and others who prepare and/or isolate new molecular and extended solids, single crystal and powder diffraction methods are a critical tool. These methods require relatively little material, give detailed structural information (including information on stereochemistry for single crystals), are relatively fast, and give these structures with more confidence than do other more "sporting" methods of structure determination such as NMR or MS. In addition, a substantial majority of such determinations proceed in a relatively routine fashion. This means that novices, especially when properly trained and with a suitable support system, can successfully solve most such structures (when they can't they can go to more experienced people in the ADSC for help). Data collection can be done at a host site with the more challenging and scientifically interesting part of the project taking place on a personal computer in their home institution. Indeed, crystallographic projects are one of the few reliable ways that a novice can start a project and take it all the way to submission for publication in one semester. For these reasons, basic structure determinations are expected to be a significant majority of the number of diffraction studies carried out under this project. These studies can be carried out at all of the host institutions but most ADSC undergraduate faculty and student participants are expected to be done at the MS level host institutions which have more liberal instrument access policies, no direct user charges to undergraduate faculty and students, and faculty who have a strong interest in advising and/or collaborating on these studies. In cases where these novices are not able to successfully collect an adequate data set (e.g., because they have a very weakly diffracting sample) or to solve for a reasonable structure (e.g., because their crystal is twinned or the space group is non-obvious) they will be able to rely on access to the advanced diffractometers and skilled crystallographer present at the ADSC host institutions.

Routine structural studies often form a small, but important, part of other research projects that have a different primary focus (e.g., a synthetic chemistry program). In other cases, crystallography forms a central focus of an ongoing research program. Both types of crystallography will be supported by this consortium. Potential mentors for routine structural studies include: Allen Hunter and Tim Wagner at YSU, Margaret Kastner at Bucknell University, Bryan Craven at Indiana University of Pennsylvania, and David Grossie at Wright State University. In addition, they and other ADSC faculty have sustained research programs with a major crystallography focus. Several representative examples of "routine" diffraction methods being used to solve scientific problems are described below:

C2c(i)a. Twist-twist p-Conjugated (TTPC) and Twist-twist p-Conjugated/p-Stacked (TTPC/PS) Molecules, Oligomers and Polymers: Investigations of New Conjugated Systems. Two-photon absorption (TPA), electroluminescent (EL), and non-linear optical (NLO) materials are of intense scientific and technological interest. In addition, new applications in photodynamic cancer therapy, luminescent display panels, optical limiters, materials aging, and photonics are continually being found. Fundamental advances in molecular theory and access to novel materials lead the way for these developments. For the first time, a series of molecules is available in Gano's group at the University of Toledo to study extended π-systems whose planes are held rigidly perpendicular to one another, twist-twist pi conjugated, TTPC, which have unusual properties. Typified by E-di-tert-butylstilbene, the TTPC motif is supplemented by a continuous π-stacking interaction in the TTPC/PS system Z-di-tert-butylstilbene. Metal coordination to Z-di-tert-butylstilbene offers further structural diversity. Sudden polarization and TICT (Twisted Intramolecular Charge Transfer) have been observed in structurally similar excited states. Understanding the impact of TTPC and TTPC/PS structural units on molecular properties is the goal of this project. Toward this end, the identity for the newly synthesized TTPC and TTPC/PS polymers and oligomers will be established by X-ray

methods. The primary focus will be the impact of TTPC and TTPC/PS structural features on efficient TPA, EL, and NLO properties. This project complements one by Hunter and Brower at YSU which focuses on the synthesis and photophysics of both convention NLO materials having coplanar π-systems and novel materials having organometallic centers in the chromophores as well as work at Wright Patterson Air Force Base, University of Toledo, and Case Western Reserve University where TPA, EL, and NLO properties are studied, respectively.

C2c(i)b. Fundamental Studies of Organic Reactions and Mechanisms. The chemistry of iodosylbenzene (PhI=O) and (tosyliminoiodo)benzene (PhI=NTs, Ts = *p*-toluenesulfonyl), the primary sources of oxygen atoms and tosylimino groups (nitrenes, NR) for many important transition metal catalyzed oxygenation and imination reactions, are being studied by John Protasiewicz at Case Western Reserve University. These heavily employed organoiodonium(III) ylides, unfortunately, are insoluble in all common organic media due to their polymeric and highly aggregated nature in the solid-state. Catalytic reactions which employ these reagents are therefore heterogeneous and efforts thus far to improve catalytic performance or to gain mechanistic information are both limited and difficult. New *soluble* iodonium ylides, which serve as efficient oxygen atom and nitrene precursors have been engineered to contain internal dipoles designed to disrupt the I•••N and I•••O secondary bonds that occur in ArI=X (X = O or Ts) and hence the solid-state aggregation of organoiodonium ylides which imparts dramatic increases in solubility. Structural studies guide these syntheses and confirm the predictions of computational chemistry that the *ortho*-^{t}BuS=O_2 group would enable internal secondary bonding to compete or replace intermolecular secondary bonding and hence solubilize this class of materials. Work is ongoing to examine the generality of this principle for hypervalent iodine chemistry. These new versions of PhI=O and PhI=NTs are expected to benefit studies of atom and group transfer reactions by allowing (a) reactions to be performed in homogeneous manner, with greater selectivity and efficiency, (b) enantioselective oxidants to be prepared, (c) the mechanism of reactions (especially under catalytic conditions) to be studied by conventional methods, and (d) asymmetric reactions to be performed at lower temperatures enabling increased enantioselectivities. This work typifies the use of detailed structural data to help understand organic reactions, rationally design new reagents, and determine complex stereochemical relationships and structures.

C2c(i)c. Multiply Functionalized Metallocenes. Edward Zovinka of Saint Francis College is interested in expanding the number of ligands (phosphines) that can be attached to a metallocene core beyond the commonly found two or three groups, thereby producing a multiply (greater than three donor ligands) functionalized metallocene. Materials in this general class have the ability to catalyze alkylations, arylations, hydrogenations, polymerizations, and many other reactions. While functionalized metallocenes have aroused great interest due to their catalytic nature, there is currently no method to prepare multiply functionalized metallocenes as leads to novel catalysts. Doing so is the core of this undergraduate research program. As with many organometallic and coordination compounds prepared by ADSC members, crystallography is the best, and often the only practical, method to establish molecular structures and will therefore be very widely used. For example, David Grossie at Wright State University is studying silver(I) and silver(II) transition metal complexes, Allen Hunter at YSU is studying organochromium host guest complexes of his own and organometallic derivatives related to C60 complexes with Larry Curtin at YSU, Margaret Kastner at Bucknell University is studying Fe(III), Ni(II), and Gd(III) complexes, Schiff Base complexes of first row transition metals, and mercury(II) complexes (the latter two projects in collaboration with Charles Root at Bucknell and Deborah Beboit of the College of William and Mary, respectively).

C2c(i)c. Structural Effects on Organic Reactivity. Sydnones are, in most cases, extremely stable crystalline compounds that exhibit a distinct polarity. The five-membered heterocyclic ring is subject to electrophilic substitution at the C-4 position. Only with a strongly activating group present will the 3-aryl group compete effectively for the electrophile, due to the considerable partial positive change at the 3-position of the sydnone ring. Similarly, the regioselectivity of Friedel-Crafts acylations of 1-benzenesulfonyl pyrroles are found to be dependent on the acid promoter used. For hard Lewis acids, the substitution occurs at C-3, while for soft acids it occurs at C-2. Like most crystallographers, David Grossie at Wright State University collaborates with his organic colleagues to understand such organic reactivity patterns and determine the detailed structures of synthetic and natural products. David is collaborating with Ken Turnbull and Dan Ketcha from Wright State to understand these observations using both conventional and high resolution diffraction methods. As an example of stereochemical determinations, Allen Hunter and Tim Wagner at YSU collaborate with several organic chemists, including John Jackson and Peter Norris at YSU, to determine the absolute structures of synthetic products such as organophosphorous transition state analogues and carbohydrate derivatives.

C2c(ii). High Resolution Crystallography and Charge Density Studies. If one collects a sufficiently high quality data set (e.g., free from significant systematic errors and using low temperature measurements, excellent signal to noise ratios, high angle data, and often access to neutron data) and carefully analyzes these data, one can often derive not only atomic coordinates but also direct information about the electron distribution (and derived

quantities) about the atoms and bonds. Such studies are valuable not only in their own right but also because of the relationship of their results to those from theoretical studies and a diverse range of fundamental and applied experimental techniques. Several representative high resolution diffraction projects are presented below:

C2c(ii)a Hydrogen Bonded Solids Related to Biological Molecules. Understanding the details of hydrogen bonding is one of the most important challenges on our path to being able to: predict and control structures of biologically relevant molecules such as DNA, proteins, and carbohydrates, understand important chemical phenomena such as spontaneous self assembly and host-guest chemistry, and control the microstructures of many classes of polymers. Bryan Craven, formally at the University of Pittsburgh and now at Indiana University of Pennsylvania, along with a diverse community of collaborators (including Bryan Chakoumakos) has played a leading role in understanding the detailed structures, properties, and bonding of these materials by charge density studies of model compounds. Such understanding is critical to researchers as diverse as theorists such as Janet Del Bene at YSU and protein crystallographers across our consortium. In collaboration with the neutron diffraction group at ORNL, Craven will extend his previous studies to new nucleic acids and alcohols.

C2c(ii)b. Advanced Crystallographic Studies on Energetic Materials. Explosive power and specific impulse of energetic materials as well as their shock sensitivity are related to physical parameters which are best obtained from crystallographic studies. These parameters need to be determined for known compounds and can then be coupled with theory to establish the strategy used to synthesize new and better energetic materials. An advanced crystallographic study on known materials and newly synthesized compounds will be carried out. Whereas the importance of density and crystal packing (obtained from routine X-ray crystallography) are well recognized as predictors of performance, the use of variable temperature and variable pressure single crystal X-ray diffractometry as performed at the University of Toledo is a new approach which furnishes much more detailed information directly related to mechanical properties, thermodynamic parameters, explosive characteristics, and theoretical models. Single crystal X-ray diffraction experiments will be carried out over the temperature range 10 - 350 K or over a range of pressures up to 50 kbar to determine the variation of density with temperature or pressure, the coefficient of thermal expansion or compressibility (variation of unit cell volume with temperature or pressure), the anisotropy of thermal expansion or compressibility (variation of unit cell metric with temperature or pressure, thermal expansion or compressibility tensor), and the variation of atomic displacement parameters with temperature or pressure. In addition, using very accurate low temperature diffraction data, molecular charge density distributions will be obtained for the determination of atomic charges and complete three dimensional electron density mapping (e.g., to show the deformation from spherical atoms due to chemical bonding as well as the corresponding electrostatic potentials). In addition, the defect densities will be determined from accurate rocking curve measurements and then correlations between defect density with shock sensitivity, between defect density (due to temperature cycling) with anisotropy of thermal expansion, and between expected shelf life with the thermal expansion tensor will be determined. This capability to carry out high resolution diffraction experiments under extremes of temperature and pressure and to measure defect structures will be useful to a wide range of ADSC participants including materials scientists, protein crystallographers, and theorists. These capabilities nicely complements those at the HTML at ORNL and in the labs of several other ADSC participants.

C2c(ii)c. Transition Metal Organometallics. Allen Hunter at Youngstown State University is interested in charge density studies of transition metal organometallic complexes, especially those related to single site catalysts. The commercialization of single site catalyst technology is revolutionizing the technology of vinyl polymers. The recent introduction of metallocene and related single site catalysts has enabled the economic production of high performance materials having closely controllable stereochemistry from inexpensive monomers such a propene. The mechanisms by which these catalysts produce this exceptional level of control are becoming more well understood but many fundamental questions remain, including the relative importance of steric and electronic effects in key steps. Charge densities studies on transition metal containing materials, especially molecular solids, have not been very widely employed in the past for both theoretical and practical reasons. This collaborative project with Bryan Craven at Indiana University of Pennsylvania will focus on extending high resolution charge density methods to the study of single site catalysts and model compounds and will take advantage of new crystallographic methods and theoretical approaches to handling heavy metals.

C2c(ii)d. Experimental Electron Densities and Electrostatic Potentials for c-AMP Phosphodiesterase Inhibitors. For a molecule to be of therapeutic use, it must first bind to a receptor which recognizes it. This may be thought of as a shape function - the lock and key analogy. A more sophisticated description matches the topology of the electrostatic potential (which is derived from the electron density distribution) of the drug to that of the receptor. The best pharmaceutical compound will have the closest match between its own topology and that of the receptor, hence a knowledge of the required form of the electrostatic potential will greatly assist in the rational design of new drugs. Although much effort has been expended to obtain this information from theory, the calculation of reliable

electrostatic potentials from high level *ab initio* methods is only possible for very small molecules. Until recently, the experimental determination of electrostatic potentials using X-ray diffraction data was very time consuming, even for very small molecules, and was only attempted in a small number of laboratories. It has thus found little use in the design of new drugs. With the advent of a new generation of X-ray diffractometers coupled with new cryogenic techniques and powerful workstations, this approach now becomes tractable for larger molecules and for series of molecules. A typical experiment on one compound will now take but a few days and the data analysis a few weeks. Thus a complete series of compounds of known activity can be studied in a period of a few months and new structure activity relationships based on electrostatic potentials can be developed. The Pinkerton group at the University of Toledo has initiated a new direction of research in the area of medicinal chemistry. As one component, they map the electron density distribution and the derived electrostatic potential for a series of c-AMP phosphodiesterase inhibitors and define appropriate descriptors to relate the topology of the potential to their known activities. These compounds have applications in the treatment of congestive heart failure and respiratory diseases. This study will open a new window to the understanding of the mechanism of controlling these diseases and will provide a new tool in the quest. Clearly, participation in this type of study would be an ideal approach for introducing new investigators such as undergraduate faculty and students into high resolution crystallographic research. They will then be able to apply the skills they have learned on this specific collaborative project to the study of the diverse range of organic and biological molecules related to their primary research areas. In addition, the results of all such experimental charge density studies will undoubtedly be of interest to synthetic chemists, theoreticians, spectroscopists, biochemists, structural biologists, etc., at their home institutions and elsewhere in the consortium with whom they already collaborate.

C2c(iii). Macromolecular Crystallography. The related fields of genomics, enzymology, structural biology, and rational drug design all depend on a detailed knowledge of the structures of biological molecules such as proteins, traditionally obtained in solution by NMR and in the solid by single crystal diffraction. Until recently, determining such structures was exceptionally time consuming and was limited to relatively small proteins and/or molecular assemblies. Recent advances in crystal growth methodology, computers and software, radiation sources, and detector designs have dramatically improved the relative speed, ease, and resolution of such studies. This has made many more proteins amenable to structural analysis and has given such studies relevance to a wide range of non-specialists. Several representative protein crystallography projects are presented below:

C2c(iii)a. Free Radical Induced Protein Degradation Reactions. Molecular oxygen, O_2, is kinetically unreactive but partial reduction generates a family of reactive compounds collectively known as reactive oxygen species including free radicals like superoxide ($O_2^{\bullet -}$) and hydroxyl (HO) as well as non-radicals such as singlet oxygen and hydrogen peroxide (H_2O_2). The hydroxyl radical is the most reactive with biomolecules giving essentially diffusion controlled rates. *In vivo* damage is largely due to the production of HO by the interaction of transition metals with endogenously produced H_2O_2 in a Fenton-type of reaction. For this reason, metal ions are tightly sequestered under normal physiological conditions to prevent oxidative damage. However, with increases in age, diabetes, or during periods of oxidative stress the plasma concentration of the transition metals copper and iron increases. These "free" metal ions either precipitate out of solution or bind to available biomolecules. Reaction of the bound metal ion with H_2O_2 leads to the production of HO which reacts in the immediate vicinity of its site of production. Such damage has been referred to as site-specific. Site-specific damage to proteins is characterized by the following features: (a) one or at most a few amino acid residues are modified, (b) oxidative damage is insensitive to the presence of free radical scavengers suggesting that damage is caused by radicals produced at the protein's surface and not in the bulk solution, and (c) most of the enzymes that are sensitive to metal ions and H_2O_2 require metal ions for activity. The goal of the research in Mike Serra's group at Youngstown State University is to determine structural characteristics of site-specific protein oxidative damage mediated by copper and hydrogen peroxide at atomic resolution. The specific aims are to compare the protective affects of various free radical scavengers, to determine the effects of chemical modification of specific residues on a model protein in regards to oxidative damage, and to obtain detailed structural information via X-ray crystallography on the metal-protein complex as well as the oxidized proteins to better understand the nature of site-specific damage. The latter part of this project will be carried out in collaboration with Vivien Yee at the Cleveland Clinic Foundation.

C2c(iii)b. Crystal Structures and Functions of Limulus hemocyanin. Knowledge of the three-dimensional structures of the oxygenated and deoxygenated forms of Limulus II hemocyanin has clarified hitherto unsuspected aspects of the molecular controls of function in these large copper-based oxygen-transport proteins. The native hemocyanin of Limulus consists of 48 subunits with eight distinct types of polypeptide chains. Each of the eight subunit types is capable of reversibly binding molecular oxygen at a dicopper active site. The subunit types differ markedly in primary structure, ligand affinities, and sensitivity to assorted allosteric effectors. Mechanistic ideas about how this will occur will be tested using a combination of crystallographic, biochemical, biophysical and

molecular biological techniques. The eight Limulus hemocyanin subunits interact as hexamers, dodecamers, 24-mers, and the native 48 subunit hemocyanin. These structures and their functional interactions will serve as prototypes for a large class of multisubunit assemblies that require multiple components for complete function and are being studied by the Magnus group at CWRU. For example, comparison of the structure of Limulus II hemocyanin with preliminary structural results for subunits IIIa and IV suggests that the mechanism proposed earlier for subunit II cooperativity may well be general for all arthropod-type hemocyanin subunits. The electron density map of subunit IV is sufficiently high that segments of primary structure can be determined unambiguously, aiding the determinations of the subunits gene sequences. cDNA has been isolated from a Limulus library that codes for a 24 residue peptide identical in sequence to part of the subunit a from Tachypleus sp., a southeast Asian horseshoe crab. The cDNA was used to select for other hemocyanin subunits and nine have been subcloned. Once the nucleic acid sequences for the subunits are available, construction of designed variants and smaller reversible oxygen-binding entities will be pursued. The structure of subunit IIIa is incomplete, but it is sufficiently good to see that its active site environment differs from other known hemocyanins in that two of the highly conserved phenylalanine residues are some other amino acid, providing further insight into the chemistry of the dicopper active site, that in subunit IIIa alone is capable of decomposing peroxides. Protons, divalent cations, and specific anions act as modulators of oxygen affinity in Limulus hemocyanin. Reduction of conserved disulfide bonds found in all arthropod and molluscan hemocyanins thus far examined leads to loss of their oxygen-binding capacity. This active-site disruption induced by disulfide reductants such as dithiothreitol is reversible. The well-characterized differences between Limulus hemocyanin subunits are particularly suited to allow discrimination between specific ion and aggregation effects. Disulfide bridges, oxygen, calcium, and quaternary interactions between subunits act synergistically to restrict tertiary conformational fluctuations. The appropriate geometry for oxygen binding between the two copper atoms in the active site is lost as these conformational restrictions are lifted. Changes at the active site will be compared with changes in sulfhydryl availability that reflect the conformational flexibility of the system. X-ray crystallographic studies of assorted hemocyanins in conformationally restricted states will further clarify structure/function relationships in these ancient molecules.

C2c(iii)c. Protein Crystal Growth Technologies. Gloria Borgstahl 's program at the University of Toledo in collaboration with E. Snell is dedicated to the study of protein crystal growth using various methodologies, including microgravity, and to applying these methods to the structure determination of proteins and protein/DNA complexes important to breast cancer. The general long term objective of this program is to perfect and optimize the crystallization of a number of proteins both on earth and eventually in microgravity. The specific aims are to assess crystal mosaicity by measuring rocking widths, to collect high-resolution diffraction data, to correlate crystal volume, X-ray diffraction resolution, and signal-to-noise ratios with the rocking width mosaicity measurements, to then identify the best crystallization methods, and, finally, to determine high-resolution protein structures of proteins important to breast cancer. The "rocking width" of a diffraction peak (i.e., the width at half maximum intensity) can be used to derive crystal mosaicity values. Protein mosaicity is a powerful measure of crystal quality because it is independent of the diffraction resolution, the type of detector used, and the source of X-rays. Reduction in mosaicity indicates the protein molecules within the crystal are more highly ordered. Reduced mosaicity leads to an increased signal-to-noise ratio in the diffraction data. This is particularly useful for the measurement of high resolution data since such data, important for detailed structural studies, is intrinsically weaker in intensity. Both synchrotron and lab sources are used for such studies. Crystals of biological macromolecules often diffract X-rays poorly due to misalignment of the protein molecules within the three dimensional crystal. Actually, the growth of high quality protein crystals is frequently the major "bottle neck" in the process of determining protein structure. Research into crystal growth technologies can therefore have a substantial payback. Ewa Skrzypczak-Jankun at the University of Toledo is working on several related projects including developing systematic approaches to crystal growth and solving the structures of proteins from closely related organisms to determine the effects of naturally occurring point differences in the amino acid sequences (e.g., the seven point mutations between chicken and turkey lysozyme).

C2c(iii)d. Ab Initio Molecular Replacement Method for Solving Membrane Protein Structures. Membrane proteins play a central role in many cellular and physiological processes, including active and passive transport of molecules into and out of cells and organelles, transduction of energy among various forms (light, electrical, and chemical energy), and reception and transduction of chemical and electrical signals across membranes. Despite the importance of membrane proteins, the knowledge of their high resolution structures and mechanisms of action has lagged far behind in comparison to that of water soluble proteins. As with all proteins, a key bottleneck in X-ray crystallographic structure determination remains the so-called phase problem. A new approach to dealing with this problem is being developed by Xiche Hu at the University of Toledo who is using the method of *ab initio* molecular replacement. The proposed *ab initio* molecular replacement contains two components:

prediction of the tertiary structure for a protein, followed by utilization of the predicted structure as a probe model in the framework of the molecular replacement method to resolve the crystal structure. Here, the term "*ab initio*" stems from the fact that the probe model is computationally modeled by means of protein structure prediction methods rather than the structure of a homologous protein as in the conventional molecular replacement method. The proposed *ab initio* molecular replacement method will broaden the class of solvable protein structures and speed up the process of X-ray crystallographic structure determination for membrane proteins. Since the entire world is solving crystal structures of membrane proteins at a pace of one or two proteins annually, the proposed method is very timely and promising. Moreover, the development of the *ab initio* molecular replacement method itself represents a subject of great theoretical importance. Integrated tertiary structure prediction methods for membrane proteins will be developed and tested; its successful implementation will shed light on one of the outstanding questions in the field of structural biology, i.e., protein folding.

C2c(iii)e. Calcium Dependent Transglutaminases. The transglutaminases are a family of large enzymes (≈80 kDa) which are involved in a variety of biological processes, including blood coagulation, wound healing, cell signaling, apoptosis, keratinocyte differentiation, neuronal regeneration, and erythrocyte membrane structure organization. Vivien Yee's group at the Cleveland Clinic Foundation and Case Western Reserve University is involved in structure determination studies of various calcium-dependent transglutaminases, and in their mutants which have been implicated in human disorders, and in the use of computational tools to aid in the determination of their structures. Dr. Yee has experimentally determined the first molecular structure of a transglutaminase, that of the blood coagulation transglutaminase factor XIII. Current efforts in her group are focussed on the other transglutaminases including tissue transglutaminase, keratinocyte and prostate transglutaminase, and band 4.2 protein. They are particularly interested in the development of working models of these proteins that have been computationally constructed using amino acid sequence alignments and the crystal structure of factor XIII. Katherine Kantardjieff and her group are studying a different class of proteins related to human health. In this case, they are bacterial toxins that are secreted by cells and are being studied using both multiple isomorphous replacement (MIR) and multiple anomalous dispersion (MAD) phasing techniques. The latter of these is particularly powerful and will be available to all ADSC participants through our membership in the MB-CAT team at the APS.

C2c(iii)f. Structure Determination of Colicin E3 in Complex with its Inhibitor, the Immunity Complex. Colicin E3 is a toxic protein secreted by certain strains of *E. coli* in order to eliminate related strains of bacteria living in the same ecological niche. Colicin E3 carries out three functions: it binds to a specific receptor on the target cell envelope, is internalized into sensitive cells across their inner membrane, and once inside the cell, it inactivates the protein biosynthetic machinery of the infected cell by cutting a specific bond of 16S ribosomal RNA. The toxicity of colicin E3 thus stems from its enzymatic activity. The three functions are apparently localized on three different domains of the colicin E3 molecule. The producing organism is immune to the toxicity of colicin E3 by virtue of an "immunity protein" which tightly binds to colicin E3 in a 1:1 complex, and thus renders it inactive. Colicin - immunity protein complexes are amongst the most stable protein-protein complexes ever observed. Menachem Shoham and his group at CWRU is investigating the molecular level nature of these extremely tight protein-protein interactions. Furthermore, the crystal structure will provide information on the mechanism of inhibition by the immunity protein, as well as identification of colicin E3 residues likely involved in catalysis. Detailed knowledge of the enzyme-inhibitor interactions will also shed light on the local structure of the ribosome in the vicinity of the cutting site. Three suitable heavy-atom derivatives have already been found, and more will be searched for. The electron density corresponding to the four molecules in the asymmetric unit will be averaged in order to improve the interpretability of the map. Upon completion of the structure determination, site-specific mutants of colicin E3 and of the immunity protein will be designed, to probe the contribution of specific residues to the affinity. These mutants will be characterized both structurally and functionally *in vitro* as well as *in vivo*.

C2c(iv). Materials Diffraction Studies. Solid state materials are ubiquitous in our lives and their interesting and useful properties are critically dependent on their crystalline, powder, and/or amorphous characters. These are best assessed by diffraction methods which give direct and detailed structural information. Several representative materials diffraction projects are presented below:

C2c(iv)a. Metal Nitride-Fluorides and Metal Oxides. This research project by Tim Wagner and his group at Youngstown State University focuses on the synthesis and structural characterizations of a series of nitride-fluoride powders derived from well-known oxides in the rocksalt, perovskite, and 1-2-3 high temperature superconductor systems. The proposed nitride-fluoride compositions are obtained by replacing two O^{2-} ions of the metal oxide analog with a $(NF)^{4-}$ group. Several such materials including Ca_2NF and Sr_2NF (analogs of rocksalt-type CaO and SrO) have been synthesized by students working on this project. Compounds proposed for preparation in future work include Ba_2NF, Cu_2NF, TiNF, and $Y_2(NF)_{1.5}$, which are analogs of the corresponding

binary oxides, and $CaTi(NF)_{1.5}$, which is an analog of perovskite, $CaTiO_3$. The ultimate goal of the project is to synthesize a nitride-fluoride analog to the well-known 1-2-3 high temperature superconductor, $YBa_2Cu_3O_{7-x}$. The successful preparation of this phase would be highly significant in terms of comparison of conductivity properties with the analogous oxide material. Whether or not the new material is superconducting (which cannot be predicted), valuable insight could be gained as to the role oxygen plays in the superconducting properties of the 1-2-3 oxide phase. A related project involves the preparation and single crystal diffraction analysis of β-Alumina/Magnetoplumbite type compounds. In particular, phases having Ba^{2+} present as the large cation display unusual crystal chemistries, due to the effects of the relatively large size of Ba^{2+} on the lattice, and are quite interesting to study from a fundamental crystal chemical perspective. Proposed ideal compositions for future study are $BaR_{12}O_{19}$, where R = Mg, Ti, and V.

C2c(iv)b. Diffraction Analysis of Polymeric Materials. Research to be done in collaboration with Mark Foster at The University of Akron would involve the use of small angle X-ray scattering (SAXS) in microphase segregated block copolymer systems, X-ray reflectivity of thin films, and off-specular diffuse scattering from polymer systems. SAXS is sensitive to the characteristic size of domains and to the symmetry of the morphology of microphase segregated block copolymer systems. The morphology depends upon the architecture of the block copolymer, particularly the way in which the blocks are connected. Of central interest here is the behavior of heteroarm star block polymers in which arms are connected to a single junction unit and the identity or length of the various arms may differ. The question to be investigated is how the resulting asymmetries in the architecture of the molecule affects the microphase segregated state. The study of the structure of layers of proteins adsorbed to surfaces may be undertaken with X-ray and neutron reflectivity (NR). X-ray reflectivity provides high resolution data on the thickness and structure of the adsorbed layer once a substrate is removed from contact with a protein solution and appropriately rinsed. NR can provide information on the adsorbed layer while the substrate surface is still in contact with the protein containing solution because the neutron beam can pass through a single crystal silicon substrate on which an organic surface of well-defined chemistry has been created using a self-assembled monolayer. Another topic of interest is topological correlation between interfaces of a thin film or layers of a multilayer lamellar structure. Schematic representations of thin films or lamellar ordered nanophase materials (such as those obtained with ordered block copolymers) generally depict the correlation of successive interfaces as being perfect, or nearly so. In systems where specific properties are to be obtained as nearly as possible in two-dimensional structures of nanometer thickness, deviations from such a perfectly correlated structure present limitations to ultimate performance in technological applications. Very recently diffuse X-ray scattering under glancing incidence has been applied to the study of such interface-interface correlation in polymeric materials, after having been developed first with more strongly contrasting metal and semiconducting systems. We propose to exploit this new development to quantify the correlation between interfaces in polymer thin film structures formed by polymer brushes. Prof. Foster has already made measurements of this type at the synchrotron at DESY in Hamburg, Germany.

C2c(iv)c. Materials Research for Aerospace Applications. Michael Nathal of the Materials Division at NASA Lewis and his group study advanced materials for aerospace applications including metals, alloys, intermetallic compounds, and ceramics. X-ray and electron diffraction are essential tools in all of these studies. A wide variety of projects suitable for those with interests as diverse as inorganic chemistry and metallurgy are available.

C2c(iv)d. Biomineralization. This process results in a wide array of complex materials ranging from laminate composites and ceramics such as bones, teeth, and shells to magnetic materials used as directional sensors in magnetobacteria, sea turtles, and homing pigeons to non-linear optical materials like the morphologically unique peptide coated cadmium sulfide particles produced in yeast. Additionally, biomineralization processes play important roles in the pathologies of a number of diseases including malaria. An essential ingredient to understanding these biomaterials is an examination of the molecular interactions at inorganic-organic interfaces which result in the controlled nucleation and growth of these novel materials. By adopting methods from peptide chemistry and molecular biology, it will be possible to design biomineralization templates to not only elucidate these interfacial interactions, but develop strategies to disrupt them. Such an approach being taken by David Wright's group at Duquesne will lead to novel discoveries ranging from new materials to new therapeutic advances for the treatment of disease.

C2c(iv)e. Mineralogy. Professors John Hughes and John Rakovan of the Department of Geology, Miami University, are mineralogists and thus study the atomic structures of naturally-occurring materials. Both researchers undertake studies of bulk crystallography using x-ray diffraction techniques, including single-crystal and Rietveld studies. Professor Rakovan is also interested in investigating the surface structure of materials. Using

Atomic Force Microscopy, Professor Rakovan investigates the surface structure of materials and studies how the bulk crystallography relaxes at the surface. Such studies are particularly important in the investigation of reactions between minerals and fluids in natural environments. This work is closely related to studies by Tim Wagner and Ray Beiersdorfer at YSU who are studying metamorphic materials to better understand their histories and the processes that shaped them.

C2c(iv)f. Advanced Microwave Dielectric Materials. With the current world wide explosion in the development of microwave-based communications technologies, the production of dielectric resonators has emerged as one of the most rapid growth areas in electronic ceramic manufacturing. This will require the development of new ceramics with higher dielectric constants and lower dielectric losses. Cam Hubbard and his group at ORNL are investigating this system and their work has focused on the solid solutions $Ba_{6-3x}Ln_{8+2x}Ti_{18}O_{54}$ (Ln = La-Gd) that are used as components in various wireless applications. They are also working on many related projects including those on high energy permanent magnet and solid oxide fuel cell materials.

