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PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 01-2					FOR NSF USE ONLY	
NSF 01-7					NSF PROPOSAL NUMBER	
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DMR - MAJOR RESEARCH INSTRUMENTATION						
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Youngstown State University			Youngstown State University			
AWARDEE ORGANIZATION CODE (IF KNOWN)			410 Wick Avenue			
0031450000			Youngstown, OH. 445550001			
NAME OF PERFORMING ORGANIZATION, IF DIFFERENT FROM ABOVE			ADDRESS OF PERFORMING ORGANIZATION, IF DIFFERENT, INCLUDING 9 DIGIT ZIP CODE			
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IS AWARDEE ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions) <input type="checkbox"/> FOR-PROFIT ORGANIZATION <input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> WOMAN-OWNED BUSINESS						
TITLE OF PROPOSED PROJECT RUI-MRI: Acquisition of a Powder X-Ray Diffractometer System						
REQUESTED AMOUNT \$	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE			
170,310	12 months	08/15/01				
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW						
<input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.A)			<input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.C.11) IACUC App. Date _____			
<input type="checkbox"/> DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C)			<input type="checkbox"/> HUMAN SUBJECTS (GPG II.C.11)			
<input type="checkbox"/> PROPRIETARY & PRIVILEGED INFORMATION (GPG I.B, II.C.6)			Exemption Subsection _____ or IRB App. Date _____			
<input type="checkbox"/> NATIONAL ENVIRONMENTAL POLICY ACT (GPG II.C.9)			<input type="checkbox"/> INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED _____			
<input type="checkbox"/> HISTORIC PLACES (GPG II.C.9)			<input type="checkbox"/> HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.E.1)			
<input type="checkbox"/> SMALL GRANT FOR EXPLOR. RESEARCH (SGER) (GPG II.C.11)						
PI/PD DEPARTMENT		PI/PD POSTAL ADDRESS				
Department of Chemistry		Youngstown, OH 44555				
PI/PD FAX NUMBER		United States				
330-742-1579						
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CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

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

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

Name (Typed)	Signature	Social Security No.*	Date
PI/PD Timothy R Wagner	Signature Not Required	*ON FASTLANE SUBMISSIONS* SSNs are confidential and are not displayed	
Co-PI/PD Raymond E Beiersdorfer	Signature Not Required		
Co-PI/PD Allen D Hunter	Signature Not Required		
Co-PI/PD			
Co-PI/PD			

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 01-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U. S. Code, Title 18, Section 1001).

In addition, if the applicant institution employs more than fifty persons, the authorized official of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of Grant Policy Manual Section 510; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflict which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Debarment Certification

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

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency?

Yes

No

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding \$100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding \$150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

- (1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.
- (3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

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

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) Dr. Peter Kasvinsky/Graduate Dean	Electronic Signature	Feb 7 2001 3:48PM
TELEPHONE NUMBER 330-742-3091	ELECTRONIC MAIL ADDRESS pjkasvin@cc.ysu.edu	FAX NUMBER 330-742-1580

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SECTION A. PROJECT SUMMARY

Funds are requested for the purchase of a powder X-ray diffractometer system which will support the research needs of faculty, master's level students, and undergraduate research students at Youngstown State University. The instrument would also be available to support research projects of faculty and students at other colleges, who already are part of a consortium of users affiliated with the single crystal X-ray facility at YSU. The proposed instrument would provide data of sufficiently high quality to enable structure determinations of powder samples, which is not possible with the multi-wire detector currently used for powder analysis. Like all research-grade equipment at YSU, the proposed instrument will be available on a hands-on basis to students in upper-level laboratory courses, and thus will also positively impact educational efforts at YSU and other colleges.

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Section	Total No. of Pages in Section	Page No.* (Optional)*
Cover Sheet (NSF Form 1207) (Submit Page 2 with original proposal only)		
A Project Summary (not to exceed 1 page)	1	_____
B Table of Contents (NSF Form 1359)	1	_____
C Project Description (plus Results from Prior NSF Support) (not to exceed 15 pages) (Exceed only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)	15	_____
D References Cited	5	_____
E Biographical Sketches (Not to exceed 2 pages each)	6	_____
F Budget (NSF Form 1030, plus up to 3 pages of budget justification)	3	_____
G Current and Pending Support (NSF Form 1239)	5	_____
H Facilities, Equipment and Other Resources (NSF Form 1363)	3	_____
I Special Information/Supplementary Documentation	13	_____
J Appendix (List below.) (Include only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)	_____	_____
Appendix Items:		

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

SECTION C: PROJECT DESCRIPTION

C1. RESULTS FROM PRIOR NSF SUPPORT

The PI and co-PIs have actively pursued NSF support for their research, instrumentation, and educational project needs during the past several years. A common goal of many of the previous grant proposals (as well as the current one) is to establish and maintain a state-of-the-art infrastructure to support not only faculty research efforts, but also hands-on training of undergraduate and master's level graduate students, who are encouraged to utilize research-grade equipment in their own projects. The most relevant NSF-funded projects that the PI's have been involved in over the past five years are summarized below.

