NSF Division of Chemistry

Research Sites for Educators in Chemistry, RSEC, Program

(and Parallel OBoR Investment Fund and Action Fund Applications)

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

An Outline of the Consortial Proposal

Final Draft for Circulation to Consortium Members

Based on Comments on the First and Second Drafts and on the December 12th Organizational Meeting

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PLEASE FEEL FREE TO MAKE DETAILED SUGGESTIONS FOR ADDITIONS, DELETIONS, AND CHANGES

THESE WILL BE INCORPORATED INTO THE FINAL PROPOSAL.

Highlights of the NSF RFP and Hence the Core of This RSEC Proposal:

The NSF RFP for the RSEC program gives a series of specific directions on the goals of the program and how the proposals will be evaluated. To give us the maximum chance of success, the proposal I outline below follows these very closely, including:

- ♠ The ***Deadline Date for electronic submission of a proposal to this program is January 11th 1999 (i.e., use of the FastLane system is required for the RSEC program)***. I plan on submitting the proposal January 6th and therefore will need everything in my hands by January 4th especially the letters of commitment from the PhD schools and the Biographical Sketches and Current and Pending Support forms from the senior participants.

- ♠ According to the program officer at NSF, Dr. Osteryoung, review will be as expeditious as possible. The complexity and length of the review process will depend on the number of applications submitted. She said to assume a June 1st starting date for planning purposes (i.e., they would like to consortia to begin their activities this coming summer).

- ♠ The *five* consortia to be funded from this program, hopefully including our crystallographic/diffraction consortium, must be appropriate to serve as a national models.

- ♠ Our emphasis is on collaboration between faculty at research universities (i.e., defined as schools offering PhDs in Chemistry), undergraduate institutions (defined in this proposal as schools offering 2 year, BS, MS programs in Chemistry), and high schools and researchers in government and industry labs. In addition, there is an emphasis on collaborations between these institutions.

- ♠ A emphasis on a regional and sustainable groupings of institutions is mandatory. Here our history of previous and ongoing collaborations is very important. In this area, we will show that the size of the consortium described in the proposal is appropriate – the we have a reasonable ratio of research mentors to participants and that a critical mass will develop.

- ♠ The proposed research projects must clearly be of fundamental importance and have attained, or be capable to reaching, national prominence. To this end, I think we can get a boost from the strong credentials of the co-PIs and other Senior Personnel and their national prominence in diffraction research and/or education.

- ♠ A central emphasis on *development, training, and integrating undergraduate school faculty into the "national research enterprise" (i.e., th world of advanced chemical research)* is mandatory and *the most important part of the program* according to the RFP and the program director. This will directly benefit their research and indirectly benefit their teaching.

- ♠ A central emphasis on *research experiences for undergraduates, especially those from non-PhD schools,* is mandatory according to the RFP and the program director. We will include some direct support for this in the later years of this RSEC proposal. However, a major part of this will come in the form of (senior) research projects in crystallography for which data will be collected at the host institutions and solved at the home institutions (e.g., as crystallographic communications or as part of synthetic papers). In addition, I plan on writing a REU application in the summer *from the consortium* (i.e., with several sites but all focused on crystallographic projects) and organizing a list of possible student ROA supervisors.

- ♠ An important emphasis on the *inclusion of members of underrepresented groups* is suggested by the RFP and this will be a major part of our proposal. Does anyone have access to good statistics to underline this need (e.g., the proportion of minorities in our region vs. in our universities and graduate programs and faculties). There must be numbers available from NSF and our university planning offices.

- ♠ I have tried to emphasize that we will be developing a seamless pipeline into the "national research enterprise", starting with efforts at the pre-college level, focusing strongly on undergraduate crystallographic education, and leading through post-graduate training opportunities in diffraction methods for both faculty and students into productive research collaborations. Critical to all of this is the faculty and teacher development and training initiatives in crystallography and the direct involvement of more faculty and teachers in diffraction research.

- ♠ An emphasis on the integration of crystallographic/diffraction research and undergraduate education at all involved institutions and particularly the development of new curricular materials and approaches for teaching diffraction methods and integrating it into our curricula will give us a unique angle.

- ♠ The primary focus of the proposal is supposed to be in areas supported by Chemistry Division with multidisciplinary overlap outside of chemistry allowed. I have asked the program officer specifically about the inclusion of protein and materials structural studies by diffraction and allied methods and she indicated that this was entirely appropriate. I would like to keep a strong balance between these areas, all of which have components funded by NSF and the Chemistry Division.

- A budget of up to **$400,000 per year (overhead included) for 5 years from NSF (i.e., $2,000,000), additional external moneys (e.g., from the OBoR Action Fund), plus internal matches** is allowed. To focus on the program goals, it is essential that this money primarily benefit research and training for faculty and students from predominantly undergraduate schools. To this end, the large majority of the proposed budget is for Fellowships and research and training funds for them. To help ensure that NSF and the reviewers will clearly perceive that we are mainly interested in these goals (and not just supporting current graduate and postdoctoral research programs – which the program officer made clear was not the purpose of this program), significant money that might be construed as primarily supporting current research efforts at the PhD schools will have to be carefully justified. Two areas where we will have to be very careful on are major equipment purchases and salary/maintenance lines, particularly at the PhD granting host institutions, which will require significant match funds and extensive justification. Details on this and other budgetary issues are presented in detail in the Budget Section at the end of this proposal.

- Although the NSF RSEC grant is for 5 years, Dr. Osteryoung has indicated that it would be reasonable and acceptable to extend our activities into the sixth year as a one year no-cost grant extension. Since the consortium's activities will just get started in the summer of 1999 (primarily in terms of ordering equipment and getting it in place), I think it makes sense to schedule activities in the 6th summer and them use that Fall to write up the final report on the activities funded by the grant.

- The establishment of regional chemistry research facilities *accessible to the faculty and students of predominantly undergraduate schools* is key Here it is important that we clearly spell out the instrument access policies/costs for undergraduate faculty and students and for educational offerings, especially for instrumentation partially funded through this RSEC grant. The role of YSU and other host institutions on providing both on-site access across our region and remote access is very important.

- Use of the internet for access to equipment, teleconferencing and virtual meetings, and on-line sharing of library and other resources is suggested in the RFP. Here I think we need to show practical ways that faculty/students from remote sites can access the diffraction facilities. We need to think of how long-distance collaborations can be facilitated, perhaps through "web cams" at each site. We need to think about sharing of library (OhioLink does this for Ohio and Pennsylvania is just beginning to set up a similar system) and other resources (e.g., crystallographic data bases) and how the accessibility barriers to these for those at predominantly undergraduate schools can be overcome. We need to discuss how the costs for these efforts will be born. This can also include distance education opportunities.

- A detailed Evaluation/Assessment plan will be very, very, critical in how this proposal is judged. We need to tie in both internal and external methods. I am proposing that the Project Director be primarily responsible for collecting this data which will be evaluated both internally and by and external assessment committee. We must ensure that clearly adequate funds for these purposes are set aside. I am proposing an external advisory panel composed of interested outsiders who will provide continuing monitoring and advice and have also contacted the ACA Continuing Education Committee for their assistance.

- A detailed Dissemination plan will also be very, very, critical in how this proposal is judged. We need to tie in a variety of methods. I am proposing that the Project Director be heavily involved in this effort which will also be evaluated both internally and by the external assessment committee. We must ensure that clearly adequate funds for these purposes are set aside. Types of dissemination tools will include: talks, papers, and books/manuals, new courses and course materials, and faculty newly qualified to teach diffraction methods at their home departments. These individuals will initially be almost entirely from our region but by the end of the 5 years I expect that they will largely be drawn from a national pool. The summer courses in diffraction methods will be the most important and novel component of our dissemination effort.

- Having a detailed and clearly viable plan for the continued funding of the consortium's activities after the end of the five year period will also be critical in getting this grant funded. This plan will include internal funding and integration into the national research enterprise via conventional external training and research grants. We must set up a strong mechanism to facilitate this process.

- To ensure that the scientific goals outlined in this project will be evaluated as exciting and viable, they are being set up as parallel to those of the research programs of the PIs and other Senior Applicants who are all recognized US and world leaders in crystallography/diffraction methods research, or are newer faculty members already building strong reputations in this area.

- To ensure that the educational goals outlined in this project will be evaluated as exciting and viable, I have attempted to choose several participants with nationally recognized credentials in the area of crystallographic education who are from outside the consortium's region.

Dr. Janet Osteryoung (the Director of the NSF Division of Chemistry and the Program Officer for the RSEC proposals) and I have discussed the broad outlines of this proposal and specific questions several times. She seems very interested in, and supportive of, the idea. She approved my rationale for having myself, a faculty member from a predominantly undergraduate school, as the PI and Project Director. She also supported my reasoning for having YSU, a predominantly undergraduate institution, designated the lead institution. Unfortunately, the letter of the RFP says that the formal managing institution must be a PhD school. To work around this, we will designate a PhD school (i.e., Case) the *formal* managing institution with YSU as the subcontractor for ≈99% of the project. She approved this model and, the geographic distribution I proposed for the consortium, and the broad outline of the scientific breadth of the proposal I presented as appropriate. She was especially interested in my idea of integrating the faculty development/training component of the summer schools as the vital link between pre-college and undergraduate education and the "national research enterprise".

Note: in subsequent parts of this outline where institutions' or individuals' names are followed by a single question mark it means that they have not yet been successfully contacted but that they are expected to participate (however, they might decline) based on their past records and/or recent conversations on related topics. Additional question marks imply that they have not yet been contacted and their number indicates the level of difficulty that I have in estimating whether they would like to participate. In both cases, these individuals/institutions are included to help give a broad outline of the concept behind the proposal and its scope and not to imply/prejudice their decisions.

Rationale for our Approach to Undergraduate Faculty and Students Training and Integrating them into the National Research Enterprise

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 to us. It includes a range of X-ray, neutron, and electron diffraction techniques that are used on single crystal and powdered (polycrystalline and amorphous) samples. To keep our consortium focussed, we will concentrate on X-ray techniques and supporting neutron methods. The information from these methods are best understood in the context of complementary analytical, physical, spectroscopic, thermochemical, theoretical, and reactivity studies. [Note: Although these are generally not discussed in detail (for space reasons) in the following outline, the participating institutions have a wide range of strong people in these areas. If you feel any faculty, at your school or elsewhere, with whom you collaborate in these areas should be explicitly mentioned, then please let me know.]

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* increased the quality of this data. The difficulty in using this new diffractometer hardware and crystallographic software has also rapidly decreased. This increased pace and increased ease 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 and more often 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. It has been widely noted, and succinctly summarized by Bryan Craven, that "more and more structures are being done and more and more structures are being done badly" by methods that strongly resemble "black box crystallography." Responding to the challenges posed by these trends in a positive and productive fashion is central to what we are attempting with this grant application.

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 and at professional conferences and 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 pro forma discussion of Bragg's law in several undergraduate courses along with, perhaps, the odd powder diffraction lab, 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, some excellent. 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. [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 problems 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 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, publishing, and getting funded competitive research projects. 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 the 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 and software 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.

Institutions Involved in the Proposed Diffraction Consortium

As with the other sections of this outline, please feel free to make suggestions for additional institutions, individuals, roles, etc. In particular, individuals initially placed in one of the personnel categories (often largely on my intuition of their likely wishes) may actually desire to be placed in another.

- ♠ The proposed consortium is composed of schools in a band running along the south shore of Lake Erie from Toledo to Pittsburgh, namely those in northern Ohio and western Pennsylvania. I have attempted to keep the consortium as regionally concentrated as possible because this is one of the key instructions in the RFP. In addition, this will help us to retain our intellectual focus and to keep our limited resources concentrated into a critical density.

- ♠ Note: I have considered expanding our consortium to institutions having strong crystallography credentials just outside our "boundaries" (e.g., Penn State, U. Michigan Ann Arbor, SUNY Buffalo, the Hauptman Woodward Institute, and OSU). However, I have not done so to help us keep our focus. The consortium already has a relatively large set of participants in terms of institutions and individuals. In addition, I think that the current participants are appropriate in terms of our budget.

- ♠ I have expanded the consortium's boundaries somewhat for predominantly undergraduate institutions where these and/or their faculty have a history of collaborations with the host institutions. To help us reach our goal of more fully integrating underrepresented minorities, I have also included 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.

- ♠ There seems to be a strong consensus on making the *Lead Institution Youngstown State University*. I have talked extensively to the program officer and NSF Chemistry Division head about this and she has said that this

makes "excellent sense" in terms of the program goals. Because of the RFP language, YSU can not be the formal managing institution, we discussed this and she suggested making one of PhD school participants the formal managing institution with YSU subcontracting almost the whole project. I am working with John Mieyal and the administration at Case to finalize their role.

- The consortium will have institutional members that fit into two 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" from which the bulk of the undergraduate faculty and students will come. There will be some overlap in these two categories, especially for institutions who's 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.

- 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
  - Duquesne University
  - Kent State University
  - The University of Akron
  - University of Pittsburgh
  - University of Toledo (the home of the Ohio Crystallography Consortium diffraction instrumentation)

- 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
  - Youngstown State University

- We will also include the following *Non-University Host Institutions* at which some of the collaborative research projects will take place and/or which are the home bases of some of our research mentors.
  - Advanced Photon Source MB-CAT beam line team from the Cleveland Center for Structural Biology, CCSB.
  - Cleveland Clinic (via its involvement in the CCSB)
  - NASA Lewis Research Center
  - Oak Ridge National Lab
  - Wright-Patterson Air Force Base?

- The following is a listing of the *participating 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 who's

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 participating institutions will generally not be required to provide any materials for inclusion in the proposal beyond a letter indicting their willingness to have their faculty and students participate in Consortial activities. The undergraduate schools in our region will be listed in the proposal as sites from which faculty and students will be eligible to apply for funding.

Please feel free to fill in additional suggestions. The ? marks indicate these schools have not yet been contacted or have not yet responded. Any that do not respond by the time the proposal is submitted will not be named in it but their faculty and students will still be eligible to participate if the grant is funded.