C2d. Plan for Institutionalizing the ADSC Activities. The ADSC has developed a detailed plan to expand the activities of the consortium during the five years of the RSEC grant by seeking additional funding and providing it with continuing funding after this time, both from conventional sources. As a consortium and/or its components, we plan on applying for the following supplemental/replacement funding (specific agencies/titles can be found on the Current and Pending Support Forms):

C2d(i). For Instrumentation: the Ohio Board of Regents Instructional Equipment Fund (an application is already pending), Ohio Board of Reagents Action and Investment Fund (two applications are already pending), NSF research equipment funding (especially to the CHEM-CRIF, DMR-IMR, and NSF-MRI programs and for the undergraduate schools the RUI versions of these programs), NSF instructional equipment funding (i.e., the CCLI program), and the Dreyfus Foundation Special Research Grants Program in Chemistry.

C2d(ii). For Educational and Professional Development Initiatives: NSF funding (i.e., the CCLI program for crystallographic instructional tool development and dissemination efforts related to the old undergraduate faculty enhancement projects), the Dreyfus Teacher/Scholar program, minority student funding initiatives (i.e., for minority student enhancement programs: Council for Undergraduate Research, CUR, Summer Fellowships in geology, chemistry, and biology; NSF-SURE Summer Undergraduate Research Experience for geology; Student Achievement in Research and Scholarship, STARS, program funded by OBoR (currently in place at Cleveland State and John Carroll Universities) targets academically gifted students from groups which are under-represented in higher education; the Minority Work program at Youngstown State University and similar programs at other institutions, and the ACS SEED program used to fund high school students.); the Eisenhower Grant Program (for pre-college teacher development activities); and to the NSF REU program (i.e., as a distributed site for undergraduate student research).

C2d(iii). For research grants: The NSF ROA program will be used heavily to support ongoing collaborations developed initially through RSEC funding. Such funds require only a very short application and the success rate is relatively high. ROA supplements provide funding for both undergraduate faculty and students to participate in collaborative research with holders of major federal grants. Research Corporation and ACS-PRF funding will also be sought by individual undergraduate faculty and NSF RUI funding will be sought to support more mature research programs/collaborations.

To help build both the rate of grant applications by undergraduate faculty participants and their success rate, the ADSC has developed several strategies. The ADSC Grants Committee has been established and contains a group of individuals with proven records at writing external grant proposals to assist interested individuals in writing proposals and to provide friendly internal proposal review where this is requested. Access to the facilities provided by the ADSC and the collaborative research experiences to be funded out of this grant will help undergraduate faculty members sharpen their research skills and develop preliminary research results to support their proposals. As a condition to accepting undergraduate faculty research support from the consortium these individuals will also have to commit to submitting at least one external individual or collaborative grant on a related topic in the following year. Many of these will initially be for ROA supplements, to the Research Corporation or the ACS PRF, or to the NSF CCLI program. If these proposals are not funded, the Grants Committee will help these individuals rewrite them to address the reviewers comments for resubmission the following year. The resulting flow of new and revised grants should get many participating undergraduate faculty onto the first leg of externally funded research. Indeed, the relatively high success rates of these programs (typically 25 to 40% and much higher for the ROA program) means that the majority of undergraduate faculty participants are likely to receive such funding after one or several tries. Once they have a history of success/results, we will help them apply for larger scale funds to foundations and federal agencies such as NSF, DOE, and NIH.

C3. Human Resource Development

C3a. Overview of Human Resource Development. The primary focus of the RFP and our primary focus as a consortium is on undergraduate faculty and student development, training, and integration into the national research enterprise. This training will enable these faculty and students to more quickly become productive members of the national research enterprise. In addition, this will also invigorate the teaching of crystallography/diffraction methods at their home institutions. Finally, this training and collaborative research experience will help these individuals get funding for their research from more conventional channels.

The major methods the ADSC will use to support these goals for faculty from predominantly undergraduate schools are: (a) summer and sabbatical research support for undergraduate faculty to work in cutting edge crystallography labs, as collaborative partners, and/or as individual researchers, (b) the development of long term collaborations between undergraduate faculty and faculty at the host institutions and between groups of undergraduate faculty, (c) long term, convenient, and affordable access to conventional X-ray, intermediate/advanced X-ray, and the most advanced X-ray and neutron diffraction facilities (the conventional diffraction facility will be available for both "hands on" data collection and remote submission of samples), (d) stable funding to "kick-start" their collaborative and independent research projects, (e) the availability of the various summer crystallography short courses will facilitate their research and teaching, and (f) the availability of support for grant writing.

The major methods the ADSC will use to support these goals for students are: (a) summer research experiences in crystallography as members of a research group at home and host institutions, (b) these research experiences will typically be done collaboratively with a faculty sponsor from their home department, (c) these student research experiences will be designed to proceed smoothly from their course work to undergraduate research at their home institutions and, if desired, through to either MS and/or PhD research or to industrial employment, (d) crystallographic "basic training" summer schools for students to be held at Youngstown State University and at other sites, (e) once more undergraduate faculty complete their course work in crystallography and get involved in crystallographic research it is expected that their students will typically get more crystallography in their courses at the home institutions, and (f) interested BS and MS students (and PhD students on a space available basis) will also be eligible to take the advanced crystallography courses.

C3b. Summer Schools in Diffraction Methods.

C3b(i). Overview. The consortium will sponsor a series of intensive "hands on" summer short courses during the summers of 2000-2004 (i.e., for the 2nd through 5th years of the grant and in the summer immediately after the 5 year term of the grant expires). At least two basic courses will be offered each summer along with one or two more advanced courses. These courses are modeled on the excellent ACA summer school in crystallography which was previously offered by several ADSC members at the University of Pittsburgh and is now offered by B. C. Wang (on the ADSC Oversight and Assessment Committee) and his team at the University of Georgia. These courses will be offered in association with the Pittsburgh Diffraction Society (the past, current, and future presidents of which are part of this proposal). Most of the basic courses (i.e., those designed for relative novices) will be offered at the beginnings of the summers to help participants prepare for their summer research. The basic courses will usually meet for their first one or two weeks at Youngstown State University with the final portion of the course being offered at dispersed sites near the participants home institutions and/or by the internet. Each of these courses will include both the fundamentals and practical aspects of diffraction methods with a very strong emphasis on "hands on" practice during and after the course. The basic courses will typically consist of a first phase having 20 to 40 hours of "lectures" and 60 to 40 hours of "labs" scheduled over two weeks followed by a dispersed phase at multiple sites spread over several months. The more advanced courses will typically be for shorter periods of time and will be more directly tied into specific research projects/groups in the second phase. All courses will be taught in small classes and with high instructor to participant and instrumentation to participant ratios. Course instructors with demonstrated interest and skills in crystallographic education will be drawn primarily from participating BS and MS level schools for the more basic courses and from the PhD level institutions for the more advanced courses. While the more basic courses will typically be taught at YSU, at least for their first phases, the advanced courses will often be taught at participating research universities and institutions. The advanced courses will focus on cutting-edge crystallographic techniques and will be run by acknowledged experts in each research area. Due to their nature, the advanced courses will typically draw their participants from a wider geographic region than will the more basic courses.

To insure that the skills learned in the courses are put into practice, all course participants from predominantly undergraduate schools will be provided with the same books/manuals, instructional software, and crystallographic software that they used in the course to take back to their home institution where they will be able to use it in both teaching and research. Each course will have an explicit emphasis on the teaching of crystallography to

undergraduates and/or graduate students and other relative novices in scheduled courses and in research. This will include presentations on, and practice with, topics/labs which can be quickly adapted by faculty participants to teaching in their home institutions. Several guest lecturers with expertise in more advanced methods will typically contribute to the second week of lectures and/or labs. At the end of each summer course, participants will be asked to give short presentations of their preliminary results. In addition, each year, as part of the annual Pittsburgh Diffraction Society, PDS, fall meeting, summer school participants will be invited to present their final results as posters or talks. This will be in a special session devoted to ADSC activities where summer school and research participants will be eligible for the current PDS awards. In addition, the most meritorious faculty and student presentations will be selected for presentation at national conferences with travel funds to be provided by the ADSC RSEC grant as part of our dissemination efforts.

For most courses, the first priority for admission will be faculty participants drawn initially from our region and later from across the nation. However, for good pedagogic and practical reasons, it is expected that the typical classes will be composed of about 1/3 to 1/2 students, especially in the later years of this grant. These courses will be available for graduate or undergraduate transfer credit from YSU or the offering university. There will be no registration fee for these courses at YSU for faculty and student participants and the RSEC budget will fund their housing in new air conditioned dorm rooms on campus for the duration of the course. It will also fund reasonable travel costs for course participants.

C3b(ii). Basic Single Crystal Diffraction Methods. This course will focus on the fundamental and practical aspects of diffraction methods for use in "routine" structure determination studies on small molecules and simple extended solids. The initial text will be the excellent book "Crystal Structure Analysis for Chemists and Biologists" written by Glusker, Lewis, and Rossi and the new laboratory manual will be "Allen Hunter's Youngstown State University X-Ray Structure Analysis Laboratory Manual: A Beginner's Introduction," written by the PI of this proposal (270 pages, currently being reviewed by one dozen crystallographers for electronic release in January, 1999) which broadly reflect the level and approach of the course. It will be a general course introducing crystallography to novices and those seeking a "refresher" in modern methods. This course will be presented at an appropriate level to allow practicing chemists, biochemists, structural biologists, materials scientists, geologists, etc., to carry out "routine" structure determinations with only occasional assistance from more experienced crystallographers when they are finished. It will also enable these faculty to integrate modern crystallography into courses at their home schools. It will involve a two week intensive program involving about 30 hours of lectures and about 40 hours of "hands on" laboratory time at Youngstown State University and then a dispersed component at various satellite sites and over the internet. Labs will teach the skills used in various stages of data collection from crystal growth through measuring data for absorption corrections.

This course will be taught in small classes and with high instructor to participant ratios (typically one/five or six). Ample diffractometer experience via a small diffractometer to participant ratio will be provided using the two current Siemens P4 diffractometers at Youngstown State University and the CCD diffractometer to be purchased from this budget. YSU also has two new computer labs that will be used, one with 12 Windows NT machines and one with 24 Windows 95 machines that will be used. Typical class sizes will be 15 to 20 students and for most diffractometer exercises the students will work in pairs. This arrangement will give about 40 days of data collection time, enough for two data sets per participant team (i.e. each participant team having one data set collected on a conventional diffractometer for 2 to 3 days and one on a CCD system for one day). The students will also be exposed to the value of film methods using the Film Diffractometer to be funded from this grant (e.g., Weissenberg and Precession techniques on single crystal samples to evaluate crystal quality and for space group and unit cell determinations and powder methods to confirm that the crystal solved is crystallographically and chemically representative of the bulk sample).

After the two week "on site" phase of the course is over, the participants will be paired with a crystallographic facility and participating faculty member from close to their home institution or with whom they would like to collaborate (i.e., usually Youngstown State University, Bucknell University, Indiana University of Pennsylvania, or Wright State University) where they will have the rest of the summer to complete their data collections to higher resolutions and/or signal to noise ratios. It is expected that these dispersed interactions will form the basis for long term collaborations and instrument access. During the course, the student will be taught the methods for solving routine crystal structures and how to recognize non-routine structures (for which ADSC participants will provide assistance). They will also be exposed to the use of crystallographic data bases which will be available to them after the course is over through Youngstown State University and other sites and to the writing of crystallographic results for electronic submission to journals such as *Inorganic Chemistry* and *Acta. Cryst*. By the end of the course, it is expected that each team will have one or two structures collected and solved and in a format suitable for publication.

Instructors with demonstrated interest and skills in crystallographic education will be drawn primarily from participating BS and MS level schools. Allen Hunter will be the main lecturer and the Diffraction Laboratory Scientist at YSU will help with the laboratory components. Other individuals who have expressed an interest in instructing the on site and/or dispersed aspects of this course include: Alan Jircitano of Penn State Erie - The Behrend College, Bryan Craven of IUP, David Grossie of Wright State University, Guy Crundwell of Central Connecticut State University, John Hughes of Miami University, and Margaret Kastner of Bucknell University. In addition, Katherine Kantardjieff from Cal. State Fullerton will offer her on line course in diffraction methods (which she has offered several times to faculty in the Cal. State system) as a supplement to this on site course. Guest lecturers (i.e., with expertise in more advanced methods such as charge density and protein studies and including representatives from instrument vendors) will typically contribute to the second week of the course.

C3b(iii). Basic Powder Diffraction Methods. The basic powder course will closely resemble the single crystal course described above being two weeks long with about 30 scheduled lecture and 40 schedules laboratory hours in the first phase of the course at Youngstown State University. The lecture part of this course will have substantial sections on solid state chemistry, defect structures, the symmetry of solids, space group assignments, and macro- and microscopic properties of crystals. These topics will fill approximately the first half of the lecture sequence. Thus, this course would be a true crystallography course while the basic single crystal one described above is more of a structure solution course. In the second half of the course, these crystallography topics will be combined with a discussion of powder instrumentation including thin film methods and surface methods, the use of powder methods in sample identification (i.e., using the JCPDS) and in new structure characterization, and a basic introduction to Rietveld analysis. For the labs, the students would learn how to collect and analyze powder data using both automated diffractometers and film methods (including Guinier or Debye-Scherrer methods) for the identification of unknowns and new materials using the diffractometers at YSU for about 1/3 to 1/2 of their laboratory time (depending on the student's interests). In addition, there will be a series of "computer exercises" on solid state chemistry and symmetry (the latter provided by Margaret Kastner), exercises on using basic Rietveld methods, and afternoon "field trips" to specialized materials characterization facilities in our region, including those set up for surface analysis, analysis under extreme conditions, polymer analysis, etc., especially at the University of Akron Polymer Science Institute. As with the single crystal course, at the end of the first phase each course participant will be paired with an institution having a powder diffractometer and a participating faculty member at that school. The student will have the rest of the summer to complete a special project related to their research and/or teaching interests (e.g., in mineralogy, solid state chemistry, materials science, and crystallography). This course would be taught by several individuals, including: Tim Wagner from Youngstown State University, John Hughes from Miami University, and Margaret Kastner from Bucknell University. Mark Foster of the Akron Polymer Science Institute has agreed to serve as a guest lecturer for the materials diffraction component of this course.

C3b(iv). Protein Crystallography. There is an acute need for advanced training in the crystallographic methods employed with macromolecules such as proteins for both aspiring crystallographers and biologists, biochemists, and chemists wishing to better understand this increasingly important technique. A course in protein crystallography targeted to this audience will be offered approximately every other year. It will typically assume a background in crystallography equivalent to the basic single crystal course described above and at least one course in structural biochemistry. Vivien Yee and Karen Magnus from Case Western Reserve University have volunteered to offer the first section of this course at Case Western Reserve University during the summer of 2000. It will be based on their graduate level protein crystallography course but tailored to meet the needs of our audience. As with the basic courses, it will supply participants with the knowledge and skills (as well as a basic software suite) to understand protein crystallography. The second phase of this course (for those participants wanting a deeper understanding of protein diffraction methods) will be offered in the dispersed mode at participating research institutions as part of ongoing research projects. Additional individuals who are likely to be involved in this course include Katherine Kantardjieff from Cal. State Fullerton and Ewa Skrzypczak-Jankun from the University of Toledo. In some years, a more advanced/specialized version of this course may be offered depending on demand.

C3b(v). High Resolution Crystallography and Charge Density Studies. One of the most exciting recent developments in crystallography is the use of high resolution diffraction data and advanced refinement and computational strategies to derive information about the electron distribution around the atoms in molecules. Several of the key participants in this consortium are world leaders in this area and will be involved in teaching an advanced short course on the opportunities and pitfalls in the collection of the requisite high resolution data, the theory of charge density studies, and practical aspects of refining and interpreting charge density results. This course will have as prerequisites, the basic single crystal course and experience in routine diffraction methods. It will be taught several times over the course of this grant (perhaps alternating with the protein diffraction course).

Bryan Craven of Indiana University of Pennsylvania has volunteered to organize this course which will be taught by a team of senior RSEC participants.

C3b(vi). Solid State Structural Methods for High School Teachers. This course is optimized for the professional development of high school chemistry teachers and will be offered multiple times over the course of this grant. This course is particularly timely, and desirable from high school teachers perspectives, because of increasing state requirements for post-graduation teacher "content" certification. This course will be a two week short course analogous to the broader structural methods for teachers course (which focussed more on "sporting methods" such as NMR) which Allen Hunter taught at YSU several years ago and is similar to a course that Margaret Kastner has taught several times at Bucknell University. It will have about 30 hours of lecture/discussion time, typically broken down so that about two hours is scheduled first thing each morning to discuss theory and about one hour at the end of the day is used to discuss curricular implications. It will also have about 40 hours of laboratory time, including: two afternoons on a single crystal diffractometer where the students will collect rotation photographs and the procedures for data collection will be demonstrated (with the assistance of the instructor, the class as a group will collect and analyze one or more complete data sets), one or two afternoons on the powder diffractometer where the students will learn to collect and analyze powder data, two afternoons on strategies for growing single crystals of organic molecules and inorganic salts, one or two afternoons on mineral crystals (taught by one of our geologist participants), one afternoon on biomolecular structures (e.g., proteins, DNA, and RNA), including the use of "freeware" molecular drawing programs to view structures downloaded from the Protein Data Bank, three or four afternoons in the computing labs learning how to solve a variety of "routine" data sets (i.e., to get a feel for where molecular structures come from) and learning solid state symmetry from Margaret Kastner's "Crystallographic CourseWare" package. This course is one that seems particularly suitable for cloning and offering at several sites around our region on alternating years.

This course will have a strong emphasis on relevance to the pre-college curriculum. The teacher participants will be required to develop at least one new lesson outline out of their coursework for possible integration into their school the following year. Those participants who elect to work further on this outline and actually test it and distribute it to other participants will be eligible for further course credit. Teacher participants will be provided with the requisite books/manuals, instructional software, and crystallographic software for use at their home schools. The cost of this program will be born initially out of this grant. Funding to continue/expand this program will be sought from the Eisenhower program. This course will be closely allied to our efforts to develop crystallographic units suitable for inclusion in the pre-college and early undergraduate curricula. Many of its graduates will be actively involved in developing these materials (as a graduate level course in instructional materials development), with testing them in the classroom, and with disseminating them to the national teacher audience.

C3b(vii). Distance/Electronic Diffraction Courses. Margaret Kastner at Bucknell University has developed some excellent software for teaching the basic vocabulary of crystallography and the symmetry of crystals (i.e., "Crystallographic CourseWare"). Katherine Kantardjieff at the CMolS laboratory at Cal. State Fullerton has experience offering diffraction methods instruction to remote sites of the Cal. State system which we will extend to our consortium. Allen Hunter has written, and is currently updating, a student's guide for solving routine crystal structures which is currently being reviewed by over a dozen skilled crystallographers including several of our consortium members. This experience will be used to develop electronic course components and courses which are ideally suited to wide scale dissemination efforts. These are tied in with several other "distributive" aspects of the ADC's human resource development and research initiatives, including: the second distributed phases of the courses, the provision for remote access to the data bases at YSU, the well established OhioLink program for research and educational library resource sharing, and the use of electronic communication methods to run the consortium.

C3b(viii). Other Summer School Courses. There are many possibilities for other advanced courses ranging in length from two or three days to two weeks. The choices of which ones will be offered and when will be made based on surveys of ADSC participants interests, the availability of volunteers to host/teach them, and the availability of supplemental funding. Possible advanced course topics which ADSC members have suggested, include: the use of synchrotron data and MAD phasing in macromolecular structure determinations, the integration of diffraction data with that from complementary "sporting" methods such as NMR, line shape analysis in crystallography and materials science, crystallography under conditions of extreme temperature and/or pressure, advanced Rietveld methods, materials diffraction studies, systematic approaches to growing single crystals, dealing with intractable data sets, etc. These courses will be offered both as regular summer courses and at other times in the year (i.e., in conjunction with the annual PDS meeting).

C3b(ix). Continuing Faculty Development Initiatives. In addition to these regular courses, the ADSC will provide a range of continuing faculty development opportunities. These include long term collaborative

relationships with the faculty and instructors from the summer schools and research projects. Remote access will be provided to data collection facilities at the YSU Diffraction Laboratory and to a web of resource people that are active members of the ADSC. In addition, remote access to crystallographic data bases at YSU and to Library resources through OhioLink will be made available.

C3c. Diffraction Related Curriculum Materials Development Initiatives. In addition to conventional research involving diffraction methods, the ADSC budget will be used to supply seed funding for research into crystallographic and related education. For example, during the term of this grant, Allen Hunter will work with faculty and students from both undergraduate and graduate institutions to develop crystallographic/diffraction methods materials for integration into the undergraduate and graduate curricula. This will include new laboratory experiments, computer exercises, new units for lectures, new demonstrations, and other teaching materials. Several of the faculty participants have experience in this area. Another focus will be on developing materials for laboratory oriented courses focussing on diffraction methods that are suitable both for schools with their own diffractometers and for those without in-house diffraction facilities. There will also be efforts at developing materials useful in courses such as general chemistry. Allen has already approached Bruker AXS for their support in this area and he will write a NSF CCLI proposal to help fund this effort.

C3d. Undergraduate Faculty Research Support Programs. Research support will be offered to a total of 50 undergraduate faculty participants over the 5 years of the grant. These will be front loaded into the early years of the grant as such a distribution will have the maximum impact on the overall program goals. Each fall, the ADSC will prepare and distribute a list of faculty at the host institutions willing to host undergraduate faculty collaborators along with a description of their research interests. It will also prepare and distribute a list of interested undergraduate faculty who have expressed interest in applying for participant support along with a description of their research interests. This will be done prior to the annual Fall meeting of the ADSC/PDS. Where ongoing collaborations have not previously been established, the Director will introduce undergraduate and host faculty with similar research interests who are geographically close to one another. Every effort will be made to ensure that each host site that desires to do so will receive at least one undergraduate faculty participant and that no more than 20% go to any one site. This is to ensure that both the benefits and costs inherent in hosting external researchers are spread throughout the consortium.

Applicants will typically make joint applications with their chosen host researcher for these participant support positions. These written applications will be sent to the Consortium Director for subsequent distribution to the Operational Oversight Committee for review and decision. The proposals must be submitted one month before the first annual scheduled meeting of this committee and will be decided on the day of that meeting. Any participant support awards not awarded in the first round may be applied for one month before subsequent meetings. The faculty participant support awards will initially be usable at host institutions for collaborative projects. It is particularly noteworthy that those who hold most federal research grants may apply for Research Opportunity Award supplements (or similar programs from other Federal agencies) to support such researchers and their incremental costs. These grants may be obtained by sending in a short application, they are typically for $10,000 to $15,000, and they are an underutilized resource. Because of this, they should typically be the first choice for those having current federal money who face exceptional research costs. More importantly, they are a way of funding longer term collaborations with faculty and students from predominantly undergraduate schools on a continuing basis (i.e., after the participant support awards or this grant expires). They will, therefore, be requested when there is sufficient notice of a pending collaboration or to continue one past the first year. This will free up funds to support additional undergraduate faculty, students, and other purposes of this consortium.

Each faculty member will normally be eligible for funding as a Fellow for only two years. Each year will require a separate application. Those who have applied for ROA, RUI, PRF, Research Corporation, etc., funding for projects related to the ones for their participant support awards will be given "bonus points" on their applications, especially for their second year. If one of these external grants is awarded, the participant support award may still be awarded at a reduced amount. However, if there are less applications in a given year than there are support funds, the Operational Oversight Committee may chose to award funding for additional year(s) or to use this money for other consortial purposes. All Faculty Research Support Participants will be required to apply for external research grants as a condition of continued RSEC support. It is expected that after two years faculty will "graduate" from this program to support from more conventional sources such as ROA supplements from NSF and ACS-PRF and Research Corp. funding.

Summer (and prorated sabbatical) support will be provided as participant support awards from an account administered by Youngstown State University. These participant support awards are meant to be competitive and prestigious and will be for a fixed sum of $7,500 per summer. If funds are available, this amount may be supplemented and/or supplanted by home institutions, host institutions, and/or from grants. Undergraduate faculty

may have part of this amount as research, rather than summer, support if they chose. To support the research to be carried out by these faculty participant support awards, they will be paired with research funds averaging $7,000 per fellow (i.e., $2,000 to support research at the home institution, $2,000 to support research at the host institution, and an average of $3,000 per fellow to support extraordinary research costs). Undergraduate faculty who do not require summer salary support may apply to this fund for research cost only.

C3e. Student Research Support Programs. Support for student research will be awarded in the form of student participant support award tenable at host institutions and/or home departments while working on collaborative research projects. These will be available to undergraduate and MS students and to high school science teachers. Written applications will be sent to the Consortium Director for distribution to the Operational Oversight Committee which will review the applications and award the participant support awards. The proposals must be submitted one month before the first annually scheduled meeting of this committee and will be decided on the day of that meeting. These applications would commonly, although not exclusively, be accompanied by one from a faculty partner who is also applying for a faculty participant support award so that the student and faculty member can work together in the same research group. Any student participant support awards not distributed in the first round will be available for application one month prior to the next meeting. The rate is set at $2,500 per summer (which can be supplemented by host department funds where these are available) and the 30 student participant support awards to be funded from this grant would be "back loaded" into the later years of the RSEC program. It is expected that once undergraduate faculty become more involved in research they will be able to support many additional students from other sources. One source that the ADSC will explore is a NSF REU application from the ADSC. This will be a topically focussed proposal on diffraction methods that will have the students start the summer at a summer school on diffraction methods and end the summer at a regional student research conference to present their results. They will spend the majority of the summer engaged in diffraction research at the host sites that decide to participate.

C3f. Minority Participant Development Initiatives. This RSEC grant will provide funding in this area as well as facilities and a collaborative framework. Dr. Sherri Lovelace-Cameron in the Youngstown State University Chemistry Department will head this initiative as she has extensive experience and interest in this area. She is being appointed as the Coordinator of Minority Enhancement Programs for the Consortium. This program will be designed to attract students to college programs in the natural sciences and engineering. There will be a suitable instructional component to help these high school students to understand their parts of the diffraction projects. These will be developed in concert with teachers who have gone through the course and will include activities such as growing single crystals and computer laboratory activities on the nature of symmetry, diffraction analysis, etc. This course will be taught at the beginning of the summer for participants that will be carrying out research at all of the schools. There will also be a post research conference day for them to present their results and discuss their experiences. This instruction will be followed by research projects in collaboration with the faculty of any of the participating institutions involving crystal growth, data collection, and analysis of new materials. This program will be based on current experiences with programs such as the ACS project SEED and ongoing collaborations with inner city school systems in our region. Initially, we will fund this minority enhancement program for high school students for $5,000 per year while integrating those minority students who are already in college into our current programs. We can also apply for internal and external funding to expand this program. Dr. Lovelace-Cameron will be in charge of coordinating these efforts with the assistance of interested consortium faculty. She is also coordinating our interactions with historically black colleges from outside our immediate region in this collaboration.

C4. Goals, Outcomes, and Assessment

C4a. Goals of the Advanced Diffraction Studies Consortium. The central *Goal* of the Advanced Diffraction Studies Consortium is to serve as a national model of inter-institutional collaboration while attempting to:

C4a(i). Integrate Crystallographic/Diffraction Methods into Teaching and Research. Through various consortium sponsored efforts including the intensive summer schools, distance education programs, curriculum development initiatives, a developed sense or community, and model educational efforts, the ADSC will assist efforts by faculty at all participating institutions to more fully integrate crystallography/diffraction methods into their undergraduate curricula, from the freshmen to the senior level. These efforts will also extend to the pre-college curriculum and graduate education and the developed materials and approaches will be disseminated nationally. The faculty development effort will also focus on expanding the use of these methods to solve scientific problems at both the home and host institutions.

C4a(ii) Integrate Faculty and Students of Predominantly Undergraduate Universities into the Mainstream of the National Research Effort. The consortium has established a sequenced series of initiatives to more fully develop the research activities at undergraduate institutions. Initially, this will be done through consortium funded summer research collaborations with more experienced research mentors at the host schools. This will be followed with assistance to develop nationally competitive externally funded research programs, both individual and collaborative. This will typically be through ROA, ACS-PRF, Research Corporation, etc., support in the first instance, often to be followed through larger proposals under the NSF-RUI program and related initiatives.

C4a(iii) Educational Pipeline Initiatives. The consortium is committed to improving the quality, quantity, and diversity of students moving through the educational pipeline, especially into research areas relying on crystallographic/diffraction methods. These efforts will include: increased training of undergraduate faculty which should feed back into their teaching, outreach efforts at the high school level to improve the quality of science instruction there and identify and encourage potential scientists, a strong focus on research experiences at the undergraduate level, and all of these efforts having a special emphasis on students and faculty from historically under-represented groups.

C4a(iv) *Integration of Research and Teaching.* Both research and teaching are enhanced by their integration, especially at the undergraduate level. Efforts to enhance teaching and research in crystallography at all educational institutions and to provide materials to enhance this effort nation wide. We will emphasize the uniquely suitable model that diffraction methods can play in this area because of the low data collection to data analysis ratio diffraction entails and its suitability for both novice and advanced student projects.

C4a(v) *Critical Mass.* To attain and maintain a critical mass, these efforts are to initially focus on faculty and students drawn from predominantly undergraduate institutions in northern Ohio and western Pennsylvania. As the consortium develops, our activities will be broadened to our larger regional area and then to the nation arena.

C4b. Timeline for the Advanced Diffraction Studies Consortium RSEC project. The expected starting date for the grants funded under the RSEC program is June 1 st of 1999. The project proposed by the Advanced Diffraction Studies Consortium for the RSEC is planned for 5 years (i.e., until June 1 st, 2004). We are also planning on using some funds from the 5th year of the RSEC budget to fund activities in the following year via a 1 year no-cost project extension (i.e., so that our project has until June 1 st, 2005 to be totally completed). This will allow us to extend some consortium activities for a 5th full summer (e.g., the summer schools) and will allow for a more orderly termination of the project. Following is a brief timeline of the consortium's activities:

Year 0 1998-1999 Establishment of the ADSC building upon a complex web of preexisting collaborations. Development of a long range plan of activities, including other grant opportunities, collaborative interactions, summer schools, and planning for the hoped RSEC award.

Year 1 1999-2000 Award of grant, purchase of instrumentation, installation of ADSC Crystallography Laboratory at YSU including hiring of Laboratory Manager and diffraction facilities at other participants, initiation of collaborative research projects, award of summer support for participating faculty and students for the summer of 2000, application for NSF-REU grants to support additional undergraduate collaborators, NSF-CCLI grants to fund additional educational initiatives, and Dreyfus teacher/scholar grant.

Year 2 2000-2001 About 15 undergraduate faculty and 6 students will participate in collaborative research projects at host schools funded by summer support for participating faculty and students, 1st year of summer schools, award of support for summer of 2001, 1st intensive evaluation cycle, application for external grants by all undergraduate faculty having support that summer, application for additional external funding opportunities by consortium.

Year 3 2001-2002 About 15 undergraduate faculty and 6 students will participate in collaborative research projects at host schools funded by summer support for participating faculty and students, 2nd year of summer schools, award of support for summer of 2002, 2nd intensive evaluation cycle and 1st dissemination cycle, application

for external grants by all undergraduate faculty having support that summer, application for additional external funding opportunities by consortium.

Year 4 2002-2003 About 12 undergraduate faculty and 18 students will participate in collaborative research projects at host schools funded by summer support for participating faculty and students, 3rd year of summer schools, award of support for summer of 2003, 3rd intensive evaluation cycle and 2nd dissemination cycle, application for external grants by all undergraduate faculty having support that summer, application for additional external funding opportunities by consortium.

Year 5 2003-2004 About 8 undergraduate faculty will participate in collaborative research projects at host schools funded by summer support for participating faculty and students, 4th year of summer schools, award of support for summer of 2003, 4th intensive evaluation cycle and 3rd dissemination cycle, application for external grants by all undergraduate faculty having support that summer, application for additional external funding opportunities by consortium.

Year 6 2004-2005 Completion of RSEC project, 5th year of summer schools, final evaluation and dissemination cycles, application for external grants by participating undergraduate faculty having had support from the RSEC, application for additional external funding opportunities by consortium, final reports to NSF and all participants.

C4c. Expected outcomes of the Advanced Diffraction Studies Consortium Project.

C4c(i). Faculty Development Outcomes. At the end of this RSEC grant it is expected that undergraduate faculty in our region will much more fully integrate diffraction methods into both their teaching and research. They will have received a modern "hands on" education in both basic and advanced diffraction methods suitable to their teaching and research interests. They will have a web of colleagues with whom they have been interacting for the better part of 5 years, including both peers at other smaller colleges and those at major research universities and institutions. They will have excellent access to instrumentation, data bases and software, expertise, and support to help meet their continuing needs.