C1.a. NSF DUE 9551683: "Integration of GC-MS into the Undergraduate Curriculum."

This *DUE-ILI* grant (\$34,450, \approx \$50,000 match, 1995-96, J. Jackson, PI and A. Hunter, S. Schildcrout, R. Falconer, and T. Wagner, Co-PIs) was used to purchase a Finnigan 1020 Gas Chromatograph-Mass Spectrometer, which has subsequently (Dec. 1999) been upgraded with a new system controller, data system, and software. This instrument is now fully integrated into student research, senior level Organic Synthesis, Organic Analysis, Physical, and Inorganic Lab courses (i.e., 50 students a year), and into the Sophomore Organic sequence (i.e., \approx 200 students a semester, primarily from the natural sciences, engineering, and pre-medicine). In each case, it has facilitated a new collaborative learning/discovery-oriented approach. Our success with integrating this and related instruments into our teaching and student research sufficiently impressed an Ohio Board of Regents Investment Fund review panel that they recently helped fund a new LC-MS on campus (A. Hunter, YSU PI).

C1.b. NSF DUE ILI 9851107: "Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment." These *DUE-ILI* grant funds (\$44,600, over \$44,600 YSU match, 1998-2001, A. Hunter, PI and S. Brower, T. Kim, D. Mincey, and T. Wagner, Co-PIs) have been stretched to purchase more capable instrumentation than originally proposed, including: (a) a TA Instruments 2910 DSC, a 2050 TGA, a data system, and an upgrade of our older Dupont DSC/DMA/TMA data system, (b) a Cannon CT-518 constant temperature bath, and (c) a GBC Instruments/Polymer Labs GPC-SEC-HPLC system (i.e., autosampler, isocratic/gradient pump, column oven, RI and diode array UV-visible detectors, and data system) as well as additional equipment (authorized by Susan Hixson, DUE program officer, January 1999) including: (d) a Jasco 410 FT-IR (0.9 cm^{-1}) and (e) a basic Vacuum Atmospheres HE-43-2 inert atmosphere glove box with the residual funds. These instruments have now been/are being integrated into six upper division Chemistry and Chemical Engineering courses and into undergraduate research, and over the coming months its integration into several lower division Chemistry courses and into the Condensed Matter Physics course will be completed. These efforts are facilitating interdepartmental collaborations as well as the integration of materials science into non-specialist courses.

C1.c. NSF DUE-CCLI-EMD-POC: "X-Ray Diffraction Analysis Throughout the Curriculum: A Powerful Tool for Understanding Molecular Structure and Bonding."

This *DUE Educational Materials Development Grant* (\$74,707, 2000-02, A. Hunter, PI) had a May 1st, 2000 starting date. This project proposed the development of new documentation (texts and/or Adobe PDF), online annotated crystallographic database, software, and other teaching

materials to enhance the integration of single crystal diffraction methods into the undergraduate curriculum. The work is being carried out by a team that includes half a dozen high school chemistry teachers. It is on schedule for completion by its April 30th, 2002 completion date.

C1.d. NSF DUE-CCLI-A&I 9981040: “Integration of Computer Technology into the General Chemistry Curriculum.” This *DUE Adaptation and Implementation Grant* (\$94,945, \$103,956 YSU match, 2000-02, **T. Wagner**, PI and J. Mike, Co-PI) had a July 1st, 2000 starting date. During summer 2000, thirty LabWorks II workstations were purchased for the purpose of introducing computer data acquisition capability into the freshman chemistry laboratory. The workstations were used for the first time during the Fall, 2000 semester in the General Chemistry I Laboratory course, and are now being integrated into the General Chemistry II Laboratory course. The general chemistry laboratory curriculum has been almost completely revised to incorporate the new technology, and the second semester course will culminate in discovery-based, independent projects where students will use the workstations for data collection, storage, analysis, and tabulation/reporting of data. Students have or will use the workstations to collect and analyze temperature, pH, conductivity, colorimetric, and titration data. Following the Fall 2000 semester, students filled out customized questionnaire forms on-line at the NSF-supported site: *Student Assessment of Learning Gains*, centered at the University of Wisconsin–Madison. The assessment results indicated an overall positive impact of the equipment in their laboratory experiences. For further assessment of the project, students will be interviewed (on video tape) on a voluntary basis following completion of the second semester course.