- In this category I include the following *PhD granting participating universities.*
  - Cleveland State University

- I suggest we may include as many of the following *BS granting participating colleges* as possible:
  - Allegheny College
  - Ashland University (does anyone have a contact there)?
  - Bowie State University?
  - California State of PA
  - Carlow College (I have left a phone message for Craig Johnson there)?
  - Central State University (Sherri is contacting them)?
  - Chatham College (I have left a phone message for Lisa Lambert there)?
  - Clarion State University
  - College of Wooster (does anyone have a contact there)?
  - Defiance College (suggested by Jim Gano, does anyone have a contact there)?
  - Edinboro College (I have not got a usable phone number (i.e., not 814-938-2485) for Donald Penn there)?
  - Gannon University
  - Geneva College (I have left a phone message with David Badger there)?
  - Grove City College (this institution may will accept any federal funds and so they can not be listed on the proposal)
  - Hiram College
  - Janiata College (I have sent an e-mail message here)?
  - John Carroll University
  - Lake Erie College (I have sent an e-mail message here and I expect that they will wish to participate)?
  - Lincoln University
  - Malone College (I have sent an e-mail message here and I expect that they will wish to participate)?
  - Mercyhurst College
  - Morgan State University
  - Mount Union College

- Notre Dame College (in Cleveland, does anyone have a contact here???)
- Oberlin College (I am particularly interested in the participation of Oberlin as they have just received a new powder diffractometer and have recently hired several excellent materials people from NIST)
- Ohio Northern University
- Penn State Erie, The Behrend College
- Saint Francis College
- Slippery Rock University
- Thiel College
- University of Pittsburgh at Johnstown (Bryan please contact or get me the contact information)?
- Walsh University (I have sent an e-mail message here and I expect that they will wish to participate)?
- Washington and Jefferson College
- Westminster College

- I suggest we may want to include as many of the following *two year community colleges participants* as possible:
  - Cuyahoga Community College (sp??? Does anyone have contacts there)?
  - Kent State University-Stark Campus
  - Penn State Beaver (I have sent an e-mail message here and I expect that they will wish to participate)?
  - Penn State Shenango?
  - Loraine County Community College
  - Wayne College Community College of UA

- Individual school districts and teachers ???
  - I have begun to contact several high school teachers in the Youngstown area with whom I have close contacts (i.e., they have been my students in the past) and who I expect will want to participate in my efforts in the high school area.

- I have also begun to approach *Industrial partners* both because I feel that their involvement will be valuable in its own right (if for no other reason than that they will employ some of our graduates) and because Dr. Osteryoung indicated that consistent with the program guidelines they would be considered "a big plus and would significantly strengthen the proposal. Included on this list are the major diffraction equipment vendors at which I have contacts. **Please send me lists of your contacts or, better yet, make the initial contacts yourselves and send me the results.**
  - Abbott Labs (I have already contacted them and am awaiting their response, I have also asked J K-B who collaborates with them to contact them on our behalf)?
  - Amoco/BP (I have contacted James Kaduk at Amoco in Chicago but he hasn't gotten back to me yet, does anyone have a contact at BP in Cleveland) ?
  - Bruker AXS (Sue Byram, Chuck Campana, and Bob Sparks are my primary contacts here)
  - Delphi Packard Electric (Paul Shiller)
  - Dow AgroSciences (Scott Thornburgh via Zoltan Benko) ?
  - Ferro Corp. (Jim Kinder is our contact)

- Genencor (I will contact an old friend, Tony Day, who works there) ?
- General Motors, Lordstown (they are sending a letter of support)
- Goodyear (very strong support, our contact is Matt Muir)
- Monarch Analytical (Toledo, suggested by Jim Gano, Ernie Lippert 419-897-9000, Jim will you contact them???)?
- MSC/Rigaku (Cindy Overbey is my primary contact here)
- Nonius (I will contact them about their participation)
- Pfiser (I will contact one of our ex-students who works in the analytical group there) ?
- Phillips (I will contact them about their participation)
- Proctor and Gamble (I have asked J K-B who collaborates with them to contact them on our behalf) ?
- Ricerca, Inc. (Cleveland, suggested by Jim Gano, Tony Gallacher 216-357-3462, at UT PhD, Jim will you contact them???)?
- RP-Rorer (Andrew Allen via Katy Van Kirk)?
- Zirconia (Gale Graves)
- **Please use you industrial contacts an ask corporations with a strong technology component in our region to "sign on board." Examples in our region include PPG, Chrysler (Toledo), BP…. Does anyone have good contacts at these?**

- *The consortium described in the current RSEC proposal has grown out of a range of current collaborations/interactions.* These will be discussed in the text to show that the proposed consortium has not grown out of thin air. In addition, by linking to them we show that we are part of a larger web of research interests. Those of you with strong contact in these and other regional groups, please let me know so that we can add them in. The following come immediately to mind:
  - ACA Crystallographic Summer School Alumni
  - MatNet
  - Ohio Crystallography Consortium, OCC.
  - Ohio NMR Consortium (which has a large structural biology component)
  - OhioLink Library Network
  - Pittsburgh Diffraction Society
  - YSU Center for Photon Induced Processes
  - YSU Public/Private Alliance (includes 10 undergraduate schools in our region)
  - YSU Structure Center

Faculty Involved in the Proposed Diffraction Consortium

- *Principle Investigators* I have asked Dr. Osteryoung, who is the program officer for this proposal, about what number of Co-PIs is reasonable. She said that NSF only records 5 people on their records of a grant, the PI and four co-PIs. We therefore need to pick four individuals out of the many highly qualified people in our consortium to serve as co-PIs. The PI and co-PIs, like the other Senior Personnel, will be asked to submit the full, two page, Biographical Sketches and Current and Pending Support Forms for the grant application.

  I will chose four people from amongst the list of people in the Other Senior Personnel category as the co-PIs. With this number, we need individuals to represent both the research and geographic breadth of the consortium. I also will consider factors like a mix of sizes of institutions, public vs. private institutions, etc. In addition, these people should

have strong national credentials and grant histories on crystallographic/diffraction topics to lend our proposal the maximum "weight" with reviewers

- Allen Hunter (YSU-Chemistry, PI and Program Director, my interests are mainly in the educational aspects of this proposal, I also will begin doing charge density studies on organometallics in collaboration with Bryan Craven soon)
- Bryan Craven (IUP-Chemistry, charge density studies and diffraction education).
- Mark Foster (Akron-Polymer Science, materials diffraction)
- Vivien Yee (CWRU and Cleveland Clinic, protein crystallography)
- Wild card person drawn from any of these areas

- *Other Senior Personnel* As defined by NSF, these individuals will be making *substantial* contributions to the consortial effort. This includes researchers, mostly at the PhD schools, having firm plans described in the proposal to host faculty and students from predominantly undergraduate schools in their research groups. It also includes individuals with established reputations in crystallographic/diffraction education and/or those who will be centrally involved in the crystallographic summer schools. After each individual's name, I give their affiliation and possible suggestions of their primary area(s) of responsibility with respect to this proposal. These individuals will be asked to submit the full, two page, Biographical Sketches and Current and Pending Support Forms, and short descriptions of their research interests. I have discussed with Dr. Osteryoung what she considers a reasonable total number of such Senior Personnel for our project/proposal. She said "we need to strike a balance between having all of the people we need to clearly present our proposal and the space limitations of the proposal." Although the list is a long one, remember that the consortium will fund about 50 Faculty Fellowships and this will require the participation of a significant number of research collaborators. For space reasons in the proposal this list may need to be shortened.

  - Those individual indicated below by * have major federal grants and have indicated an interest in hosting undergraduate faculty via ROA supplements. **If you have such a grant and would be willing to host an undergraduate student of faculty member on an ROA, please let me know.**
  - Alan Pinkerton (UT-Chemistry, CCD technology applied to advanced problems and charge density studies of high energy molecules)
  - Bryan Chakoumakos (Oak Ridge-Solid State Chemistry Division, single crystal and powder studies on HIFIR and a Bryan Craven collaborator)
  - Bryan Craven (IUP-Chemistry, structure determination by X-ray diffraction and charge density studies of small molecules, crystallographic education)
  - Cam Hubbard (Oak Ridge National Labs, diffraction studies under extreme conditions for many extended inorganic solids (and minerals?) and neutron and synchrotron diffraction methods)
  - Casey Raymond (Kent-Chemistry, inorganic/materials chemistry and crystallography)?
  - David Grossie (Wright State University-Chemistry, small molecule crystallography)
  - Gloria Borgstahl (UT-Chemistry, protein crystallography)
  - Jim Gano (UT-Chemistry, OCC Director, NLO materials)
  - John Protasiewicz* (Case-Chemistry, small molecule diffraction)
  - John Rosenberg (Pitt-Biological Sciences, protein crystallographer)
  - Katherine Kantardjieff (Cal. State Fullerton, CMolS crystallography center, protein crystallography and crystallographic education)
  - Margaret Kastner (Bucknell-Chemistry, small molecule diffraction studies and computer aided crystallographic instructional tools)
  - Mark Foster (U Akron-Polymer Institute, materials crystallography)
  - Mike Nathal (NASA-Lewis, Advanced Materials)
  - Omar Steward (Duquesne-Chemistry and Biochemistry, small molecule crystallography)
  - Partha Basu (Duquesne-Chemistry and Biochemistry, metallo-enzymes)

- Sherri Lovelace Cameron (YSU-Chemistry, Coordinator of Minority Enhancement Programs)
- Shih-Chi Chang (Duquesne-Physics, organometallic structures and kinematic diffraction theory)
- Tim Wagner (YSU-Chemistry, extended inorganic solids, diffraction methods, instruction)
- Vivien Yee (Case-Center for Structural Biology and the Cleveland Clinic, protein crystallography)
- Xavier Lee (Case-Biochemistry and Cleveland Clinic, X-ray and neutron crystallography)
- Xiche Hu (UT-Chemistry, the theoretical prediction of protein structures)

- *Auxiliary Personnel* As defined by NSF, these individuals will typically hold faculty appointments and for our proposal they may be at both research institutions and undergraduate schools. They will be making *significant* contributions to the consortial effort, often as a collaborator for structural studies, via their expertise in non-crystallographic methods, or their contributions to the teaching. After each individual's name, I give their affiliation and possible suggestions of their primary area(s) of contribution/interest with respect to this proposal. They will be asked to submit the brief, one page, Biographical Sketches and I think that they need only submit Current and Pending Support Forms if their support is directly relevant to this proposal. I also ask that they indicate in a few sentences what their likely areas of research interest will be. I have talked with Dr. Osteryoung about this category. They only should submit the brief, 1 page, Biographical Sketches as they do for equipment grant proposals but that they don't need to submit Current and pending support forms. [Special note: Please feel free to suggest other people in our region.]

  - Alan Jircitano (Penn State Erie, The Behrend College-Chemistry, small molecule crystallography and crystallographic education)
  - Bob Stewart (CMU-Chemistry, theoretical basis for experimental charge density studies)
  - Bradford Braden (Bowie State, protein crystallography) ?
  - Constance Schall (Toledo-Chemical & Environmental Engineering, protein crystal growth)
  - David Wright (Duquesne-Chemistry and Biochemistry, area?)
  - Gale Graves (Zirconia)
  - Guy Crundwell (Central Connecticut State University, structural analysis of solid state materials)
  - Janet Del Bene (YSU-Chemistry, theoretical studies of hydrogen bonding)
  - Jeanette Krause Bauer (UC-Chemistry-Staff Crystallographer, small molecule crystallography and crystallographic education)
  - John Andrews (Hiram College-Chemistry, thermal analysis and crystallographic instruction)?
  - John Hughes (Miami University-Geology, diffraction analysis of minerals, crystallographic education)
  - Menachem Shoham (Case-Center for Structural Biology, protein crystallography)
  - Mike Burnett (Oak Ridge, neutron diffraction analysis)??
  - Mike Hopkins (Pitt-Chemistry, theoretical studies of inorganic structures)
  - Mike Meador (NASA-Lewis, Chief of Polymers Division, I have contacted him and he was interested in the proposal)
  - Paul Shiller (Packard Electric)
  - Phillip Fanwick (Purdue-Chemistry-Chemical Crystallographer, small molecule crystallography and crystallographic education)
  - Robert Towns (CSU-Chemistry, X-ray crystallography)???
  - Ronald Baker (CSU-Chemistry, X-ray crystallography)
  - Shih-Chi Chang (Duquesne-Physics, area?)
  - Steve Geib (Pitt, small molecule crystallography and crystallographic education)

- *Other Personnel Having Exceptional Qualifications* As defined by NSF, these non-faculty individuals can be at both research institutions and undergraduate schools (typically the host institutions). They will be making significant contributions to the consortial effort. After each individual's name, I give their affiliation and possible suggestions of their primary area(s) of contribution to this proposal. They would be listed in the proposals with their special qualifications/expertise described but will not need to provide Biographical Sketches. [Special note: Please feel free to suggest other people.]
  - Ewa Skrzypczak-Jankun (UT-Chemistry, protein crystallography)
  - Ray Hoff (YSU-Chemistry, electronic instrument technician)

- *Identified Faculty Participants* These individuals are largely drawn from the predominantly undergraduate schools or from PhD granting institutions having minimal diffraction facilities. They have expressed an interest or are expected to in participating in the summer school courses and/or as future Research Fellows at the host institutions. For the advanced summer school courses, participants will include a larger proportion of faculty from PhD granting departments including PhD students. These faculty participants will be listed in the proposal along with their affiliations and the consortial research areas in which they have the most current interest but will not need to provide Biographical Sketches. [Special note: Please feel free to suggest other people in our region.]
  - Andrew Burns (Kent State Stark)
  - Art Murdock (Mount Union College-Chemistry)
  - Bruce Armitage (Thiel)
  - Carl Hultman (Gannon)
  - Chase Smith (ONU-Chemistry, organic crystallography)
  - Clyde Clen Daniel (Cal State of PA)
  - Colleen Fried (Hiram College)?
  - Craig Johnson (Carlow) ?
  - Donald Mitchell (Janiata College) ?
  - Donald Penn (Edinboro) ?
  - Donghai Chen (Malone College)?
  - Edward Zovinka (Saint Francis College)
  - Fred Beil (Gannon)
  - Greg Gould (Cal. State of PA) ?
  - Jayne Giniewicz (IUP-Physics, crystallography)
  - Jeff Smiley (YSU-Chemistry, protein crystallography)
  - Jim Andrews (YSU-Physics, condensed matter physics)
  - John Simpson (Penn State Beaver) ?
  - John Woolcock (IUP-Chemistry, inorganic crystallography)
  - Kathy Frantz (Thiel) ?
  - Ken Long (Westminster)
  - Larry Curtin (YSU-Chemistry, inorganic crystallography)
  - Lisa Lambert (Chatham) ?
  - Mark Harris (Washington and Jefferson)
  - Marty Serra (Allegheny-Chemistry)
  - Michael Nichols (John Carroll)