C4c(ii). Student Pipeline Outcomes. At the end of this RSEC grant, we will have dramatically increased the percentage of students in our region who are exposed to crystallography/diffraction methods in both teaching and research. This seamless pipeline will extend from our high schools through the undergraduate years into graduate and continuing education efforts. These efforts will focus particularly on enhancing the participation of historically under-represented groups. The resulting educational materials will be disseminated nationally for broader impacts.

C4c(iii). Research Outcomes. At the end of this RSEC grant it is expected that at least one faculty member from all participating institutions will have been involved in diffraction/crystallographic research. This will initially focus on collaborative efforts and later on both collaborative project and individual projects where the diffraction serves research focussing on other topics (e.g., synthetic chemistry). Through a programmed series of steps, faculty participants will establish research and granting histories and activities that will make them active members of the national research enterprise.

C4d. Dissemination of the Advanced Diffraction Studies Consortium Project Results. The dissemination activities of the ADSC will have several components. One of the most innovative of these will be our series of intensive summer short courses and distributed educational activities that by the end of the 5th year will be attracting participants from across the nation. The consortium will participate in a regional conference by the Pittsburgh Diffraction Society in which our educational and research results will first be aired to be followed by presentations at national crystallography, chemistry, materials science, molecular biology, etc., meetings, with support from our RSEC travel budget. The results of RSEC funded research and teaching initiatives will be published in the appropriate professional journals and through the submission of external grant proposals.

C4e. Assessment of the Advanced Diffraction Studies Consortium Project. The value of no project can be adequately determined if it has not been carefully assessed. We have a three stage program for our consortium.

C4e(i). Internal Assessment Strategies for the ADSC project. The Director of the ADSC will be responsible for continual assessment of all ADSC activities and will write a detailed annual report. This will first be circulated to the Operational Oversight Committee and then to the membership of the ADSC for comment and correction.

C4e(ii). Assessment for the ADSC project by the External Advisory Committee. The completed report will then be passed to the External Advisory Committee of the ADSC. This group will have a sufficient budget (i.e., $5,000 annually) to independently assess the ADSC, both by distance methods and through on-site visits. They will suggest to the ADSC membership and governing structure any strengths, weaknesses, and opportunities they detect and then monitor the action taken on these.

C4e(iii). Assessment of ADSC activities by External Organizations. Finally, external organization will be asked to monitor our performance. The Pittsburgh Diffraction Society has agreed to do this, most intensively through the presentation of our results at their annual meeting. In addition, we have requested that the Continuing Education Committee of the American Crystallographic Association audit our assessment reports and make recommendations.

C5. Organizational Structure and Operating Procedures of the Consortium

C5a. Overview. Coordinating the proposed activities of a large and diverse group such as the Advanced Diffraction Studies Consortium, ADSC, will require a substantial and effective organizational structure. To this end, the ADSC was formally inaugurated at a meeting at Youngstown State University on December 12th, 1998, where its purpose and rationale, plans for research and educational activities, goals, draft Bylaws, organizational, and management structure, were approved. The purposes and rationales for the ADSC are described in section C1, above, the plans for ADSC activities were described in sections C2 and C3, above, and the goals of the ADSC were described in section C4, above. This information, along with current membership lists, will also be available from the ADSC WEB site at http://www.as.ysu.edu/~adhunter/ADSC/index.html. The organizational structure and management plan for the ADSC are established in its Official Bylaws. Those components relevant to this RSEC proposal are described below.

C5b. Membership. The initial membership in the Advanced Diffraction Studies Consortium is centered in northern Ohio and western Pennsylvania and is composed of 6 PhD and 4 MS level institutions, three federal labs, several dozen two and four year colleges, and about a dozen industrial partners. The institutional members may be *research universities* (i.e., universities granting PhD degrees in chemistry), *predominantly undergraduate institutions* (i.e., granting MS, BS, or two year Associate degrees as their highest degrees in chemistry), *non-profit research institutions*, or *corporations*. The institutional membership includes: *Host Institutions* are places where faculty and students from predominantly undergraduate schools may go to conduct individual or collaborative research and/or to attend professional development courses in crystallography/diffraction, *Home Institutions* are the predominantly undergraduate institutions whose faculty and students this consortium is meant to serve (some MS granting institutions fall into both categories). *Associate members* are individual schools, school districts, and high school teachers. *Industrial Partners* are industrial organizations with which consortium members have productive partnerships or which are vendors of diffraction equipment. The individual membership includes faculty and those holding similar permanent appointments at institutions of higher learning or research. They may join the ADSC independent of the membership status of their employers. The ADSC institutional membership at the time this proposal was submitted are listed above. Its current membership is listed on its WEB page.

The ADSC is open to new members who will be added if their membership will strengthen the ADSC in carrying out its goals. Prospective individual, institutional, associate, and industrial members may apply for admission to the Director of the ADSC. After review of their applications, they may be given temporary memberships until the next meeting of the ADSC Operational Oversight Committee approves their permanent membership. Membership in the Advanced Diffraction Studies Consortium may be revoked if a majority of the members of the Operational Oversight Committee concludes in a secret ballot that the member in question is no longer meeting their responsibilities to the consortium.

There will be an annul meeting of the fully ADSC membership held in conjunction with the annual Pittsburgh Diffraction Society conference each fall. During this meeting, research and educational results from the past year's activities will be presented and priorities and activities for the coming year will be set.

C5c. Director of the ADSC. The Director of the Advanced Diffraction Studies Consortium will be responsible for the day to day operation of the consortium following the policy guidelines set out by the Operational Oversight Committee. The Director will be responsible for calling meetings of the Consortium's various committees, providing recommendations to the committees, surveying the Consortium's membership, and coordinating and disseminating the results. The Director will be responsible for administering the Consortium's budget and, in particular, this NSF RSEC grant for which he is the PI. The Director will be responsible for various additional functions to be decided by the Operational Oversight Committee, including: organizing the summer school program in crystallographic/diffraction methods, surveying the membership to gather assessment and planning information, coordinating external grant proposals to be submitted by the Consortium, drafting the annual assessment document and annual and final grant reports (which will be approved by the Operational Oversight Committee and forwarded to the External Advisory Committee for comment and critical review). The first Director will be Dr. Allen D. Hunter of the Chemistry Department of Youngstown State University. His (initial) term will extend from January 1st, 1999 to June 1st, 2005 (i.e., the expected 5 year life of the RSEC grant plus one year to assess and report the results). Subsequent Directors will be chosen by secret ballot of the Operational Oversight Committee following a survey of the membership for nominations. The Director may be removed for non-performance of duties by a two thirds vote of the Operational Oversight Committee and the ADSC membership. [So that he has the time available to carry out these duties, YSU is committed to reducing his teaching load by 100% in the first and 50% in each subsequent year of the grant.]

C5d. Operational Oversight Committee. The Operational Oversight Committee, OOC, is the official governing body of the consortium and is charged with strategic planning, allocation of funds and equipment, policy

development, and leadership of the ADSC with a particular charge of ensuring that the Consortium is operating according to its founding principles, meeting the needs of is target groups, and is making adequate progress to becoming self-supporting at the end of the 5 year RSEC grant period. This committee will meet several scheduled times each calendar year to discuss these issues (i.e., in August/September, December/January, and May/June). A quorum for these meetings will be 50% of the committee's members. To ensure that this committee contains an appropriate balance it will have ten members, including: three Senior Research Personnel drawn from the host institutions, three faculty from the predominantly undergraduate schools, one representative from each of the national research labs and industry, and the Director of the ADSC and the Coordinator of Minority Enhancement Programs as *ex officio* members. With the exception of the *ex officio* members, no more than two Operational Oversight Committee members will be drawn from any one institution. The Director of ADSC will be the committee's chair. The three research personnel will be chosen to represent a cross section of primary research areas (i.e., high resolution crystallography of small molecules, materials characterization crystallography, and protein crystallography) and geographic regions.

The initial Senior Personnel members are: Bryan Craven (Indiana University of Pennsylvania, high resolution crystallography, PA), Vivien Yee (Cleveland Clinic foundation and Case Western Reserve University, protein crystallography, northeast Ohio), and James Gano (University of Toledo and Director of the Ohio Crystallography Consortium). The initial members from predominantly undergraduate institutions are: Alan Jircitano (Penn State Erie-The Behrend College), Edward Zovinka (Saint Francis College), and Marty Serra (Allegheny College). The initial representatives from the federal research labs and industry are: Mike Nathal (NASA Lewis Research Center) and Matt Muir (Goodyear), respectively.

These initial members will serve a 1 or 2 year term which will extend from January 1st, 1999 until December 31st, 2000 or 2001 (i.e., staggered terms). If any of these members resigns before the end of their term, their replacements will be elected from a slate nominated by the rest of the members of the Operational Oversight Committee by a secret ballot of the individual members of the Advanced Diffraction Studies Consortium. In subsequent years, the members of the OOC will serve 2 year terms. These committee members will be elected by secret ballot of the active faculty members of the Advanced Diffraction Studies Consortium from a slate of nominees for each category prepared by the OOC.

The Operational Oversight Committee will evaluate all applications to the ADSC for undergraduate faculty and student research participant support and other supplemental funding proposals. The OOC will also be centrally involved in assessing and disseminating consortium activities and results, facilitating collaborations between ADSC members, writing future grant proposals, monitoring access policies and costs on instrumentation funded by RSEC funds, and planning future consortium activities.

C5e. Coordinator of Minority Enhancement Programs. The Coordinator will be responsible for organizing and overseeing the consortium's efforts meant to enhance research and educational opportunities for high school students and individuals from groups that have historically been underrepresented in science and engineering. The Coordinator's responsibilities will include organizing the summer research programs for high school students and outreach activities to faculty and students from historically black colleges and universities. This Coordinator will be supported by the Operational Oversight Committee with required organizational and financial support (i.e., initially $5,000 per year). The Goals and Objectives of the Coordinator are to advance the diversity, quality, and quantity of students in the pipeline for research by targeting African, Latin, Native, and Disabled Americans. The Coordinator will also be the lead individual on our external grant applications to fund our minority enhancement programs, examples include: Council for Undergraduate Research, CUR, Summer Fellowships in geology, chemistry, and biology, NSF-SURE Summer Undergraduate Research Experience for geology, Student Achievement in Research and Scholarship, STARS, program funded by OBoR (currently in place at Cleveland State and John Carroll Universities) which targets academically gifted students from groups which are under-represented in higher education, the Minority Work program at YSU, and the ACS SEED program used to fund high school students. Sherri Lovelace-Cameron from YSU will be appointed to this position for the five year term of the grant. If she resigns, or after a five year term, this position would be elected by the faculty members of the consortium from individuals nominated by the Operational Oversight Committee.

C5f. Consortium Grants Committee. The purpose of this committee is to identify suitable grant opportunities and to facilitate external research grant applications by consortium members, to aid them in preparing and internally reviewing proposals, and to help them join the mainstream of nationally funded research. It will also help them with educational grants related to crystallography/diffraction. This committee will be supported by the Operational Oversight Committee with required organizational and financial support. It will be composed of Consortium members with records of receiving and evaluating educational and research grants, especially members of the

Operational Oversight Committee. The two *ex officio* members of this committee will be the Consortium Director and the Coordinator of Minority Enhancement Programs.

C5g. External Advisory Committee. The purpose of the External Advisory Committee is to directly contact a representative sample of the Consortium membership and/or visit a representative selection of the Consortium institutions throughout the year and to annually review the assessment documents provided by the Consortium. It will be support by $5,000 in funds annually from the RSEC budget. Based on this information, this committee is to make recommendation to the Consortium on it successes, potential or actual problems, and opportunities for future growth. It's membership will be three individuals from outside our region having national credentials in crystallography/diffraction, ideally in both research and teaching. The following individuals who strongly support the ideas embodied in our proposal and have agreed to act in this role are: Phil Fanwick (Purdue University, staff crystallographer, very active in the ACA, crystallographic education expert), B. C. Wang (University of Georgia, protein crystallographer and current head of the ACA summer school in crystallography), and John Ricci (University of South Maine, Portland, a member of the Chemical Crystallography Group at Brookhaven, strong undergraduate crystallography experience). The initial members of the External Advisory Committee will have terms that expire on December 31st of 2004. At the end of their terms, or if any member resigns, their replacement(s) will be selected by a majority vote of the Operational Oversight Committee. Additional support and information for this committee will be provided by the ACA Continuing Education Committee which we have approached through Jeanette Krause, who serves on this group, to assist in the evaluation and oversight of our consortium's activities.

C5h. Allocation of Funds and Equipment. During the organization of the ADSC via phone, e-mail, and surface mail and in its initial meeting on December 12th, the ADSC set up a priority system for the budget of this RSEC proposal. It was decided to ensure that the maximum proportion of the RSEC funds went to directly support research by, and human resource development activities for, undergraduate faculty and student participants.

The *PhD level and national laboratory host institutions* that are members of this consortium are already well equipped with the advanced and national resource level instrumentation required to carry out the most demanding diffraction methods studies and have the experience and resources to augment their facilities through conventional channels. For this reason, only minimal funding was requested in the budget (i.e., $54,000, Budget items D4 and D7 in the Budget Justification section for the Protein Diffraction Data Systems and MB-CAT Beamline Components at APS). Undergraduate faculty and student participants will carry out the majority of their advanced research projects in collaboration with the senior researchers at these institutions using the facilities which are already in place. The incremental costs of accessing these facilities and carrying out these collaborative research projects are provided in the budget by an allowance of $7,000 per undergraduate faculty research participant to cover incremental research costs.

In contrast to the more advanced crystallographic projects, the more routine diffraction projects will generally be carried out using the diffraction facilities of the four *predominantly undergraduate host institutions*. There are multiple reasons for this, including: the very heavy internal usage rates on the diffractometers at the research institutions means that only limited time is available on them to outside users (especially to novices who tend to use much longer blocks of time to collect their data than do more experienced users), these institutions generally have cost recovery policies that make their diffractometers relatively expensive to use on the small research and teaching budgets typical of undergraduate institutions, and the goals of research institutions typically result in the efficiency of instrument usage being measured primarily in terms of quality data sets collected, solved, published, and supported by grants. In contrast, instrumentation facilities at predominantly undergraduate institutions typically have lower internal usage rates which means that much more diffractometer time is available to external users, particularly those from other predominantly undergraduate institutions. Similarly, such undergraduate host institutions in the ADSC will not have any direct charges for the utilization of their diffraction facilities by users from other predominantly undergraduate institutions (i.e., these costs will be covered by internal funds). The goals of predominantly undergraduate institutions tend to emphasize the importance of "hands on" training of novices, especially for undergraduates, more heavily than do research institutions. For this reason, they often measure the efficiency of instrument utilization more broadly than do research institutions. For example, at Youngstown State University we use both of our P4 diffractometers almost *exclusively* during the Spring quarter for the approximately 10 to 12 undergraduate and MS students taking our "hands on" Solid State Structural Methods course. This is very inefficient in terms of pure research productivity but it is a very efficient way of integrating advanced methods into a course which blends research and teaching. Finally, the goals, administrative structures, experiences, scales of research activity, teaching loads, etc., of the faculty at the predominantly undergraduate host and home institutions are very similar.

For a combination of the reasons cited above, the four predominantly undergraduate host institutions that are part of the ADSC are expected to be used for the large majority of the more routine single crystal and powder diffraction research and teaching. As described in sections H (i.e., Facilities, Equipment, and other Resources) and F (Budget Justification), Youngstown State University, Bucknell University, Indiana University of Pennsylvania, and Wright State University are all currently equipped with some diffraction facilities. The consortium has decided to spend the majority of its equipment request (i.e., $237,000) from NSF on upgrading the diffractometers at Youngstown State University, Bucknell University, and Wright State University (i.e., Indiana University of Pennsylvania is in the process of purchasing a new powder diffractometer which was recently funded by NSF, DMR-9802781). With the provision of the requested equipment, these institutions will be able to fulfill the large majority of the routine single crystal and powder diffraction requirements for teaching and research by undergraduate faculty and students. They will also be able to do so with *convenient and generous access policies* and at *no direct cost to participants from undergraduate institutions*. In addition, the CCD instrumentation at Youngstown State University and the new powder diffractometers at YSU and Indiana University of Pennsylvania will also be useful for some types of more advanced experiments such as high resolution data collections for charge density studies, preliminary protein structure determinations, and powder structure determinations by Rietveld methods. To demonstrate the extremely high level of support for their proposed role in the ADSC, this group of predominantly undergraduate institutions has committed a total cash match of $449,000 (i.e., 65%) towards the purchase of $686,000 worth of instrumentation (i.e., a NSF request of $237,000) to be placed at their sites. In addition to this cash matching for the equipment purchase, these schools have dedicated substantial additional funds to ensure that this equipment is well maintained and fully utilized. For example, YSU has committed at total personnel match to this proposal of $792,283 and a match for diffractometer maintenance and diffraction laboratory renovation of $95,000 against the NSF equipment request for instrumentation to be placed at YSU of $172,000.

After the equipment to be purchased from this grant is in place, there will be a modernized single crystal diffractometer at Bucknell University, a single crystal and a powder diffractometer at Indiana University of Pennsylvania, a new single crystal diffractometer at Wright State University, and a complete diffraction facility at YSU. All undergraduate faculty and student participants in the ADSC will be able to use these diffractometers "on site" for both educational purposes and for research both during the school year and the summer. In addition, they will be able to send samples by mail or courier to the YSU Diffraction Laboratory where the Diffraction Laboratory Scientist (2/3 funded by NSF and 1/3 funded by Youngstown State University) will mount them, collect the data, where requested determine the structure, and send the results back to the undergraduate faculty or student member who submitted them. Based on the expected utilization rates of these instruments, significant time will be available not only to ADSC members but also to the larger national community, especially during the academic year. In this context, the priority for samples sent to the YSU Diffraction Laboratory will be: 1st undergraduate faculty and students from within our region, 2nd undergraduate faculty and students from outside our region but in the US, 3rd PhD faculty and students from within our region, and 4th PhD faculty and students from outside our region but within the US. All participants from undergraduate institutions will be provided cost free access (they will be charged only for expensive consumables such as cryogens for low temperature runs) while participants from research institutions will be charged a small fee to offset maintenance costs and staff time. Industrial participants will have access to this facility on a time available basis with full cost recovery. If their project is carried out in collaboration with a participating faculty member and student, their work will have a higher priority and the cost recovery will be reduced.

If during the course of the RSEC grant, any institution requests minor equipment not specified i n the grant (e.g., for X-ray tube replacements), these requests will be evaluated by the Operational Oversight Committee and the PI of the grant/ADSC Director and then to the NSF Program Officer (where required).

D. References

Leading references to both the research and educational aspects of this proposal are presented in the Biographical Sketches section, E, following. For the sake of brevity, they will not be repeated here.

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

***. Results of Prior NSF Support.** Since 1994, Dr. Hunter was a PI or co-PI on an X-ray Diffractometer grant (co-PI, RUI DMR-9403889), a GC-MS grant (co-PI, ILI-IP DUE 9551683), a grant for GPC and DSC/TGA instrumentation (PI, ILI-IP DUE 9851107), and a grant to develop investigative approaches to science labs for non-science majors (co-PI, DUE-IWR 9850079). These funds have helped dramatically change both teaching and research at YSU which is now one of the premier MS level institutions in the country. The first two projects have now been fully implemented and their final reports submitted. The GPC and DSC/TGA systems have just been ordered and their integration into our program will begin this winter, initially with the polymer, inorganic, and instruments lab courses. The first pilot sections of the new lab course for non-science majors is now being taught as the first step to its university wide introduction with our new general education program in the Fall of 2000.

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, and the American Physical Society. Dr. Hunter has extensive experience in synthetic chemistry of inorganic, organometallic, and polmer 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 including his recent book (i.e., *Allen Hunter's Youngstown State University X-Ray Structure Analysis Lab Manual: A Beginner's Introduction*, 2nd Edition, Fall 1998 Version F98D1 © 1997, 1998, 270 pages) which is currently being reviewed by over one dozen crystallographers for electronic release in January/February, 1999.

Since 1994, he has developed a strong emphasis on conventional 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 38 refereed journal publications, including 19 since 1992. His 5 publications most closely related to this proposal (1-5) and 5 other significant publications (6-10) are below.

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. Landis, K. G.; Hunter, A. D.; Wagner, T. R.; Curtin, L. S.; Filler, F. L.; Jansen-Varnum, S. A: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt ($Ph_2PCH_2CH_2PPh_2$)M(Maleonitriledithiolate) Congeners," *Inorganica Chimica Acta*, **1998**, *282*, 155-162.
3. Hunter, A. D.; Shilliday, L.; Furey, W. S.; Zaworotko, M. J.: "A Systematic X-ray Crystallographic Study of the Structural Manifestations of the π-Donor and π-Acceptor Substituent Effects in Substituted (η^6-Arene)$Cr(CO)_3$ Complexes," *Organometallics*, **1992**, *11*, 1550-1560.
4. Chukwu, R.; Hunter, A. D.; Santarsiero, B. D.; Bott, S. G.; Atwood, J. L.: "Synthesis and Characterization of Polyaromatic Azine Derivatives of (η^5-C_5H_5)$Fe(CO)_2$ and (η^5-C_9H_7)$Fe(CO)_2$: X-ray Crystal Structures of 4-[(η^5-cyclopentadienyl)irondicarbonyl]-7-chloroquinoline, 2-[(η^5-cyclopentadienyl)irondicarbonyl]-3-chloroquinoxaline, and 2-[(η^5-indenyl)irondicarbonyl]-3-chloroquinoxaline," *Journal of Organometallic Chemistry*, **1996**, *526*, 1-14.
5. 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.
6. Hunter, A. D.; Guo, X. A.: "Organometallic Polymers, Fluoroarylene Bridged (Rigid Rods to Segmented Chains)," *The Polymeric Materials Encyclopedia, Volume 6*, CRC Press, **1996**, 4813-4822.
7. Guo, X. A.; Sturge, K. C.; Hunter, A. D.; Williams, M. C.: "Molecular Weight Determination and Establishment of a Rod-Like Structure for Organonickel Polymers -$[Ni(PR_3)_2Ar^F]_n^-$," *Macromolecules*, **1994**, 27, 7825-7829.
8. Macdonald, P.M.; Hunter, A. D.; Lesley, G.; Li, J.: "Solid State Distortions of Linear Mono-, Bi-, and Trimetallic Bis(Tri-n-ButylPhosphine) Nickel and Palladium Complexes Having 1,4-Tetrafluorophenylene Bridges as Observed Via ^{31}P CP/MAS NMR Spectroscopy," *Solid State Nuclear Magnetic Resonance*, **1993**, *2*, 47-55.
9. 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.
10. Chukwu, R.; Hunter, A. D.; Santarsiero, B. D.; Bott, S. G.; Atwood, J. L.: "Synthesis and Characterization of Polyaromatic Azine Derivatives of (η^5-C_5H_5)$Fe(CO)_2$ and (η^5-C_9H_7)$Fe(CO)_2$: X-ray Crystal Structures of 4-[(η^5-cyclopentadienyl)irondicarbonyl]-7-chloroquinoline, 2-[(η^5-cyclopentadienyl)irondicarbonyl]-3-chloroquinoxaline, and 2-[(η^5-indenyl)irondicarbonyl]-3-chloroquinoxaline," *Journal of Organometallic Chemistry*, **1996,** *526*, 1-14.

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), Stanislaus Tsai, PhD 1995 (University of Alberta), 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.

Biographical Sketch for Bryan M. Craven

Indiana University of Pennsylvania

***. Results of Prior NSF Support.**

none

A. Vitae.

Place of Birth: Wellington, New Zealand. (Citizen, USA).

Education:

University of New Zealand	B.Sc.	1953	Chemistry
University of New Zealand	M.Sc.	1954	(1st Class Honors, Chemistry)
University of New Zealand	Ph.D.	1957	Chemistry

Positions:

Senior Research Fellow, Indiana University of Pennsylvania	1997-
Chairman, Dept. of Crystallography, University of Pittsburgh	1974-76, 1985-97
Research Collaborator, Brookhaven National Laboratory	1976-
Professor of Crystallography, University of Pittsburgh	1971-1997
Associate Professor of Crystallography, University of Pittsburgh	1970-71
Associate Research Professor, University of Pittsburgh	1966-69
Rothmans Senior Research Fellow, University of Sydney	1963-65
Assistant Research Professor, University of Pittsburgh	1959-66
Research Associate, University of Pittsburgh	1958-59
Instructor of Chemistry, University of Pittsburgh	1957-59

Professional activities:

NIH Molecular and Cellular Biophysics Study Section, 1979-83.

National Steering Committee for an Advanced Neutron Source, 1986-1994.

Program Advisory Committee for the High Flux Beam Reactor at Brookhaven National Laboratory, Member 1992-pres., Chair, 1994

USA National Committee for Crystallography, 1987-90

General Chairman, Pittsburgh Diffraction Conference; 1968, 1974, 1985, 1987, 1994.

President, Pittsburgh Diffraction Society, 1988, 1995.

Chair, Gordon Conference on Electron Density Distributions and Chemical Bonding, 1989. [Session Chair, 1978, 1983; Speaker, 1980, 1985, 1995]

President, American Crystallographic Association, 1989. [Vice-President, 1988; Chair, Publications Committee, 1977; Chair, Small Molecule Special Interest Group, 1982; Chair, Neutron Scattering S. I. G. 1987; Editor, Transactions of the ACA, Vol. 23, "Symposium on Neutron Diffraction"]

Local Chair, Joint Meeting of the American Crystallographic Association and Pittsburgh Diffraction Society; Pittsburgh, 1992.

Executive Director and Lecturer, ACA Summer Course in Crystallography (Pittsburgh), 1992-1996.

US Co-Editor, Acta Crystallographica, 1988-present.

B. Refereed Journal Publications.

Publications related to this project:

1. The Neutron Crystal Structure at 198K of Polymorph II of 5,5-Diethylbarbituric Acid (Barbital).
R. K. McMullan, R. O. Fox & B. M. Craven,
Acta Cryst. B34, 3719-3722 (1978).
2. The Electrostatic Potential for the Phosphodiester Group Determined from X-ray Diffraction.
W. T. Klooster & B. M. Craven,
Biopolymers 32, 1141-1154 (1992).
3. Molecular Electrostatic Potentials from Crystal Diffraction: The Neurotransmitter g-Aminobutyric Acid.

R. F. Stewart & B. M. Craven,
Biophys. J. 65, 998-1005 (1993).
4. Molecular Structure of (Bicyclo[3.3.1]nona-2,6-diene)dichloropalladium(II)
J. C. Woolcock, M. Niederhut & B. M. Craven.
Aust. J. Chem., 49, 977-980 (1996).
5. Electrostatic properties of ammonium fluoride and deuterated ice-I
C. G. van Beek, J. Overeem, J. R. Ruble & B. M. Craven,
Can. J. Chem. 74, 943-950 (1996).

Other publications:
1. The Crystal Structure of Cholesterol Monohydrate.
B. M. Craven,
Nature 260, 727-729 (1976).
2. Energies of Molecular Interactions from Bragg Diffraction Data.
M. A. Spackman, H. P. Weber & B. M. Craven,
J. Am. Chem. Soc. 110, 775-782 (1988).
3. Internal Vibrations of a Molecule Consisting of Rigid Segments. I. Non-interacting Internal Vibrations.
X. M. He & B. M. Craven,
Acta Cryst. A49, 10-22 (1993).
4. Hexamethylenetetramine at 298K: New Refinements.
M. Terpstra, B. M. Craven & R. F. Stewart,
Acta Cryst. A49, 685-692 (1993).
5. Effects of H/D Substitution on Thermal Vibrations in Piperazinium Hexanoate-(h_{11},d_{11}).
J.-Q. Luo, J. R. Ruble, B. M. Craven & R. K. McMullan,
Acta Cryst. B52, 357-368 (1996).

C. Other Collaborators.
The P.I. has been senior collaborator with Drs X.-M. He, W. T. Klooster, J. R. Ruble and R. Srinivasan since 1991 and with 9 others before then. He also has ongoing collaborations with Profs R. F. Stewart and T. M. Sabine.

D. Graduate Students.
Bryan Craven has been thesis advisor for J. Luo , S. P. Kamperman and L.-R. Chen who obtained the PhD since 1991 and for 17 others who graduated before then.

E. Advisors.
The P.I.'s mentors were Prof Sir John Llewellyn (deceased) and D. Hall (Univ. of New Zealand) and G. A. Jeffrey (Univ. of Pittsburgh).

Biographical Sketch for Mark D. Foster

Institute of Polymer Science, University of Akron, Akron, OH 44325-3909
Telephone: (330) 972-5323

***. Results of Prior NSF Support.**

Prof. Foster was the recipient of a 2 year Research Initiation grant through the CTS program in the engineering directorate of NSF (CTS91-10110). That funding supported research on the structure and interlayer interdiffusion in Langmuir-Blodgett multilayers containing both layers of classical short chain amphiphiles and layers of "hairy-rod" polyglutamate polymers. Results of that work appeared in a total of six refereed publications.

A. Vitae.

Education

B.S., Chemical Engineering, Washington University, St. Louis, 1981, (magna cum laude);German minor.
Ph.D., Chemical Engineering, University of Minnesota, Minneapolis, 1987.

Experience

Associate Professor, Department of Polymer Science, The University of Akron, Akron, Ohio, 07/1995-present.
Assistant Professor, Department of Polymer Science, The University of Akron, Akron, Ohio, 11/1990-06/1995.
Research Associate, Polymer Lab, University of Minnesota, Minneapolis, Minnesota, 11/1989 -11/1990 with Prof. F. S. Bates.
Temporary staff scientist, Max-Planck-Institut für Polymerforschung, Mainz, Germany, 11/1988 - 11/1989 with Prof. E. W. Fischer.
Postdoctoral Researcher, Max-Planck-Institut für Polymerforschung,Mainz, Germany, 11/1986 - 11/1988 with Prof. E. W. Fischer.

Honors

National Merit Scholarship, 1977-1981
Chancellor's Scholarship, 1977-1981
Alcoa Scholarship, 1979-1980
Tau Beta Pi, 1980
Corporate Fellowship, 1981-1983

Research Interests

Interfacial segregation and its effects on surface and thin films properties
Bulk microstructure and phase behavior of block copolymers
Interdiffusion at polymer interfaces
Protein adsorption at interfaces
Langmuir-Blodgett deposited and self-assembled ultrathin films
X-ray, neutron and visible light scattering characterization techniques including:SAXS, SANS, reflectometry, ellipsometry, and grazing incidence scattering

B. Refereed Journal Publications.

Five Publications Most Closely Related to the Proposed Project:

1. M. D. Foster, " X-ray Scattering Characterization of Polymer Interfaces," *Critical Reviews in Analytical Chemistry* **24**, 179-241, 1993.
2. C.M. Turner, N.B. Sheller, M.D. Foster, B. Lee, S. Corona-Galvan, R.P. Quirk, B. Annis, J.-S. Lin, "Effect of Chain Topology on Ordered Structure in Block Copolymers: Comparison of a Heteroarm A_2B_2 Star with its Linear Diblock Analog," *Macromolecules* **31**, 4372-4375, 1998.
3. H. Yim, M.D. Foster, D. Balaishis, I. Manners, "Structural Study of Monolayers of Alkyl Side Chain Substituted Poly(ferrocenylsilane)," *Langmuir* **14**, 3921-3925, 1998.
4. N. B. Sheller, S. Petrash, M.D. Foster, "Atomic Force Microscopy and X-ray Reflectivity Studies of Albumin Adsorbed onto Self-Assembled Monolayers of Hexadecyltrichlorosilane,"*Langmuir*, **14**, 4535-4544, 1998.