C1.e. NSF INT 0086313: “Structural Investigations of Main Group Heterocyclic Rings and Cages.” This *RUI - International Division Cooperative Activities* grant (\$13,200 with \$84,000 in YSU and St. Andrews match, A. Hunter, PI) is partially funding one of the Co-PI's (ADH) 2000/2001 academic year sabbatical at St. Andrews University in Scotland (which concludes on June 31st, 2001) with professors Derek Woollins and Alex Slawin as hosts. It was recommended for funding (Dec 5th, 2000) by the program officer and had a February 1st, 2001 starting date. The emphasis of the proposed work is on diffraction methods, and it has both chemical education and chemical disciplinary research components. The educational component involves the writing of a “step-by-step” and very “hands-on” text, with supporting electronic materials, on routine single crystal diffraction studies targeted for undergraduates. The disciplinary component involves the charge density diffraction analysis of a series of organic and inorganic derivatives of nitrogen-sulfur heterocyclic rings and chains and molecular modeling studies of these species. This project is presently current with its projected timeline. A portion of the research plans presented (see section C2.2) by Dr. Hunter pertaining to the present powder X-ray diffractometer proposal is related to this funded project.

C1.f. Two of the applicants (TRW & ADH) have been involved in two NSF initiatives just recently awarded:

i. NSF REU-CHEM 0097682: “Research Experience for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities.” This Research Experience for Undergraduates grant (\$180,000, \$186,810 YSU match, D. Mincey, PI and **A. Hunter**, J. Jackson, S. Lovelace-Cameron, and **T. Wagner**, Co-PI's) will fund 10 undergraduate researchers each summer for the next three summers (i.e. 2001-2003). Some of these undergraduate researchers (i.e. any who choose to work on projects described herein) will be impacted by the proposed powder X-ray diffractometer system.

ii. **NSF DUE-CCLI-A&I 0087210: “WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions.”** This *DUE-CCLI Adaptation and Implementation Grant* (\$200,000, \$200,182 YSU match, 2001-04, **A. Hunter**, PI, L.M. Hoistad, A.J. Jircitano, **T.R. Wagner**, and E.P. Zovinka, Co-PI's) had a January 15th, 2001 starting date. The grant will fund a new Bruker APEX CCD single crystal diffractometer (or an analogous model from a different vendor). This instrument, along with our two current Bruker AXS P4 diffractometers, will be housed in a newly remodeled, ≈1,200 square foot diffraction facility. NSF and matching funds will also be used to equip the diffraction facility so that anyone in the world with WEB access will be able to watch lab and instrument operations via fixed and pan/tilt/zoom WEB cameras. If they have a WEB camera on their own computer, they will also be able to video-conference with the operators or faculty and students in this lab. A new stereo polarizing microscope to be placed in this lab will be equipped with a color WEB camera, so that students at remote sites will be able to view the crystal selection and mounting operations. The grant also provides funds to upgrade the two current P4 diffractometers with new computer hardware and software so that they can be remotely controlled over the WEB. The new CCD instrument will have this capability as well. The proposal specifies YSU as the Hub of a consortium of 27 other Predominantly Undergraduate Institutions (PUIs), which have indicated their interest in utilizing this facility to integrate diffraction methods into their undergraduate teaching and research programs.

C1.g. Educational and Research Impacts of These and Other Successful NSF Grants

The instrumentation projects described above, along with others funded by NSF over five years ago, have had a significant impact on both educational and research initiatives at Youngstown State University. First, the successful acquisition of research-grade instrumentation, made possible largely through NSF support, has played a key role in faculty successes in attracting outside funding (up by over an order of magnitude in the past decade) for their research and educational projects, from agencies such as PRF, Research Corporation, the Ohio Board of Regents, and NSF. Second, these projects have led to a number of peer-reviewed publications in the last few years, with several more in preparation. The improved education outcomes, along with the significantly improved instrumentation facilities, have translated into dramatically increased undergraduate participation in research, in a rapidly growing masters program, and in a rising national prominence for our *Predominantly Undergraduate Institution* chemistry program. At the undergraduate and even the master's levels, there is really no clear distinction between a student's education and their research, since these components interact in a synergic fashion with one another. This has led to a substantial increase in both the quantity and quality of student research being carried out at YSU.