- Mike Bucholtz (Gannon University)
- Mike Dunphy (Walsh University)
- Mike May (Central State) ?
- Mike Serra (YSU-Chemistry, protein crystallography)
- Neil Walsh (Ohio Dominican University)
- Ray Beiersdorfer (YSU-Geology, mineral crystallography)
- Robert Benz (Lake Erie College)?
- Robert Hinds (Slippery Rock University)
- Saligrama Subbarao (Lincoln College-Chemistry)
- Santosh Mandal (Morgan State, organometallic crystallography)
- Shane Brower (YSU-Physics, condensed matter physics and NLO materials)
- Terry Green (LCCC)
- Timothy Wooster (Westminster)
- Todd Trout (Mercyhurst)
- Tom Kim (YSU-Chemistry, protein crystallography and computer aided instruction)?
- W. Faye Hollaway (Mount Union College)
- William Krugh (Clarion State)

Organizational Structure and Operating Procedures of the Proposed Diffraction Consortium

According to the RFP, this section is limited to 4 pages in the proposal. The development of an effective and functional management structure, including its evaluation/assessment and dissemination sub-components, for our consortium will have a dominant influence on both getting it funded and ensuring that, if funded, it meets its goals and objectives. As set out in the RFP, the appropriateness and anticipated effectiveness of the management plan, including the organizational and management abilities of the proposed management team, will be amongst the evaluation criteria. Below, I outline possible compositions for key committees and their general charges. Budgets to support ADSC activities via the RSEC grant are presented in the following budget section.

Draft bylaws for the ADSC were circulated to interested parties in two documents in November/December of 1998. These were discussed at the December 12th, 1998 organizational meeting of the ADSC held at Youngstown State University. The overall plan presented below was approved in principle. There were several "friendly" amendments proposed that were adopted and have been included below. **These bylaws are being circulated in this version of the outline for final comment. Based on this comment, an draft set of bylaws will be prepared and distributed to the ADSC membership for acceptance/rejection in early January.**

- The official *Bylaws* of the Advanced Diffraction Studies Consortium are described below. Once the proposal is funded, they may be amended by circulation of the proposed amendments to institutional and individual members for comment and a two thirds vote of the responding membership and the Operational Evaluation Committee.

- The central *Goals* of the Advanced Diffraction Studies Consortium are to serve as a national model of inter-institutional collaboration while attempting:
  - To advance the integration of crystallographic/diffraction methods into the teaching and research of faculty at predominantly undergraduate institutions.

- To advance the integration of the faculty and students of predominantly undergraduate universities into the mainstream of the national research effort.
- To advance the quality, quantity, and diversity of students moving through the educational pipeline into research areas relying on crystallographic/diffraction methods.
- To advance the integration of undergraduate teaching and research in crystallography at all educational institutions and to provide materials to enhance this effort nation wide.
- 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.

- The *membership* of the Advanced Diffraction Studies Consortium is initially composed of the founding members (i.e., those who participated in the 1999 RSEC proposal) plus those members admitted later.
  - 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 come to conduct individual or collaborative research and/or to attend professional development courses in crystallography/diffraction.
    - *Home institutions* are the predominantly undergraduate institutions who's faculty and students this consortium is meant to serve.
    - Some MS granting institutions fall into both categories.
  - The individual membership includes faculty and those holding similar permanent appointments at institutions of higher learning or research. Any faculty member, whether at a member institution or not, may become an individual member of the ADSC by application to the ADSC (i.e., if their membership will strengthen the research and/or educational missions of the consortium).
  - Prospective new institutional members will be added after application to the ADSC in writing (i.e., if their membership will strengthen the research and/or educational missions of the consortium).
  - Associate membership can be granted to individual schools or school districts and to individual high school teachers by the Director of the Advanced Diffraction Studies Consortium.
  - 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 they are no longer meeting their responsibilities to the Advanced Diffraction Studies Consortium.

- The *Director* of the Advanced Diffraction Studies Consortium
  - **Charge:** 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 Consortiums membership, and coordinating and disseminating the results.
  - The Director will be responsible for administering the Consortium's budget and, in particular, reporting the results from the 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 (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 December 31st, 2005 (i.e., the expected life of the RSEC grant).

- 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.

- *Operational Oversight Committee*

  - **Charge:** The Operational Oversight Committee 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 Advanced Diffraction Studies Consortium 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 of members 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 federal 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 Advanced Diffraction Studies Consortium (initially Allen Hunter) will be an *ex officio* member of this committee and its chair.

    - The Coordinator of Minority Enhancement Programs (initially Sherri Lovelace-Cameron) will be an *ex officio* member of this committee.

    - Three of the Senior 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 slate of members I propose are:

      - Bryan Craven, IUP (high resolution crystallography, PA)

      - Vivien Yee, Cleveland Clinic and CWRU (protein crystallography, northeast Ohio)

      - Volunteers??? (materials crystallography and/or the rest of Ohio would be ideal)

    - There should be three additional members from predominantly undergraduate institutions. The initial slate of members I propose are (if they agree):

      - Alan Jircitano, Penn State Erie-The Behrend College

      - Marty Serra, Allegheny College

      - W. Faye Hollaway, Mount Union College

    - In addition, there should be one addition representative from one of the federal research labs and one from industry. I would suggest the following individuals (if they agree):

      - Mike Nathal, NASA Lewis Research Center

      - Matt Muir, Goodyear

  - The initial membership of the Operational Oversight Committee is as set out in the 1999 RSEC proposal. They will serve a 1 or 2 year term which will extend from January 1st, 1999 to December 31st, 2000 or 2001 (i.e., staggered terms). If any of these members resigns before the end of their term, they will be elected from a slate

nominated by the rest of the members of the Operational Oversight Committee by secret ballot of the individual members of the active members of the Advanced Diffraction Studies Consortium.

- In subsequent years, the members of the Operational Oversight Committee 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 Operational Oversight Committee.
- Fellowship and supplemental funding proposals will be evaluated by the Operational Oversight Committee.

- The *Coordinator of Minority Enhancement Programs*, will be responsible for organizing and overseeing the consortial efforts meant to enhance research and educational opportunities for individuals from groups that have historically been underrepresented in science.
  - The Coordinator's responsibilities will include organizing the summer research programs for high school students from historically under-represented groups in science and engineering.
  - 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 Kent State, Cleveland State, and John Carroll Universities) targets academically gifted students from groups which are under represented in higher education.
    - Minority Work program at YSU
    - ACS SEED program used to fund high school students.
  - I propose that Sherri Lovelace-Cameron from YSU be initially 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.

- *Consortium Grants Committee*
  - **Charge:** The purpose of this committee is 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 the Consortium Director and Consortium members with records in receiving and evaluating educational and research grants who volunteer to help in this important area.
  - The initial members will include:
    - Allen Hunter, the Consortium Director
    - Sherri Lovelace-Cameron, the Coordinator of Minority Enhancement Programs
    - Volunteers are eagerly awaited!

- *External Advisory Committee*
  - **Charge:** The purpose of the External Advisory Committee is to directly contact a representative selection 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. 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.

- I suggest that its **membership** be three individuals. The members should be from outside our region and should have national credentials in crystallography/diffraction, ideally in both research and teaching. I would suggest the following individuals who strongly support the ideas embodied in our proposal and have agreed to act in this role:
  - Phil Fanwick, Purdue University (staff crystallographer, very active in the ACA, and crystallographic education expert)
  - B. C. Wang, in Georgia (protein crystallographer and current head of the ACA summer school in crystallography)
  - 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 a term that expires on December 31st of 2005. At the end of their term, 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 probably will be provided by the ACA Continuing Education Committee which I have approached through Jeanette Krause, who serves on this committee, to assist in the evaluation and oversight of our consortium.

- *Target groups*
  - The two key target groups will initially be drawn from schools in our region and are:
    - Faculty and students from predominantly undergraduate institutions and
    - Faculty and students from under-represented groups
  - We need to 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 they and their faculty mentors to more fully join the mainstream of the "national research enterprise".
  - As the consortium matures, we should open it up to a broader definition of our region and eventually open it up nationally to these target groups. This could be done via proposals/applications from interested participants/institutions which would be evaluated in light of available space, facilities, and funding and how they would fit into our consortium goals. I would expect that for the first three years, almost all participants in consortium funded activities will come from our region. I believe that at this point 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 could be increased.

Diffraction Facilities and Other Relevant Equipment at Host Institutions

Where the following information is in error, please correct it. In addition, please provide information on current and proposed access policies to these instruments for faculty and students from predominantly undergraduate schools (and at what cost). It would also be useful to find out how diffraction/crystallographic methods is currently introduced into the undergraduate and graduate courses at each site.

- *Host Site:* Youngstown State University
  - YSU has extensive experience acting as the "middle person" in collaborations between predominantly undergraduate schools and PhD schools, including in the Ohio NMR and Crystallography Consortia.
  - YSU has two 4 year old P4 diffractometers
    - The one with a Mo sealed tube source is used entirely for single crystal work.

- The one with a Cu sealed tube source also has a multiwire area detector and is currently used most heavily for powder studies.

- With these current systems, we have made available some diffractometer time to non-YSU users and this will continue. However, these instruments are kept quite busy for teaching and research by YSU faculty, MS students, and especially undergraduates and very little time is available during the spring and summer quarters for "outsiders." With the provision of the proposed CCD upgrade (which will decrease typical single crystal data collection times by an order of magnitude) and the proposed dedicated powder diffractometer (which will release significant diffractometer time on our Cu machine for single crystal work and add new powder capabilities), YSU will be able to dedicate large amounts of instrument time for teaching and research by consortium members. In particular, these new and upgraded instruments will also allow YSU to collect data "remotely" on samples sent from other undergraduate schools.

- The CCD upgrade and dedicated powder instruments will also be sought via the OCC application to the current round of the OBoR Investment Fund.

- Departmental instructional computer facilities:

  - One new computer lab with 12 new NT machines that will be running SHELXTL by January of 1999.

  - One computer lab with 24 new Windows 95 machines on which we plan to install SHELXTL in early 1999.

  - Three 3 year old SGI INDY computers and several Wintel boxes in the X-ray lab that will be available full time for the consortium's use. In addition, several other UNIX machines are available in the Chemistry Department for more occasional use.

- We will order a new NSF funded DSC and TGA system by January 1999 and expect to order an Inert Atmosphere Glove Box by then for crystal preparation and mounting (models???).

- Siemens model 102 Transmission Electron Microscope.

- CWRU and the Cleveland Center for Structural Biology are developing a proposal to buy a share in a new X-ray beam line on the Advanced Photon Source (i.e., as part of the MB-CAT team). YSU has provided matching funds in this RSEC grant to join this team and YSU has committed more limited cash for a smaller share of the team. This ultra high intensity X-ray source has readily tunable wavelengths that have revolutionized the collection of data for protein structures (i.e., via MAD phasing) and also for very weakly diffracting crystals.

- *Host Site:* Wright State University

  - An aging CAD4 diffractometer that will be upgraded as part of this RSEC grant (i.e., the OBoR matching funds).

  - The principle crystallographic research interests of Wright State faculty include: crystal and molecular studies of new tetra-nitrogen macrocyclic ligands and their transition metal complexes, structural studies of coordination compounds of biological or catalytic interest, crystallographic studies relating to the selective functionalization of N-protected indoles and pyrroles, crystallographic studies of fused ring sydnones, mesoionic C- nucleosides and S=S and S=C compounds, and structural analysis of polymer precursors with NLO and conductive properties.

- *Host Site:* Indiana University of PA

  - CAD4 diffractometer with low temperature capabilities from Bryan Craven's group at Pitt.

  - A new powder diffractometer is on order (model???).

  - A new DSC in on order (model???).

  - Bryan Craven is currently helping other faculty and students there get involved in crystallographic research.

- *Host Site:* Bucknell University

  - Bruker R3 Diffractometer for small molecule crystallographic studies which will be upgraded as part of this proposal.

- Computer labs having PCs and two SGI workstations are available in Chemistry for crystallographic instruction and research (the consortium is planning on putting SHELXTL, or the equivalent, on these).
- Extensive experience in computerized crystallographic instructional methods development.
- Free dorm rooms available over the summer (i.e., as a Bucknell matching grant) for research and summer school participants. Faculty, students, and high-school teachers from other schools would be welcome to work here.
- Proposal from Marj Kastner to prototype a summer school program on crystallographic methods. We need to talk about how this will integrate with the rest of our courses.

- *Host Site:* University of Pittsburgh
  - Pitt has a P3 diffractometer with low temperature capabilities in chemistry (which is totally saturated now).
  - Pitt has a rotating anode (i.e., AFC5R with Cu anode) with a Bruker area detector, a MAR Imaging Plate equipped diffractometer, and possibly a third diffractometer in biochemistry (??? Is this correct???) under the care of John Rosenberg's protein diffraction group.

- *Host Site:* Duquesne University
  - Duquesne University has a Rigaku AFC7R rotating anode system with low temperature capabilities. They have two Weissenberg, two Debye-Scherrer, and one Laue camera for this instrument.
  - Duquesne University has two Rigaku D/MAX-B powder diffractometers (one with a horizontal and one with a vertical generator).
  - Duquesne University has a SGI workstation with teXsan software.

- *Host Site:* Carnegie Mellon University
  - Materials, Biochemistry Equipment (??? Does anyone have any information on this ????)