5. H. Yim, M.D. Foster, K. McCreight, X. Jin, S.Z.D. Cheng, F.W. Harris, "Structural Study of monolayers of alkyl side chain substituted polyimides," POLYMER, **39**, 4675-4678, 1998

Five Other Significant Publications

1. S. Petrash, A. Liebmann-Vinson, M. D. Foster, L. Lander, W.J. Brittain, C. F. Majkrzak, " Neutron and X-ray Reflectivity Studies of Human Serum Albumin Adsorption onto Functionalized Surfaces of Self-Assembled Monolayers", *Biotechnology Progress*, **13**, 635-639, 1997.
2. S. Petrash, N. Sheller, W. Dando, M.D. Foster, "Variation in Tenacity of Protein Adsorption on Self-Assembled Monolayers with Monolayer Order as Observed by X-ray Reflectivity",*Langmuir* **13**, 1881-1883, 1997.
3. T. R. Vierheller, M.D.Foster, A. Schmidt, K. Mathauer, W. Knoll, G. Wegner, S. Satija, C.F. Majkrzak, "Structure and Stability of Two Component Langmuir-Blodgett Multilayers Containing Cadmium Arachidate and Polyglutamate Determined by Reflectivity,"*Langmuir* **13**, 1712-1717, 1997.
4. T.R. Vierheller, M.D. Foster, H. Wu, A. Schmidt, W. Knoll, S. Satija, C.F. Majkrzak, "Stability of Cadmium Arachidate Langmuir Blodgett Multilayers as Determined by Neutron and X-ray Reflectometry," *Langmuir* **12,** 5156-5164, 1996.
5. M. D. Foster, M. Sikka, N. Singh, F. S. Bates, S. K. Satija, C. Majkrzak, "Structure of symmetric polyolefin block copolymer thin films," *J. Chem. Phys.* **96**, 8605, 1992.

C. Other Collaborators.

Henning Menzel
Wayne Mattice
Ernst von Meerwall
Adel Halasa
Edward Kramer
David Trowbridge
Ken Shull
Craig Hawker

D. Graduate Students.

Graduate Advisees:

Timothy R. Vierheller
Hong Wu
XiaoQing Li
Nuntita Sirikup
April Harrison -Boddie
C. Michele Turner
Nina Sheller
Stas Petrash
Hyun Yim
Adriana Paiva
David Teale
Zhihao Chen
Carmen Greenberg
Wei Li
Teresa Zook
Alison Szczecinski
Tricia Cregger

Postgraduate Advisees:

Andrea Liebmann-Vinson

E. Advisors.

Klavs Jensen, MIT
Erhard Fischer, MPIP, Mainz
Frank S. Bates, U. Minnesota

Biographical Sketch for Alan Pinkerton

Department of Chemistry, University of Toledo, Toledo, OH 43606
Ph: 419-530-4580, FAX: 419-530-4033, APinker@UofT02.UToledo.Edu

***. Results of Prior NSF Support.**

none

A. Vitae.

Education

FRSC	1997	Royal Society of Chemistry
Ph.D.	1971	University of Alberta, Canada
A.R.I.C.	1968	Brighton College of Technology, UK
G.R.I.C.	1966	Brighton College of Technology, UK
HNC	1964	Oxford College of Technology, UK

Professional Experience

Chairman, Department of Chemistry	
Professor, University of Toledo, Dept. of Chemistry	1989-present
Associate Professor, University of Toledo, Dept. of Chemistry	1985-1989
Assistant Professor, University of Toledo, Dept. of Chemistry	1984-1985
University of Toledo, Dept. of Medicinal and Biological Chemistry, joint appointment	1986 - present
University of Toledo, Dept. of Physics and Astronomy, joint appointment	1996 - present
Privat-Docent, University of Lausanne, Switzerland, Dept. of Chemistry	1978-1986
Maître-Assistant, University of Lausanne, Switzerland, Dept. of Chemistry	1978-1984
Research Associate, University of Lausanne, Switzerland, Dept. of Physics	1976-1978
Research Associate, University of Nice, France, Dept. of Chemistry	1974-1976
Research Associate, University of Lausanne, Switzerland, Dept. of Chemistry	1972-1974
Research Associate, University of Sussex, UK, Dept. of Chemistry	1971-1972

B. Refereed Journal Publications.

Related Publications

λ/2 Contamination in CCD Area Detector Data. Kirschbaum, K.; Martin, A.; and Pinkerton, A.A.; *J. Appl. Cryst.*, 1997, *30*, 514-516.

Charge Density Studies Using CCD Detectors - Oxalic Acid at 100 K Revisited. Martin, A.; and Pinkerton, A.A.; *Acta Crystallogr.*, 1998, *B54*, 471-478.

Characterization of Actinide Bonding in $Th(S_2PMe_2)_4$ by Synchrotron X-Ray Diffraction. Iversen, B.B.; Larsen, F.K.; Pinkerton, A.A.; Martin, A.; Darovsky, A.; and Reynolds, P.A.; *Inorg. Chem.*, 1998, *37*, 4559-4566.

An Open Flow Helium Cryostat for X-ray Diffraction. Hardie, M.J., Kirschbaum,. K., Martin, A; and Pinkerton, A.A., *J. Appl. Cryst.*, 1998, *31*, 815-817.

A Variable Temperature X-ray Diffraction Study of 4,7-Dioxatricyclo[3.2.1.$0^{3,6}$]octane and Characterization of the High Temperature (> 268 K) Plastic Crystalline Phase. Pinkerton, A.A., *J. Mol. Cryst. Liq. Cryst.*, in press.

Other Significant Publications

Charge Densities and Electrostatic Potentials for Energetic Materials. Pinkerton, A.A.; and Martin, A., *Mat. Res. Soc. Symp. Proc.*, 1996, *418*, 49-53.

Energetic Materials - The Preparation and Structural Characterization of Three Biguanidinium Dinitramides. Martin, A.; Pinkerton, A.A.; Gilardi, R.D.; and Bottaro, J.C., *Acta Crystallogr.*, 1997, *B53*, 504-512.

Dithiophosphinate Complexes of the UO_2^{2+} Ion Containing a Coordinated Water Molecule - Solid State Structures and Stereochemical Rigidity in Solution. Pinkerton, A.A.; Ahlers, F.-P.; Greiwing, H.F.; and Krebs, B.; *Inorg. Chim. Acta*, 1997, *257*, 77-81.

Quaternary Complexes of Tantalum and Niobium with Chloride-, Sulphide- and Oxideligands: Synthesis and Crystal Structure of (Tetrachloro)bis(disulfido)-(μ-η^2 : η^2-disulfido)(μ-oxo)bismetallates $[Cl_2(S_2)Ta(\mu\text{-}O)(\mu\text{-}S_2)Ta(S_2)Cl_2]^{2-}$ and $[Cl_2(S_2)Nb(\mu\text{-}O)(\mu\text{-}S_2)Nb(S_2)Cl_2]^{2-}$ as their tetraphenylphosphonium salts. Bösing, M.; Conrad, O.; Hommerich, B.; Kirschbaum, K.; Kövari, E.; Krebs, B.; Pinkerton, A.A.; and Steinforth, W.; *Inorg. Chim. Acta*, 1998, *274*, 251-256.

Energetic Materials: The Preparation and Structural Characterization of Melaminium Dinitramide and Melaminium Nitrate. Tanbug, R; Kirschbaum, K.; and Pinkerton, A.A.; *J. Chem. Crystallogr.*, in press.

C. Other Collaborators.
Prof. D. Schwarzenbach (Université de Lausanne, Switzerland),
Prof. P. Vogel (Université de Lausanne, Switzerland),
Prof. B. Krebs (University of Münster, Germany),
Prof. R.G. Cavell (University of Alberta, Canada),
Prof. A.J. Pearson (Case Western Reserve University),
Prof. A.B. Kunz (Michigan Technological University).

D. Graduate Students.
Dr. R. Klein (Micron, Boise, Idaho)
Dr. S. Uhlenbrock (Micron, Boise, Idaho)
Dr. A. Martin (University of Toledo)
Dr. K. Kirschbaum (University of Toledo)
Dr. M.J. Hardie (Monash University)
Dr. D.C. Finnen (Bowling Green State University)

E. Advisors.

Graduate:	Prof. R.G. Cavell, University of Alberta
Post-doctoral:	Dr. J.F. Nixon, University of Sussex

Biographical Sketch for Menachem Shoham

Department of Biochemistry, Case Western Reserve University, Cleveland, OH 44106-4935
Ph: 216-368-4665, FAX: 216-368-4544

***. Results of Prior NSF Support.**

MCB90-18333 $300,000 5/1/91 - 4/30/94 "Crystal Structure of the Immunity Protein and its Complex with Colicin E3." The crystal structure of the immunity protein to colicin E3 (Im3) has been solved to a resolution of 1.75Å by MIR phasing. (Tables I and II). All 11932 reflections to a resolution of 1.75 Å (no cutoff applied) have been used to refine the structure to an R-factor of 0.196. The deviations from ideal values are 0.02 Å and 2.2° for r.m.s. bond lengths and bond angles, respectively. The secondary structure of Im3 consists of a four-stranded antiparallel β-sheet flanked by three α-helices on one side of the sheet which resembles that of RNA-binding proteins which contain the RNP motif, such as the U1A spliceosomal protein.

A. Vitae.

Education:

1966	B.S., Bar-Ilan University, Israel, Chemistry
1973	M.S., Weizmann Institute,Israel, Chemistry
1978	Ph.D., Weizmann Institute, Israel, Protein Crystallography
1978-1981	Postdoctoral Fellow in the laboratory of Dr. Thomas A. Steitz at Yale University
1981-1989	Senior Scientist, The Weizmann Institute of Science, Rehovot, Israel
1987-1988	Visiting Scientist, E.I. du Pont de Nemours & Co., Experimental Station, Wilmington,DE
1989-present	Associate Professor, Department of Biochemistry, Case Western Reserve University

B. Refereed Journal Publications.

1. D. Zhao, A. Djebli, A. Zappala and M. Shoham. Crystal structure of colicin E3 immunity protein: an inhibitor to a ribosome-inactivating RNase. *Submitted for publication.*
2. M. Shoham and A. Djebli. Structural Studies on Colicin E_3 and its Immunity Protein. NATO ASI Series H, Vol. 65 "Bacteriocins, Microcins and Lantibiotics", pp. 203-214. Springer Verlag, 1992.
3. F. Frolow and M. Shoham. Crystallization and Preliminary X-ray Investigation of Colicin E_3 and its Immunity Protein. *J. Biol. Chem.* 265:10196-10197, 1990.
4. F. Frolow, M. Harel, J.L. Sussman, M. Mevarech, and M. Shoham. Insights into protein adaptation to a saturated salt environment from the crystal structure of a halophilic 2Fe-2S ferredoxin. *Nature Structural Biology* 3:451-457, 1996.
5. R.L. Walter, S.E. Ealick, A.M. Friedman, P. Proctor, R.C Blake II, and M. Shoham. Multiwavelength Anomalous Diffraction (MAD) Crystal Structure of Rusticyanin: A Highly Oxidizing Cupredoxin with Extreme Acid Stability. *J. Mol. Biol.* 263:730-751, 1996.
6. L. Kuttner-Kondo, W. Brodbeck, M.E. Medof and M. Shoham. Molecular Modeling and Mechanism of Action of Human Decay Accelerating Factor. *Protein Engineering*, 9:1143-1149, 1996.
7. M. Shoham. Crystal Structure of an Anticholera Toxin Peptide Complex at 2.3Å. *J. Mol. Biol.* 232:1169-1175, 1993.
8. M. Shoham, T. Scherf, J. Anglister, M. Levitt, E. Merritt, and W. G. J. Hol. Structural diversity in a conserved cholera toxin epitope involved in ganglioside binding. *Protein Science* 4:841-848, 1995.
9. J. Jentoft , M. Shoham, D. Hurst, and M. Patel. Structural Model for Human Dihydrolipoamide Dehydrogenase. *Proteins: Structure, Function and Genetics* 14:88-101, 1992.
10. A. Djebli, P. Proctor, Robert C. Blake II, and M. Shoham. Crystallization and Preliminary X-ray Crystallographic Studies of Rusticyanin from *Thiobacillus ferrooxidans. J. Mol. Biol.* 227: 581-582, 1992.

C. Other Collaborators.

Karen Jakes, Albert Einstein College of Medicine; Robert Blake II, Xavier University, New Orleans; Bryan Roth, John Schreiber, Mark Tykocinski; Case Western Reserve University

D. Graduate Students.

Peter Proctor, Lisa Kuttner-Kondo, Alvin Changco, Karen Mroz, Bandaru Viswanath, Abdellah Djebli, Dong Zhao, Chunmin Li, David Sahapiro. Five graduate students, four postdoctoral fellows.

E. Advisors.
Aaron J. Gilboa, Israel Pecht, Wolfie Traub, Thomas A. Steitz

Biographical Sketch for Partha Basu

Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA 15220

***. Results of Prior NSF Support.**

A. Vitae.

Education and Appointments

1998-present	Assistant Professor, Duquesne University
1994-1998	Assistant Research Scientist, University of Arizona
1992-1994	Postdoctoral Research Associate, University of Arizona
1991-1992	Postdoctoral Research Associate, Indian Association for the Cultivation of Science, India
1986-1991	Research Fellow, Indian Association for the Cultivation of Science, India
1991	Jadavpur University, Calcutta, W.B., India (Ph.D., Chemistry)
1985	Calcutta University, Calcutta, W.B., India (M.Sc., Chemistry)
1982	Calcutta University, Calcutta, W.B., India (B.Sc.w/Honors, Chemistry)

Honors and Awards

1986-1991	Research Fellowship, University Grants Commission and Council of Scientific and Industrial Research, New Delhi, India
1991-1992	Associateship, Department of Science and Technology, Government of India and Council of Scientific and Industrial Research, New Delhi, India
1992	Affiliate member, International Union of Pure and Applied Chemistry
1992	Young Scientist, Indian National Science Academy
1998	Research Innovation Award, Research Corporation

Professional Affiliations

American Chemical Society
International EPR (ESR) Society
International Union of Pure and Applied Chemistry
Society of Biological Inorganic Chemistry

B. Refereed Journal Publications.

1. P.. Basu, A.M. Raitsmring, J.H. Enemark, F.A. Walker "Oxomolybdenum(V)/Iron(III)Porphyrinate Complexes The effect of Axial Ligand Plane Orientation on Complex Stability, Reduction Potential, NMR and EPR Spectra," *Inorg. Chem.* **36**, 1088-1094 (**1997**).

2. A. Pacheco, P. Basu, P. Borbat, A.M. Raitsimring, J.H. Enemark, "Multi-Frequency ESEEM Spectroscopy of Sulfite Oxidase in Phosphate Buffer: Direct Evidence for Coordinated Phosphate," *Inorg. Chem.* **35** 7001-7008 (**1996**).

3. P. Basu, N.V. Shokhirev, F. Ann Walker and J.H. Enemark, "NMR Studies of Hindered Ligand Rotation, Magnetic Anisotropy, Curie Behavior, Proton Spin Relaxation and Ligand Exchange in some Novel Oxomolybdenum(V)/Iron(III) Porphyrinate Complexes," *J. Am. Chem. Soc.*, **117**, 9042-9055 (**1995**).

4. P. Basu, A. M. Raitsimring, M.J. LaBarre, I.K. Dhawan, J.L. Weibrecht and J.H. Ememark, "Covalently Coupled Oxo-Molybdenum(V) and Iron(III) Porphyrin Centers: Synthetic Models for the Molybdenum-Iron Interaction in Sulfite Oxidase," *J. Am. Chem. Soc.*, **116**, 7166-7176 (**1994**).

5. P. Basu, S. B. Choudhury, S. Pal and A. Chakravorty, "Chemistry of Ferro- and Ferriverdins. Iron Redox and Geometrical Stereodynamism," *Inorg. Chem.*, **28**, 2680-2686 (**1989**).

C. Other Collaborators.

Berthold Fischer, Ruhr University, Germany
Martin L. Kirk, University of New Mexico
F. Ann Walker, University of Arizona
Carl J. Carrano, Southwest Texas State University
Arnold M. Raitsimring, University of Arizona

Nadine E. Gruhn, University of Arizona

D. Graduate Students.

Undergraduate Students: Michael Burchianti, Scott Davie, Kate Welt, Graduate Students: Matt Moore, Postdoctoral Scholars: Sujit Mondal

E. Advisors.

Postdoctoral Director: Professor John H. Enemark, University of Arizona
Ph.D. Thesis Director: Professor Animesh Chakravorty, IACS, Calcutta, W.B., India

Biographical Sketch for Gloria E.O. Borgstahl

Department of Chemistry, University of Toledo

***. Results of Prior NSF Support.**

A. Vitae.

Education

The University of Iowa	B.S.E.	1985	Biomedical Engineering
The University of Iowa	Ph.D.	1992	Biochemistry

Experience

1982 - 86	Research Assistant, Biomechanics Laboratory, The University of Iowa
1987	Teaching Assistant, Biochemistry Laboratory, The University of Iowa
1988	Teaching Assistant, Dental Biochemistry, The University of Iowa
1989	Guest Lecturer, Molecular Modeling Techniques, The University of Iowa
1992 - 94	Postdoctoral Research Associate, The Scripps Research Institute
1994	Senior Research Associate, The Scripps Research Institute
1994 - 96	Postdoctoral Research Associate, Los Alamos National Laboratory
1996 -present	Assistant Professor, The University of Toledo

Fellowships and Awards

Institutional, Predoctoral Fellowship in Biotechnology; National Research Service Award, Postdoctoral Fellowship; URAF Summer Research Fellowship

Patents

Invention Disclosure CHM00497 "A Lanthanide-Binding Peptide Fussed to the N- or C- Terminus of Any Recombinant Protein" Jeffrey Ohren and Gloria Borgstahl, filed 6/5/97

B. Refereed Journal Publications. (Publications: 9 published or accepted; Presented Papers: 13)

"The Structure of Human Manganese Superoxide Dismutase Reveals a Novel Tetrameric Interface of Two 4-helix Bundles". Borgstahl, G. E. O.; Parge, H. E.; Hickey, M. J.; Beyer, W. F.; Hallewell, R. A. and Trainer, J. A. *Cell*, 71, 107-118, **1994.**

"The 1.4A Structure of Photoactive Yellow Protein, a cytosolic photoreceptor: Unusual Fold, Active site and Chromophore". *Biochemistry*, **34**, 6278 - 6287, (1995)

"Human Mitochondrial Manganese Superoxide Dismutase Polymorphic Variant lle58Thr Reduces Activity by Destabilizing the Tetrameric Interface". Borgstahl, G. E. O.; Parge, H. E.; Hickey, M. J.; Boissinot, M.; Hallewell, R. A.; Lepock, J. R.; Cabelli, D. E.; Tainer, J. A. *Biochemistry*, **35**, 4287-4297, **1996**

"Quantitative Analysis of Time-resolved Laue Diffraction Patterns". Ren, Z.; Ng, K.; Borgstahl, G. E. O.; Getzoff, E. D. Moffat, K. *J. Appl. Cryst*. **29**, 246-260, **1996**

"Millisecond Time-Resolved Laue Crystallography: Structure of a Protein Photocycle Intermediate". Genick, U.K.; Borgstahl, G. E. O.; Ng, K.; Ren, Z.; Pradervand, C.; Burke, P. M.; Srajer, V.; Teng, T. Y.; Schildkamp, W.; McRee, D. E.; Moffat, K.; Getzoff, E. D. Science Accepted. (**1997**)

"Crystal Structure of Y34F Mutant Human Mitochondrial Manganesse superoxide Dismutase and the Functional Role of Tyrosine 34", *Biochemistry* **37**, 4722-4730 (1998)

C. Other Collaborators.

D. Graduate Students.

E. Advisors.

Biographical Sketch for Janet E. Del Bene

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

***. Results of Prior NSF Support.**

The results of ab initio calculations on hydrogen bonding and proton transfer which were supported by NSF grant CHE-9505888 have been reported in 10 papers, including an invited chapter in a book, a paper in a special issue on theoretical spectroscopy, and an encyclopedia article. In addition, the results of this research have been presented at both national and international meetings.

A. Vitae.

Professor of Chemistry, Youngstown State University

Current joint appointment: Research Professor of Biochemistry and Molecular Biology (1977-), Northeastern Ohio Universities College of Medicine

Other professional experiences:
DOE external examiner at Pacific Northwest National Laboratory, Richland, Washington, March, 1998
Consultant to the Goodyear Tire and Rubber Company, Molecular Modeling Group, Akron, Ohio (1995 -)
Consultant with NIH Laboratory of Chemical Physics, NIDDK, December, 1993
Member of NSF Review Panel, November, 1990
Consultant to NIH-NIGMS Study Section BBCA, February, 1988
Member of the Statewide Users Group of the Ohio Supercomputer Center (1986 -); Chair (1988-1989)
Member of the Medical Research Committee of St. Elizabeth Health Center, Youngstown, Ohio (1985 -)

Education:
NIH Postdoctoral Fellow (1969-1970), Mellon Institute
Postdoctoral Fellow (1968-1969), Theoretical Chemistry Institute, University of Wisconsin
Ph.D. (1968), University of Cincinnati
B.A. (1965) & B.S. (1965) Summa Cum Laude, Youngstown State University

Sabbatical leaves:
1980-1981: Mellon Institute, with Dr. John A. Pople
1988-1989: The Ohio State University, with Dr. Isaiah Shavitt
1996-1997: Department of Chemistry, University of Cambridge, England, & Quantum Theory Project, University of Florida

Grants, honors, and awards:
National Science Foundation Grant CHE-9873815 (1999-2002); $247.000.
National Science Foundation Grant CHE-9505888 (1995-1998); $316,000.
Ohio Board of Regents for the Ohio Molecular Computation and Simulation Network (1995); $57,000.
National Institutes of Health - NIGMS research grant (1985-1987); $225,000.
National Institutes of Health - NIGMS research grant (1980-1983); $79,000.
Camille & Henry Dreyfus Foundation Teacher-Scholar (1974-1979); $20,000.
National Institutes of Health - NIGMS research grant (1974-1977); $84,000.
American Chemical Society PRF Type G starter grant (1974-1977); $7,500.
Distinguished Alumni Award, U. of Cincinnati College of A&S, May, 1994
First CERFnet (California Education and Research Federation Network Award for Excellence in Networked Applications (Physical Sciences), June, 1991
Fellow of the American Association for the Advancement of Science, (elected May, 1985)
Agnes Fay Morgan Research Award given triennially by Iota Sigma Pi (1972)
NIH Postdoctoral Fellowship (1969-1970); NIH Predoctoral Fellowship (1966-1968); NSF Summer Research Fellowship (1966)

B. Refereed Journal Publications. (10 most recent)

1. "A Comparative Study of Vibrational Anharmonicity in the Bihalide Ions XHX^-: X = F, Cl, Br" J. E. Del Bene and M. J. T. Jordan, invited article for a special issue of Spectrochimica Acta entitled "Theoretical Spectroscopy: State of the Science" (in press).
2. "A Comparative Study of Anharmonicity and Matrix Effects in the Complexes $XH:NH_3$, X = F, Cl, and Br" J. E. Del Bene and M. J. T. Jordan, J. Chem. Phys. 108, 3205 (1998).
3. "An Ab Initio Study of Anharmonicity and Matrix Effects on the Hydrogen-Bonded $BrH:NH_3$ Complex" J. E. Del Bene, M. J. T. Jordan, P. M. W. Gill, and A. D. Buckingham, Mol. Phys. 92, 429 (1997).
4. "Ab Initio Theoretical and Matrix Isolation Experimental Studies of Hydrogen Bonding. IV. The HBr:Pyridine Complex" K. Szczepaniak, P. Chabrier, W. B. Person, and J. E. Del Bene, J. Mol. Struct. 436-437, 367 (1997).
5. "Resolving Discrepancies between Theory and Experiment: IR Spectrum of the Proton-Shared HBr:Pyridine Complex" J. E. Del Bene, K. Szczepaniak, P. Chabrier, and W. B. Person, J. Phys. Chem. A, 101, 4481 (1997).
6. "Ab Initio Theoretical and Matrix Isolation Experimental Studies of Hydrogen Bonding: Evidence of a Dramatic Effect of the Matrix on the Structure and Vibrational Spectrum of HBr:3,5-dichloropyridine" J. E. Del Bene, K. Szczepaniak, P. Chabrier, and W. B. Person.Chem. Phys. Lett. 264, 109 (1997).
7. "Ab Initio Theoretical and Matrix Isolation Experimental Studies of Hydrogen Bonding: II. Ab Initio Investigation of Distances, Force Constants, and Vibrational Frequencies in Complexes between Hydrogen Halides and 4-Substituted-Pyridines" J. E. Del Bene, W. B. Person, and K. Szczepaniak, Molecular Physics. 89, 47 (1996).
8. "Ab Initio Quantum Chemical and Matrix Isolation Experimental Studies of Hydrogen Bonding. Vibrational Consequences of Proton Position in 1:1 Complexes of HCl and 4-X-Pyridines" J. E. Del Bene, W. B. Person, and K. Szczepaniak, Chem. Phys. Lett. 247, 89 (1995).
9. "The Quest for Reliability in Calculated Properties of Hydrogen-Bonded Complexes" (invited chapter) J. E. Del Bene and I. Shavitt, in Molecular Interactions: From Van der Waals to Strongly Bound Complexes. S. Scheiner, ed. John Wiley and Sons, Inc., Sussex. pg. 157-179 (1997).
10. "Hydrogen Bonding" (invited article) J. E. Del Bene, in The Encyclopedia of Computational Chemistry. P. v. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer, III, P. R. Schreiner, eds. John Wiley & Sons, Chichester, UK, 1998, Vol. 2, pp. 1263-1271.

C. Other Collaborators.

Dr. Rodney J. Bartlett, Dr. Michael J. Tubergen

D. Graduate Students.

E. Advisors.

Dr. Hans H. Jaffe', Dr. John E. Harriman, Dr. John A. Pople

Biographical Sketch for James E. Gano

Department of Chemistry, University of Toledo

***. Results of Prior NSF Support.**

A. Vitae.

Experience:

1967 - 71	Assistant Professor, Department of Chemistry, University of Toledo
1971 - 76	Associate Professor, Department of Chemistry, University of Toledo
1976 - Present	Professor, Department of Chemistry, University of Toledo
1974 - 75	Visiting Scholar, University of California at Los Angeles
1987 - 88	Associate Chairman, Department of Chemistry, University of Toledo
1994 - Present	Director, Instrumentation Center in A & S, Univ. of Toledo
1995 - Present	Director, Ohio Crystallography Consortium

Education:

Miami University	A.B.	1963	Organic Chemistry
University of Illinois	M.S./Ph.D.	1966/1967	Organic Photochemistry

Honors:

Phi Beta Kappa, Alpha Chi Sigma, Phi Lambda Upsilon, University of Toledo, Exceptional Merit Award, 1987-88, President of UT Chapter of Sigma Xi , 1988-89, Dean's Merit Award, 1996.

Patents:

J. E. Gano (PI) and P. Sekher "Substituted Stilbenes with Adjacent Chromophors,", Patent Disclosure. CHM00794, August 1996: Submitted to UT Patent Office, Pending.

B. Refereed Journal Publications.

Publications: 46 (including pending) in refereed journals; Abstracts at meetings: 42; Invited presentations at academic institutions: >70.

34. Gano, J. E.; Park, B.-S.; Subramaniam, G.; Lenoir, D.; Gleiter, R. "Unusual, Cofacial Structure of Sterically Congested Stilbene: (*Z*-2,2,5,5-Tetramethyl-3,4-diphenyl-3-hexene: *J. Org. Chem.* **1991**, *56*, 4806-4808.
35. Gano, J. E.; Skrzypczak-Jankun, E.; Kirschbaum, K.; Lenoir, D.; Frank, R. "Z-Perchlorostilbene," *Acta Crystallogr, Sect. C., Cryst. Struct. Commun.* **1993**, 1985-1988.
38. Laali, K. K.; Gano, J. E.; Lenoir, D.; Gundlach, C. W. III "Electrophilic Chemistry (Protonation, Nitration, Bromination) of Crowded (*Z*)-2,2,4,4-Tetramethyl-3,4-diphenyl-3-hexene; Formation of Phenanthrenium Ions by Facile Ring Protonation/Transannular Cyclization in Superacid Media; p,p'-Dinitration and p,p'-Dibromination with $NO_2^+BF_4^-$ and Br_2/SO_2" *J. Chem. Soc. Perkin Trans. 2* **1994**, 2169-2173.
40. Gano, J. E.; Kirschbaum, K.; Sekher, P "(*E*)-2,2,5,5-Tetramethyl-3,4-di[4-(tribromomethyl)phenyl]hex-3-ene" *Acta Crystallogr, Sect. C52, Cryst. Struct. Commun.* **1996**, 2334-2337.
41. Gano, J. E.; Jacob, E. J.; Subramaniam, G.; Eriksson, L. A.; Lenoir, D. "Effects of Steric Congestion on Stilbene Radical Anions and Dianions/ DFT Calculations in the Interpretation of Stilbene Radical Anion ESR Spectra" *J. Org. Chem.* **1996**, 6739-6743.
43. Gano; J. E.; Garry, P. A.; Sekher, P.; Schliesser, J.; Lenoir, D. "Double Stereochemical Labeling in Stilbene Photochemistry: Distinctly Different Reaction Pathways for Formation of the *Z*- and *E*-Products" *J. Am. Chem. Soc.* **1996**, Accepted.
44. Cheng, J.; Sekher, P.; Gano, J. E.; Morgan, A. R. "A New Method for the Synthesis of 1,2-Bis(Pyrrol-2-yl)ethenes" *Synth. Commun.* **1996**. In Press.

C. Other Collaborators.

D. Graduate Students.

Thesis directed: 8; Thesis in progress: 1.

E. Advisors.

Biographical Sketch for Jayne R. Giniewicz

Department of Physics, Indiana University of Pennsylvania

***. Results of Prior NSF Support.**

none

A. Vitae.

Place of birth: Weymouth, Massachusetts (USA citizen).

Education:

Wheaton College	B.A.	1982	Physics
Pennsylvania State University	M.A.	1985	Solid State Science
Pennsylvania State University	Ph.D.	1991	Solid State Science

Positions:

Indiana University of Pa.	Assistant Prof. (Physics), 1992-
Pennsylvania State University	(Materials Research Lab.) Research assistant, 1982-1992
Sophia University, Tokyo;	Fujitsu General, Ltd., Kawasaki, Visiting researcher, 1987

B. Refereed Journal Publications.

1. J. R. Giniewicz. "An Investigation of the Lead Scandium Tantalate-Lead Titanate Solid Solution System." Ph. D. Thesis, Pennsylvania State University, University Park, PA. (December, 1991).
2. J. R. Giniewicz, A. S. Bhalla & L. E. Cross. "An Investigation of the Structural and Dielectric Properties of the Solid Solution System (1-x) Pb $(Sc_{1/2}\ Ta_{1/2})O_3$ - (x) $PbTiO_3$." *Ferroelectrics Letters*, **12**(2), 35-42. (1990).
3. J. R. Giniewicz, A. S. Bhalla & L. E. Cross. Pyroelectric Response and Depolarization Behavior of (1-x) Pb $(Sc_{1/2}\ Ta_{1/2})O_3$ - (x) $PbTiO_3$." *Materials, Ferroelectrics*, **118**, 157-164. (1991).
4. J. R. Giniewicz, A. S. Bhalla & L. E. Cross. "Lead Scandium Tantalate-Lead Titanate Materials for Field-Stabilized Pyroelectric Device Applications." *Ferroelectrics Letters*, **14**, 21-30. (1992).
5. J. R. Giniewicz, D. A. McHenry, T. R. Shrout, S.-J. Jang, A. S. Bhalla & F. A. Ainger. "Characterization of (1-x) Pb $(Mg_{1/3}\ Nb_{2/3})O_3$ - (x) $PbTiO_3$ and Pb $(Sc_{1/2}\ Ta_{1/2})O_3$ Transparent Ceramics Prepared by Uniaxial Hot-Pressing." *Ferroelectrics*, **109**, 167. (1990).
6. D. A. McHenry, J. R. Giniewicz, T. R. Shrout, S.-J. Jang & A. S. Bhalla. "Electrical and Optical Properties of Relaxor Ferroelectrics." *Ferroelectrics*, **102**, 161-171. (1990).
7. K. Ohmura, Y. Murai, K. Uchino & J. R. Giniewicz. "A New Type of PLZT Light Valve for an Image Projector." *Conference Record of the 1988 International Display Research Conference*, 137-141. (1988).

C. Other Collaborators.

D. Graduate Students.

Jayne Giniewicz has been co-advisor for Colin L. Metz who obtained his M.S. degree in Physics in May 1996 and is currently advisor to Lorelei L. Winsheimer and William L. Powell, Jr. candidates for the M.S. at IUP.

E. Advisors.

Dr. L. E. Cross (Ph.D. advisor, Pennsylvania State Univ.), Dr. A. S. Bhalla (Ph.D. co-advisor, Pennsylvania State Univ.), Dr. R. E. Newnham (M.S. advisor, Pennsylvania State Univ.), Dr. Kenji Uchino (supervisor at Sophia University, currently at Pennsylvania State Univ.) and Dr P. Wilson (B.A. thesis advisor, Professor emeritus from Wheaton College).