- *Host Site:* Kent State University and its Liquid Crystal Institute
  - A remanufactured 1st generation Bruker CCD detector on a new SMART diffractometer is on order.
  - A Bruker D-5000 powder diffractometers is on order.
  - The Liquid Crystal Institute has a D-5000 powder diffractometer equipped with a rotating anode source.
  - Funding is being sought in this proposal to upgrade the current camera facilities to add a modern film facility that will be dedicated to the consortium.

- *Host Site:* University of Toledo
  - UT is the home of the Ohio Crystallography Consortium instrumentation.
  - The OCC has one Siemens CCD equipped diffractometer (i.e., 1K SMART CCD with cryostat for liquid nitrogen and Mo).
  - The OCC has one imaging plate system equipped with a rotating anode source.
  - Alan Pinkerton has a Siemens CCD equipped diffractometer (i.e., 2K SMART CCD with cryostat for liquid nitrogen and Ag, Mo, or Cu sources) equipped for low temperature studies down to 20K with He cooling.
  - A grant application is pending for a "materials diffractometer.".
  - The Chemical Instrumentation Center has a Scintag XDS 2000 powder diffractometer with Cu source, thin film attachment, and Buhler oven for high temperature experiments.
  - CWRU and the Cleveland Center for Structural Biology are developing a proposal to buy a share in a new X-ray beam line on the Advanced Photon Source (i.e., as part of the MB-CAT team). Toledo has provided matching

funds in this RSEC grant to join this team. This ultra high intensity X-ray source has readily tunable wavelengths that have revolutionized the collection of data for protein structures (i.e., via MAD phasing) and also for very weakly diffracting crystals.

- *Host Site:* Case Western Reserve University and the Cleveland Clinic
  - The Chemistry Department has a P4 diffractometer that has been upgraded from a P3.
  - The Cleveland Center for Structural Biology has a Rigaku rotating anode source with MSC focussing mirrors, a R-Axis2 imaging plate detector, and a Oxford Cryostream crystal cooling system.
  - The Cleveland Clinic has a Rigaku rotating anode source with MSC focussing mirrors, a R-Axis4 imaging plate detector, and a MSC X-stream crystal cooling system.
  - There are 2 SGI workstation in each of the 4 research groups.
  - CWRU and the Cleveland Center for Structural Biology are developing a proposal to buy a share in a new X-ray beam line on the Advanced Photon Source (i.e., as part of the MB-CAT team). YSU and Toledo have each provided matching funds in this RSEC grant to join this team and YSU has committed more limited cash for a smaller share of the team. This ultra high intensity X-ray source has readily tunable wavelengths that have revolutionized the collection of data for protein structures (i.e., via MAD phasing) and also for very weakly diffracting crystals.

- *Host Site:* Oak Ridge National Labs
  - Our gateway to access to synchrotron sources, neutron sources, and extreme conditions studies as well as extensive thermal analysis capabilities.
  - The High Flux Isotope Reactor, HFIR, as a neutron source.
  - The High Temperature Materials Laboratory, HTML, for extreme conditions studies.
  - The Shared Research Equipment, ShaRE, center.
  - Access through Oak Ridge to the other national diffraction facilities.

- *Host Site:* NASA Lewis Research Center
  - The Materials Research Group currently employs X-ray diffraction as an essential tool.
  - They are most interested in inorganic solids including metals, alloys, intermetallic compounds, and ceramics.
  - They are particularly interested in hosting students and/or faculty at their facility for extended periods, to collaborate on research projects. They feel confident that they can set up projects that are both beneficial to their organization and provide learning experiences.

- *Host Site:* The University of Akron and its Polymer Science and Engineering Center.
  - Peter Rinaldi has an excellent solids NMR and is a valuable resource person. [Note: Is a NMR set up to do single crystal NMR studies available in our area ?????????? Help ????????]
  - They have excellent electron microscopy facilities in the Polymer center.
  - Wiley Youngs in chemistry has a conventional diffractometer with low temperature capabilities. (Wiley, please send me the Model #)
  - Mark Foster in Polymer Science has interests in materials diffraction and an excellent range of materials diffractometers in their polymer characterization center and in his research group, including:
    - A rotating anode generator used with a custom reflectometer.
    - A second rotating anode generator used with a custom surface spectrometer (i.e., suitable for studying horizontal surfaces and for simultaneous grazing incidence diffraction with a linear PSD and Evanescent Wave Induced X-Ray Fluorescence).

- In January he will get a new pinhole SAXS setup with focussing optics and 1-D PSD.
- Both Wiley and Mark have been on sabbatical in Europe (Mark has now returned).

Overview of Crystallographic Methods to be Integrated into Various Aspects of This Proposal

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, which may be mundane to the skilled crystallographer, 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 who's 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 then solving for their structures must remain the first stage of our educational and research programs. Until undergraduate faculty and students feel comfortable doing routine studies, they will not be ready to begin more advanced diffraction studies. The consortium must also provide facilities at which these undergraduate faculty and students can conveniently, quickly, and at little for no cost collect such data. I propose that Youngstown State University play the central role in this area for the "basic" courses on diffraction methods. We plan on offering such access, through the consortium, to undergraduate faculty and student users on single crystal diffractometers equipped with both serial and area detectors and on a powder diffractometer. They will be able to access these capabilities either by bringing their samples to YSU or by sending them here by mail and having the YSU Diffraction Lab Scientist collect the data. They can then either solve the structures themselves or do so collaboratively with either one of the YSU staff or another researcher in the consortium. This proposal is structured such that they should have quick access at no direct cost to themselves for ambient temperature data collections (for the expected number of samples). Indeed, I expect that there will be sufficient capacity on these new diffractometers that almost immediately they will be available for use by faculty and students from undergraduate institutions across the US.

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 the consortial Research Fellowships. After two years of this fellowship support it is expected that these individuals will be fully productive members of the collaborative teams and that their further collaborative or individual participation in these projects should be fundable by conventional granting channels.

The specific types of diffraction studies to be carried out are outlined below:

Please feel particularly free to suggest additions, deletions, and corrections to this section.

- *Quality Conventional Single Crystal X-ray Diffraction Studies*

This type of studies will represent a substantial majority of single crystal samples for which data will be collected and analyzed. 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. With funding of the equipment upgrades in the proposed budget, Youngstown State University will be able to fulfill a large part of this requirement for offsite undergraduate faculty and students. The consortium will offer "basic training" courses in single crystal methods at our YSU summer school and will provide an appropriate structure solution software package to its graduates. Various consortium members will provide advice and consultation for dealing with problem structures. These types of studies can be done on conventional "lab" diffractometers equipped with serial detectors. Data collection times can be decreased, signal to noise ratios improved, 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. Where even area detectors and rotating anode sources fail to produce data of sufficient quality (i.e., where one has particularly small and/or otherwise weakly diffracting crystals), one can turn to extremely bright synchrotron sources. If one is interested in 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 the participation of ORNL and the proposed MB-CAT beam line team. With funding of the equipment purchases in the proposed budget, Youngstown State University, Bucknell, and Wright State will be able to fulfill a significant

part of this requirement for no-cost access to undergraduate faculty and students. In addition, YSU will provide a free service for remote data collection. The consortium will offer "basic training" courses in single crystal methods at our summer school and will provide an appropriate single crystal diffraction package to its graduates. Various consortium members will provide advice and consultation for dealing with problem structures.

♠ *Quality Conventional Powder X-ray Diffraction Studies*

This type 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 no-cost access to undergraduate faculty and students. In addition, YSU will provide a free service for remote data collection. The consortium will offer "basic training" courses in powder methods at our summer school and will provide an appropriate powder diffraction package to its graduates. 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.

♠ *Very High Resolution Single Crystal Structural 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 this 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 "lab" diffractometers. These are typically fitted with some combination of a high intensity X-ray source (e.g., a sealed tube X-ray source using Gobel 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. Access to facilities for high resolution data collection will be available a most of the host institutions. In addition, YSU will provide no-cost access to its proposed CCD diffractometer for these purposes (users will have to pay for their cryogens). 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 synchrotron radiation sources. Such sources are only available at the national labs but access can typically be arranged at little or no cost (other than travel and lodging) to users from predominantly undergraduate schools if one applies for beam line time (i.e., via the YSU share at the proposed MB-CAT beamline). The consortium will assist in this process through the provision of funding for travel and lodging to collect such data.

♠ *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.

♠ *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 Cam Hubbard of the High Temperature Materials Lab at Oak Ridge. It also requires skill with using specialized software and analytical tools.

♠ *Line Shape Analysis of Diffraction Peaks*

The analysis of line shapes of diffraction data 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, etc. Such studies require diffraction data that have been carefully collected to be optimized to reduce the instrumental line width and also requires skill using specialized software and analytical tools.

- *Protein Diffraction Studies*

Proteins and related macromolecules have tremendous significance to both scientific and biomedical research and we have a growing number of experts in their study in our region. They will form a cornerstone of our proposal. The equipment required for these studies is similar to that for other high resolution single crystal methods (i.e., one needs high intensity sources and area detectors, commonly imaging plate systems). The use of synchrotron sources (which allow MAD phasing) are of growing importance here.

- *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. Casey Raymond is going to write a section on layered hybrid inorganic/organic materials. Mark Foster has suggested we include surface structure and amorphous materials analysis which I think is an excellent idea.

Primary Advanced Research Areas

Most of the diffraction studies useful to undergraduate faculty and students fall into the "routine" powder and single crystal categories. Our primary advanced research areas seem likely to be high resolution crystallography of small molecules, materials characterization crystallography of both polymeric and inorganic materials, and protein crystallography. Under the 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 their teaching and research at their home institution. In cases where the undergraduate faculty member is more experienced, the role of the PhD hosts will typically be more focused on providing instrument access and advice, although collaborative arrangements are still encouraged.

I had a long talk with Dr. Osteryoung about the best way to arrange the research section of the grant. She noted that "group" proposals that look like they have been "stapled together" by a half dozen people, each talking about their own area are generally received poorly. After discussing several options with her, she commented that the strongest group proposals can have different structures but all read as a seamless whole. For a consortium like ours, she preferred an organization I suggested for the proposal in which we would talk about each of our main research areas in terms of their general descriptions, challenges, opportunities, and impacts and then at the end of each list those senior and auxiliary personnel and faculty associates that would be contributing to solving these challenges. These projects will be the central core of the *Scientific Activities of Project* section of the grant proposal. She strongly indicated that all of these should be written by the same person (at least in the final draft) to ensure stylistic consistency and consistency of content and approach. I would be willing to put together a draft of these for all of us to edit and comment on. Alternately, one or more of you might volunteer to send me a first draft of the sections most closely related to your research interests. **In either case, please send me information (e.g., parts of grant proposals, descriptions of research interests, purpose written documents) from which I can begin to put together these sections.**

Each of the following classes of materials of fundamental technological and scientific interest are currently being studied by the research groups at one or more of the host institutions. Excellent research proposal topics could clearly built around each.

Please feel particularly free to suggest additions, deletions, and corrections to this section, the specific ideas are there largely to serve as a starting point for our discussions.

- *High Resolution Diffraction (Charge Density) Studies of Molecular Solids*
  - *Organic molecules that have unusual and/or important structures and bonding.*
    - Molecules who's bonding has been the topic of dispute/interest.
  - *Oriented organic materials of interest in electronic and photonics applications.*
    - NLO organic materials.

- Organic metals.

- *Organic and bio-organic molecules of biochemical and biomedical interest.*
  - Hydrogen bonded complexes related to DNA, RNA, and Proteins.
  - High hydrates of alcohols and other hydrogen bonded systems.
  - Small molecules with interesting biological activities.
  - Enzyme inhibitors and transition state analogues.
- *High energy organic molecules related to explosives*
  -
- Transition metal coordination and organometallic complexes related to high performance catalysts.
  - Organometallic carbonyls.
  - Organometallic π-complexes.
  - Molecules related to single site catalysts.

- *High resolution macromolecular crystallography of molecules of biomedical importance.*
  - ***Please suggest specific systems***

- *Materials Diffraction Studies*
  - *Extended Inorganic Solids*
    - Solids related to electronic, optical, sensor, high performance structural, and catalytic materials.
    - Measurements at both ambient conditions and extremes of temperatures and pressures.
    - Metal oxides such as Perovskites and the 123 superconductors.
    - Aluminosilicates such as Zeolites.
    - Semiconductors.
    - Inorganic NLO materials.
    - Sensor materials.
    - Minerals.
- *Crystallographic Characterization of Polymeric Materials*
  - Morphology
  - Defects

Primary Areas of Faculty and Student Development and Training

There will be a central focus on faculty development in this grant, especially for participants from predominantly undergraduate institutions and on undergraduate student training. 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.

This section will form the core of the *Human Resource Development* section of the NSF proposal. I particularly welcome your ideas on how this thrust of our consortial efforts can be strengthened.

- *The primary focus of the RFP and our primary focus as a consortium is on undergraduate faculty development, training, and integration into the national research enterprise.*
  - Summer and sabbatical research support for undergraduate faculty to work in cutting edge crystallography labs, as collaborative partners and/or as individual researchers.
  - Development of long term collaborations between undergraduate faculty and faculty at the host institutions and between groups of undergraduate faculty.
  - Long term, convenient, and affordable access to conventional X-ray, advanced X-ray, synchrotron X-ray, and neutron diffraction facilities. The conventional diffraction facility will be available for both "hands on" data collection and remote submission of samples.
  - Source of stable funding to "kick-start" their collaborative and independent research projects.
  - Availability of the various summer crystallography short courses will facilitate their research and teaching.
  - Availability of support for grant writing.

- *Student training initiatives.*
  - Summer research experiences in crystallography as members of a research group at home and host institutions.
  - These research experiences will typically/often be done collaboratively with a faculty sponsor from their home department.
  - 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.
  - Crystallographic "basic training" summer schools for students to be held at Youngstown State University (on a space available basis, see below for details) and at other sites. This course will be available for undergraduate or graduate transfer credit.
  - 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.
  - Interested BS and MS students (and PhD students on a space available basis) will also be eligible to take the advanced crystallography courses.

- Introductory *"basic training course in single crystal diffraction methods"* as an intensive summer school to be held at *Youngstown State University* (mainly for undergraduate faculty and students).
  - This course will typically be offered once each summer. Although the grant awards are supposed to be announced by June 1st of 1999, I don't think we would easily be able to start this course until the summer of 2000.
  - This course is modeled on the excellent ACA summer school in crystallography. I have discussed ACA affiliation for this and the following courses with B. C. Wang and his team in Georgia. They recommended that we not pursue this option until our program is well established (because of the administrative headaches that would result and the regional focus of our proposal). The Georgia team (i.e., B. C. Wang, John Rose, and Gary Newton) commented that we are proposing "a very nice program" and are willing to assist us with the proposal. In addition, B. C. has agreed to serve on our external advisory and assessment committee.
  - The Georgia people did suggest more local affiliation might be more appropriate for this and the other courses. I think that we should approach the Pittsburgh Diffraction Society about this. This should be easy because its past, current, and future presidents are on this proposal!

- The current 12 day ACA summer school in Georgia is substantially over subscribed. It had 60 registrants this past summer, only 45 of which participated in the lab component (in a large part because of crowding on the diffractometers)! To meet the growing interest in this course from aspiring protein crystallographers, it is planned that it will expand to 16 days next summer, 8 on small molecules and 8 on macromolecular studies.
- Our basic training course will be available for graduate or undergraduate transfer credit from Youngstown State University for 3 or 4 semester hours of credit. The students will only have to pay low "general fees" if they want to get this credit. I am exploring how even these fees might be waved.
- The undergraduate faculty participants will have first priority for these courses with faculty participants being 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 undergraduate and MS students, especially in the later years of this grant.
- This course will focus on the fundamentals 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 text "Crystal Structure Analysis for Chemists and Biologists" written by Glusker, Lewis, and Rossi.
- 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 the courses at their home schools.
- It would probably make sense to schedule some of these classes directly before or after ACS and chemical education meetings with sensitivity to undergraduate instructional schedules.
- This course will be taught in small classes and with high instructor to participant ratios (typically one/five or six).
- Ample diffractometer experience and small diffractometer to participant ratios will be provided. Based on my experience with the ACA summer course, if we use our two current P4 diffractometers, this class would be best taught with about 10 or 12 students. This is because such a high diffractometer to student ratios will allow us to give the students extensive hands on experience and allow each to collect data of publishable quality on one or two different samples. Over two week and with two diffractometers this will give each student two to three days of diffractometer time (this is sufficient for a publishable structure if one has a relatively small molecule and decent crystals). However, if one or more of the diffractometers is upgraded to give it increased capabilities (i.e., as I propose in the budget section) then the class size could be substantially expanded and each of the students would still be able to collect both more and/or better quality data sets.
- 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 crystallographic assistant/technician will help with the lab components. Other individuals who have expressed an interest in being involved with this course include:
  - Margaret Kastner from Bucknell University
  - Bryan Craven from IUP
  - Guy Crundwell from Central Connecticut
  - Alan Jircitano from Penn State Erie
  - Volunteers???
- This course will have as one emphasis the teaching of crystallography to undergraduates 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.
- This course will involve a two week intensive program involving about 30 hours of lectures and at about 40 hours of "hands on" lab time.
- During this two week period our two modern single crystal diffractometers and a crystallographic computing lab having twelve workstations will be dedicated to supporting this course. If funding is provided by NSF for a CCD upgrade, this area detector system will be used extensively in this course and the students will have hands on experience with data collection on both serial and area detector systems. I expect that each student/team will typically collect one data set using a serial detector and one using the CCD system.

- Lectures will be taught emphasizing both the fundamentals of crystallography and how to avoid the most common novice mistakes.
- Labs will teach the skills used in various stages of data collection from crystal growth through measuring data for absorption corrections.
- Students and faculty will typically work in pairs on their new structures.
- By the end of each course, it is my plan that least one data set will be collected, analyzed, and typically prepared for publication *on a new structure* for each team. Based on my experience with the current ACA summer school, it seems likely that with the proposed diffractometer to student rations, each team will collect data on about two to three structures (i.e., about 2 to 3 days per data set).
- Course participants will be provided with the same books/manuals, instructional software, and crystallographic software used during the course for use in teaching and research at their home institutions.
- This course will typically be taken by undergraduate faculty and students just before they start with one of the research collaborations.
- Mat Muir at Goodyear pointed out that these types of short courses would likely be of great interest to industrial participants who would be very interested in sending some of their staff to these courses as refreshers or to gain new skills. They noted that their companies have no problem paying for these courses.
- This course is designed to produce at least one paper on their results for each team. For those who wish it, we will help them prepare their results for electronic submission to Acta Cryst.
- In many ways these courses resemble things funded by the old NSF Undergraduate Faculty Enhancement Project which has now been absorbed into the CCLI program.
- I am exploring a version of this course where the first part(s) would be taught at YSU and at the end of this time the students would be associated with one of the host institutions near their homes (e.g., Wright State and Bucknell have volunteered and I am asking for who else would like to do so) for the rest of the summer where they would complete their data collections and solutions. In other words, the course would include about two intense weeks at YSU followed by a more leisurely follow up time at multiple sites. I can see several advantages for such an approach, especially for faculty participants.
- There will include a section on film methods in crystallography.
    - The development of modern, automated single-crystal and powder diffractometers has greatly advanced the use of X-ray diffraction techniques. However, the cost of these advances has been the loss of some basic knowledge, particularly related to film techniques.
    - For single crystals, the most common methods utilize the Weissenberg or Precession cameras. The Weissenberg technique allows the determination of cell constants and space group and the alignment of a crystal. The Precession method provides an undistorted representation of the reciprocal lattice, unlike the Weissenberg technique. However, both allow the geometry and symmetry of the reciprocal lattice to be visualized on film.
    - For powdered samples, the most common methods utilize Guinier or Debye-Scherrer cameras. Powder X-ray diffraction techniques are underutilized. These techniques allow rapid analysis for bulk samples for comparison to the one single crystal that was used for structure determinations.
    - All of these techniques provide alternatives to automated systems for routine analysis of crystalline materials. The films can quickly be compared to reagents and undesired products without waiting in line for more powerful automated systems.
    - The use of modern area detectors is replacing many of the traditional 4-circle goniometers, which creates difficulties discussing the diffraction experiment. Film techniques allow students to obtain much greater insight into the theory and practice of X-ray diffraction.
    - These techniques also provide methods to confirm lattice parameters and space group assignments, without monopolizing heavily used automated systems.

- Introductory *"basic training in crystallography and powder diffraction methods"* to be held as a summer school (mainly for undergraduate faculty and students) to be held at *Youngstown State University and other sites.*

- The structure of this powder course will closely resemble that of its single crystal analogue. Thus, its admission criteria and administrative features of this course will be similar to those described above.
- If this course focussed solely on the most basic powder methods it might be only 2 to 3 days long. However, I think this might leave participants asking "where's the beef."
- I propose that the lecture part of this course 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 alone would easily fill a week long lecture sequence. Thus this course would be a true crystallography course which the basic single crystal one would not be. If these crystallography topics were combined with a discussion of powder instrumentation including thin film 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 one would have the makings of an excellent two week lecture series.
- For the labs, I propose that the students would learn how to collect and analyze powder data for the identification of unknowns and new materials using the powder diffractometers on site for about 3-4 days. In addition, there would be a series of "computer exercises" on solid state chemistry and symmetry (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.
- As with the single crystal course, there will be instruction in the use of film methods in crystallography.
- It might very well make sense to have this course in two parts: a self contained course in the first part that was relatively basic and a more advanced unit as a separate course the following week for a total of 3 or 4 semester hours of graduate credit.
- This course would be taught by a mixture of individuals, including:
  - Tim Wagner from YSU
  - John Hughes from Miami University
  - Margaret Kastner from Bucknell University for the section on symmetry
  - Other Volunteers

- *Advanced crystallographic summer school for students and faculty.*
  - These courses will likely be held at both YSU and several of the other host institutions depending on who volunteers to teach them and can make the appropriate facilities available.
  - They will be available for graduate transfer credit from YSU (for 1 to 4 semester hours of credit) or from the other host site (if that institution prefers).
  - They are designed to bring participants "up to speed" for the advanced parts of their collaborative research projects and to provide "special topics" for the teaching of crystallographic methods at their home institutions.
  - It will focus on "cutting edge" crystallographic methods and new techniques and methods.
  - These courses will be run by the acknowledged experts in the selected topics.
  - These advanced courses will use a varying mixture of lectures, lab experiences, and exercises. For example, some courses might also have a very strong "hands on" lab experience, some might involve the whole class collecting a single quality data set over the period of the course to learn its general principles, while others might be based entirely on lectures and data analysis exercises. The reasons for these differences will arise from both differences in the natures of differences and the intrinsically time demanding nature of some of the techniques.
  - These courses will be intensive three days to two week courses (the most appropriate value will vary for these courses).
  - Course participants will be provided with the requisite books/manuals, instructional software, and crystallographic software for use at their home institutions.
  - It would probably make sense to schedule at least some of these directly before or after ACS and ACA meetings.

- There are many possible choices for advanced courses. The choices of which ones will be offered and when will be made based on surveys of undergraduate faculty interests, the availability of volunteers to host/teach them, and the availability of supplemental funding. Possible advanced course topics include (please feel free to volunteer your self and your institution for the following):
  - Charge density studies using very high resolution crystallographic data.
    - Bryan Craven
    - Other volunteers?
  - Protein and macromolecular crystallography.
    - Katherine Kantardjieff from Cal. State Fullerton
    - Vivien Yee (for parts????????????)
    - Other volunteers?
  - Analysis of neutron, multi-wavelength, and synchrotron data, MAD phasing.
    - Volunteers?
  - Line shape analysis in crystallography.
    - Volunteers?
  - Crystallography under extreme conditions (e.g., temperature and pressure).
    - Volunteers?
  - Advanced Rietveld analysis of powder data.
    - Volunteers?
  - Materials Diffraction Studies
    - Mark Foster (Guest lectures on surface scattering, grazing incidence techniques, reflectometry, and/or small angle scattering)
  - Systematic approaches to growing single crystals.
    - Allen Hunter for small molecules
    - Volunteers for proteins
  - Dealing with intractable data sets and new methods of solving the "Phase Problem" in single crystal studies.
    - Volunteers?
  - Working with minerals in single crystal and powder methods.
    - Volunteers?

- Distance/electronic education courses and instructional materials are mentioned specifically in the RFP, we have some participants in this proposal with interests in these areas that should be explored:
  - Marj Kastner at Bucknell has developed some excellent software for teaching the symmetry of crystals.
  - Katherine Kantardjieff at the CMolS Cal. State Fullerton has experience offering diffraction methods instruction to remote sites of the Cal. State system which we might extend to our consortium.
  - Allen Hunter has written and is currently updating a students guide to solving routine crystal structures which is currently being reviewed by over a dozen skilled crystallographers including several of our consortium members.

- *Support for grant seeking by predominantly undergraduate faculty.*
  - Participation in the crystallography courses and collaborative research projects will help in developing the skills and pedigrees needed for individual grant seeking activities by these undergraduate faculty.
  - The consortium will set up Consortium Grants Committee to act as a resource for those participants who would like help developing and sharpening grant proposal writing skills.
  - Long term collaborations that develop could be supported through NSF Research Opportunity Awards, ROA (i.e., as supplements to the grants of researchers at the host institutions), and similar programs from other agencies.
  - One of the requirements of the Faculty Fellowships will be that the fellows submit at least one external grant proposal (i.e., in teaching or research) related to crystallography during the term of their grant. We will help them do so.

- *Crystallography/diffraction methods integrated into the undergraduate curriculum*
  - During the term of this grant, Allen Hunter will work with faculty and students from both undergraduate PhD students to develop crystallographic/diffraction methods materials for integration into the undergraduate and graduate curricula. This will include new lab experiments, computer exercises, new units for lectures, new demonstrations, and other teaching materials. Several of the faculty participants have experience in this area.
  - The other focus will be on developing materials for lab 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 will write a NSF CCLI proposal to help fund this effort.

- *Crystallography in pre-college curriculum.*
  - This RSEC grant will provide seed funding in this area as well as facilities and a collaborative framework.
  - A *"solid state structural methods for teachers"* course optimized for the professional development of high school chemistry teachers. This is particularly important, and desirable from their perspective, with increasing state requirements for postgraduate teacher certification.
  - It will carry 3 semester hours of graduate credit from Youngstown State University. The students will be responsible only for their relatively low general fees.
  - This course will be a two week short course analogous to the structural methods for teachers course Allen Hunter gave several years ago.
    - 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.
      - Typically about one hour at the end of the day is used to discuss curricular implications.
    - It will have about 40 hours of lab time.
      - There will be *an afternoon* 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 data on one new sample for publication.
      - There will be *an afternoon* on the powder diffractometer where the students will learn to collect and analyze powder data.
      - There will be two afternoons on strategies for growing single crystals of organic molecules and inorganic salts.
      - There will be one or two afternoons on mineral crystals (ideally taught by one of our geologist participants).

- There will be 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.
- There will be about three or four afternoons in the computing labs learning how to solve a variety of "routine" data sets (i.e., to get a feel of where molecular structures come from) and learning solid state symmetry from Marj Kastner's software.

- It will have a strong emphasis on relevance to the pre-college curriculum.
- The teacher participants will be expected to develop at least one new lesson outline out of their coursework for integration into their school the following year. Those students 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 (i.e., ADH will develop and teach it as part of his directors duties along with one or two others) at minimal incremental cost. Funding to continue this program will be sought by ADH from the Eisenhower program.
- This course is one that seems particularly suitable for cloning and offering at several sites around our region on alternating years.

- Stipends for the high school teachers to get involved in the research programs at any of the participating schools will be available on a competitive basis, initially from the same funding pool as the undergraduate and MS students.
- Development of crystallographic experiments and materials suitable for high school facilities, teachers, and students will be part of the goals of this program.
  - Some of the interested teachers who have taken this course will be asked to participate in this effort through our teaching Practicum in Chemistry course as YSU has done before for other instrumental techniques.
  - YSU is in the process of implementing a MS in Chemistry with an emphasis on Chemical Education. This is designed primarily for high school chemistry teachers (a group we have been serving with our current "general purpose" MS up to now). We also will soon apply for a new program (i.e., a MS in Natural Science) that will be suitable for middle and high school science teachers with broader interests. These groups will mostly take the basic courses and it is expected that some will choose to do their research projects in the area of crystallographic education.
- Allen has already approached Bruker for their support in this area and will write a NSF CCLI proposal to help fund this effort.