Biographical Sketch for David A. Grossie.

Department of Chemistry, Wright State University, Dayton, OH, 45435.

***. Results of Prior NSF Support.**
none

A. Vitae. David A. Grossie received a BS degree in Chemistry in 1977 from Texas Lutheran College. In 1982 he received a PhD degree in Chemistry from Texas Christian University under Dr. W. H. Watson. He worked as a postdoctoral fellow with W. O. Milligan and D. F. Mullica in the Department of Chemistry at Baylor University, carrying out single crystal X-ray diffraction studies of simple complexes of the lanthanide elements, transition metal complexes, and organic molecules. In September of 1986, Dr. Grossie joined the faculty at Wright State University, holding an appointment as an Assistant Professor. He was promoted to Associate Professor at WSU in the fall of 1992. He is a member of the American Chemical Society and the American Crystallographic Association. Dr. Grossie has extensive experience the characterization of organic compounds and transition metal complexes by X-ray crystallography. In 1994, Dr. Grossie initiated and supervised the acquisition of a used Enraf-Nonius CAD4 X-ray diffractometer.

Dr. Grossie's teaching has included lecture and laboratory courses at both the undergraduate and grad uate levels on a wide range of topics, including: Chemistry for Non-Science Majors, General Chemistry, Inorganic Chemistry, Physical Chemistry, and X-Ray Crystallography.

He current research interests center around the synthesis and characterization of co mplexes of silver(II) as well as structural chemistry in general.

B. Refereed Journal Publications. Dr. Grossie has had 34 refereed journal publications. His 5 publications most closely related to this proposal are below.

1. David A. Grossie and William H. Watson, "Nitrato(Triphenylphosphine oxide)Silver(I), $Ag(C_{18}H_{15}PO)NO_3$," *Acta Crystallogr. Sec. C, Crystal. Struct. Commun.*, **C45**, 1998-2000 (1989).

2. David A. Grossie, Albert V. Fratini, and W. Wade Adams, "Single-Crystal Diffraction analysis of 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline," Technical Report WRDC-TR-89-4120 (1989).

3. David A. Grossie and Kenneth Turnbull, "5-Hydroxy-5-methylsydno[3,4-a]indole," *Acta Crystallogr. Sec. C, Crystal. Struct. Commun.*, **C48**, 377-379 (1992).

4. David A. Grossie and D. M. Ketcha, "1-Benzenesulfonyl-3-methyl-2-oxo-2,3-dihydroindol-3-yl Acetate," *Acta Crystallogr. Sec. C, Crystal. Struct. Commun.*, C48, 1718-20 (1992).

5. Daniel M. Ketcha, Qin Zhou, and David Grossie, "Manganese(III) Acetate Oxidation of Alkyl Substituted 1-(Phenylsulfonyl)indoles," *Synth. Commun.*, **24**, 565-74 (1994).

C. Other Collaborators.
Dr. S. R. Hall, University of Western Australia.
Dr. J. M. Stewart, Naval Research Laboratory.
Drs. W. A. Feld and V. Katovic at WSU.

D. Graduate Students. Beverly Schwind, MS, 1993. I have served as the principle advisor for 1 MS student, and 4 undergraduate researchers.

E. Advisors. W. H. Watson, Texas Christian University.

Biographical Sketch for Xiche Hu

Department of Chemistry, University of Toledo, Toledo, OH 43606

A. Vitae.

Xiche Hu received his B.S. degree in chemistry in 1982 from Wuhan University, China. He graduated with a Ph.D. degree in chemistry in 1991 from Wayne State University under Dr. William L. Hase, undertaking dissertation research entitled "Molecular Dynamics Studies of the Role of Microscopic Solvation in Chemical Reactions". From 1991 to 1994, he worked as a postdoctoral research fellow with Dr. Craig C. Martens at University of California at Irvine, studying chemical dynamics of intercluster association reactions and multidimensional optimization of polyatomic molecules. From 1994 to 1998, he was a postdoctoral research fellow with Klaus J. Schulten at University of Illinois at Urbana-Champaign where his research has focused on protein structure prediction, computational modeling of proteins, and X-ray crystallographic computing for macromolecular structure determination.

One of the most important scientific contributions that Dr. Hu has made was prediction of the three-dimensional structure of the bacterial light harvesting complex II (LH-II) and the subsequent determination of the crystal structure of LH-II utilizing the computationally modeled structure as a probe in the framework of the molecular replacement method. This work represented a major methodology advance in X-ray crystallographic computing, and he was responsible for all aspects of protein sequence analyses, 3D model building, and the subsequent X-ray crystallographic computing. The determination of the crystal structure of LH-II has laid an important structural foundation for studying primary energy transfer processes in bacterial photosynthesis, and will greatly impact our understanding of interactions of light and matter for many years to come.

In August 1998, Dr. Hu joined University of Toledo as an assistant professor of chemistry. He has established a computational biochemistry program in advanced biomolecular modeling and protein structure determination. Currently his research interests are focused on the following research areas: (1) developing the *ab initio* molecular replacement method for X-ray crystallographic structure determination of membrane proteins; and (2) modeling computationally the three dimensional structure of the bacterial photosynthetic unit, and performing theoretical and computational studies of the dynamics of the primary energy transfer process in the bacterial photosynthetic unit.

Dr. Hu's teaching interests include the general area of physical chemistry, theoretical and computational chemistry, and biophysics. In particular, he is in the process of developing a web-based computational quantum chemistry course to be offered at both undergraduate and graduate levels. He is a member of the American Chemical Society and the Biophysical Society.

B. Referenced Journal Publications.

Dr. Hu has published 23 articles in peer-reviewed journals. Listed below are 5 publications [1-5] that are most closely related to this proposal, along with 5 other significant publications [6-10].

1. X. Hu, A. Damjanovic, T. Ritz and K. Schulten, "Architecture and Function of the Light Harvesting Apparatus of Purple Bacteria", *Proc. Natl. Acad. Sci. USA*, **1998**, 95, 5935.
2. X. Hu and K. Schulten, "A Computationally Modeled Structure for the Light Harvesting Complex I of Rb. sphaeroides", *Biophysical Journal*, **1998**, 75, 683.
3. J. Koepke, X. Hu, C. Muenke, K. Schulten, and H. Michel, "The Crystal Structure of the Light Harvesting Complex II (B800-850) from Rhodospirillum molischianum", *Structure*, **1996**, 4, 581.
4. X. Hu, D. Xu, K. Hamer, K. Schulten, J. Koepke and H. Michel, "Predicting the Structure of the Light Harvesting Complex II of Rhodospirillum molischianum", *Protein Science*, **1995**, 4, 1670.
5. X. Hu, W.L. Hase, T. Pirraglia, "Vectorization of the General Monte-Carlo Classical Trajectory Program VENUS", *Journal of Computational Chemistry*, **1991**, 12, 1014.
6. MG. Cory, M.C. Zerner, X. Hu, and K. Schulten, "Electronic Excitations in Aggregates of Bacteriochlorophylls", *Journal of Physical Chemistry B*, **1998**, 102, 7640-7650.
7. X. Hu and K. Schulten, "How Nature Harvests Sunlight", *Physics Today*, **1997**, 50, 28.
8. X. Hu, T. Ritz, A. Damjanovic and K. Schulten, "Pigment Organization and Transfer of Electronic Excitation in the Purple Bacteria", *Journal of Physical Chemistry B*, **1997**, 101, 3854.
9. X. Hu & C. C. Martens, "Atom-Cluster Interaction Potential and Thermal Collision Rates", *Journal of Chemical Physics*, **1993**, 99, 2654.
10. X. Hu & W.L. Hase, "Use of Micro-clusters to Simulate Cage, Trapping, and Chaperon Effects in Association Reactions", *Journal of Physical Chemistry*, **1992**, 96, 7535.

C. Other Collaborators.

Dr. Hartmut Michel, Max-Planck Institute at Frankfurt, Germany
Dr. Michael Zerner, University of Florida

D. Graduate Students.
Dr. Hu has established a computational biochemistry laboratory since joining the faculty of The University of Toledo in August 1998. He will be leading an active research group including graduate and undergraduate students, as well as postdoctoral research associates.

E. Advisors.
Dr. Hu's Ph.D advisor was Dr. William L. Hase at Wayne State University, and his postdoctoral advisors were Dr. Klaus Schulten at University of Illinois at Urbana-Champaign and Dr. Craig C. Martens at University of California at Irvine.

Biographical Sketch for Camden R. Hubbard

Leader, Diffraction and Thermophysical Properties Group, High Temperature Materials Section, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6064

***. Results of Prior NSF Support.**
none (i.e., funding has been from DOE)

A. Vitae.
Education:
Ph.D. (Physical Chemistry/Crystallography) Iowa State University, 1971
B.S. (Chemistry) University of California, Berkeley, 1966

Societies and Professional Activities:
American Ceramic Society
American Chemical Society
American Crystallographic Association
International Centre for Diffraction Data (Board of Directors Member (1980-1986, 1996-2000), Vice Chairman (1982-1986), Technical Committee Chair (1998 --))
Materials Research Society
Neutron Scattering Society of America

Scope of Research:

Cam Hubbard is leader of the ORNL research group responsible for the activities in the Residual Stress, Diffraction, and Physical Properties User Centers within the High Temperature Materials Laboratory. He is principle investigator on two multidisciplinary ORNL development projects "Development and Demonstration of Residual Stress Mapping by Neutron and X-ray Diffraction Methods" and "Three Novel Neutron Based NDE Techniques for Materials Characterization".

The Diffraction and Thermophysical Properties Group consists of 8 professional staff, 3 professional contractors, 2 postdocs, and a secretary. The overall Group budget is approximately $3M per year, primarily from DOE programs but also including funding from industry and other agencies. The major programs relevant to crystallography and use of diffraction methods are listed below:

• Diffraction User Center - $375,000 per year FY88-FY99. Provides US industry and academic scientists and engineers access to state-of-the-art in situ diffraction facilities for studies of behavior of materials as a function of temperature and environment. Facilities include laboratory and synchrotron x-ray diffractometers and utilize the ORNL neutron diffraction facilities.

• Thermophysical Properties User Center - $500,000 per year FY88-FY99. Provides industry and academic scientists and engineers access to an exceptional array of thermophysical properties instruments including DSC, STA, TG, dilatometers, laser flash thermal diffusivity and four unique instruments for thermal transport measurements of value.

• Residual Stress User Center - $1,000,000 per year FY94-FY99 plus $500,000 in capital equipment. This user center utilizes x-ray and neutron diffraction facilities to measure macro and micro residual stresses at the surface and through thickness.

•Materials Microcharacterization Collaboratory - $150,000 per year FY97-FY99. The collaboratory is a collection of DOE and industrial laboratories working to test and demonstrate use of the internet for remote instrument operation and scientific collaboration. Emphasis for the Neutron Residual Stress Facility is to incorporate web based tools to improve user access and enhance collaboration over the internet using web based tools such as remote instrument control, electronic notebooks, video conferencing, and security tools to protect the instruments and intellectual results.

•Development of New Dielectric Ceramics - $37,500 per year FY98-FY99. This project lead by Dr. Rawn is trying new synthesis routes for making bulk quantities of a new dielectric ceramic previously prepared only in small single crystal form. If successful the new material should have outstanding properties based on the crystal structure and crystal chemistry models for temperature dependence of properties.

•Lower Temperature Oxygen Conductors - $75,000 per year FY98-FY00. This project lead by Dr. Payzant is using crystal chemical approaches to develop a lower temperature oxygen ion conductor for use in solid oxide fuel cells.

• Materials for Kraft Recovery Boilers - $150,000 per year FY97-FY00. The ORNL team includes efforts in materials properties, corrosion, microstructure, modeling, and residual stress analysis. The latter component involves the Diffraction and Thermophysical Properties Group. Stress analysis is used as starting boundary conditions for finite element modeling (FEM) of the boiler as well as verification of FEM predictions.

B. Refereed Journal Publications.

Dr. Hubbard has had over 150 publications and reports as well as certified 5 Standard Reference Materials for powder diffraction. The 5 publications most closely related to this proposal (1-5) and 5 other significant publications (6-10) are listed below:

1. "High Temperature Phase Transformation in Rhombohedral Bismuth Strontium Oxide", E.A. Payzant, W.D. Porter, C.R. Hubbard, Thermochemica Acta (accepted).
2. "Interlamellar Residual Stresses in Single Grains of NiO-ZrO_2 (cubic) Directionally Solidified Eutectics", E.C. Dickey, C.R. Hubbard and V.P. Dravid, *J. Amer. Ceram. Soc.* **80** 2773-2780 (1997)
3. "High Temperature X-ray and Calorimetric Studies of Phase Transformation in Quasicrystalline Ti-Zr-Ni Alloys", R.M. Stroud, K.F. Kelton, and S.T. Misture, *J. Mater. Res.* **12**, 434-438 (1997)
4. "Characterization of Innovatively Synthesized Low Cost NZP Powders". Cutis, J. A., Nageswaran, R., Limaye, S. Y., Hubbard, C. R., Porter, W. D., and Misture, S. T. Proc. 21st Annu. Cocoa Beach Conf./Expo. on Composites, Advanced Ceramics, Materials and Structures, American Ceramic Society, 1997.
5. "Sulfated Zirconia Catalysts: The Crystal Phases and Their Transformations", R. Srinivasan, T.R. Watkins, C.R. Hubbard, and B.H. Davis, *Chem. Mater.* **7**, 725-730 (1995)
6. "Neutron Diffraction Measurements of the Residual Stresses in Al_2O_3-ZrO_2 Ceramic Composites", X.-L. Wang, C.R. Hubbard, K.B. Alexander, P.F. Becher, J.A. Fernandez-Baca, and S. Spooner, *J. Amer. Ceram. Soc.* **77** 1569-1575 (1994)
7. "Crystallographic Strain Measurements of Modified Lead Magnesium Niobate using Neutron Diffraction", S.T. Misture, J.C. Hicks, C.T. Blue, E.A. Payzant, C.R. Hubbard, Applied Physics Letters, **72**, 1042-1044 (1998).
8. "Epitaxial Growth of Cu(111) Films on Si(110) by Magnetron Sputtering: Orientation and Twin Growth", H. Jiang, T.J. Klemmer, J.A. Barnard, W.D. Doyle, and E.A. Payzant, *Thin Solid Films* **315**, 13-16 (1998)
9. "Experimental Determination of the Residual Stresses in a Spiral Weld Overlay Tube", X.-L. Wang, E.A. Payzant, B. Taljat, C.R. Hubbard, J.R. Keiser, and M.J. Jirinec, *Mater. Sci. Eng*. **A232** 31-38 (1997)
10. "The Materials Microcharacterization Collaboratory: Scientific Collaboration over the Internet", M. C. Wright and C. R. Hubbard, published by Argonne National Laboratory at: http://www.aps.anl.gov/xfd/bcda/nobugs/proceed/MMC.html (1998).

C. Other Collaborators.

D. Graduate Students.

Professionals in the Diffraction & Thermophysical Properties Group include:

Dr. Ralph Dinwiddie, Dr. Andrew Payzant, Mr. Wally Porter, Dr. Claudia Rawn, Dr. Steve Spooner, Dr. Hsin Wang, Dr. Xun-Li Wang, Dr. Thomas Watkins

Postdocs Advised	*University of PhD*	*Current Position*
Christina Hoffmann	University of Bern, Switzerland	ORNL Postdoc
David Wang	The Open University, Britain	ORNL Postdoc
E. Andrew Payzant	Univ. of Western Ontario	ORNL Senior Staff
Claudia J. Rawn	Univ. of Arizona	ORNL Senior Staff
Dudley Raine	University of Virginia	SAIC
Hsin Wang	Alfred University	ORNL Senior Staff
Xun-Li Wang	Iowa State University	ORNL Senior Staff
Xiaojing Zhu	University of Denver	Materials Data, Inc.
Scott T. Misture	Alfred University	Prof at Alfred University

E. Advisors.

Biographical Sketch for John M. Hughes

Dept. of Geology, Miami University, Oxford, OH 45056

***. Results of Prior NSF Support.** Since 1992, the following NSF grants have been held by Hughes as P.I. or Co-P.I.: **NSF EAR-9804768** "Determination of site occupancy in multiply-occupied atomic sites", **NSF EAR-9627222** "Experiments in X-ray crystallography: Rare Earth elements in titanite, disorder in $LaNi_{5-y}Sn_y$ intermetallics, and Rare Earth elements in naturally-occurring perovskites", **NSF EAR-9218577** Supplement, "REU Supplement for crystal structure studies of rare earth bearing minerals, to support Jennifer M. Bell", $2,000, 5/95-8/95, **NSF EAR-9403194**, "Acquisition of an automated powder X-ray diffractometer", **NSF EAR-04397** "Petrologic and geochemical investigation of the Wrangell Volcanic Field, Alaska", $109,298, 6/93-5/98, Substitute P.I. of record after W.K. Hart accepted temporary position at NSF; original PI = W.K. Hart, **NSF EAR-9218577**, "Crystal structure studies of common rare earth bearing minerals". The grants supplied continuous support for equipment and faculty/student research in x-ray crystallography and powder diffractometry; several of the grants included a co-P.I. in the Department of Chemistry, Miami University. As noted below, 26 papers have been published since 1992, as well as 26 conference abstracts/presentations; virtually all those papers were supported by the above grants.

A. Vitae.

Education:

Ph.D., Dartmouth College, 1981; Resident Predoctoral Fellow, Carnegie Institution of Washington, Geophysical Laboratory, 1980, A.M., Dartmouth College, 1978; A.B., Franklin and Marshall College, 1975

Academic Employment History:

1992-Present:	Chair, Department of Geology, Miami University
1992-Present:	Professor, Department of Geology, Miami University
1987-1992:	Assistant Chair, Department of Geology, Miami University
1986-1992:	Associate Professor, Department of Geology, Miami University
1981-86:	Assistant Professor, Department of Geology, Miami University
1980:	Predoctoral Fellow, Geophysical Laboratory, Carnegie Institution of Washington
1976-81:	Research and Teaching Fellow, Department of Earth Sciences, Dartmouth College
1975-76:	Research Associate, Department of Geology, Franklin & Marshall College

Committees to Render Scientific Judgement:

Associate Editor, *American Mineralogist*, 1990-1993.
NSF Panel Member, ILI Program, 1991.
Associate Editor, *The Canadian Mineralogist*, 1996-1998; re-appointed 1999-2001.

Societal Fellowships, Memberships, and Committees:

Fellow, Mineralogical Society of America (elected to Fellowship, 1993)
Member, Research Grant Committee, 1990-1991
Member, Nominating Committee, 1987-88
Member, Kraus Crystallography Award Committee, 1997, 1998
American Geophysical Union
Sigma Xi
Mineralogical Association of Canada
Member, Hawley Medal Committee, 1993
Mineralogical Society of Great Britain and Ireland

B. Refereed Journal Publications.

Professor Hughes has had 59 referreed journal publications (published, in press, submitted), including 26 since 1992. His 5 publications most closely related to this proposal (1-5) and 5 other significant publications (6-10) are listed below.

1. Foley, J.A., J.M. Hughes, and J.W. Drexler (1997) Redledgeite, $Ba_x([Cr(III),Fe(III),V(III)]_{2x}Ti(IV)_{8-2x})O_{16}$, a new space group and elucidation of the Markovian sequence of Ba cations. *The Canadian Mineralogist, 35,* 1531-1534.
2. Foley, J.A., and J.M. Hughes (1997) The atomic arrangment of of brackebuschite, redefined as $Pb_2(Mn^{3+},Fe^{3+})(VO_4)_2(OH)$, and comments on Mn^{3+} octahedra. *The Canadian Mineralogist, 35,* 1027-1034.
3. Hughes, J.M., E.S. Bloodaxe, J.M. Hanchar, and E.E. Foord (1997) Incorporation of rare earth elements in titanite: stabilization of the *A*2/*a* dimorph by creation of antiphase boundaries. *American Mineralogist,* 82, 512 - 516.
4. Ni, Y. and J.M. Hughes (1996) The atomic arrangement of nanpingite, $CsAl_2(AlSi_3)O_{10}(OH)_2$, a 2:1 $2M_2$ dioctahedral mica. *American Mineralogist,* 81, 105-110.
5. Hughes, J.M., J.S. Cantrell, and R.C. Bowman (1997) Positional disorder in $LaNi_{5-y}Sn_y$ intermetallic phases? *International Journal of Hydrogen Energy*, 22, 347-349.
6. Hughes, J.M., E.E. Foord, J. Jai-nhuknan, and J.M. Bell (1996) The atomic arrangement of iimoriite, $Y_2(SiO_4)(CO_3)$, and comments on silicate-carbonate structures. *Canadian Mineralogist,* 34, 817-820.
7. Hughes, J.M., E.S. Bloodaxe, K.D. Kobel, and J.W. Drexler (1996) The atomic arrangement of ojuelaite, $ZnFe_2^{3+}(AsO_4)_2(OH)_2 \cdot 4H_2O$. *Mineralogical Magazine, the Journal of the Mineralogical Society of Great Britain and Ireland,* 519-521.
8. Ni, Y., J.M. Hughes, and A.N. Mariano (1995) The crystal chemistry of monazite and xenotime. *American Mineralogist,* 80, 21-26.
9. Hughes, J.M., E.E. Foord, M.A. Hubbard, and Y. Ni (1995) The crystal structure of cheralite-(Ce), (LREE, Ca, Th, U)$(P,Si)O_4$, a monazite-group mineral. *Neues Jahrbuch Mineralogie,* H. 8, 344-350.
10. Ni, Y., J.M. Hughes, and A.N. Mariano (1995) The crystal chemistry of monazite and xenotime. *American Mineralogist,* 80, 21-26.

C. Other Collaborators.

W.W. Adams	S.M. Cline	A.-M. Fransolet
Paul B. Moore	Z. Yang	Mellissa Brown (Mitchell)
T.M. Cooper G. Geister	C. Regan	J. Zemann
Peter Bayliss	Kevin D. Crowley	J. Hanchar
J. Ronsbo	R.C. Bowman, Jr.	Yongshan Dai
D. Jarosch	W. Schreyer	Maryellen Cameron
John W. Drexler	Akira Kato	D.B. Sullenger
Joseph S. Cantrell	Eugene E. Foord	

D. Graduate Students (Past 5 Years).

Jennifer M. Bell	Mollie A. Hubbard	Brian C. Payne
Jaran Jai-nhuknan	Harold D. Rowe	Kyle D. Kobel
Seth Hortsmeyer		

E. Advisors.

Richard W. Birnie	Robert M. Hazen	Larry W. Finger
Richard E. Stoiber		

Biographical Sketch for Alan J. Jircitano
Penn State Erie, The Behrend College

***. Results of Prior NSF Support.**
none

A. Vitae.
Education
B.S., Chemistry, Niagara University, 1977
Ph.D., Inorganic Chemistry, University of Kansas, 1982

Experience
Assistant Professor, 1984-present, Penn State Erie, the Behrend College
Postdoctoral Research Associate, 1982-84, Ohio State University
Teaching Assistant, 1977-1980, University of Kansas
Teaching Assistant, 1975-1977, Niagara University

Professional Society Memberships
American Chemical Society
American Crystallographic Association
Concil on Undergraduate Research

B. Refereed Journal Publications. 29 publications, including:
"The Self-Condensation of a Derivative of *o*-Aminobenzaldehyde: The Structure of the Polycyclic, Bisanhydro-Trimer, " A.J. Jircitano, S.O. Sommerer, J.J. Shelley, B.L. Westcott, and I.-H. Suh, *Acta Cryst., Sec. C.*, C50, 445-447, (1994).

"The Synthesis and Structure of Two Metal-Di-2-Pyridyl Ketone Oxime Dimers," S.O. Sommerer, B.L. Westcott, A.J. Jircitano, and K.A. Abboud, *Inorg. Chim. Acta*, 238, 149-153, (1995).
"Crystal Structures of *trans*-[Ru(dppe)$_2$(CO)(Cl)](BF$_4$)·toluene and *trans*-[Ru(dppm)$_2$ (CO)(Cl)](BF$_4$).CH$_2$Cl$_2$: A Study of the Steric and Electronic Ligand Effects of *trans*-Positioned Diphosphine Ligands," L.F. Szczepura, J. Giambra, R.F. See, J. Lawson, R.S. Janik, A.J. Jircitano, M.R. Churchill, and K.J. Takeuchi, *Inorg. Chim. Acta*, 239, 77-85, (1995).

"*trans*-Bis[4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole-N1,N']copper(II) Bis(tetrafluoroborate)," A. J. Jircitano, S. O. Sommerer and K. A. Abboud, *Acta Cryst. Sec. C.*, C53, 434 - 436, (1997).

"*trans*-Diaquabis(2-thienyl 2-pyridyl ketone-O,N)copper(II) Tetrafluoroborate," S. O. Sommerer, T. L. Friebe, A. J. Jircitano, C. E. MacBeth and K. A. Abboud, *Acta Cryst. Sec. C.*, C54, 178 - 179, (1998).

C. Other Collaborators.
Shaun O. Sommerer - Formerly of Barry University (Miami Shores, FL)
Khalil H. Abboud - University of Florida

D. Graduate Students.
none

E. Advisors.
Kristin Bowman-James - Formerly Kristin B. Mertes, University of Kansas
Daryle H. Busch - Formerly Ohio State University now at University of Kansas

Biographical Sketch for Margaret E. Kastner

Department of Chemistry, Bucknell University

***. Results of Prior NSF Support.**

1985 NSF-CSIP $21,054 (Bucknell matched) Instrumentation Grant - X-ray Precession Camera
1988 NSF-ILI - $69,500 (Bucknell matched) Instrumentation Grant, X-Ray Diffractometer
1990 NSF-REU (3 years) $120,000 Departmental Grant for summer support for undergraduates
1992 NSF Undergraduate Faculty Enhancement Workshops at the 13th Biennial Conference on Chemical Education 1993-95 $55,000 88 faculty members in six, three-day workshops

Highlights of the results these grants, related to potential success of proposed RSEC grant, are: The 1985 grant: For publication 21 this instrument was used to get cell constants and space groups of the several compounds prior to sending them out for data collection elsewhere. Additionally, J. Chem. Ed., 1989, 66, 968-969 describes how the instrument was being used in the physical chemistry course and J. Chem. Ed., 1989, 66, 969 is short note describing a video tape on how to use the instrument. This video is currently distributed by PolyCrystal Book Services, which also distrutes a video-tape Overview of X-ray Crystallography that was made using the diffractometer purchased under the 1988 grant. Both of these instruments are still in use with undergraduate students and several publications 22-27 would not have been possible without the latter grant. The 1990 grant to the department supported several undergraduates working with me doing synthetic work and learning crystallography. The experience I had teaching students in the summer research format will be built upon should I serve as host for students under the proposed grant. The 1992 grant allowed one workshop on crystallography lead by Prof. Glusker as well as five other workshops. I currently have under review by J. Chem. Ed: Software a series of computer programs I wrote to teach symmetry and crystallography. Although the development costs have been supported by grants from Pew and Dreyfus, the project would not be possible without the 1988 NSF grant.

A. Vitae.

Education

University of Notre Dame	Ph.D. 1979	Inorganic Chemistry
Indiana University at South Bend	B.S. 1972	Education

Professional Background

June 1990 - present:	Associate Professor of Chemistry Bucknell University
September 1984 to May 1990:	Assistant Professor of Chemistry Bucknell University
September 1980 to August 1984:	Instructor of Chemistry Boston University

B. Refereed Journal Publications.

Five most recent publications

23. Tang, K.; Kastner, M.E.; Cooper, J.N.; Kanaskie, M. and Monoski*, A., "Structure of cis and trans Bis(ethylenediamine)(isothiocyanato)(thiosulfato)cobalt(III), Acta Cryst. C, 1993, 49, 1265-1267.
24. Kastner, M.E.; Tang, K. and Birdsall, W.J., "Structures of a Monomeric and a Dimer Ni(II) Complex Containing 2-Acetylpyrrole," Inorganica Chimica Acta, 1994, 227, 159-162.
25. Bebout, D.C.; Ehmann, D.E.; Trinidad, J.C.; Crahan, K. K.; Kastner, M.E. ; Parrish, D.A., “Preparation of Mercury(II) Complexes of Tris[(2-pyridyl)methyl]amine and Characterization by X-ray Crystallography and NMR Spectroscopy,” Inorg. Chem. (1997), 36(19), 4257-4264
26. Bebout, D.C.; DeLanoy, A.E.; Ehmann, D.E.; Kastner, M.E.; Parrish, D.A.; Butcher, R.J., “Characterization of Mercury(II) Complexes of Bis[(2- pyridyl)methyl]amine by X-ray Crystallography and NMR Spectroscopy,” Inorg. Chem. (1998), 37(12), 2952-2959.
27. Bebout, D.C., Bush, J.F., II, Crahan, K.K., Kastner, M.E., Parrish, D.A., “Correlation of a Solution State Conformational Change between Mercuric Chloride Complexes of Tris[(2-(6-

methylpyridyl))methyl]amine with X-ray Crystallographic Structures", Inorg. Chem. (1998), 37(18), 4641-4646

Five additional publications

3. Kastner, M.E.; Scheidt, W.R.; Mashiko, T. and Reed, C.A., "Molecular Structure of Diaqo-α, β, δ , γ-Tetraphenylporphinatoiron (III) Perchlorate and Perchloro-α, β, δ-Tetraphenylporphinatoiron (III). Two New Structural Types for Iron (III) Porphyrins," Journal of the American Chemical Society, 1978, 100, 666-667.
5. Reed, C.A.; Mashiko, T.; Bentley, S.P.; Kastner, M.E.; Scheidt, W.R.; Spartalian, K. and Lang, G., "The Missing Heme Spin State and a Model for Cytochrome c'. The Mixed S=3/2,5/2 Intermediate Spin Ferric Porphyrin: Perchlorateo(mesotetraphenylporphinato)iron(III)," Journal of the American Chemical Society, 1979, 101, 1948-1958.
15. Kastner, M.E.; Fackler, P.H.; Podbielski, L.; Charkoudian, J. and Clarke, M.J., "A Dissymetric μ-oxo Technetium Complex," Inorganica Chimica Acta, 1986, L11-L15.
21. Kastner, M.E.; Smith, D.A.; Kuzmission, A.G.; Cooper, J.N. and Tyree*, T., "Structural trans Effect in Some Bis(ethylenediammine)cobalt(III) Complexes," Inorganica Chimica Acta, 1989, 158, 185-199.
22. Birdsall, W.J.; Long, D.P.; Smith*, S.P.E.; Kastner, M.E.; Tang, K. and Kirk*, C., "Steric Influences in the Formation of Ni(II) Complexes Containing Schiff Base Derivatives of 1-Acetylpyrrole with Primary Amines," Polyhedron, 1994, 13, 2055-2060.

C. Other Collaborators.

William Birdsall
Deborah C. Bebout, College of William and Mary

D. Graduate Students.

Dan Smith, MS, 1988
Mark Woomer, MS, 1993
Kai Tang, MS, 1994
Damon Parrish (current)

E. Advisors.

Graduate Advisor (January 1975 - January 1979) Robert Scheidt, University of Notre Dame
Post-Doctoral Advisor (February 1979 - August 1980) Michael Clarke, Boston College

Biographical Sketch for Sherri Lovelace-Cameron

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

***. Results of Prior NSF Support.**

None

A. Vitae.

Sherri R. Lovelace-Cameron earned a B.S. in Chemistry from Drexel University in 1986. She then enrolled in the chemistry graduate program at the University of Pittsburgh. Under the direction of Dr. N. John Cooper, she completed her Ph.D. thesis in Inorganic Chemistry in 1992. Her thesis title was "Electrochemical Studies of Reduced Manganese Complexes with Arene, Cyclopentadienyl and Indenyl Ligands". In the fall of 1992, Dr. Lovelace joined Professor William E. Geiger's' group, in the Department of Chemistry, at the University of Vermont as a postdoctoral research assistant. In the fall of 1995, Sherri began her current position as Assistant Professor in the Department of Chemistry at Youngstown State University.

Sherri received a Citibank Postdoctoral Fellowship for (1993-94). During her graduate studies she received an NAACP Sutton Education Scholarship (1991-92) and a Department of Education Fellowship (1989-90). As an undergraduate she was awarded a Gulf Oil Scholarship (1981-85).