- *College research experiences for high school juniors/seniors from under-represented groups.*
  - This RSEC grant will provide seed funding in this area as well as facilities and a collaborative framework.
  - The emphasis will be on individuals from historically under-represented groups.
  - I have asked Sherri Lovelace-Cameron in the YSU-Chemistry Department to 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 an suitable instructional component to help these high school students to understand their parts of the crystallographic 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 lab 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.
- Initially, we can fund this minority enhancement program for $5,000 per year while integrating those minority students who are in college into our current programs. We can also apply for internal and external funding to expand this program. Sherri will be in charge of coordinating these efforts with the assistance of interested consortium faculty.
- We are also seeking to develop ways to include historically black colleges from outside our immediate region in this collaboration.

- *Completion of courses by undergraduate faculty will "check them out" for data collection on consortial diffractometers (with appropriate oversight and consistent with institutional access policies).*
  - Currently, these undergraduate faculty officially have access to most of these diffractometers but it is seldom used for a wide range of reasons.
  - This training will help give them the confidence to want to use these instruments and the skills to do so more efficiently.
  - They will probably use the facilities at YSU for a substantial fraction of their needs for "routine" single crystal and powder data, both on site and through remote submission of samples.

- *Development of teaching materials to aid the integration of crystallography throughout the curriculum and in special crystallography courses for chemistry and allied disciplines and to facilitate research by students and faculty from predominant undergraduate schools.*
  - The curriculum development efforts will be developed from, and facilitated by, the variety of crystallography courses which will be offered. They will be honed by experience and the most successful ones described in detail to act as national models.
  - J. Chem. Ed. articles will be prepared on new curricular materials.
  - Articles in general circulation science and educational journals will be prepared on new curricular materials.
  - Continued revisions and updating of the ADH-YSU manual on crystal structure determination for novices will be done.
  - Other manuals on basic and advanced topics will grow out of the summer schools.
  - A WEB site of annotated data sets and crystallographic teaching resources is being prepared at YSU.
  - Any educational software developed will be distributed.
  - There will be presentations at regional and national meetings of the ACS, ACA, PDS, CUR, General Education, etc.

Budget

These budget numbers are still rough estimates and will certainly change somewhat over the next two weeks but are of the right close order of magnitude. We especially need to find more information on other internal matches and sources of external funds.

Budget Summary

Budget Category and Detailed Information ALL PRICES BELOW ARE ESTIMATES BASED ON RECENT SELLING PRICES. Overhead rate is 42% on salaries only (shown in double underlined italics). Expected OBoR Action Fund matches are in **bold** (i.e., 1:1:1 NSF/OBoR Action Fund/host school). YSU matching funds are underlined.	**External Funds** NSF and **OBoR** ($ in thousands)	**Internal Match** ($ in thousands)	**Total Funds** ($ in thousands)
A. Major and Minor Equipment (total)			
(1) YSU CCD Single Crystal Diffractometer	101 + **101**	101	303
(2) YSU Powder Diffractometer	51 + **51**	51	153
(3) Film Diffraction System (YSU (and Kent???))	20 + **20**	10 + 10	60
(4) Protein Crystallography Data System (Cleveland Clinic/CWRU and YSU)	20 + **20**	10 + 10	60
(5) Wright State Single Crystal Diffractometer	40 + **40**	40	120
(6) Bucknell Diffractometer Upgrade	25	25	50
(7) MB-CAT Beamline Contribution	34 + **34**	17 + 17	102
(8) Mount Union College	1	1	2
(Subtotals)	(292 + **266**)	(292)	(850)
B. Recent/Current Crystallographic Investments (as capital match??? , a share proportionate to ADSC involvement)			
(1) YSU (P4 upgrades (5K?), Wintel labs (part of 200K?))		65	
(2) Kent (Raymond startup????)		xxx	
(3) CWRU and Cleveland Clinic (MB-CAT (400-500K) + new Protein Diffractometers???)		xxx	
(4) IUP		xxx	
(5) Duquesne		xxx	
(6) Toledo		xxx	
(7) Other schools???		xxx	
(8)		xxx	
(Subtotals)		(xxx)	(xxx)
C. Direct Maintenance and Operating Expenses (as non-capital match, a share proportionate to ADSC involvement)			
(1) YSU (All diffractometers maintenance budgets)		75	
(2) Kent (Raymond and Huang startup)		xxx	
(3) CWRU and Cleveland Clinic		xxx	
(4) MB-CAT Annual Operating Expenses (a share of 50K)		xxx	
(5) IUP		xxx	
(6) Duquesne (service contract)		xxx	
(7) Toledo		xxx	
(8) Wright State		xxx	
(9) Other schools???		xxx	
(10)		xxx	
(Subtotals)		(xxx)	(xxx)
D. Crystallographic Software and Data Bases	60	xxx	60 + xxx

E. Project Director (ADH) (1) Academic Year Salary and Benefits (1/2 time for 4 years and full time for 1 year) (2) Summer Salary (2/9, 1999-2004) (3) Research Support (5 years)	 *85* 25	 210 	320
F. Minority Enhancement Programs (1) Coordinator (SLC) Academic Year Salary and Benefits (1/6 time for 5 years) (2) Coordinator Summer Salary (1/9, 2000-2004) (3) Seed Money (4) YSU minority student summer support (Project SEED, other funds) (5) Other schools??? (6) (Subtotals)	 *25* 25 (50)	 60 xxx xxx xxx (xxx)	110 + xxx
G.. Diffraction Lab Scientist (a *new position* at the post-doctoral level, average salary 36K + benefits)) to run remote data collections, assist with onsite studies, manage data base access, etc.	*100*	150	250
H. Faculty Reassigned Time (to ADSC and related research) (1) YSU 2 x 1/3 reassigned each year (e.g., TRW and MS)) (2) Other schools??? (3) (4) (5) (Subtotals)		 200 xxx xxx xxx xxx (xxx)	 (xxx)
I. Technical support staff (1) YSU Clerical support (*new position*, 25%) (2) YSU Ray Hoff (electronics instrumentation specialist, 25% of salary and benefits) (3) YSU (computer networking support, Bob Hogue, 5%, + students) (4) Other schools??? (5) (6) (7) (8) (Subtotals)		 35 90 20 xxx xxx xxx xxx xxx (xxx)	 (xxx)
J. Undergraduate Faculty Fellowships (50 in total) (1) Stipend (7.5K for 2/9 summer + academic year reassigned time (salary and benefits, 1/9 year average, 8K average value each)) (2) Home expenses grants (2K each) (3) Host expenses grants (2K each) (4) Extraordinary Expenses Grants for Undergraduate Faculty Research Programs (materials, supplies, travel for data collection, annual 40K pool) (5) (Subtotals)	 *375* 100 100 200 (775)	 400 xxx xxx xxx (xxx)	 (xxx)
K. BS, MS, and Teacher Stipends (annual 25K pool)	*125*		125
L. Summer School Costs (1) Stipends for instructors (2) Instructor expenses and consumables costs (3) Student Expenses (4) YSU tuition fee wavers	 *50* 50 50 	 45 xxx	150 + xxx
M. Direct Charges for ADSC Evaluation and Dissemination Costs	125		125
N. Overhead (calculated at 32/42% of salaries totaling ≈ $600K)	190???		190

Totals	1977	xxx	xxx

- *Budget: General Considerations*
  - I had a very long discussion with the program officer on November 17th about general budgetary issues. She said that the project budget was somewhat flexible but we needed to be very careful that all budget items were fully justified and were clearly *justifiable* in terms of the program objectives (i.e., predominantly undergraduate faculty development, enhancement of teaching and research in the undergraduate institutions, integration of the undergraduate faculty into competitive research, and widening and diversifying the educational pipeline). She most strongly cautioned me about anything that even hinted at what has happened to often in the past on such programs (i.e., toys for the boys and most of the money ending up supporting current research powerhouses rather than directly supporting the undergraduate faculty enhancement initiatives).
  - As to the question of how much equipment funding was appropriate for this program, she answered that "it depends on what is justified" and "whatever you need to do the job" but that the equipment not be more than what is required to meet the program objectives. In the budget proposed above, we are asking for about 15% of the NSF money to be used for equipment purchases (i.e., $292,000). This is to be match by $266,000 from the Ohio Board of Regents, OBoR, Action fund and $292,000 from the institutions asking for the equipment (i.e., $850,000 in total for equipment for the project).
  - In terms of timing, it seems clear to me that the equipment should be "front loaded" into the budget (i.e., almost all in the first year). One very strong rationale for this is that a May/June announcement and nominal June 1st start would make it challenging to get the summer courses and research assistance programs going at a steady state pace. In addition, the hardware has to be in place for the research to be carried out.
  - Several people have also pointed out that it makes the most sense to have the Faculty Fellowships front loaded (e.g., 20, 15, 10, and 5 being awarded in the summers of 2000, 2001, 2002, and 2003, respectively) while the Student Fellowships would be back loaded (e.g., 5, 10, 15, and 20, respectively). This is because it makes sense to first train faculty and get them involved in research so that the undergraduates coming up can be better trained and research involved at their home institutions. Also, many faculty should be getting their own individual or collaborative grants (i.e., Research Corp., PRF, RUI, ROA, etc.) in later years and this should also support more students. Also, if we can get a consortial REU grant for the ADSC then some of the programmed student money can be used to support extra Faculty Fellows or other purposes.
  - One advantage of this late start is that there should be some money left for the summer of 2004 (i.e., as a no cost extension) to wind the project up and transition the ADSC to full self funding.

- *<u>Item A, above:</u> Capital Diffraction Equipment (purchases and upgrades) to be included in the budget*
  - $850,000 in total: $292,000 from NSF, $266,000 from OBoR, and $292,000 from universities.
  - To date, I have had a number of requests for minor equipment, equipment upgrades, and major equipment items that appear to be well justified in terms of the program goals.
  - During the ADSC organizational meeting on December 12th 1998, we discussed this budget component in detail and agreed on the items to be included in this RSEC proposal. In particular, we decided to include those items most consistent with the RFP and the ADSC goals.
  - Where allowable by the program guidelines, these capital items have been included in the OBoR Action Fund application from YSU (i.e., to get a 1/3 capital match from the state of Ohio).
  - The capital equipment match policy is we only ask NSF for 1/3 of the price for major items and 1/2 for smaller items).
  - Access policy to instruments purchased with RSEC money: undergraduate faculty and collaborative projects priority for the majority of the instrument time on instruments so purchased and no direct user charges for these instruments are to be charged to them.
  - The following items were requested and are included in the budget [Note: All prices are my estimates based on recent selling prices of similar systems. The specified vendors and models are illustrative and do not represent a commitment to these specific choices.]:

- ♠ Item A1, above: CCD Single Crystal Diffractometer System (YSU and ADSC), a Bruker AXS SMART 1000 system with PLATFORM goniometer, sealed tube generator, heat exchanger, Oxford Cryostream low temperature system, Capillary optics, data system, and SHELXTL site license (the site includes all of the undergraduate institutions in the ADSC without their own diffractometers who collect their data on the YSU system). $303,000 in total with $101,000 requested from NSF, $101,000 from the OBoR Action Fund, and $101,000 from YSU.
- ♠ Item A2, above: Powder Diffractometer (YSU and ADSC), a Bruker AXS D8 powder diffractometer with sealed tube generator, heat exchanger, sample changer, and data system. $153,000 in total with $51,000 requested from NSF, $51,000 from the OBoR Action Fund, and $51,000 from YSU.
- ♠ Item A3, above: Film Diffraction System(s) (Kent State and YSU), new X-ray generator(s) (i.e., the current ones are unreliable and don't meet radiation safety standards) and cameras for Weissenberg, Precession, Guinier, and Debye-Scherrer methods, approximately 60K in total with a 2/3 match (1/3 OBoR Action Fund, 1/6 Kent State University, and 1/6 YSU).
- ♠ Item A4, above: Protein Crystallography Data System(s) (Cleveland Clinic/CWRU and YSU), SGI workstation(s) for collaborative protein structure determinations, approximately 60K in total with a 2/3 match (1/3 OBoR Action Fund, 1/6 Cleveland Clinic/CWRU, and 1/6 YSU).
- ♠ Item A5, above: Wright State Replacement diffractometer, approximately 120K with a 2/3 match (i.e., 1/3 OBoR Action Fund and 1/3 Wright State). Nonius MACH3 diffractometer with low temperature system and data system.
- ♠ Item A6, above: Bucknell, modernize the R3, approximately 50K with a 50% match from Bucknell.
- ♠ Item A7, above: YSU and Toledo, $102,000 for a 20% nominal share in the CWRU MB-CAT beamline team at the APS. The 10% YSU share of the time will also be available to faculty from other predominantly undergraduate schools in the ADSC.
- ♠ Item A8, above: Mount Union College - Chemistry and Geology: Upgrade to their new Phillips 3710 powder diffractometer to add a track for mounting cameras. I will guess a total cost of $2,000 with a 50% match from them.

♠ ***I want to clearly reiterate here that all of the YSU equipment funds will build additional capacity to carry out new single crystal and powder studies to be funded by this RSEC grant. They will be fully used to support the research and teaching of undergraduate faculty and their students. In spite of this commitment, we will be asking NSF for only 1/3 of the money, with OBoR (Action Fund), and YSU providing the rest. This money will support not only on-site studies but also data collection at a distance – a major aspect of our Consortium's support for undergraduate institutions.***

♠ *The 1999 OBoR Investment Fund Equipment Application from the Ohio Crystallography Consortium, OCC, and This RSEC Proposal*. Some PhD institutions have outlined clear needs for equipment that would be hard to justify in terms of the RSEC program goals (i.e., these goals and my discussions with the program officer have been very specific on what the RSEC program is likely to fund). These equipment requests make good sense to ask for as a central part of the OBoR Investment Fund grant application this winter from the OCC and some of are being included there. In addition, some of the equipment requested by the predominantly undergraduate schools in Ohio will be included in the OBoR Investment Fund application. Indeed, a major part of this OCC Investment Fund application parallels the thinking of the current RSEC proposal.

♠ *Items B, above: Recent/Current Crystallographic Investments (as other capital matching funds)*

- ♠ I need information from participating schools that currently have diffraction facilities and have recently made capital investments in these or are in the process of planning to do so over the 5 year life of the grant. We may be able to include some or all of these investments as matching funds for this RSEC grant proposal.
- ♠ Item B1, YSU: YSU has spent/will spend $5,000 to upgrade the diffraction lab over 1998/99, will spend an additional $20,000 to renovate a lab to hold the proposed diffractometers (tentatively identified by the chair of Chemistry, Daryl Mincey, as Room 5025 in Ward Beecher Hall adjacent to our current diffraction lab), including attached office space for the Diffraction Lab Scientist, and has spent/is spending $200,000 over 1998/99 for the two computer labs to be used in the instructional courses ($40,000 of which is directly related to diffraction methods). This adds up to an additional capital match of $65,000 from YSU.
- ♠ Other Schools???

- *Items C, above: Direct Maintenance and Operating Expenses (as non-capital match)*
  - This include the funds required to keep the instruments to be purchased with this grant operating. I can also use information from participating schools that currently have diffraction facilities and have will make non-capital investments over the 5 year life of the grant to keep them running (i.e., maintenance budgets and contracts, parts budgets, etc). We may be able to include some or all of these investments as matching funds for this RSEC grant proposal.
  - Item C1, YSU: The diffractometer maintenance budget for YSU will be increased by $10,000 per year to a total value of $75,000 over 5 years to keep the current and new diffractometers operating in top form. Since we have a skilled electronics person, see below, to do the repairs/maintenance, this amount will be sufficient to cover repairs/breakage/etc.
  - Other Schools???

- *Item D, above: Crystallographic Software and Data Bases*
  - $60,000 in total from NSF over the life of the RSEC project.
  - It is essential that the students get copies of the software that they learn in the summer schools to take home so that it will be more readily integrated into their teaching and research.
  - I am also trying to convince Bruker AXS (with the assistance of Bob Sparks) to make a version which has been "stripped down" (e.g., so that it can only solve structures in a few space groups and lacks the XPREP and XCIF functions) available for wider distribution and use in early undergraduate and high school data analysis experiments at a very low cost (since this is all most school districts can afford).
  - It is difficult to estimate this total software cost in detail. However, much of the advanced software is in the public domain or is available at little or no charge to academic users (e.g., SHELXL and SHELXS). However, for novices, these packages typically have a relatively non-intuitive and hard to learn interface. In contrast, some of the commercial crystallography/diffraction packages are much easier for students to pick up (e.g., teXsan, Crystallographica, and SHELXTL-XSHELL, SnB).
  - Some of the software packages I expect to include are:
    - A user friendly package for routine single crystal structure determinations:
      - SHELXTL for single crystals: I have included a site license for SHELXTL from Bruker AXS included in the capital budget (i.e., item A1, above). This license includes the undergraduate members of the ADSC that collect their data at YSU and don't have their own diffractometers in the YSU site license.
      - teXsan for single crystals: I have gotten a quote bulk pricing for the teXsan package ($2,500 for the first copies, and then a sliding scale eventually approaching $200 for each additional copy). Considering that we may require 100 copies, these prices are a challenge but the software has an excellent user interface. There is also the option of buying a copy or copies to go on workstations which others may access via X-windows.
      - The Nonius package????
    - Crystallographica and molecular graphics packages????
    - Powder diffraction software packages:
      - Reitveld package…….
    - Protein diffraction software packages: Vivien Yee's information on protein software and costs to go into full proposal. In general, they are free or of low cost – estimated total only several thousand dollars.
  - Timely access to the various crystallographic data bases is essential for both routine and advanced crystallographic research. The cost of this access is a burden on even PhD departments and is entirely beyond the means of undergraduate institutions. A major service to the faculty and students from these schools by the consortium will be us giving them easy access to these databases.
  - Some of the Data Bases I expect to include are:
    - Cambridge Crystallographic Data Base: ≈$500 per year.

- Inorganic Crystal Structure Data Base: ≈$800 per year.
- PCPDF-Powder Diffraction Files: ≈$1,250 per year (1st year included in item A2, above).

- Direct costs of a server, etc., to provide these data bases to undergraduate faculty and students at remote sites. These data bases will be made available to all consortium participants on the YSU host site. They will also be made available to off site users at predominantly undergraduate schools via Internet and/or mail requests to be carried out by the diffraction technician. (i.e., assisted by the Diffraction Lab Manager)..

- *Item E, above: Project Director (Allen Hunter)*
  - $320,000 in total: $210,000 from YSU and $110,000 from NSF.
  - Academic year reassigned time equivalent to 1/2 of my contractual teaching load will be provided by YSU for 4 years and for my full teaching load for 1 year as a match to enable me to manage the day to day activities of the consortium. Salary and benefits for 3 years, $210,000 as a YSU match.
  - I am requesting summer support of 2/9 of my academic year salary and benefits from this NSF grant for 1999-2004. Salary and benefits for these summers, $85,000 from NSF.
  - Since I will be the primary teacher at several of the summer schools, most of this money would otherwise be spent on stipends, travel, and lodging costs for their instructors.
  - I will carry out all of the administrative duties described above for the Project Director
  - I will direct and lead additional grant seeking/writing efforts by the consortium and this will be my main grant writing effort for the next five years.
  - I am also requesting support for consumables and research travel to support my high resolution crystallographic research at the rate of $5,000 per year from NSF(i.e., less than the average rate will be for the Consortium Fellows).

- *Item F, above: Minority Enhancement Program (Director: Sherri Lovelace-Cameron)*
  - $110,000 + xxx in total: $50,000 from NSF, $xxx from YSU, $xxx from other schools.
  - Dr. Sheri Lovelace-Cameron of YSU to head this effort. She is being appointed as the Coordinator of Minority Enhancement Programs.
  - I am asking for reassigned time equivalent to 1/6 of Sherri's normal teaching load each academic year to support her efforts. Match value of $60,000 from YSU.
  - I am asking NSF for summer support for Sherri equivalent to 1/9 of her annual salary to support her efforts. Cash value from NSF of $25,000.
  - The Consortium will provide seed money of $5,000 per year to support this initiative. Cash value from NSF $25,000.
  - However, this program will require significant funds for summer student wages. Fortunately most schools already have funds available for this purpose and others from foundations, the ACS SEED project, the NSF REU program, etc., are relatively easy to obtain. Specific contributions that have been identified by school, include:
    - YSU, $xxx from ACS Project SEED, its YSU match, and YSU funds for minority students that can be reprogrammed to support this initiative. Match value $xxx from YSU.
    - Other schools?????
    -
    -
  - I suggest that a representative from each participating institution approach the person at their department/campus who is involved/responsible for these programs and ask them to designate one or two of

their current slots to support placing student from underrepresented groups in crystallographic groups. This should easily produce 15 or 20 slots for minority students.

- We are actively encouraging minority faculty members from outside our immediate region to participate in our programs, especially those at historically black colleges.

- <u>*Item G, above:*</u> *Diffraction Lab Scientist*
  - This person will be critical to handle a large load of submitted samples, to help with increased diffractometer maintenance, and to ensure efficient instrument utilization.
  - After discussion at the ADSC organizational meeting it was decided that this position will be at the postdoctoral level and that an average salary of about $36,000 would be sufficient to attract good candidates. With benefits, this corresponds to about $50,000 per year..
  - I think it would be too hard to justify full support from NSF for this project. I am asking YSU for a 60% match for this *new position* and am asking NSF for the other 40% (i.e., for $150,000 from YSU and $100,000 from NSF).
  - Since this person will assist with the summer course labs, their availability will lower the cost to NSF and the consortium of providing these schools.
  - This person will be assisted by trained undergraduate and MS students, as required, to meet demand.
  - They will mount crystals and collect data on crystals submitted by faculty and students at other sites. They will also assist people who come to YSU to collect data.
  - By doing analyses for industrial customers, they might generate sufficient funds to partially cover YSU's portion of their salary and to defray increased maintenance costs.
  - This person would assist faculty and students from YSU and other predominantly undergraduate schools with their personal research.
  - This individual would have some time available to institute a collaborative research project if they so desire.
  - I plan on applying for funding to convert this position into a Dreyfus Teacher/Scholar position or some similar program. The first application will be in the summer of 1999.

- <u>*Item H, above:*</u> *Faculty Reassigned Time to Support/Assist/Participate in this Proposal*
  - To get the maximum benefit from this proposal for our research and teaching programs, institutions may be willing to commit faculty time/resources. These faculty will be involved in the instructional component of this proposal, in assisting visiting faculty and students, in carrying out collaborative research with external faculty and students, in (further) developing crystallographic research programs, etc. These would not be new budget lines but rather an acknowledgement of the time these people will spend on the project (typically counted as a share of salary and benefits proportional to reduced teaching loads).
  - YSU is willing to strongly support this effort by designating two faculty members each year who would have an average of 1/3 reassigned time each for this project. The candidates in the Chemistry department for 1999/2000 would be Tim Wagner and Mike Serra. The matching value of this reassigned time would be a minimum of $40,000 each year for $200,000 in total over 5 years..
  - Other schools????

- <u>Item I, above:</u> Technical Support Staff
  - <u>Item I1, above:</u> It was pointed out to me by my Dean of Graduate Studies and Research, Peter Kasvinsky (a protein crystallographer), that the Directorship of this consortium will be a real administrative headache and will require significant clerical support. Since our current departmental secretary is saturated, we will need to develop new clerical support. We have administration support to dedicate a ***new*** *25% time clerical position* or the equivalent to support this effort at a cost of about $7,000 per year (this may be through a part time secretary or though the employment of one or more skilled student clerical assistants) for a total of $35,000 over 5 years.

- Item I2, above: For the NSF proposal to succeed, we need to demonstrate that we have committed sufficient personnel and funds for diffractometer and computer maintenance. In addition to routine instrument maintenance duties to be performed by the new Diffraction Lab Scientist, instrument maintenance will be carried out by the departmental electronic instrumentation specialist. *Ray Hoff* is very skilled in this area with about ten years experience on advanced chemical instrumentation and we will dedicate *25% of his time* to support the diffraction lab at an annual cost to YSU of $18,000, *about half of this is a new commitment*. This represents a total match of $90,000 over 5 years.
- Item I3, above: The College of Arts and Science *computer networking expert*, Bob Hogue, (and/or equivalent YSU staff) will dedicate *5% of his time* at an annual cost to YSU of $3,000 to supporting the consortial research and teaching effort. In addition, our departmental computer labs are continually staffed by skilled student assistants. During the summer courses their assistance will increase the *new cost to YSU by $250 per week*. In addition, the YSU Chemistry Department will make its new Windows NT computer lab, having 12 work stations, and our new Windows 95 lab, having 24 workstations, available for use in the courses and by visiting researchers and students as it will our 3 three year old SGI INDY workstations.
- Note: through OhioLink, participating Ohio colleges and universities have free online access to Elsevier and Academic Press journals and to interlibrary loans of other crystallographic journals and books. YSU is developing good holdings in this area.
- Other Schools????

- *Item J. above: Undergraduate Faculty Fellowships*
  - Undergraduate Faculty Fellows, general information
    - A total of about 50 Faculty Fellowships be awarded over 5 years. It make sense to front load these fellowships into the early years of the grant. Thus, we might award something like 15-20 Faculty Fellowships for the summer of 2000 and only around 5 the summer of 2003. Such a distribution seems likely to have the maximum impact on the program goals, see above.
    - 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 fellowships along with a description of their research interests. This will be done prior to the annual Fall meeting of the ADSC. Where ongoing collaborations have not previously been established, the Director will introduce undergraduate and host faculty with similar research interests and that 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 of Faculty Fellows 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 though the consortium.
    - Prospective Fellows will typically make joint applications with their chosen researcher host for these Fellowship 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 Fellowships not awarded in the first round may be applied for one month before subsequent meetings.
    - With the suggested stipends and allowances to home and host institutions this would total $575,000. This would represent about one third of the annual non-overhead budget which is consistent with the goals of our program.
    - The Faculty Fellowship 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 I am told that they are usually **relatively easy to get** and NSF feels that they are underutilized. 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 collaborations with faculty and students from predominantly undergraduate schools on a continuing basis (i.e., after the fellowships or this grant expires). They should therefore be asked for when there is sufficient notice of a pending collaboration or to continue one to the next 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 Fellowships will be given "bonus points" on their applications, especially for their second year. If one of these external grants is awarded, the Fellowship may still be awarded at a reduced amount. However, if there are less applications in a given year than there are Fellow positions, the Operational Oversight Committee may chose to give Fellowship funding for additional year(s) or to use this money for other consortial purposes.
- All Faculty Fellows 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.