Dr. Lovelace is a member of the American Chemical Society (Inorganic Division) and is currently serving the Local chapter as Chair-elect. Sherri is also a member of the Association of Women in Science, the Council on Undergraduate Research, Iota Sigma Pi, the National Organization for the Professional Advancement of Black Chemist and Chemical Engineers, and the Society of Electroanalytical Chemistry.

B. Refereed Journal Publications.

(1) Teen T. Chin; Sherri R. Lovelace; William E. Geiger; Craig M. Davis; Russell N. Grimes: "Infrared Spectroelectrochemistry of Boron-Hydrogen Stretches: A Tool for Diagnosis of Delocalization in Mixed-Valent Metallacarborane Complexes." *J. Am. Chem. Soc*. **1994**, 116, 9359.

(2) Lee, S.; Lovelace, S. R.; Cooper, N. J.: "Two-Electron and One-Electron Reduction of the Indenyl Complex $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]$ and Reversible Counterion-Controlled Comproportionation of $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]$ and $[Mn(\eta^3\text{-}C_9H_7)(CO)_3]^{2-}$ To Give $[Mn(\eta^5\text{-}C_9H_7)(CO)_3]^-$." *Organometallics* **1995**, 14, 1974.

(3) Lee, S.; Lovelace, S. R.; Arford, D. J.; Geib, S. J.; Weber, S. G.; Cooper, N. J.: "Reductively Induced Dimerization of the Ligated Benzene in $[Mn(\eta^6\text{-}C_6H_6)(CO)_3]^+$: Formation of the Initial C-C Bond by Anion/Cation Addition." *J. Am. Chem. Soc.* **1996**, 118, 4190.

(4) Koeslag, M. A.; Baird, M. C.; Lovelace, S. R.; Geiger, W. E.: "Synthesis and Properties of the 17-Electron, Tantalum-Centered Radical $Ta(CO)_4(Ph_2PCH_2CH_2PPh_2)$." *Organometallics* **1996**, 15, 3289.

(5) Rulkens, Ron; Lough, Alan J.; Manners, Ian; Lovelace, Sherri R.; Grant, Casey; Geiger, William E.: "Linear Oligo (ferrocenyldimethylsilanes) with between Two and Nine Ferrocene Units: Electrochemical and Structural Models for Poly (ferrocenylsilane) High Polymers.". *J. Am. Chem. Soc.* **1996**, 118, 12683.

C. Other Collaborators.

Fola Ladipo, University of Kentucky.

D. Graduate Students.

Gretchen Metz, MS 1997 (YSU)

E. Advisors.

(1) Ph.D. Advisor. Dr. N. John Cooper, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260.
(2) Postdoctoral Advisor. Dr. William E. Geiger, Department of Chemistry, University of Vermont, Burlington, VT 05405.

Biographical Sketch for Karen Magnus

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***. Results of Prior NSF Support.**

The properties and regulation of functions of macromolecular complexes are of fundamental importance to biology. Substantial progress occurred during the grants MCB 9004561 (Karen A. Magnus, P.I.) and later MCB 9305250 - "Crystal Structures and Functions of Limulus Hemocyanin", September 1, 1993 to August 31, 1999, P.I. Dr. Karen Magnus, Case Western Reserve University directing crystal structure studies and co-P.I. Dr. Celia Bonaventura, Duke University, directing functional studies. Hemocyanins are copper-containing proteins that effect cooperative oxygen transport in mollusks and arthropods. The largest known arthropod hemocyanin, from horseshoe crab, Limulus polyphemus, is comprised of 48 subunits, each of molecular weight about 73 kDa. The long term goal of our project is to understand in atomic detail how this large molecule functions. We determined the structures of oxygenated and deoxygenated forms of a subunit II and are attempting the whole molecule structure in its oxygenated and deoxygenated states. The following publications resulted from the current NSF-funded project: Papers (10), Abstracts (13), Book Chapter (1), Review (1), PhD Thesis (1), MS Thesis (1), Lab Manual (1), and PDB Deposits (4).

A. Vitae.

Education

B.S. University of California, Davis 1974 majored in Biological Sciences and in Chemistry
Ph.D. Johns Hopkins University 1980 Biophysics

Professional Experience

Postdoctoral Fellow, Department of Biophysics and Theoretical Biology, University of Chicago 1980-1981 (Dr. Paul Sigler, advisor).
Postdoctoral Fellow, Department of Biophysics, Johns Hopkins University School of Medicine 1981-1985 (Dr. Eaton E. Lattman, advisor).
Research Associate, Department of Biophysics, Johns Hopkins University School of Medicine 1985-1989.
Instructor in Physiology, Marine Biological Laboratory, Woods Hole, Massachusetts, 1989.
Guest Assistant Biophysicist, Biology Department, Brookhaven National Laboratory, 1991-1993.
Secondary Appointment, Assistant Professor, Department of Physiology and Biophysics, Case Western Reserve University School of Medicine, 1994-present.
Assistant Professor, Department of Biochemistry, Case Western Reserve University School of Medicine, 1989-1998.
Associate Professor, Department of Biochemistry, Case Western Reserve University School of Medicine, 1998-.

Honors and Awards

Individual National Research Service Award GM07985, Karen A. Magnus, Research Fellow, (Paul B. Sigler and Eaton E. Lattman, sponsors). 1980-1983.
Minority Research Initiation Award NSF DMB90-04561, Karen A. Magnus, P.I. 1990-1993.

B. Refereed Journal Publications.

(1) Magnus, K.A., Lattman, E.E., Volbeda, A. and Hol, W.G.J. (1991) Hexamers of Subunit II from Limulus Hemocyanin (a 48-mer) Have the Same Quaternary Structure As Whole Panulirus Hemocyanin Molecules. Proteins 9: 240-247.
(2) Hazes, B., Magnus, K.A., Bonaventura, C., Bonaventura, J., Dauter, Z. Kalk, K. and Hol, W.G.J. (1993) Crystal Structure of Deoxygenated Limulus polyphemus Subunit II Hemocyanin at 2.18 Å Resolution: Clues for a Mechanism for Allosteric Regulation. Protein Science. 2: 579-619.
(3) Fedorov. A.A., Magnus, K.A., Graupe, H., Lattman, E.E., Pollard, T.D. and Almo, S.C. (1994) X-ray Structures of the Actin Binding Protein Profilin that Differ in Their Affinity for Polyphosphoinositides. PNAS (USA) 91: 8638-8640.

(4) Magnus, K.A., Ton-That, H. and Carpenter, J.E. Recent Structural Work on the Oxygen Transport Protein Hemocyanin. Chem. Rev. 94: 727-735 (1994).
(5) Magnus, K.A., Hazes, B., Ton-That, H., Bonaventura, C., Bonaventura, J. and Hol, W.G.J. (1994) Crystallographic Analysis of Oxygenated & Deoxygenated States of Arthropod Hemocyanin Shows Unusual Differences. Proteins 19: 302-309.
(6) Challen, P.R., Peapus, D.H. and Magnus, K.A. (1997) A Niobium (V) Complex with Mixed O,S Donor Ligands. Synthesis, Structure and Properties of the Anion Tris(2-mercapto-4- methylphenolato) niobate (V) Polyhedron 16(9): 1447-1451.
(7) Liu, S., Federov, A.A., Pollard, T.D., Lattman, E.E., Almo, S.C. and Magnus, K.A. (in press J. Structural Biol.) Crystal Packing Induces a Conformational Change in Profilin-I from Acanthamoeba castellanii.
(8) Liu, S. and Magnus, K.A. (accepted pending revision Bioch. Bioph. Acta) Preliminary Crystallographic Studies of Limulus polyphemus Hemocyanin Subunits IIIa, IIIb and IV.
BOOK CHAPTER: Magnus, K.A., Ton-That, H. and Carpenter, J.E. (1993)

C. Other Collaborators.

Steven Almo, Albert Einstein; Celia Bonaventura, Duke; Joseph Bonaventura, Duke; Paul Carey, Case Western Reserve; Paul Challen, John Carroll; David Ewing , John Carroll; Martin Feiters, Nijmegen; Bart Hazes, Edmonton; Wim Hol, Washington; Kenneth Karlin, Johns Hopkins; Eaton Lattman, Johns Hopkins, Vance Lemmon, Case Western Reserve; Nelson Phillips, Case Western Reserve; Thomas Pollard, Salk Institute; David Samols, Case Western Reserve; Edward Solomon, Stanford; Robert Sweet,Brookhaven..

D. Graduate Students.

Students

Hoa Ton-That, Ph.D., Peter Proctor, Ph.D., Alvin Changco, Dejan Zivkovic

Postdoctoral Fellows

Diane Peapus, Ph.D., Shenping Liu, Ph.D

E. Advisors.

Warner E. Love, graduate, Johns Hopkins University; Paul B. Siglar, postdoctoral, then at University of Chicago; Eaton E. Lattman, then at Johns Hopkins University School of Medicine, postdoctoral and research associate, Thomas D. Pollard, then at Johns Hopkins University School of Medicine, research associate.

Biographical Sketch for John D. Protasiewicz

Department of Chemistry, Case Western Researve University

***. Results of Prior NSF Support.**

A. Vitae.

Education:

Cornell University, Ph.D. Inorganic Chemistry, 1990
Michigan Technological University, B.S. Chemistry, 1985
Massachusetts Institute of Technology, Postdoctoral Associate, 1990-93, with S. J. Lippard

Professional Activities and Awards:

1998-: Graduate Assistance in Areas of National Need (GAANN) Program Administrator
1998 ACS Cleveland Section By-Laws Chairman
1996- AXΣ Chemistry Fraternity Advisor
1996- Chemistry department liaison to ChemVL project and other Library issues related to Chemistry
1996-97: Glennan Fellows Teaching Award
1995-97: Chair, Chemistry Graduate Admissions Committee
1994-1996: Chemistry Department Executive Committee
1994-1995: American Chemical Society, CWRU, Student Affiliate Chapter, Advisor.
1993- Director CWRU Chemistry X-ray Facility
1985- Member, American Chemical Society

B. Refereed Journal Publications.

Urnezius, E.; Shah, S.; Protasiewicz, J. D. "Diphosphene and Phosphoranylidenephosphine Formation from a Terminal Phosphinidene Complex" *Phosphorus, Sulfur* **1998**, in press.

Shah, S.; Yap, G. P. A.; Protasiewicz, J. D. "'Phospha-Wittig' Reactions Using Isolable Phosphoranylidenephosphines ArP=PR_3 (Ar = 2,6-$Mes_2C_6H_3$ or 2,4,6-$Bu^t_3C_6H_2$)" *J. Chem. Soc. Chem. Commun.* **1998**, 1585-1586.

Shah, S.; Burdette, S. C.; Swavey, S.; Urbach, F. L.; Protasiewicz, J. D. "Alkali Metal Induced Rupture of a Phosphorus-Phosphorus Double Bond. Electrochemical and EPR Investigations of New Sterically Protected Diphosphenes and Radical Anions [ArPPAr]-" *Organometallics* **1997**, *16*, 3395-3400.

Boucher, M.; Macikenas, D.; Ren, T.; Protasiewicz, J. D. "Secondary Bonding as a Force Dictating Structure and Solid-State Aggregation of the Primary Nitrene Sources (Arylsulfonylimino)iodoarenes (ArINSO$_2$Ar')" *J. Am. Chem. Soc.* **1997**, *119*, 9366-9376.

Cicero, R. L.; Zhao, D.; Protasiewicz, J. D. "Polymorphism of (Tosyliminoiodo)*o*-toluene: Two New Modes of Polymeric Association for ArINTs" *Inorg. Chem.* **1996**, *35*, 275.

C. Other Collaborators.

Arnold Rheingold, University of Delaware
Malcolm E. Kenney, Case Western Reserve University

D. Graduate Students.

Eugenijus Urnezius
Shashin Shah
Bindu V. Meprathu
Dainius Macikenas

E. Advisors.

PhD: Klaus H. Theopold, Cornell University and now at the University of Delaware
Postdoctoral: Stephen J. Lippard, MIT

Biographical Sketch for Michael A. Serra

Department of Chemistry, Youngstown State University, One University Plaza, Youngstown, OH 44555
Ph: 330-742-3667

***. Results of Prior NSF Support.**
none

A. Vitae.
Education
1990Ph. D. in Molecular, Cellular and Developmental Biology from the Dept. of Biochemistry and Biophysics, Iowa State University, Ames, Iowa
1984 B.S. Biology, B.A. Mathematics, and a minor in Chemistry from Adrian College, Adrian, Michigan

Work Experience
1994-presentAssistant Professor of Chemistry, Chemistry Department, Youngstown State University, Youngstown, Ohio
1992-1994 Assistant Professor of Chemistry, Chemistry Department, Hiram College, Hiram, Ohio
1991-1992 Visiting Assistant Professor of Chemistry, Department of Chemistry, Hope College, Holland, Michigan
1990 Research Associate, Department of Chemistry, Michigan State University, East Lansing, Michigan
1984-1990 Research Assistant, Department of Biochemistry and Biophysics, Iowa State University, Ames, Iowa

B. Refereed Journal Publications.
"Correlation Between Antioxidant Defenses and Intensity of Systemic Inflammatory Response Following Aortic Surgery", Cornu-Labat, G., Serra, M. A., Smith, A. H., McGregor, W. E., Hirko, M. K., Turner, J. J., and Rubin, J. R. (in preparation).

"Crystal Structure of Adenylosuccinate Synthetase from Escherichia coli: Evidence for Convergent Evolution of GTP Binding Domains", Poland, W. B., Silva, M. M., Serra, M. A., Cho, Y., Kim, K. H., Harris, E. M. S., and Honzatko, R. B. (1993) *J. Biol. Chem.* **268**, 25334.

"Structure of an Adenine-Hydrogen Peroxide Adduct", Serra, M. A., Dorner, B. K., and Silver, M. E., (1992) *Acta Crystallo*. C**48**, 1957.

"Preliminary X-ray Crystallographic Study of Adenylosuccinate Synthetase from *Escherichia coli*", Serra, M.A., Bass, M.B., Fromm, H.J., and Honzatko, R.B. (1988) J. Mol. Biol. **200**, 753.

"Structure of 1-(p-Nitrobenzylidineamino)guanidinium Chloride", Serra, M.A. and Honzatko, R.B. (1986) *Acta Crystallo.* **C42**, 1755.

C. Other Collaborators.
Dr. Cornu-Labat, Northside Medical Center
Mr. Brian DelFraino, undergrad. research asst.
Ms. Erica Eliser, undergrad. research asst.
Ms. Phyllis Haugabook, undergrad. research asst.
Dr. Mark Hirko, Northside Medical Center
Dr. Walter McGregor, Northside Medical Center
Dr. Jeffrey Rubin, Northside Medical Center
Mr. Arthur Smith, undergrad. research asst.
Dr. John Turner, Northside Medical Center
Dr. Vivien Yee, Cleveland Clinic Foundation

D. Graduate Students.
Masters: AntoinetteVargallitto and Kathleen Kwolek

E. Advisors.
PhD: Dr. Richard B. Honzatko, Dept. of Biochemistry, Biophysics and Molecular Biology, Iowa State University, Ames, IA.
Post-doctoral: Dr. Alexander Tulinsky, Dept. of Chemistry, Michigan State Univeristy, East Lansing, MI. He has since retired.

Biographical Sketch for Omar W. Steward

Department of Chemistry, Duquesne University

***. Results of Prior NSF Support.**

none

A. Vitae.

Omar W. Steward received his B.Sc. and Ph.D. degrees in Chemistry from the University of Delaware in 1953 and The Pennsylvania State University in 1957 respectively. His Ph.D. dissertation entitled, "Organosilicon Monomers and Polymers Having Functional Groups Linked to Silicon in the β- and δ-Relations to Silicon" was directed by Dr. Leo H. Sommer. After graduation, he worked for Dow Corning Corporation, Midland, Michigan for five years with Dr. Ogden R. Pierce on the synthesis of fluoroalkylsiloxane polymers. In 1962, he received as a National Science Foundation Postdoctoral Fellowship and worked with Dr. Colin Eaborn at the University of Leicester studying the stereochemistry of the cleavage of aromatic rings from silicon. In 1963 and 1964, Dr. Steward obtained temporary teaching positions at the University of Illinois, Urbana, and Southern Illinois University, Carbondale. Dr. Steward joined the faculty of Duquesne University in September 1964 as an Assistant Professor in the Department of Chemistry. In 1966, he was promoted to the rank of Associate Professor, and in 1972, he became a full professor. He has been a member of the American Chemical Society since 1951.

Dr. Steward's teaching has included lectures and laboratory courses at both the undergraduate and graduate levels covering a wide range of topics including: chemistry for science and pharmacy majors, chemistry for nursing students, inorganic chemistry for both undergraduate and graduate students, organometallic chemistry, inorganic reaction mechanisms, and chemistry of the group 14 elements. He has directed the theses of six master candidates and the dissertations of eight doctoral candidates. A number of undergraduate students have worked in his laboratory both during the school year and during the summer. Dr. Steward has extensive experience in both synthesis and mechanistic studies in the areas of organosilicon and organometallic chemistry. Since 1985, he has used routinely single crystal X-ray diffraction in his research on magneto-structural relationships of carboxylato complexes of the first transition series. Currently, Dr. Steward is collaborating with Dr. Tadashi Tokii , Saga University, Japan, on these magneto-structural studies.

Currently, structural studies on the geometry of transition-metal carboxylato complexes form the viewpoint of the steric effects of both the carboxylato ligands and amine bases are in progress. Aromatic nitrogenous bases substituted in the α-position tend to yield five-coordinate complexes. Recently, we have observed that steric effects can be used to force formation of five-coordinate polymeric complexes with chain structures. Magneto-structural relationships for these complexes are under investigation. Some of the self-assembled clusters we have studied simulate the structures of the carboxylato-bridged centers in metalloenzymes.

B. Refereed Journal Publications.

Dr. Steward has 40 journal publications, with 12 of the last 13 published since 1986 in the area of structural chemistry. His five publications most closely related to this proposal (1-5) and five other significant publications (6-10) are listed below.

(1) "Manganese(II) Triphenylacetate Hydrate, a Manganese(II) Complex with a Chain Structure", Yaukey, T. S.; Steward, O. W.; Chang, S.-C. *Acta Crystallogr. Sect. C*, **1998**, *C54*, 1081.

(2) "Structural and Magnetic Studies of Copper(II) 2,2-Diphenylpropanoato and Triphenylacetato Complexes with Oxygen-Donor Ligands. The Cage Geometry of Dimeric α-Phenyl Substituted Carboxylates", Steward, O. W.; Johnston, B. S.; Chang, S.-C.; Harada, A.; Ohba, S.; Tokii, T.; Kato, M. *Bull. Chem. Soc. Jpn.*, **1996**, *69*, 3123.

(3) "Structural, Magnetic, and Spectroscopic Characterization of the Pyridine Complexes of Copper(II) Triphenylacetate: a Dimeric Copper(II) Triphenylacetate-Pyridine Complex with Distorted Trigonal Bipyramidal Geometry Around Copper", Steward, O. W.; Kato, M.; Chang, S.-C.; Sax, M; Chang, C.-H.; Jury, C. F.; Muto, Y.; Tokii, T.; Taura, T.; Pletcher, J. F.; Yoo, C. S. *Bull. Chem. Soc. Jpn.*, **1991**, *64*, 3846.

(4) "Correlation of Electron Density and Spin Exchange Interactions in Dimeric Copper(II) Formates, Acetates, and Silanecarboxylates", Yamanaka, M.; Uekusa, H.; Ohba, S.; Saito, Y.; Kato, M.; Tokii, T.; Muto, Y.; Steward, O. W. *Acta Crystallogr. Sect. B*, **1991**, *B47*, 344.

(5) "Carboxysilanes and -germanes. 5. Copper(II) Complexes of Carboxysilanes and -germanes: Structure and Magnetic Properties. Crystal Structure of Tetrakis(α-phenyldimethylsilane-carboxylato([bis(aquacopper(II)]", Steward, O. W.; Chang, S.-C.; McAfee, R. C.; Piskor, S. R.; Schreiber, W. J.; Jury, C. F.; Taylor, C. E.; Pletcher, J. F. *Inorg. Chem.*, **1986,** *25*, 771.

(6) "Characterization of Dimeric Copper(II) Trichloroacetato Complexes By Electron Spin Resonance, Infrared, and Electronic Reflectance Spectra. Correlation of Spectral Properties with Molecular Geometry", Muto, Y.; Horie, H.; Tokii, T.; Nakashima, M.; Koikawa, M.,; Steward, O. W.; Ohba, S.; Uekusa, H.; Husebye, S.; Suzuki, I.; Kato. M. *Bull. Chem. Soc. Jpn.*, **1997**, *70*, 1573.

(7) "Dimeric Copper(II) 2-Methyl-2-phenylpropanoate Adducts with Water or 2,6-Lutidine and a Monomeric Copper(II) Triphenylacetate with 2,6-Lutidine", Fujita, T.; Ohba, S.; Tokii, T.; Jury, C. F.; Steward, O. W.; Kato. M. *Acta Crystallogr. Sect. C*, **1993**, *C49*, 2095.

(8) "Crystal Structure and Magnetic Properties of Binuclear Copper(II) Complexes with Alkoxo and Benzoato or Silanecarboxylato Bridges", Kawata, T.; Yamanaka, M.; Ohba, S.; Tokii, T.; Jury, C. F.; Steward, O. W.; Kato. M. *Bull. Chem. Soc. Jpn.*, **1992**, *65*, 2739.

(9) "Magneto-Structural Correlations of Dimeric Copper(II) Trichloroacetates", Uekusa, H.; Ohba, S.; Tokii, T.; Muto, Y.; Kato, M.; Husebye, S.; Steward, O. W.; Chang, S.-C.; Rose, J. P.; Pletcher, J. F. *Acta Crystallogr. Sect. B*, **1992**, *B48*, 650.

(10) "Structure Comparisons Between Copper(II) Triorganosilanecarboxylate, -germanecarboxylate, and -acetates", Uekusa, H.; Ohba, S.; Saito, Y.; Steward, O. W.; Tokii, T.; Muto, Y. *Acta Crystallogr. Sect. C*, **1990**, *C46*, 1805

C. Other Collaborators.

D. Graduate Students.

E. Advisors.

Biographical Sketch for Timothy R. Wagner

Department of Chemistry, Youngstown State University, Youngstown, Ohio 44555
Ph: (330) 742-1960, FAX: (330) 742-1579, e-mail: trwagner@cc.ysu.edu

***. Results of Prior NSF Support.** In the past five years, Dr. Wagner has been PI or co-PI on the following NSF grants: (1) NSF-RUI DMR-9403889 (PI). Funds were awarded ($71,199) towards the purchase of a single crystal X-ray diffractometer. With a university overmatch of $154,951, the awardees were able to purchase two diffractometers (Siemens P-4 models), and a multi-wire area detector (Siemens X-1000). Since they were installed in mid-1995, the instruments have supported the work of several faculty and students from YSU as well as other local colleges. For Dr. Wagner specifically, the facility has supported the work of nine of his undergraduate research students, and one graduate student. He has had three publications resulting from his diffractometer work so far, with results for at least two other papers completed. Dr. Wagner recently was successful in obtaining funding from Research Corporation, due in part to preliminary results obtained using the NSF-supported X-ray facility; (2) NSF-ILI-IP DUE 9551683 (co-PI). This grant provided funds towards the purchase of GC-MS, for teaching and research purposes; and (3) NSF-ILI-IP DUE 9851107 (co-PI). This grant will be used towards purchase of GPC and DSC/TGA instrumentation. No other NSF grants are pending.

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

In the spring of 1988, Dr. Wagner joined Professor Lawrence Marks' group in the Department of Materials Science at Northwestern University, Evanston, Illinois, as a postdoctoral fellow. At Northwestern University, Dr. Wagner conducted HREM studies of electron and ion-stimulated surface reactions & damage in oxides. In the Fall of 1990, Dr. Wagner joined the faculty of the Chemistry Department at the Illinois Institute of Technology, Chicago, Illinois, as a Visiting Assistant Professor. He remained at IIT for two years, and then began his tenure at Youngstown State University as Assistant Professor of Chemistry in the Fall of 1992. He was promoted to Associate Professor in Fall, 1997.

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

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

B. Refereed Journal Publications.

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

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

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

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

189-203.

(5) Wagner, "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type Barium Hexagallate", *J. Solid State Chem.*, **136** 120-124 (1998).

(6) **T.** Wagner and *T. Styranec, "Preparation and Crystal Structure Analysis of $Ba_2BiGa_{11}O_{20}$", *J. Solid State Chem.*, **138**, 313–320 (1998).

(7) K. Landis, A. Hunter, T. Wagner, L. Curtin, F. Filler and S. Jansen-Varnum, "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt Congeners", *Inorganica Chimica Acta,* **282**, 155–162 (1998).

C. Other Collaborators.
None.

D. Graduate Students.
(1) Ma'en Amad, M.S., 1994.
(2) Joseph Potkinicky, M.S., 1997.

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

Biographical Sketch for John C. Woolcock

Department of Chemistry, Indiana University of PA

***. Results of Prior NSF Support.**

none

A. Vitae.

Education:

Southern College, Collegedale, TN 1978 B.Sc. Chemistry
University of California at Riverside 1984 Ph.D. Chemistry
Research advisor: Michael Rettig
Dissertation title: Nucleophilic Attack on Diolefin Complexes of Palladium(II) and Platinum(II).

Positions:

Associate Professor, Indiana University of PA (IUP); August 1984-present
Temporary Faculty, Loma Linda University, La Sierra, CA; 1981-82

Professional Activities (related to grant proposal)

1. National Science Foundation, Undergraduate Faculty Enhancement Workshop. Molecular Structure by X-Ray Crystallography was at Bucknell University, August 2-4, 1994. The presenters were Jenny Glusker and Horace Carrell (Fox Chase Cancer Center) and Miriam Rossi (Vassar College).

2. NSF Chautauqua Course: Superconductors, Semiconductors and Metals: Bringing Solids Into Introductory Chemistry Courses. held at University of Pittsburgh, May 17-19, 1995. The presenters were Arthur Ellis (University of Wisconsin) and George Lisensky (Beliot College).

3. American Crystallographic Association Course in Crystallography at University of Pittsburgh, August 2-15, 1995. This course was organized and presented in part by Bryan Craven in the Department of Crystallography at the University of Pittsburgh. Other instructors in the course were: Carolyn Brock (University of Kentucky), Robert Sparks (Siemens), Charles Strouse (UCLA) and B. C. Wang (University of Georgia).

4. National Science Foundation, Undergraduate Faculty Enhancement Workshop. PC-Based X-Ray Crystallographyö, at Clemson University, August 2-4, 1996 with Wallace Cordes (University of Arkansas) the presenter.

B. Refereed Journal Publications.

1. Rakowsky, M.H.; Woolcock, J.C.; Wright, L.L.; Green, D.B.; Rettig, M.F.; Wing, R.M. In-Plane Coordinated Double Bonds. Molecular Structures, Spectroscopy and Stability of 5-Methylenecyclooctene and 5-methylenecycloheptene Complexes of Platinum(II)ö, *Organometallics*, **1987**,*6*, 1211-1218.

2. Rakowsky, M.H.; Woolcock, J.C.; Rettig, M.F.; Wing, R.M. Chemistry of In-Plane Coordinated Double Bonds. Coordinated Alkyl and Aryl Migration to Adjacent Exocyclic Olefin in Alkyl (or Aryl) Halo[5-methylenecycooctene]platinum(II)ö, *Organometallics*, **1988**, *17*, 2149-2158.

3. Hung, A.C.H.; Woolcock, J.C.; Rettig, M.F.; Wing, R.M.: ôCyanide Exchange of the Methyltricyanoplatinate(II) Dianion: Temporal Resolution of Cis and Trans Cyanide Exchange; *Inorganic Chemistry*, **1992**, 810-812.

4. Woolcock, J.C.; Zafar, A.; Microscale Techniques for Determination of Magnetic Susceptibility;*Journal of Chemical Education*, **1992**, A176-A179.

5. Woolcock, J.C.; Niederhut, M.; Craven, B. M. ôMolecular Structure of (Bicyclo[3.3.1]nona-2,6-diene)dichloropalladium(II); *Australian Journal of Chemistry*, **1996**, *49*, 977-980.

C. Other Collaborators.

1. P. W. Jennings, Montana State University, summer 1987.
2. Bryan Craven, Indiana University of PA, 1995-present.

D. Graduate Students.

1. Herman Carl (M. A., 1988)

2. Yi Liu (M. S., 1995)
3. Elly Wijaya (M. S., 1998)

E. Advisors.

1. Ph. D. Advisor: Michael Rettig, Department of Chemistry, University of California at Riverside, Riverside, CA 92521

2. Ph. D. Dissertation Committee: Richard Wing, Department of Chemistry, University of California at Riverside, Riverside, CA 92521 (retired)

3. Ph. D. Dissertation Committee: M. Mark Midland, Department of Chemistry, University of California at Riverside, Riverside, CA 92521

Biographical Sketch for David W. Wright

Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA 15282-1530
Ph: 412-396-4222, FAX: 412-396-5683, wrightd@duq3.cc.duq.edu

***. Results of Prior NSF Support.**

A. Vitae.

Education

Massachusetts Institute of Technology — Cambridge, MA
Ph.D. degree in Bioinorganic Chemistry, December, 1993 on the "Aspects of the Structure and Function of the Enzyme Nitrogenase" under Professor W. H. Orme-Johnson.

Tulane University — New Orleans, La
B. S. degree in Chemistry, Magna cum Laude. June 1988.
B. A. degree in Classical Languages and Ancient History, Magna cum Laude. June 1988.

Professional and Research Experience

Assistant Professor	August 1997-current	Duquesne University
Adjunct Professor	1996-1997	Boston College
Postdoctoral Fellow	1994-1997	Boston College
Imperial Chemical Company	1988	Wilton, England

Fellowships and Award

National Foundation for Infectious Diseases-Young Investigator	1998
Johnson Matthey Research Award ($3000)	1995
MIT Norris Chemistry Department Fellow	1988-1990
NSF Graduate Fellowship Supercomputer Grant	1988
American Institute of Chemistry Undergraduate Student Research Award	1988
Phi Beta Kappa (Tulane University)	1988
Judah Touro Award for Excellence in Classics	1988
American Chemical Society (member)	1988-current
American Association for the Advancement of Science (member)	1989-current

B. Refereed Journal Publications.

Jim Ziegler, Richard T. Chang, and David W. Wright. Multiple-Antigenic Peptides (MAP's) of Histidine-Rich Protein II of *Plasmodium falciparum*: A Novel Family of Peptide Dendrimers with Protein-Like Activity. Accepted *J. Am. Chem. Soc*. January 9. 1999.

U. Bergmann, M. M. Grush, C. R. Horne, P. DeMarois, J. E. Penner-Hahn, C. F. Yocum, D. W. Wright, C. E. Dube, W. H. Armstrong, G. Christou, H. J. Eppley, and S. P. Cramer. Characterization of the Mn Oxidation States in Photosystem II by Kβ X-ray Fluorescence Spectroscopy. *J. Chem. Phys. B* **1998**, 102, 8350-8352.

Christopher E. Dubé, David W. Wright, Peter Bonatatebus, Samundranil Pal, and William. H. Armstrong. Tetranuclear Manganese-Oxo Aggregates Relevant to the Photosynthetic Water Oxidation Center. *J. Am. Chem. Soc*. **1998**, 120, 3704-3716.

David W. Wright, Henry J. Mok, Christopher E. Dubé, and William. H. Armstrong. Implications For the Solution State Structure of Dinuclear Manganese-Oxo Aggregates: A ^{1}H NMR Study with Magnetic Correlations. *Inorg. Chem.* **1998**, 37, 3714-3718.

Christopher E. Dubé, David W. Wright, and William H. Armstrong. Multiple Reversible Protonations of the Adamantane-Shaped $\{Mn_4O_6\}^{4+}$ Core: Detection of Protonation Stereoisomers at the $\{Mn_4O_4(OH)_2\}^{6+}$ Level. Accepted *J. Amer. Chem. Soc.* **1996**, 118, 10910.

David W. Wright, Richard T. Chang, Sanjay K. Mandal, William H. Armstrong, and William H. Orme-Johnson. A Novel Vanadium (V) Homocitrate Complex: Synthesis, Structure, and Biological Relevance of $[K_2(H_2O)_5][(VO_2)_2$ (R,S-Homocitrate$)_2]\cdot H_2O$. *J. Biol. Inorg. Chem.* **1996**, 1, 143.

David W. Wright, Patricia A. Humiston, William H. Orme-Johnson, and William M. Davis. A Unique Coordination Mode for Citrate to a Transition Metal: $K_2[V(O)_2(C_6H_6O_7)]_2\ 4H_2O$. *Inorg. Chem.* **1994**, 34, 4194.

C. Other Collaborators.

D. Graduate Students.

E. Advisors.
W. H. Orme-Johnson

Biographical Sketch for Vivien C. Yee

Department of Molecular Cardiology, Cleveland Clinic Foundation, Cleveland, OH 44195

***. Results of Prior NSF Support.**

none

A. Vitae.

Educational Background

University of British Columbia	Ph.D. 1990	Chemistry
University of British Columbia	B.Sc. 1986	Chemistry

Professional Background

July 1997 – present, Assistant Staff, Molecular Cardiology, Cleveland Clinic Foundation
July 1997 – present, Assistant Professor, Pharmacology, Case Western Reserve University
July 1995 – June 1997, Research Assistant Professor, Biochemistry, University of Washington
January 1992 – June 1995, Senior Fellow, Biological Structure, University of Washington
April 1990 – November 1991, Research Associate, Chemistry, Michigan State University

B. Refereed Journal Publications.

Five most recent publications

28. S.E. Iismaa, L. Chung, M.-J. Wu, D.C. Teller, V.C. Yee, and R.M. Graham. The Core Domain of the Tissue Transglutaminase G_h hydrolyses GTP and ATP. *Biochemistry*, 36, 11655-11664 (1997).
29. E. Laiho, J. Ignatius, H. Mikkola, V.C. Yee, D.C. Teller, K-M. Niemi, U. Saarialho-Kere, J. Kere, and A. Palotie. Transglutaminase 1 mutations in autosomal recessive congenital ichthyosis: Private and recurrent mutations in an isolated population. *Am. J. Hum. Gen.*, 61, 529-538 (1997).
30. O.V. Mitkevich, J.R. Shainoff, P.M. DiBello, V.C. Yee, D.C. Teller, G.B. Smejkal, P.D. Bishop, I.S. Kolotushkina, K. Fickenscher, and G.P. Samokhin. Coagulation factor XIIIa undergoes a conformational change evoked by glutamine substrate. Studies on kinetics of inhibition and binding of XIIIa by a cross-reacting anti-fibrinogen antibody. *J. Biol. Chem.*, 273, 14387-14391 (1998).
31. T.P. Ugarova, D.A. Solovjov, L. Zhang, D.I. Loukinov, V.C. Yee, L.V. Medved, and E.F. Plow. Identification of a novel recognition sequence for integrin $\alpha_M\beta_2$ within the γ-chain of fibrinogen. *J. Biol. Chem.*, 273, 22519-22527 (1998).
32. C.A. Behnke, V.C. Yee, I. Le Trong, L.C. Pedersen, R.E. Stenkamp, S.S. Kim, G.R. Reeck, and D.C. Teller. Structural determinants of the bifunctional corn Hageman factor inhibitor: X-ray crystal structure at 1.95 Å resolution. *Biochemistry* 37, 15277-15288 (1998).

Five additional publications

17. L.C. Pedersen, V.C. Yee, P.D. Bishop, I. Le Trong, D.C. Teller, and R.E. Stenkamp. Transglutaminase factor XIII uses proteinase-like catalytic triad to crosslink macromolecules. *Protein Science*, 3, 1131-1135 (1994).
18. V.C. Yee, L.C. Pedersen, I. Le Trong, P.D. Bishop, R.E. Stenkamp, and D.C. Teller. Three Dimensional Structure of a Transglutaminase: Human Blood Coagulation Factor XIII. *Proc. Nat. Acad. Sci.*, 91, 7296-300 (1994).
20. V.C. Yee, L.C. Pedersen, P.D. Bishop, R.E. Stenkamp, D.C. Teller. Structural Evidence that the Activation Peptide Is Not Released upon Thrombin Cleavage of Factor XIII. *Throm. Res.*, 78, 389-397 (1995).
23. V.C. Yee, I. Le Trong, P.D. Bishop, L.C. Pedersen, R.E. Stenkamp, and D.C. Teller. Structure and function studies of factor XIII A-subunit by X-ray Crystallography. *Seminars in Thrombosis and Haemostasis*, 22, 377-384 (1996).
24. V.C. Yee, K.P. Pratt, H.C.F. Cote, I. Le Trong, D.W. Chung, E.W. Davie, R.E. Stenkamp, and D.C. Teller. Crystal structure of a 30 kDa C-terminal fragment from the γ chain of human fibrinogen. *Structure* 5, 125-138 (1997).

C. Other Collaborators.

Paul Bishop, ZymoGenetics Inc.

Robert Graham, Victor Chang Cardiac Research Institute
Daniel Hohl, Hôpital de Beaumont (Lausanne, Switzerland)
Akitada Ichinose, Yamagata University School of Medicine
Aida Inbal, Tel Aviv University
Aarno Palotie, University of Helsinki
Edward Plow, Cleveland Clinic Foundation
John Shainoff, Cleveland Clinic Foundation
Graham Standen, Bristol Royal Infirmary

D. Graduate Students.

David Hyatt	(postdoctoral fellow, 1997 – 98)
Sadasivan Chittalakottu	(postdoctoral fellow, 1997 – present)
Sanjoy Bhattacharya	(postdoctoral fellow, 1997 – present)

E. Advisors.

David Teller	(postdoctoral advisor, University of Washington, 1992-1997)
Ronald Stenkamp	(postdoctoral advisor, University of Washington, 1992-1997)
Alexander Tulinsky	(postdoctoral advisor, Michigan State University, 1990-1991)
James Trotter	(graduate advisor, University of British Columbia, 1986-1990)

Biographical Sketch for Edward P. Zovinka

Department of Chemistry., Mathematics, and Physical Science, Saint Francis College
Loretto, PA 15940-0600
Ph: 814-472-3373, FAX: 814-472-3937, ezovinka@sfcpa.edu

***. Results of Prior NSF Support.**
none

A. Vitae.
Birthdate: 6/15/65

Education:
Ph.D., Chemistry, University of California, Davis , Davis, CA, 1992
B.S., Chemistry, cum laude, Roanoke College, Salem, VA 1987

Professional Positions:
Saint Francis College: Associate Professor of Chemistry 8/94-present
Assistant Professor of Chemistry, 8/94-8/98
Davidson College, Visiting Assistant Professor, 1/94-5/94
North Carolina State University, Postdoctoral Associate, 1/93-5/94

Professional:
Member of the American Chemical Society
Member of Project Kaleidoscope, Scientist in Residence 1998
Member of the Council on Undergraduate Research

Awards:
Bittle Scholar-1983-1987
Analytical Chemistry Award-1986
American Institute of Chemists Student Award-1987
Senior Scholar-1987
Clorox Graduate Assistant Teaching Award-1990
Chancellor's Teaching Fellow-1992
Who's Who Among America's Teachers-1996, 1998
CASE Pennsylvania Professor of the Year – 1997
Swatsworth Faculty Award - 1997

B. Refereed Journal Publications.
14. Cornman, C.R.; Zovinka, E.P.; Boyajian, Y.D.; Olmstead, M.M. Noll, B.C. Synthesis and Structure of a Vanadium (IV)-amide Metallacyclic Complex accepted by Inorganica Chimica Acta.

13. Howard, R.J.; Ropp, J.A.; Wasil, C.; Zovinka, E.P. Rural Outreach Chemistry for Kids (R.O.C.K.) A Service Project to Involve More than Chemistry Majors in a Chemistry Club" The Chemical Educator http://journals.springer-ny.com/chedr 1997, 2

12. Balch, A.L.; Koerner, R.; Latos-Grazynski, L.; Lewis, J.E.; St. Claire, T.N.; Zovinka, E.P. Coupled Oxidation of Heme without Pyridine. Formation of Cyano Complexes of Iron Oxophlorin and 5-Oxaporphyrin (Verdoheme) from Octaethylheme Inorg. Chem. 1997, 36, 3892-3897.

11. Crowder, M.; Wang, Z.; Franklin, S.L.; Zovinka, E.P.; Benkovic, S.J..; Characterization of the Metal-binding Site of β-Lactamase from Bacteroides fragilis Biochemistry 1996, 35, 12126-12132.

10. Cornman, C.R.; Zovinka, E.P., Meixner, M.H. Vanadium Complexes of the Active-Site Peptide of Protein Tyrosine Phosphatase 1B: $V^{IV}O(VHCSAG\text{-}NH_2)_n$ Inorg. Chem. 1995, 34, 5099-5100.

9. Cornman, C.R.; Zovinka, E.P. Chpt 14 "Mechanistic Aspects of the Chemistry of N-Alkyl Porphyrins" in Mechanistic Bioinorganic Chemistry ACS Advances in Chemistry Series #246, Thorp, H.H. and Pecoraro, V.L.(eds.) 1995, 373-403.

8. Cornman, C.R.; Zovinka, E.P.; Boyajian, Y.D.; Geiser-Bush, K.M.; Boyle, P.; Singh, P Structural and EPR Studies of Vanadium Complexes of Deprotonated Amide Ligands: Effects on the ^{51}V Nuclear Coupling Constant Inorg. Chem. 1995, 34, 4213-4219.

7. Balch, A.L.; Latos-Grazynski, L.; Noll, B.C.; Szterenberg, L.; Zovinka, E.P.The Chemistry of Iron Oxophlorins II. Oxidation of Iron(III) Octaethyloxophlorin Dimer and Observation of Stepwise, Two Electron Oxidation of the Oxophlorin Macrocycle J. Am. Chem. Soc. 1993, 115, 11846-11854.

6. Balch, A.L.; Noll, B.C.; Phillips, S.L.; Reid, S.M.; Zovinka, E.P. Structural Characterization of Nickel (II) Complexes of Octaethyloxophlorin Dianion and Octaethyloxophlorin Radical Dianion Inorg.Chem. 1993, 32, 4730-4736.

5. Balch, A.L.; Noll, B.C.; Reid, S.M.; Zovinka, E.P. Coordination Patterns for Oxophlorin Ligands:Pyridine Induced Cleavage of Dimeric Manganese(III) and Iron(III) Octaethyloxophlorin Complexes Inorg. Chem.1993, 32, 2610-2611.

C. Other Collaborators.

D. Graduate Students.

none

E. Advisors.

SUMMARY PROPOSAL BUDGET YEAR 1

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

ORGANIZATION: **Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**386,750**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**386,750**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**386,750**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **% of MTDC (Rate: 53.00, Base: 25000)**					
TOTAL INDIRECT COSTS (F&A)				**13,250**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** 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 COMMENTS - Year 1

**** G-5 Subcontracts**
Youngstown State University
**** I- Indirect Costs**
The CWRU indirect cost on this grant is 53% of the first $25,000 of the grant

SUMMARY PROPOSAL BUDGET YEAR 2

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

ORGANIZATION
Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**400,000**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**400,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**400,000**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **% of MTDC (Rate: 0.00, Base: 0)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*
Allen D Hunter

DATE

ORG. REP. TYPED NAME & SIGNATURE*

DATE

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

SUMMARY PROPOSAL BUDGET COMMENTS - Year 2

**** G-5 Subcontracts**
Youngstown State University

SUMMARY PROPOSAL BUDGET YEAR 3

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

ORGANIZATION: **Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**400,000**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**400,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**400,000**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **% of MTDC (Rate: 0.00, Base: 0)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** 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

SUMMARY PROPOSAL BUDGET COMMENTS - Year 3

**** G-5 Subcontracts**
Youngstown State University

SUMMARY PROPOSAL BUDGET YEAR 4

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

ORGANIZATION
Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**400,000**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**400,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**400,000**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **% of MTDC (Rate: 0.00, Base: 0)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE*
DATE

FOR NSF USE ONLY
INDIRECT COST RATE VERIFICATION

Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET COMMENTS - Year 4

**** G-5 Subcontracts**
Youngstown State University

SUMMARY PROPOSAL BUDGET YEAR 5

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

ORGANIZATION
Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**400,000**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**400,000**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**400,000**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **% of MTDC (Rate: 0.00, Base: 0)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE*
DATE

FOR NSF USE ONLY
INDIRECT COST RATE VERIFICATION

Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET COMMENTS - Year 5

**** G-5 Subcontracts**
Youngstown State University

SUMMARY PROPOSAL BUDGET

Cumulative

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

ORGANIZATION
Case Western Reserve 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 - none**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5. **Menachem Shoham - none**	**0.00**	**0.00**	**0.00**	**0**	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
TOTAL EQUIPMENT				**0**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**0**	
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				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**1,986,750**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**1,986,750**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**1,986,750**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**13,250**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**2,000,000**	
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)				$ **2,000,000**	$

M. COST SHARING PROPOSED LEVEL $ **0** 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

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

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

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**	$ **11,667**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**4**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**2.00**	**11,667**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**1**) POST DOCTORAL ASSOCIATES	**5.30**	**0.00**	**0.00**	**16,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**27,667**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**6,870**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**34,537**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
1. CCD Single Crystal Diffractometer $ **101,000**					
2. Powder Diffractometer **51,000**					
3. Film Diffraction System **20,000**					
Others (See Budget Comments Page...) **119,000**					
TOTAL EQUIPMENT				**291,000**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**10,000**	
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				**29,593**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**10,000**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**39,593**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**375,130**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 27667)**					
TOTAL INDIRECT COSTS (F&A)				**11,620**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**386,750**	
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)				$ **386,750**	$

M. COST SHARING PROPOSED LEVEL $ **750,369** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE* DATE

FOR NSF USE ONLY

INDIRECT COST RATE VERIFICATION

Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET COMMENTS - Year 1

**** B-1 Post Doctoral Associates**
For all budget years, Diffraction Lab Scientist, senior postdoctoral/research associate level, NSF contribution 2/3, YSU contribution 1/3 ($36,000 annual salary). In year 1, this appointment is for a total of 8 months.
**** C- Fringe Benefits**
For all budget years, the YSU fringe benefit rate is 32% for the academic year and 15% for the summer for 9 month appointments, 32% for the calendar year for 12 month appointments, and 1% for students.
**** C- Total Salaries, Wages and Fringe Benefits**
For all budget years, matching contributions for salaries, wages, and benefits for other project participants are summarized in the Budget Justification section.
**** D- Equipment**
1. CCD Single Crystal Diffractometer (Amount: $ 101000)
The total purchase price for the system is $303,000 with a $202,000 match.
2. Powder Diffractometer (Amount: $ 51000)
The total purchase price for the system is $153,000 with a $102,000 match.
3. Film Diffraction System (Amount: $ 20000)
The total purchase price for the system is $60,000 with a $40,000 match.
4. Protein Crystallography Data System (Amount: $ 20000)
The total purchase price for the system is $60,000 with a $40,000 match.
5. Single Crystal Diffractometer (Amount: $ 40000)
The total purchase price for the system is $120,000 with a $80,000 match.
6. Diffractometer Upgrade (Amount: $ 25000)
The total purchase price for the system is $50,000 with a $25,000 match.
7. MB-CAT Beamline Components at APS (Amount: $ 34000)
The total purchase price for these components is $102,000 with a $68,000 match.

The total permanent equipment is for equipment costing $848,000 with a $557,000 match to the $291,000 request.

SUMMARY PROPOSAL BUDGET COMMENTS - Year 1

**** E-1 Domestic Travel**
For all budget years, anticipated travel is to US destinations by car or economy air fare.
**** E- Travel**
For all budget years, this amount for travel to assess and disseminate results and for the instructors at the summer courses.
**** F-1 Stipends**
For the subsequent 4 budget years this category includes funds for undergraduate faculty and student research participants in ADSC funded research programs.
**** G-1 Materials and Supplies**
This amount includes $20,000 in total for software and data base packages and $9,593 for ADSC materials and supplies.
**** G-2 Publication Costs/Documentation/Dissemination**
For all budget years, this amount includes funds for non-travel assessment and dissemination activities (e.g., telephone, printing, postage, conference registrations, publication costs).
**** G- Total Other Direct Costs**
For all budget years, matching contributions to other direct costs are summarized in the Budget Justification section.
**** I- Indirect Costs**
For all budget years, the YSU overhead rate is 42% of total salaries and wages.

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**	$ **12,250**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **Sherri R Lovelace-Cameron - Coordinator**	**0.00**	**0.00**	**1.00**	**4,991**	
5. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**3.00**	**17,241**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**1**) POST DOCTORAL ASSOCIATES	**8.00**	**0.00**	**0.00**	**24,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**41,241**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**10,267**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**51,508**	
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)				**10,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **127,500**					
2. TRAVEL **10,000**					
3. SUBSISTENCE **10,000**					
4. OTHER **105,000**					
(**81**) TOTAL PARTICIPANT COSTS				**252,500**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**48,671**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**10,000**	
3. CONSULTANT SERVICES				**10,000**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**68,671**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**382,679**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 41241)**					
TOTAL INDIRECT COSTS (F&A)				**17,321**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **319,657** 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 COMMENTS - Year 2

**** B-1 Post Doctoral Associates**
This appointment is for a total of 12 months with 1/3 YSU match.
**** F-1 Stipends**
15 faculty and 6 student research participants, 40 summer course participant, and 20 high school participants.
**** F-2 Travel**
For all subsequent budget years, this amount for travel for ADSC participants to collect data at remote sites (e.g., the federal labs), to disseminate their results, and to attend the summer courses.
**** F-3 Subsistence**
For all subsequent budget years, this amount includes funds for ADSC participants at the intensive summer diffraction methods courses and at remote data collections.
**** F-4 Other**
For all subsequent budget years, this amount includes ADSC participants' materials and supplies.
**** G-1 Materials and Supplies**
This amount includes $20,000 in total for software and data base packages and $28,671 for ADSC materials and supplies.
**** G-3 Consultant Services**
For all subsequent budget years, this amount includes stipends for the instructors at the intensive summer diffraction methods courses.

SUMMARY PROPOSAL BUDGET YEAR 3

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. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **Sherri R Lovelace-Cameron - Coordinator**	**0.00**	**0.00**	**1.00**	**5,240**	
5. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**3.00**	**18,103**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**1**) POST DOCTORAL ASSOCIATES	**8.00**	**0.00**	**0.00**	**24,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**42,103**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**10,395**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**52,498**	
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)				**10,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **127,500**					
2. TRAVEL **10,000**					
3. SUBSISTENCE **10,000**					
4. OTHER **105,000**					
(**81**) TOTAL PARTICIPANT COSTS				**252,500**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**47,319**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**10,000**	
3. CONSULTANT SERVICES				**10,000**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**67,319**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**382,317**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 42103)**					
TOTAL INDIRECT COSTS (F&A)				**17,683**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **325,598** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY
Allen D Hunter		INDIRECT COST RATE VERIFICATION
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SUMMARY PROPOSAL BUDGET COMMENTS - Year 3

**** B-1 Post Doctoral Associates**
This appointment is for a total of 12 months with 1/3 YSU match.
**** F-1 Stipends**
15 faculty and 6 student research participants, 40 summer course participant, and 20 high school participants.
**** G-1 Materials and Supplies**
This amount includes $20,000 in total for software and data base packages and $27,319 for ADSC materials and supplies.

SUMMARY PROPOSAL BUDGET — YEAR 4

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**	$ **13,506**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **Sherri R Lovelace-Cameron - Coordinator**	**0.00**	**0.00**	**1.00**	**5,502**	
5. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**3.00**	**19,008**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**1**) POST DOCTORAL ASSOCIATES	**8.00**	**0.00**	**0.00**	**24,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**43,008**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**10,531**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**53,539**	
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)				**10,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **135,000**					
2. TRAVEL **10,000**					
3. SUBSISTENCE **10,000**					
4. OTHER **84,000**					
(**90**) TOTAL PARTICIPANT COSTS				**239,000**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**59,398**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**10,000**	
3. CONSULTANT SERVICES				**10,000**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**79,398**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**381,937**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 43008)**					
TOTAL INDIRECT COSTS (F&A)				**18,063**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **301,836** — AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE* — DATE

FOR NSF USE ONLY — INDIRECT COST RATE VERIFICATION

Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET COMMENTS - Year 4

**** B-1 Post Doctoral Associates**
This appointment is for a total of 12 months with 1/3 YSU match.
**** F-1 Stipends**
12 faculty and 18 student research participants, 40 summer course participant, and 20 high school participants.
**** G-1 Materials and Supplies**
This amount includes $20,000 in total for software and data base packages and $39,398 for ADSC materials and supplies.

SUMMARY PROPOSAL BUDGET

YEAR 5

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**	**4.00**	$ **29,071**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **Sherri R Lovelace-Cameron - Coordinator**	**0.00**	**0.00**	**2.00**	**11,843**	
5. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**6.00**	**40,914**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**1**) POST DOCTORAL ASSOCIATES	**10.70**	**0.00**	**0.00**	**32,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**72,914**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**16,377**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**89,291**	
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)				**20,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **60,000**					
2. TRAVEL **20,000**					
3. SUBSISTENCE **20,000**					
4. OTHER **56,000**					
(**128**) TOTAL PARTICIPANT COSTS				**156,000**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**64,086**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**20,000**	
3. CONSULTANT SERVICES				**20,000**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**104,086**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**369,377**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **42% of total salaries and wages (Rate: 42.00, Base: 72914)**					
TOTAL INDIRECT COSTS (F&A)				**30,623**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**400,000**	
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)				$ **400,000**	$

M. COST SHARING PROPOSED LEVEL $ **346,823** 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 COMMENTS - Year 5

**** B-1 Post Doctoral Associates**
This appointment is for a total of 16 months over the 5th year and into the 6th year with 1/3 YSU match.
**** F-1 Stipends**
8 faculty research participants, 80 summer course participants, and 40 high school participants.
**** G-1 Materials and Supplies**
This amount includes $20,000 in total for software and data base packages and $44,086 for ADSC materials and supplies.

SUMMARY PROPOSAL BUDGET

Cumulative

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

ORGANIZATION: **Youngstown State University**

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

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Allen D Hunter - Project Director**	**0.00**	**0.00**	**12.00**	$ **79,357**	$
2. **Bryan M Craven - none**	**0.00**	**0.00**	**0.00**	**0**	
3. **Mark D Foster - none**	**0.00**	**0.00**	**0.00**	**0**	
4. **Sherri R Lovelace-Cameron - Coordinator**	**0.00**	**0.00**	**5.00**	**27,576**	
5. **A. Alan Pinkerton - none**	**0.00**	**0.00**	**0.00**	**0**	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**5**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**17.00**	**106,933**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**5**) POST DOCTORAL ASSOCIATES	**40.00**	**0.00**	**0.00**	**120,000**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**226,933**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**54,440**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**281,373**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) **$ 291,000**					
TOTAL EQUIPMENT				**291,000**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				**60,000**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **450,000**					
2. TRAVEL **50,000**					
3. SUBSISTENCE **50,000**					
4. OTHER **350,000**					
(**380**) TOTAL PARTICIPANT COSTS				**900,000**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**249,067**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**60,000**	
3. CONSULTANT SERVICES				**50,000**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**359,067**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**1,891,440**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**95,311**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**1,986,751**	
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)				$ **1,986,751**	$

M. COST SHARING PROPOSED LEVEL $ **2,044,283** AGREED LEVEL IF DIFFERENT $

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

ORG. REP. TYPED NAME & SIGNATURE* DATE

FOR NSF USE ONLY

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)**

Budget Justification

A. Senior Personnel *A1. Dr. Allen D. Hunter:* As the Director of the ADSC, Dr. Hunter will be responsible for grant management, coordination with all other institutions, and the consortiums' organization, operation, assessment, and dissemination activities. In addition, he will be involved in his own research efforts, diffraction instructional development and summer school teaching, managing the consortium's central diffraction lab, and writing grant proposals for the ADSC. Funding is requested in the proposal for 12 months of summer support (i.e., 2/9 support in the 1st through 5th years and funds to be carried over into the 6th summer) at a total cost or $91,259 for salary and benefits. In recognition of the importance of his role to the consortium, Youngstown State University, YSU, has agreed to reduce his teaching load for the life of the grant (i.e., by 100% in its first year, 50% in each of the next 4 years and during the subsequent project completion/reporting year) for a total match of $270,336.

A2. Dr. Sherri Lovelace-Cameron: As Coordinator of Minority Enhancement Programs, Dr. Lovelace will be responsible for the consortiums research and educational activities for high school students, especially for members of historically underrepresented groups. She will also be responsible for her own research using crystallography and for writing grant proposals related to minority programs. Funding is requested in the proposal for 5 months of summer support at a total cost of $31,714 for salary and benefits. In recognition of her importance to the consortium, YSU has agree to reduce her teaching load for the life of the grant by 1/6 (i.e., one course per year) for a total match of $52,003.

A6. Other Senior Personnel: No salary support is requested from NSF for the other senior personnel involved in this project at the host institutions. To support consortium activities, YSU has agreed to assign at least two additional faculty members each year to supporting the ADSC goals with each to receive a 1/3 reduction in their academic year teaching loads. Dr. Timothy R. Wagner will be responsible for coordinating the powder diffraction activities at the YSU facility and his own crystallographic research efforts for a match value of $119,383 while Dr. Michael Serra will be responsible for coordinating the protein diffraction activities at the YSU facility and his own crystallographic research efforts for a match value of $108,958. In addition, Drs. Hunter, Wagner, and Serra will act as advisors to ADSC participants. In total, the YSU match for senior personnel is $550,680 for salaries and benefits.

B. Other Personnel *B1. Post Doctoral Associates.* The Diffraction Lab Scientist will be at the senior post doctoral level and will be responsible for the daily operation of the YSU diffraction lab. They will assist on-site users with crystal mounting, diffractometer operation, data collection, structure solution, report preparation, and data base searches. This person will perform these functions for off-site users who submit sample by mail. They will also be involved in summer school instruction. This position will be at the senior post doctoral level and will carry a 12 monthly salary of $36,000 (i.e., $11,520 in benefits). As a demonstration of its commitment to the importance of this position for the consortium's operation, YSU has agreed to provide a match of 1/3 of this person's salary and benefits (i.e., total match of $79,200 with $158,400 requested from NSF). 60 months of support from NSF and YSU are budgeted including 8 in the first year of this grant and 4 extending into the summer of the 6th year.

B2. Other Professionals. To support ADSC activities and ensure that the requested diffraction equipment is well maintained, YSU has agreed to assign a skilled electronic instrumentation specialist, Ray Hoff, to this project at 25% of his time. This has a match value of $92,687 for salary and benefits over 5 years. In addition, a computer networking specialist, Randy Ziobert, will be assigned to this project 5% of his time and additional computer lab assistants will be provided during YSU summer courses to a total match value of $22,103.

B5. Secretarial. To support it lead role in ADSC activities, YSU will provide a new 10 hour per week clerical position for the five years of the project plus the 6th year at a total match value of $47,613 for salary and benefits.

B6. Other. In total, the YSU match for other personnel is $241,603 and for all personnel is $792,283 over the life of the grant for salaries and benefits.

C. Fringe Benefits The YSU rate for fringe benefits is 32% for 9 and 12 month appointments, 15% for summer salaries on 9 month appointees, and 1% on students.

D. Equipment All of the permanent equipment requested in this grant is budgeted in the first year. All of this equipment will be available to undergraduate faculty and student ADSC participants at no direct cost for the life of the grant for 50% or more of its operating time (100% in the case of the YSU equipment). This instrumentation, plus that at Indiana University of PA, will be used for the large majority of crystallographic instruction and almost all "routine" and much of the advanced single crystal and powder research and teaching activities of undergraduate faculty and student ADSC participants. The total NSF request for this equipment is $291,000 towards a purchase cost of $848,000. The large cash match of $557,000 being offered (i.e., 66% of the total system costs) demonstrates the very high level of commitment of these institutions to its purchase.

D1. CCD Single Crystal Diffractometer. This instrument to be placed at YSU includes a Bruker AXS SMART 1000 1K CCD diffractometer system with Peltier cooling and water chiller, Mo and Cu phosphor kits, PLATFORM goniometer and goniometer heads, safety enclosure, water to water refrigerated heat exchanger, He beam path, 3 kW sealed tube X-ray generator, Cu, Mo, and Ag X-ray tubes, graphite monochromator and tubular collimator, Mono-Capillary Optics Labyrinth, video crystal mounting system, Oxford Cryostream low temperature system, diffractometer control system with SMART/ASTRO/SAINT, and off-line data system with SHELXTL site license. We have investigated upgrading one of our Siemens P4 diffractometers to this configuration. However, the total upgrade cost was only about $30,000 lower than a new purchase and there are significant limitations inherent in using area detectors on full circle goniometers. In addition, the P4 would be lost to further instructional and research use. We therefore determined that it made more sense to purchase a new system having a package price of $303,000. YSU will provide a 2/3 cash match and we are therefore requesting only $101,000 from NSF.

D2. Powder Diffractometer. This instrument to be placed at YSU includes a Bruker AXS D8 ADVANCE powder diffractometer, safety enclosure, a 3 kW sealed tube X-ray generator, water to water refrigerated heat exchanger, Cu and Co X-ray tubes, serial detector, long track for mounting our current X-1000 multi wire area detector, a complete set of filters, slits, monochromators, Ni foils, etc., both capillary and 9-position sample stages, a Gobel mirror for Cu radiation, and diffractometer control system with DIFFRAC^{plus} Basic and Search software. This has a package price of $153,000 with YSU providing a 2/3 cash match, we are requesting only $51,000 from NSF.

D3. Film Diffraction System. This instrument to be placed at YSU includes a sealed tube X-ray generator with water to water refrigerated heat exchanger, X-ray tube, and safety enclosure and Weissenberg, Precession, Guinier, and Debye-Scherrer cameras. It will replace a 30+ year old X-ray generator and Precession camera that does not meet current radiation safety standards and is no longer operable. This has a package price of $60,000 with YSU providing a 2/3 cash match, we are requesting only $20,000 from NSF.

D4. Protein Crystallography Data System. This package to be placed at Youngstown State University/Case Western Reserve University includes SGI computer(s) and peripherals to be used in solving data sets collected at consortium diffractometers to obtain protein crystal structures. All current systems are fully saturated. This has a package price of $60,000 with YSU/CWRU providing a 2/3 cash match, we are requesting only $20,000 from NSF.

D5. Single Crystal Diffractometer. This system to be placed at Wright State University includes a Nonius MACH3 single crystal diffractometer and X-ray generator, FR558SH low temperature system, and diffractometer control system and data processing computer. This system is replacing an aging CAD4 diffractometer which has reached the end of its useful life and for which spares for it and its data system are no longer available. This has a package price of $120,000 with Wright State providing a 2/3 cash match, we are requesting only $40,000 from NSF.

D6. Diffractometer Upgrade. This is for an upgrade by Bruker AXS to the R3 single crystal diffractometer at Bucknell University which has become unreliable and difficult to support due to its age. This has a package price of $50,000 with Bucknell providing a 1/2 cash match, we are requesting only $25,000 from NSF.

D7. MB-CAT Beamline Components at APS. This package includes a total contribution of $102,000 to support the construction of a new X-ray line at the Advanced Photon Source (specifically the Beamline Aperture and Collimator System) by the Molecular Biology Collaborative Access Team. This has a package price of $102,000 with YSU/University of Toledo providing a 2/3 cash match, we are requesting only $34,000 from NSF.

E. Travel The total travel request of $60,000 is designated for domestic travel and subsistence. All travel will be by car or lowest cost air fare. This travel will be for the following purposes: to collect data at remote sites (particularly national labs and to ADSC labs having area detector equipped diffractometers), to visit the many ADSC sites to assess consortium activities and disseminate results, and to disseminate consortium research and educational results at regional and national scientific meetings.

F. Participant Support Costs These funds have two purposes for the ADSC, to support participants in the ADSC summer courses in X-ray diffraction and to support the Undergraduate Faculty and Student Research Participants in the consortium's activities. To minimize the overhead costs to our budget (which for YSU cover only salaries and wages), these Research Participants (the large majority of which will be neither from, nor working at, YSU) will not be classified as YSU employees. Rather, they will be designated as visiting scientists and given performance based stipends which carry no overhead charges. Given these factors, and following the RSEC RFP and the GPG guidelines, we have decided to include the costs associated with their research to be funded by the RSEC grant under the budget lines of Participant Support Costs section.