- Item J1, above: Stipends
  - Summer (and prorated sabbatical) support will be provided as Consortium Fellowships from an account administered by YSU.
  - These fellowships are meant to be competitive and prestigious and will be for a fixed sum. A value of $7,500 per summer is very attractive for faculty from predominantly undergraduate schools. If funds are available, this amount may be supplemented and/or supplanted by home institutions, host institutions, and/or from grants. Any amounts which were supplanted would allow us to offer more Fellowships.
  - The total cost of this item is $375,000 for 50 fellows over 5 years.
- Item J2, above: Home Expense Grants
  - $2,000 will be made available to the Fellow for spending on typical levels of crystallographic and research consumables. They will be available for use at the home department without the need for a special proposal. Their spending will be at the discretion of the fellow within the policy guidelines of their home institutions for grants. Costs in excess of this amount will have to be met from internal sources, from separate external grants, and/or *as the last choice* by application to the exceptional costs fund (above).
  - It will be generally expected that home institutions provide some reasonable level of match for these funds.
  - The total cost of this item is $100,000 for 50 fellows over 5 years.
- Item J3, above: Host Expense Grants
  - $2,000 will be made available to research directors that host the Fellow for spending on typical levels of crystallographic and research consumables. They will be available for use at the host department without the need for a special proposal. Their spending will be at the discretion of the host research director within the policy guidelines of their host institutions for grants. Costs in excess of this amount will have to be met from internal sources, from current external grants, from separate external grants, and/or *as the last choice* by application to the exceptional costs fund (above).
  - These grants are meant to defray a substantial part of the *incremental costs* of hosting and undergraduate Faculty Fellow.
  - The total cost of this item is $100,000 for 50 fellows over 5 years.
- Item J4, above: Extraordinary Expense Grants
  - Requested amounts up to $4,000 per year over and above those that come automatically with the Research Fellowships will be distributed upon approval of applications from Fellows explaining the need for these *exceptionally high costs.* They may be payable to either or both of the home and host institution. This money will come from an annual pool of $40,000. These proposals will be evaluated by the Fellowship sub-committee of the Operational Oversight Committee. The proposals must be submitted to the Consortium Director two weeks before the regularly scheduled meetings of this committee and will be decided on the day of that meeting. These requests may accompany the requests for Fellowships but no more than half of the annual funding from this pool will be allocated at the first meeting. *Truly exceptional costs* might be for: unusually large scale use of cryogens, unusually

expensive chemicals, construction of special X-ray equipment, unusually extensive travel to collect data at national labs, etc.

- The total cost of this item is $200,000 for 50 fellows over 5 years.

- *Item K, above: Support of undergraduate and MS students and high school science teachers*
  - This support for research will be awarded in the form of Student Fellowships tenable at host institutions and/or home departments while working on collaborative research projects.
  - Written applications will be sent to the Consortium Director for distribution to the Operational Oversight Committee which will review the applications and award the fellowships. 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. These applications would commonly, although not exclusively, be accompanied by one from a faculty partner who is also applying for a Faculty Fellowship for the student and faculty member to work together in the same research group. Any Student Fellowships not awarded in the first round will be available for application one month prior to the next meeting.
  - The budget for this program be $25,000 per year. I further suggest an individual rate set at about $2,500 (which could be supplemented by host department funds where these are available).
  - As discussed above, these fellowships would be "back loaded" into the later years of the RSEC program.
  - I would welcome suggestions from you for sources of internal funds at your institutions that might be reprogrammed to support this effort.
  - ADH will lead a team to write a NSF REU application for the ADSC. This will be a topically focussed proposal on diffraction methods that will have the student start and end the summer at a common summer school on diffraction methods and conference to present results and spend the rest of the summer engaged in diffraction research at the host sites that decide to participate.
  - The total cost of this item is $125,000 for 50 student fellows over 5 years.

- *Item L, above: Funding for basic and advanced summer schools*
  - Allen Hunter and the diffraction technician will provide the core of the instruction for the "basic training" courses in single crystal methods and several other courses at YSU as part of their responsibilities.
  - Their will be additional instructors as appropriate for each course. The following experienced instructors have been identified for the basic courses. The instructors for the advanced courses will be selected by those willing to host them.
    - John Hughes from Miami University
    - Katherine Kantardjieff from Cal. State Fullerton
    - Margaret Kastner from Bucknell University
    - Tim Wagner from YSU
    - Vendor's representatives?
  - Item L1 and L2, above: Instructors stipends, travel and lodging expenses, and supplies totaling $20,000 per year for the basic (i.e., in basic single crystal methods, basic powder methods, and the course for high school teachers at YSU) and advanced summer courses (at various host sites) are budgeted in the RSEC grant. Additional funding from other sources including the diffractometer vendors, the Eisenhower program, and various technological/scientific educational initiatives will be sought to increase the size of the classes in these courses and the number of offerings.
  - Item L3, above: Student Expenses (for undergraduate faculty, students, and teachers) totaling $10,000 per year. This amount will cover lodging expenses while attending the summer courses.
    - For those courses to be sited at YSU, and for longer term visiting faculty and students, the YSU housing office has agreed to provide room and board in new, air-conditioned dorms two blocks from Chemistry for a rate of $25 per day double occupancy, $30 single occupancy (i.e., just covering their incremental costs). The commercial rate for such nice accommodations would be much higher (i.e., $60 to $80 per

day). The difference is shown as a YSU match (i.e., calculated based on 300 days of lodging per year, $9,000 match).

- High school science teachers are eligible to apply for participation in the basic summer crystallography courses and the Student Fellowship programs. In combination with other interested faculty, I plan on applying for Eisenhower funding to expand this program and especially to supply the stipends and expenses to those taking the courses as Eisenhower grants typically do now.

- *Item M, above: Funding for Committee Expenses and Dissemination and Evaluation Activities.*
  - I propose a total budget for the Director, the External Assessment Committee, and the Oversight and Evaluation Committee for expenses of $15,000 per year (1/3 to each group). This would fund travel and lodging expenses, postage, and phone bills needed to carry out the oversight and assessment duties of each. This money would be spent as directed by each group.
  - In addition, I propose a budget of $10,000 per year to cover miscellaneous expenses related to dissemination and evaluation activities. This money would be spent at the discretion of the Director to support these activities by himself and other consortium members. The biggest components of these costs are likely to be those involved in disseminating new printed and software crystallographic educational materials developed by consortium members and attending professional meetings to disseminate the results of our faculty and student development and research activities.

- *Item N, above: Overhead*
  - The YSU overhead rate is 32% of salaries (not including benefits). Within the above budget, approximately $600,000 are salaries which corresponds to a total overhead line of $190,000.
  - CWRU is expected to be the official managing institution (i.e., with YSU as a subcontractor for ≈ 99% of the budget). I expect that they will request some reasonable overhead or direct cost for their management role.

- *Additional external funding for related research and educational efforts.*
  - If this proposal is funded, we will need to develop additional sources of funding to expand the activities of the consortium during the first five years and provide it with continuing funding after this time. Indeed, the plan for doing so will be an integral part of what the NSF RSEC review panel will be looking at.
  - Even if this proposal is not funded, the work that has gone into putting it together will be available if we continue seeking funding for its core ideas.
  - Ohio Crystallography Consortium – Ohio Board of Reagents .
    - OBoR Action Fund for 1/3 equipment matching money for equipment going to Ohio universities.
    - OBoR Investment Fund for new equipment through OCC that is either included in, or is not fundable under, the RSEC program.
  - Internal and external sources of support for the under-represented minority program. This could include local and consortial efforts to obtain commitment of current internal funds and to raise new funds from programs such as ACS Project SEED.
  - Below, I list several sources of external funding that we should purse for the consortium and/or that I plan on pursuing for YSU and/or my personal research:
    - *Equipment funding*
      - NSF research equipment funding, especially to the CHEM-CRIF, DMR-IMR, and NSF-MRI programs. For the undergraduate schools, these programs are typically accessed through the RUI-Equipment program.
        - **CHEM-CRIF-RUI Target dates: January, July, and October 1st**
        - **DMR-IMR-RUI Deadline January 29th**

- NSF Instructional equipment funding from the **CCLI program. Deadlines June 7th and November 16th**
- Several foundations also provide partial funding for equipment:
  - **Dreyfus Foundation Special Research Grants Program in Chemistry. Deadline July 15th** for the pre-proposal.
- The Ohio Board of Research has several main types of research equipment funding:
  - **Instructional Equipment Funds** which are distributed to state supported institutions each biennium for internal allocation (YSU got our Chemistry Computing labs from these).
  - **OBoR Action Fund** which provides a 1/3 match for major external equipment grants. **Deadline date 3 weeks before proposal submission.**
  - **OBoR Investment Fund** which provides most of the money for equipment needed for consortial proposals. **Deadline date December 4th for preliminary letter (January 7th for preliminary proposals).**
- YSU is planning on applications to these programs for:
  - A powder diffractometer and other lab upgrades from DMR-IMR-RUI[1] in January.
  - The CCD upgrade/diffractometer and other lab upgrades from CHEM-CRIF-RUI in winter/spring.
  - Possible instructional diffraction equipment and support for several of the proposed education initiatives through CCLI in June.
  - Dreyfus teacher/scholar funding in July.
  - Dreyfus matching funding in July.
  - OBoR Action Fund match for the research equipment in Ohio has already been submitted (i.e., for $266,000).
- The Ohio Crystallographic Consortium will apply to the OBoR Investment Fund in January for equipment to go to Toledo and YSU.

- *Supplements to current federal research grants*
  - The NSF research grant programs for faculty at PhD schools allows them to apply for supplements under the **ROA program** to support undergraduate faculty and students for up to ≈ $15,000 per year. The NIH and other federal granting agencies have similar programs. These applications are relatively short and typically have high success rates and are an excellent way to fund collaborative research with undergraduate faculty and students. Target dates are around February 1st for this program and a similar times for other Federal agencies.
- *Research grant programs optimized for undergraduate faculty*
  - There are numerous sources of research grant support that are tailored for faculty from predominantly undergraduate schools. These include:
  - The NSF **RUI Program** in all of its research directorates. In DMR the deadline date is **November 1st**. In CHEM the target dates are **January, July, and October 1st**.
  - The **Research Corporation Cottrell College Science Awards** for up to ≈ $40,000 have Target dates of **May and November 15th**.
  - The **American Chemical Society PRF Type B Grants** of up to $30,000 have target dates of **January, July, and October 15th**.
- *Educational/Training Grants*
  - These is a variety of type of grants to support individual or consortial education and training initiatives, including:

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[1] Note: NSF-DMR-IMR-RUI partially funded our P4 diffractometers four years ago.

- The **NSF DUE CCLI** program which now allows one to integrate both equipment and/or curriculum research/development and dissemination initiatives. Deadlines **November 16th and June 7th**
  - I plan on submitting a CCLI relating to crystallographic/diffraction education in June and solicit names of those who might want to collaborate with me.
- In many ways these courses resemble things funded by the old NSF Undergraduate Faculty Enhancement Project which has now been absorbed into the CCLI program.
- The **American Chemical Society** Project SEED for minority student enhancement programs. Deadline???
- The **Eisenhower Grant Program** for pre-college faculty development activities. **Late summer/early fall deadline**
- We should apply to the **NSF REU** program as either individual schools or a Consortium as a "site" focussed on crystallographic Research Experiences for Undergraduate. In addition, supplements to current grants to support undergraduates can be applied for by anyone with an active NSF grant. Both DMR and CHEM have programs:
  - **REU supplements** with a **deadline on January 1st** for individual REU supplements
  - **REU sites** with **September 15th deadlines**.
  - I plan on applying as a REU site with a crystallographic/diffraction theme in September and I solicit names of those interested in participating.

Timeline for the proposed project

Nov. 1998	Prepare and circulate for comment outline of RSEC proposal
Dec. 1998	Send in OBoR Investment Fund letter of intent (OCC) Submit OBoR Action Fund application (YSU) On Saturday the 12th have meeting of RSEC consortium at YSU -
Jan. 1999	We need to plan on having our proposal completed by about January 6th. To this end, I need letters of commitment from each institution by January 1st and everyone's Biographical Sketch and Current and Pending Support Forms by then as well. On 1st target for RUI-Instrumentation proposals (ADH) On 1st target for RUI-Research proposals (ADH and B. Craven) (will miss target!) On 11th RSEC proposal due (ADH - RSEC Consortium) On 15th target for ACS-PRF Type B (ADH) On 29th NSF-DMR-IMR applications due (TRW)
Feb. 1999	On 17th ADH meets with program officers
May 1999	On 15th Research Corp. proposals due (ADH)
June 1999	By 1st RSEC Funded Consortia to be announced On 7th CCLI proposals due (ADH - YSU)
July 1999	Target and Due dates for NSF-RUI, Dreyfus, and PRF programs.
Sept. 1999	On 15th due date for REU proposals (ADH - RSEC Consortium)
Oct./Nov. 1999	Target and Due dates for RUI, PRF, DMR-Research, Research Corp, and CCLI grants
May/June 1999	**IF SUCCESSFUL IN GRANT COMPETITION THE RSEC CONSORTIUM WILL MEET**

Summer 1999	Order equipment to be funded from the first year of the RSEC grant.
Summer 1999	Begin first stages of educational and fellowship programs.

Timeline

The program officer at NSF, Dr. Janet Osteryoung, has stated that the expected starting date for the RSEC grants is June 1st of 1999. These RSEC grant are for 5 years (i.e., until June 1st, 2004) and, as per our discussions with Dr. Osteryoung, we plan on using the 1 year no-cost project extension that NSF provides (i.e., so that our project has until June 1st, 2005 to be totally completed). Following, is our current timeline:

Year 1	1999-2000	Award of grant, purchase of instrumentation, installation of ADSC Crystallography Lab at YSU including hiring of Lab Manager and diffraction facilities at other participants, initiation of collaborative research projects, award of Fellowships 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 20 undergraduate faculty and 5 students will participate in collaborative research projects at host schools funded by Consortium Fellowships, 1st year of summer schools, award of Fellowships for summer of 2001, 1st intensive evaluation cycle, application for external grants by all Faculty Fellows, application for additional external funding opportunities by consortium.
Year 3	2001-2002	About 15 undergraduate faculty and 10 students will participate in collaborative research projects at host schools funded by Consortium Fellowships, 2nd year of summer schools, award of Fellowships for summer of 2002, 2nd intensive evaluation cycle and 1st dissemination cycle, application for external grants by all Faculty Fellows, application for additional external funding opportunities by consortium.
Year 4	2002-2003	About 10 undergraduate faculty and 15 students will participate in collaborative research projects at host schools funded by Consortium Fellowships, 3rd year of summer schools, award of Fellowships for summer of 2003, 3rd intensive evaluation cycle and 2nd dissemination cycle, application for external grants by all Faculty Fellows, application for additional external funding opportunities by consortium.
Year 5	2003-2004	About 5 undergraduate faculty and 20 students will participate in collaborative research projects at host schools funded by Consortium Fellowships, 4th year of summer schools, award of Fellowships for summer of 2003, 4th intensive evaluation cycle and 3rd dissemination cycle, application for external grants by all Faculty Fellows, 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 all Faculty Fellows, application for additional external funding opportunities by consortium, final reports to NSF and all participants.