F1. Stipends. The stipends for 50 Undergraduate Faculty and 30 Student Research Participants to be funded by this grant are $7,500 (a flat rate not to exceed 2/9 of academic year salary) and $2,5000, respectively, for a total NSF request of $450,000. These stipends are for a minimum of two months summer research and their values are similar to, or lower than, those provided directly by external granting agencies. There will be 15, 15, 12, and 8

Undergraduate Faculty Research Participants in the 2nd, 3rd, 4th, and 5th years of the grant, respectively, and 6, 6, and 18 Student Research Participants in the 2nd, 3rd, and 4th years of the grant, respectively. The home institutions will generally be expected to reduce the teaching loads of the Undergraduate Faculty Research Participants in the year following their summer support to facilitate the integration of its results into their teaching and research and into the external grant applications that will be required of them. It is expected that an average of at least a 1/6 reduction in teaching will be offered for a value of $10,000 (salary and benefits) producing a match from these institutions of $500,000. There will be no NSF funding for stipends for the 200 attendees at the summer crystallography courses or the 100 participating high school students.

F2. Travel. NSF travel funding of $50,000 in this section will support travel by Undergraduate Faculty and Student Research Participants to remote sites to collect diffraction data (particularly the national labs and to ADSC labs having area detector equipped diffractometers), to attend conferences to disseminate their research and educational results, and for all participants in the ADSC summer courses to attend these courses.

F3. Subsistence. NSF Funding for subsistence of $50,000 will cover the housing costs of participants in the summer courses (i.e., at a rate of $10-15 per day) as well as a meal pass for visiting instructors (i.e., at a rate of $15 per day). These room rates are provided at a substantial discount from full cost recovery and commercial rates and the reduction corresponds to a match of $100,000 from YSU.

F4. Other Participant Costs. An NSF funding request totaling $350,000 is included under this heading for the materials and supplies for the Undergraduate Faculty research participants. In the budget, each of the 50 Undergraduate Faculty Research Participants is budgeted for a total of $7,000 in research support (i.e., for X-ray supplies, reagents, cryogens, and diffractometer usage charges (where applicable)) which is a modest amount to support a summer's research.

G. Other Direct Costs *G1. Materials and Supplies.* This NSF request will fund the crystallography/diffraction methods software packages and data bases which will be provided to all participants from undergraduate schools in ADSC activities (i.e., both research and teaching, $20,000 each year). It also funds X-ray diffraction supplies and consumables (e.g., cryogens, X-ray tubes, reagents) for the summer courses, and for faculty and student research projects not included in the participant support section above at a total cost of $149,067 loaded most heavily on the final years (these include faculty and students doing consortium sponsored research but not receiving consortium summer support).

G2. Publication Costs/Documentation/Dissemination. The budget includes $60,000 to cover the non-travel costs related to assessment and dissemination for the research and educational results of the ADSC efforts, including: duplicating of electronic media, printing, page charges, postage, and phone costs.

G3. Consultant Services. This category includes $50,000 to fund the stipends for the instructors in the summer courses in crystallography who will be paid approximately $1,000 per week for their instructional efforts.

G6. Other Direct Costs. To ensure that the instrumentation to be placed at YSU is fully maintained, YSU will provide a maintenance budget for the X-ray diffraction facility of $15,000 each year and will provide $20,000 to renovate the room in Ward Beecher hall in which the diffractometers will be placed for a total match of $95,000.

H/I/J/L. Total Direct Costs, Total Indirect Costs, and Total NSF Request The total of direct costs in the budget is $1,891,439. By placing all of the Undergraduate Faculty and Student Research Participants in the described categories, we have been able to keep the indirect cost contribution to this budget to $95,311 for YSU and $13,250 for CWRU out of a NSF request for $2,000,000 (i.e., 5.4%).

M. Cost Sharing Proposed Level To demonstrate the major importance placed on this proposal and its activities, the participating institutions are proposing a total match of over $2,000,000 (i.e., in excess of 100%). This includes a 66% match of $557,000 from participating institutions to go with the NSF request of $291,000 for diffraction equipment.

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: **The Ohio NMR Consortium: Phase II Development**

Source of Support: **Ohio Board of Reagents Investment Fund**
Total Award Amount: $ **3,000,000** Total Award Period Covered: **06/01/99 - 06/01/02**
Location of Project: **A consortium of 18 Ohio universities including YSU**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

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

Project/Proposal Title: **Protein Crystal Growth, X-Ray Diffraction, and the National Research Enterprise**

Source of Support: **Ohio Board of Reagents Investment Fund**
Total Award Amount: $ **786,800** Total Award Period Covered: **06/01/99 - 06/01/02**
Location of Project: **A consortium of 5 Ohio institutions including YSU**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **3.00** 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 Investment Fund**
Total Award Amount: $ **2,980,000** Total Award Period Covered: **06/01/99 - 06/01/02**
Location of Project: **A consortium of 9 Ohio institutions including YSU**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

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

Project/Proposal Title: **Advanced Diffraction Studies Consortium (ADSC): An Exciting Opportunity For Integrating Predominantly Undergraduate Institutions Into The National Research**

Source of Support: **Ohio Board of Reagent Action Fund**
Total Award Amount: $ **266,000** Total Award Period Covered: **06/01/99 - 06/01/04**
Location of Project: **A consortium of 4 Ohio institutions including YSU**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **4.00** Sumr: **0.00**

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

Project/Proposal Title: **Investigative Approaches in the Natural Sciences**

Source of Support: **NSF**
Total Award Amount: $ **183,579** Total Award Period Covered: **07/01/98 - 07/01/01**
Location of Project: **YSU**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **1.00** Sumr: **1.00**

*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: **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/Size Exclusion**

Source of Support: **NSF**

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

Location of Project: **YSU**

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

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

Project/Proposal Title: **Aquisition of a CCD Diffractometer**

Source of Support: **NSF - RUI**

Total Award Amount: $ **120,000** Total Award Period Covered: **09/01/99 - 09/01/01**

Location of Project: **YSU**

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: **Diffraction Methods in the College and Pre-College Curriculum**

Source of Support: **NSF - CCLI**

Total Award Amount: $ **200,000** Total Award Period Covered: **10/01/99 - 10/01/02**

Location of Project: **YSU**

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: **Dreyfus Teacher/Scholar at Youngstown State University**

Source of Support: **Dreyfus Foundation**

Total Award Amount: $ **100,000** Total Award Period Covered: **06/01/00 - 06/01/02**

Location of Project: **YSU**

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

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

Project/Proposal Title: **Support for the Acquisition of a Diffractometer**

Source of Support: **Dreyfus Foundation**

Total Award Amount: $ **40,000** Total Award Period Covered: **01/01/00 - 01/01/01**

Location of Project: **YSU**

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

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*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: **Bryan Craven**

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: **Aquisition of a Powder X-ray Diffractometer**

Source of Support: **NSF**

Total Award Amount: $ **162,600** Total Award Period Covered: **08/01/98 - 08/01/00**

Location of Project: **Indiana University of Pennsylvania**

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

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: **Mark Foster**	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: **In Situ Study of Protein Adsorption to Well-defined Surfaces Using Neutron Reflectometry**

Source of Support: **The Whitaker Foundation**
Total Award Amount: $ **210,000** Total Award Period Covered: **12/01/95 - 05/30/99**
Location of Project: **The University of Akron**
Person-Months Per Year Committed to the Project. Cal:**1.50** Acad: Sumr:

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

Project/Proposal Title: **Functionally Tailored Fibers and Fabrics Research**

Source of Support: **Army Research Office**
Total Award Amount: $ **267,000** Total Award Period Covered: **02/01/96 - 11/30/98**
Location of Project: **The University of Akron**
Person-Months Per Year Committed to the Project. Cal:**1.50** Acad: Sumr:

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

Project/Proposal Title: **Tackifier Interface Segregation in Pressure Sensitive Adhesives**

Source of Support: **Army Research Office**
Total Award Amount: $ **130,000** Total Award Period Covered: **08/15/95 - 02/14/99**
Location of Project: **The University of Akron**
Person-Months Per Year Committed to the Project. Cal:**1.00** Acad: Sumr:

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

Project/Proposal Title: **Blends of Linear and Branched Polymers for Useful Materials**

Source of Support: **Army Research Office**
Total Award Amount: $ **137,000** Total Award Period Covered: **03/01/96 - 01/28/99**
Location of Project: **The University of Akron**
Person-Months Per Year Committed to the Project. Cal:**1.00** Acad: Sumr:

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

Project/Proposal Title: **OBR Research Challenge Enhancement**

Source of Support: **Ohio Board of Reagents**
Total Award Amount: $ **20,000** Total Award Period Covered: **03/01/96 - 02/28/99**
Location of Project: **The University of Akron**
Person-Months Per Year Committed to the Project. Cal:**0.10** 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: **Mark Foster**	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: **Molecular Architecture Effect in Bulk and Surface Thermodynamics of Binary Blends**

Source of Support: **ACS-PRF**

Total Award Amount: $ **30,000** Total Award Period Covered: **05/01/96 - 02/28/99**

Location of Project: **The University of Akron**

Person-Months Per Year Committed to the Project. Cal:**0.20** Acad: Sumr:

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

Project/Proposal Title: **Blends of PVC with Branched Vinyl Chloride Polymers for Tailored Interfacial Properties and Improved Processibility**

Source of Support: **Edison Polymer Innovation Corporation**

Total Award Amount: $ **233,060** Total Award Period Covered: **10/01/98 - 09/30/01**

Location of Project: **The University of Akron**

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: **Integrative Graduate Education and Research Training in Interface Engineering of Polymers Integrative Graduate Education and Research Training in Interface Engineering of**

Source of Support: **NSF**

Total Award Amount: $ **782,891** Total Award Period Covered: **07/01/99 - 06/30/04**

Location of Project: **University of Akron**

Person-Months Per Year Committed to the Project. Cal:**1.00** Acad: Sumr:

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

Project/Proposal Title: **In Situ Study of Protein Adsorption to Well-defined Surfaces Using Neutron Reflectometry Transition Funding**

Source of Support: **Whitaker Foundation**

Total Award Amount: $ **70,000** Total Award Period Covered: **12/01/98 - 11/30/99**

Location of Project: **The University of Akron**

Person-Months Per Year Committed to the Project. Cal:**1.50** Acad: Sumr:

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

Project/Proposal Title: **Near Surface Behavior in Adhesives**

Source of Support: **Army Research Office**

Total Award Amount: $ **146,781** Total Award Period Covered: **02/15/99 - 01/14/02**

Location of Project: **University of Akron**

Person-Months Per Year Committed to the Project. Cal:**1.00** 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: **Mark Foster**

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: **Blends with Branched Functionalized Polymers for Controlled Surface Properties**

Source of Support: **Army Research Office**

Total Award Amount: $ **297,536** Total Award Period Covered: **02/15/99 - 01/14/02**

Location of Project: **University of Akron**

Person-Months Per Year Committed to the Project. Cal: **1.00** Acad: Sumr:

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

Project/Proposal Title: **Ohio Board of Regents Research Challenge Enhancement**

Source of Support: **Ohio Board of Regents**

Total Award Amount: $ **20,000** Total Award Period Covered: **02/15/98 - 01/14/02**

Location of Project: **The University of Akron**

Person-Months Per Year Committed to the Project. Cal: **0.10** 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.

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: **A. Alan Pinkerton**

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: **Experimental Charge Densities and Electrostatic Potentials in Energetic Materials**

Source of Support: **ONR**

Total Award Amount: $ **306,429** Total Award Period Covered: **01/08/96 - 01/08/99**

Location of Project: **University of Toledo**

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: **Advanced Crystallographic Study on Energetic Materials**

Source of Support: **ONR**

Total Award Amount: $ **75,000** Total Award Period Covered: **10/01/98 - 06/30/00**

Location of Project: **University of Toledo**

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: **Experimental Electron Densities and Electrostatic Potentials for c-AMP Phophodiesterase Inhibitors**

Source of Support: **American Heart Association**

Total Award Amount: $ **70,000** Total Award Period Covered: **07/01/99 - 06/30/01**

Location of Project: **University of Toledo**

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: **Measurement of Electron Density Distribution of Estrogens - A First Step to Advanced Drug Design**

Source of Support: **DoD**

Total Award Amount: $ **257,962** Total Award Period Covered: **07/01/99 - 06/30/02**

Location of Project: **University of Toledo**

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: **Expansion of an X-Ray Diffraction Facility**

Source of Support: **DoD + OBoR**

Total Award Amount: $ **252,500** Total Award Period Covered: **06/01/99 - 05/30/00**

Location of Project: **University of Toledo**

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

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*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: **A. Alan Pinkerton**

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: **Synthetic, Structural and Mechanistic Study of Di- and Trivalent Lanthanide Reagents**

Source of Support: **NSF**
Total Award Amount: $ **392,438** Total Award Period Covered:
Location of Project: **University of Toledo**
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:

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: **Menachem Shoham**

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: **Crystal Structure of Colicin E3**

Source of Support: **NSF**
Total Award Amount: $ **240,000** Total Award Period Covered: **02/01/98 - 01/31/01**
Location of Project: **Case Western Reserve University**
Person-Months Per Year Committed to the Project. Cal:**1.20** Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Structural Domains Required for Serotonin Receptor Pharmacology**

Source of Support: **NIH**
Total Award Amount: $ **1,146,494** Total Award Period Covered: **07/01/97 - 06/30/01**
Location of Project: **Case Western Reserve University**
Person-Months Per Year Committed to the Project. Cal:**1.80** Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Anti-iodotype-induced Immunity to Pseudomonas areuginosa**

Source of Support: **NIH**
Total Award Amount: $ **788,418** Total Award Period Covered: **07/01/96 - 06/30/01**
Location of Project: **Case Western Reserve University**
Person-Months Per Year Committed to the Project. Cal:**1.20** Acad: Sumr:

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Crystal Structure of a Thermophilic Alcohol Dehydrogenase - Augmentation Award for a Grad Student**

Source of Support: **ARO**
Total Award Amount: $ **67,075** Total Award Period Covered: **05/01/97 - 04/30/99**
Location of Project: **Case Western Reserve University**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** 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: **Parth Basu**	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: **A novel aproach towards understanding the redox properties of molybdenum**

Source of Support: **Research Corporation**
Total Award Amount: $ **33,500** Total Award Period Covered: **05/01/99 - 05/01/00**
Location of Project: **Duquesne University**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

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

Project/Proposal Title: **Design, Synthesis, Structural and Reactivity Studies of Mono-oxo-Mo(VI)**

Source of Support: **ACS-PRF**
Total Award Amount: $ **25,000** Total Award Period Covered: **07/01/99 - 07/01/01**
Location of Project: **Duquesne University**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

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

Project/Proposal Title: **Spectroscopic Analysis of Nitrate Reduction in Geobacter**

Source of Support: **NSF**
Total Award Amount: $ **377,823** Total Award Period Covered: **07/01/99 - 07/01/02**
Location of Project: **Duquesne University**
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

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

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
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: **Gloria Borgstahl**

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: **Career Development Award: Understanding the Role of Replication Protein A and RAD52 in Breast Cancer**

Source of Support: **Army BCRP-97**

Total Award Amount: $ **200,000** Total Award Period Covered: **10/01/98 - 10/01/02**

Location of Project: **University of Toledo**

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: **IDEA: Understanding the Role of Replication Protein A and RAD52 in Breast Cancer**

Source of Support: **Army BCRP-97**

Total Award Amount: $ **276,105** Total Award Period Covered: **10/01/98 - 10/01/01**

Location of Project: **University of Toledo**

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: **Reliably Tagging Recombinant Proteins with Lanthanides for Protein Purification and Solution of the Crystallographic Phase Problem**

Source of Support: **Research Corporation**

Total Award Amount: $ **35,000** Total Award Period Covered: **01/01/98 - 01/01/99**

Location of Project: **University of Toledo**

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: **Supplement to Searching for the Best Protein Crystals: Synchrotron Based Mosaicity Measurements of Crystal Quality and Theoretical Modeling**

Source of Support: **NASA**

Total Award Amount: $ **100,500** Total Award Period Covered: **11/01/97 - 11/01/00**

Location of Project: **University of Toledo**

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: **Searching for the Best Protein Crystals: Synchrotron Based mosaicity Measurements of Crystal Quality and Theoretical Modeling**

Source of Support: **NASA**

Total Award Amount: $ **361,000** Total Award Period Covered: **06/01/97 - 12/01/00**

Location of Project: **University of Toledo**

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: **Janet Del Bene**

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: **Hydrogen Bonding and Proton Transfer: A Cooperative Ab Initio Quantum Chemical and Matrix Isolation Experimental Study**

Source of Support: **NSF**

Total Award Amount: $ **316,000** Total Award Period Covered: **08/01/95 - 07/31/99**

Location of Project: **Youngstown State University & The University of Florida**

Person-Months Per Year Committed to the Project. Cal: Acad: **4.50** Sumr:

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

Project/Proposal Title: **An Ab Initio Study of Vibrational Anharmonicity and Matrix Effects on Hydrogen Bonded Complexes**

Source of Support: **NSF**

Total Award Amount: $ **247,000** Total Award Period Covered: **02/01/99 - 01/31/02**

Location of Project: **Youngstown State University & The University of Sydney, Aus.**

Person-Months Per Year Committed to the Project. Cal: Acad: **4.50** Sumr: **2.00**

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

Project/Proposal Title: **Matrix Isolation and Theoretical Study of the Mechanisms of Oxidation Processes**

Source of Support: **NSF**

Total Award Amount: $ **392,645** Total Award Period Covered: **04/01/99 - 03/31/02**

Location of Project: **University of Cincinnati and Youngstown State University**

Person-Months Per Year Committed to the Project. Cal: Acad: **2.00** Sumr: **1.00**

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:

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*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: **James Gano**

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: **Twist-Twist Pi Conjugated Linear Arrays - Synthesis and Characterization of New Materials with NLO Applications**

Source of Support: **NSF**

Total Award Amount: $ **350,755** Total Award Period Covered:

Location of Project: **University of Toledo**

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: **Protein Crystal Growth, X-Ray Diffraction, and the National Research Enterprise**

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

Total Award Amount: $ **786,800** Total Award Period Covered: **06/01/99 - 06/01/02**

Location of Project: **A consortium of 5 Ohio institutions including UT**

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.

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: **Jayne Giniewicz**

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: **Aquisition of a Powser X-Ray Diffractometer**

Source of Support: **NSF**
Total Award Amount: $ **162,600** Total Award Period Covered: **08/01/98 - 08/01/00**
Location of Project: **Indiana University of Pennsylvania**
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:

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: **David Grossie**	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: 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.

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: **Xiche Hu**

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: 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.

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: **Cam Hubbard**

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: **The Diffraction and Thermophysical Group at ORNL (Cam Hubbard leader) budget (approximate) is shown below which does not include contracts and external grants (details on**

Source of Support: **DOE**

Total Award Amount: $ **3,000,000** Total Award Period Covered: **01/01/99 - 01/01/00**

Location of Project: **ORNL**

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:

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: **John Hughes**

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: **Experiments in X-ray Crystallography: Rare Earth Elements in Titanite, Disorder in LaNi5-ySny Intermetallics, and Rare Earth Elements in Naturally-Occcuring Perovskites**

Source of Support: **NSF**

Total Award Amount: $ **12,420** Total Award Period Covered: **08/01/96 - 07/01/99**

Location of Project: **Miami University**

Person-Months Per Year Committed to the Project. Cal: Acad: **1.00** Sumr: **1.00**

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

Project/Proposal Title: **Determination of Site Occupancy in Multiply-Occupied Atomic Sites**

Source of Support: **NSF**

Total Award Amount: $ **30,302** Total Award Period Covered: **06/01/98 - 06/01/01**

Location of Project: **Miami University**

Person-Months Per Year Committed to the Project. Cal: Acad: **1.00** 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:

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*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: **Alan Jircitano**

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: **A modern FT-IR for Enhancement of the Undergraduate Laboratory**

Source of Support: **NSF-CCLI**
Total Award Amount: $ **25,715** Total Award Period Covered: **07/01/99 - 06/30/01**
Location of Project: **Penn State Erie - The Behrend College**
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:

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: **Margaret Kastner**	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: **Crystallographic CourseWare: Hypermedia Instruction in X-ray Crystallography**

Source of Support: **Camille and Henry Dreyfus Foundation, Inc.**
Total Award Amount: $ **35,000** Total Award Period Covered: **06/01/97 - 06/01/99**
Location of Project: **Bucknell University**
Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **0.00** Sumr: **2.00**

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:

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:

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*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: **Sherri Lovelace-Cameron**

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

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Investigative Approaches in the Natural Sciences**

Source of Support: **NSF**
Total Award Amount: $ **183,579** Total Award Period Covered: **07/01/98 - 07/01/01**
Location of Project: **Youngstown State University**
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: **1.00**

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:

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: **Karen Magnus**

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: **Crystal Structures and Function of Limulus Hemocyanin**

Source of Support: **NSF**

Total Award Amount: $ **510,000** Total Award Period Covered: **03/01/99 - 02/28/04**

Location of Project: **Case Western Reserve University**

Person-Months Per Year Committed to the Project. Cal: **3.00** Acad: **2.00** Sumr: **1.00**

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

Project/Proposal Title: **Crystal Structures and Functions of Limulus Hemocyanin**

Source of Support: **NSF**

Total Award Amount: $ **5,250,000** Total Award Period Covered: **09/01/93 - 08/31/99**

Location of Project: **Case Western Reserve University**

Person-Months Per Year Committed to the Project. Cal: **3.00** Acad: **2.00** Sumr: **1.00**

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:

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:

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*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: **John Protasiewicz**

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: **New Insights and Applications of Multiply Bonded Phosphorus Centers**

Source of Support: **NSF CAREER**

Total Award Amount: $ **325,000** Total Award Period Covered: **01/31/98 - 01/31/02**

Location of Project: **CWRU**

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr: **1.00**

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

Project/Proposal Title: **Soluble Iodonium Ylides as Primary Oxygen Atom and Nitrene Sources**

Source of Support: **ACS PRF**

Total Award Amount: $ **90,000** Total Award Period Covered: **06/01/99 - 08/31/02**

Location of Project: **CWRU**

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

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: **Michael Serra**

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: **Lysozyme as a Model Protein to Investigate the Site-Specific Nature of Polypeptide Fragmentation Using MCO Systems**

Source of Support: **Research Corporation**
Total Award Amount: $ **35,000** 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: Sumr:

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Oxidative Damage and Antioxidants: Structural Characteristics of Site-Specific Protein Oxidation at Atomic Resolution**

Source of Support: **American Heart Association, Ohio Valley Affiliate**
Total Award Amount: $ **65,950** Total Award Period Covered: **07/01/99 - 06/30/01**
Location of Project: **Youngstown State University**
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

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

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
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.

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: **Omar Steward**

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: 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.

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: **Timothy Wagner**

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

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

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

Source of Support: **NSF**

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

Location of Project: **YSU**

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

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

Project/Proposal Title: **Aquisition of a Powder Diffractometer**

Source of Support: **NSF**

Total Award Amount: $ **75,000** Total Award Period Covered: **01/01/00 - 01/01/02**

Location of Project: **YSU**

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

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

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

Source of Support: **Research Corp.**

Total Award Amount: $ **39,719** Total Award Period Covered: **12/31/98 - 12/31/00**

Location of Project: **Youngstown State University**

Person-Months Per Year Committed to the Project. Cal: Acad: **2.00** Sumr: **3.50**

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: **John Woolcock**

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: **Aquisition of a Powser X-Ray Diffractometer**

Source of Support: **NSF**
Total Award Amount: $ **162,600** Total Award Period Covered: **08/01/98 - 01/01/00**
Location of Project: **Indiana University of Pennsylvania**
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:

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: **David Wright**	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: **Magnetic Materials from Malaria**

Source of Support: **Research Corporation**
Total Award Amount: $ **35,000** Total Award Period Covered: **06/01/99 - 06/01/00**
Location of Project: **Duquesne University**
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

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

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
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:

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*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: **Vivien Yee**

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: **Activation an Inhibition of Blood Coagulation Enzymes: X-Ray Crystallographic Studies of Thrombin Complexes**

Source of Support: **American Heart Association**
Total Award Amount: $ **260,000** Total Award Period Covered: **01/01/99 - 12/31/02**
Location of Project: **Cleveland Clinic Foundation**
Person-Months Per Year Committed to the Project. Cal: **2.40** Acad: **0.00** Sumr: **0.00**

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

Project/Proposal Title: **Structure-function studies of the apoptotic protein tissue transglutaminase**

Source of Support: **ACS**
Total Award Amount: $ **14,700** Total Award Period Covered: **06/01/98 - 05/31/99**
Location of Project: **Cleveland Clinic**
Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **0.00** 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:

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: **Edward Zovinka**

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: **Multiply Functionalized Metallocenes**

Source of Support: **ACS-PRF**

Total Award Amount: $ **20,000** Total Award Period Covered: **06/01/97 - 06/01/99**

Location of Project: **Saint Francis College**

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:

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.

H. Facilities, Equipment, and Other Resources

H1. General

As described in section C2, above, diffraction studies can be divided into three levels of sophistication, each of which requires somewhat different levels of expertise, hardware, and software. The "routine level" is characterized by conventional single crystal and powder diffraction studies that make up the large majority of crystallographic experiments carried out in an educational context and/or to solve the structural problems of non-crystallographers. The "advanced level" requires a much more sophisticated knowledge of diffraction methods and access to advanced diffractometers equipped with high intensity sources, area detectors, and/or customized experimental apparatus. The "national resource level" also requires sophisticated knowledge and also access to specialized equipment/facilities that is sufficiently expensive that it tends to exist primarily at national labs. To assist the efficient utilization of diffraction resources, the large majority of the educational and routine crystallographic research will take place at the predominantly undergraduate host institutions (i.e., H2 to H5, below), the advanced level experiments will generally take place at the better equipped participating PhD level host institutions (i.e., H6 to H11, below), and the expert level studies will take place predominantly at participating national labs (i.e., H12 to H14, below). Each of these institutions has dedicated sufficient space, instrument time, and maintenance resources to fulfill its proposed role in the consortium.

H2. Youngstown State University

YSU is currently equipped with two Siemens P4 diffractometers. One is equipped with a Mo tube and is used for single crystal work while the other is equipped with a Cu tube and a X-1000 multiwire area detector and is used mostly for powder studies. These instruments are housed in a dedicated pair of X-ray and computing labs (500 square feet in total) and are maintained by the Chemistry Department's electronic instrumentation specialist, Ray Hoff with support from the campus electronics shop and college and campus computer centers. During Spring and Summer quarters, these instruments are almost 100% utilized for the "hands on" instruction of YSU students and for YSU research. There is currently about 50% free time available for outside users during most Fall and Winter quarters. As part of this proposal, new CCD single crystal, powder, and Film diffractometers will be placed in an adjacent 1,200 square foot laboratory (which will be renovated for this purpose) to which our current diffractometers will also be moved. These will be available full time to ADSC participants for both "hand on" data collection and the submission of samples to the Diffraction Lab Scientist who will collect the data and return it electronically. The provision of these CCD and powder systems will allow undergraduate faculty participants to carry out many of the more advanced experiments there. The YSU Chemistry Department is also equipped with two new computer labs, one having 12 Windows NT and the other 24 Windows 95 machines, as well as four lecture halls equipped with the most modern computer facilities and projection equipment. These are supported by two three year old SGI INDY computers in the crystallography lab. All of the other departmental instrumentation (e.g., on order, new, or recently rebuilt: DSC, TGA, Siemens model 102 TEM, inert atmosphere glove boxes, 400 MHz NMR, GC-MS (2), FT-IR, ICP, etc.,) that may not be available in many of the predominantly undergraduate institutions will also be available to all ADSC members. YSU has a policy of not charging undergraduate faculty and student participants for the use of any of this scientific instrumentation.

H3. Bucknell University

Bucknell is currently equipped with a Bruker R3 single crystal diffractometer and computer labs having PCs and two SGI systems. The R3 will be upgraded as part of this proposal. The resulting instrumentation will be available at no cost to undergraduate faculty and student participants.

H4. Indiana University of Pennsylvania

IUP is currently equipped with a CAD4 single crystal diffractometer and will soon receive a new Bruker AXS D8 powder diffractometer. It will make significant free time on these instruments available at no cost to undergraduate faculty and student participants.

H5. Wright State University

Wright State is currently equipped with an aging CAD4 diffractometer to which will be added a new Nonius MACH3 single crystal system as part of this grant. Wright will make 50% of the time on this instrument available at no cost to undergraduate faculty and student participants.

H6. Carnegie Mellon University

The diffraction equipment at CMU is fully committed to their research programs but Bob Stewart in Chemistry is an expert in the theoretical basis for experimental charge density studies and will collaborate with those interested in working in this area.

H7. Case Western Reserve University, Cleveland Clinic Foundation, and the Cleveland Center for Structural Biology

CWRU, CCF, and the CCSB are well equipped for advanced diffraction studies having two Rigaku rotating anode generators equipped with R-Axis2 and 4 imaging plate detectors for protein crystallography and a newly upgraded Bruker P4 diffractometer for small molecule studies. They also have a crystallization robot from Oxford Cryosystems to aid in protein crystallization studies. In addition, the lab is equipped with sufficient SGI workstations for protein structural studies by their current faculty and students.. Although these instruments are heavily used to support their research programs, time will be made available for collaborative research projects between their faculty and faculty and students from predominantly undergraduate institutions. This grant also includes funds to add additional SGI computer(s) for use in protein structural studies by ADSC visitors.

H8. Duquesne University

Duquesne has a Rigaku AFC7R rotating anode single crystal diffractometer and two Rigaku D/MAX-B powder diffractometers (one with a horizontal and one with a vertical generator). Although these instruments are heavily used to support their research programs, time will be made available for collaborative research projects between their faculty and faculty and students from predominantly undergraduate institutions.

H9. The University of Akron

The Chemistry Department has a conventional single crystal diffractometer while the Polymer Science Institute is equipped with several materials diffractometers, including one with a rotating anode generator and a custom reflectometer, one with a rotating anode generator and a custom surface spectrometer suitable for studying grazing incidence diffraction and evanescent wave induced X-ray fluorescence, and it will soon get one with focussing optics, a 1-D PSD, and a pinhole SAXS setup. It is also exceptionally well equipped for electron microscopy and for solid state NMR at 750 MHz. Although these instruments are heavily used to support their research programs, time will be made available for collaborative research projects between their faculty and faculty and students from predominantly undergraduate institutions.

H10. University of Pittsburgh

Pitt is equipped with a P3 single crystal diffractometer, a AFC5R rotating anode system with a Bruker area detector, and a MAR imaging plate equipped diffractometer. Although these instruments are heavily used to support their research programs, time will be made available for collaborative research projects between their faculty and faculty and students from predominantly undergraduate institutions.

H11. University of Toledo

UT is home to the Ohio Crystallography consortium and is equipped with a Siemens 1K SMART CCD equipped diffractometer for Mo, a rotating anode system equipped with an imaging plate detector for Cu, and a Siemens 2K SMART CCD equipped diffractometer for Cu, Mo, and Ag and for temperature studies down to 20 K. Although these instruments are heavily used to support their research programs, time will be made available for collaborative research projects between their faculty and faculty and students from predominantly undergraduate institutions.

H12. Advanced Photon Source

The CWRU/CCF/CCSB are participating with a group of 7 to 9 other major research institutions in the Midwest in developing a new X-ray line (i.e., the Molecular Biology-Collaborative Access Team, MB-CAT) on the Advanced Photon Source in Chicago. They will be putting up $500,000 to buy a 1/8 to 1/10 share in the time on this line. Through the participation of the Cleveland team in the MB-CAT, and the participation of YSU and UT in their effort, the undergraduate faculty and students participants in the ADSC will have priority access to this ultra high intensity tunable X-ray source. Access to this national resource level facility will be particularly valuable for the study of protein structures (especially using MAD phasing) and for the analysis of extremely weakly diffracting crystals.

H13. NASA Lewis Research Center

The NASA Lewis center is well equipped to study advanced solid state materials including polymers and inorganic solids. They are very interested in collaborating with undergraduate faculty and student participants.

H14. Oak Ridge National Lab

ORNL is an extremely well equipped national resource level facility that contains the High Temperature Materials Lab for diffraction studies under extremes of temperature and/or pressure, the High Flux Isotope Reactor as the most intense thermal neutron source in the western hemisphere, and the Shared Equipment Research Center. Through the involvement of ORNL, ADSC participants will also have a gateway into the other federal labs with an emphasis on diffraction methods.