C2. RESEARCH PROGRAMS OF MAJOR USERS

The Bruker D8 ADVANCE powder X-ray diffractometer system requested in this proposal provides high quality data enabling quantitative structure solution and refinement. This capability is currently not available on-site. Such an instrument is required for the successful completion of the research projects described below for the PI's and their students in the chemistry and geology departments. Even where single crystal data on individual crystals may be available, such high quality powder data is invaluable for characterizing the *bulk* phase(s).

C2.1. Dr. Tim Wagner

Dr. Wagner is an Associate Professor in the Department of Chemistry at Youngstown State University. His general research interests involve syntheses and structure characterizations of inorganic extended solids. More specifically, his major areas of interest involve studies of: (1) inorganic nitride-fluoride analogs of oxides; and (2) the crystal chemistry of oxides in the β -Alumina and Magnetoplumbite systems. Both projects would benefit significantly from the proposed equipment.

C2.1.a. Synthesis and Structural Characterizations of Nitride-Fluoride Analogs of Oxides

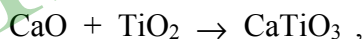
Statement of the Problem: The proposed research project focuses on the synthesis and structural characterizations of a series of nitride-fluoride compounds derived from well-known oxides, mainly in the rocksalt and perovskite systems. Here, the composition of the nitride-fluoride analog is obtained by replacing two O^{2-} ions of the metal oxide with a $(NF)^{4-}$ group. This is an area of inorganic solid state chemistry which has been largely neglected, as evidenced by the fact that fewer than forty such nitride-fluoride compounds have been reported in the literature, as compared to several thousands of inorganic oxides and hundreds of inorganic nitrides and fluorides. One reason for this is probably related to the extreme air-sensitivity of many of the nitride-fluorides already known, making them relatively difficult to prepare and characterize. Although progress has been made in recent years towards computing the likely structure of a given inorganic crystalline composition, it is still not possible at present to routinely predict from first principles whether or not a proposed composition will be the one prepared under given conditions.¹ Thus, this project is exploratory in nature, and is motivated by both the possibility of preparing new compounds with potentially useful properties, as well as expanding knowledge in the inorganic nitride-fluoride system. Such an exploratory approach to synthesis of inorganic oxides has in the past led to many materials with significant optical, magnetic, and electrical properties.

Previous Work: The previously reported nitride-fluoride compounds all contain only one metal atom, and several of these were originally prepared as analogs of rocksalt-type binary oxides. For example, nitride-fluoride compounds with compositions Ca_2NF , Sr_2NF and Ba_2NF have been reported² as analogs of CaO , SrO and BaO . Based on qualitative powder X-ray diffraction data, all three of these compounds were reported as having the rocksalt structures of their oxide analogs. Recently, however, we successfully prepared single crystalline samples of Ca_2NF and completed the structural characterization using single crystal X-ray diffraction.³ The results indicated that Ca_2NF does not have the rocksalt structure, but rather has a tetragonal structure with Ca atoms in square pyramidal coordination, similar to the structure proposed for Mg_2NF by Andersson.⁴ Qualitative analysis of powder samples of Sr_2NF synthesized in Wagner's lab suggests that Sr_2NF also has a Mg_2NF -type structure.⁵ Besides the nitride-fluorides containing Mg, Ca, Sr and Ba, the only other metals used to make inorganic nitride-fluoride compounds are apparently Ti, Zn, Zr, Tc, Th, and U.⁶⁻¹⁰ Of the approximately 40 nitride-fluoride compounds reported in these systems, less than 20 were structurally characterized, mostly by qualitative powder X-ray diffraction.

Proposed Research: The proposed research involves first synthesizing nitride-fluoride analogs of binary oxides, and then progressing to analogs of more complex oxides. Thus the first part of the project, which is already in progress, is focusing on the preparation of the following nitride-

fluoride compounds: Ba_2NF , Cu_2NF , TiNF , and $\text{Y}_2(\text{NF})_{1.5}$. These are analogs of the binary oxides BaO , CuO , TiO_2 and Y_2O_3 , respectively. The main reason these particular binary analog compositions were chosen is because they will be used as precursors in the preparation of the more complicated analogs in the next part of the project. Of these compounds, it is expected that Ba_2NF (and possibly Cu_2NF) can be characterized in single crystalline form, similarly to the Ca_2NF study recently completed. For these materials, single crystals can be made by slow cooling a mixture of the metal, M, and MF_2 from the melt under N_2 flow. The other two binary-analog compounds must be prepared in the solid state via an ammonolysis reaction, and so will be prepared as powders. The proposed nitride-fluoride analogs of the more complex oxides, discussed below, will also be necessarily prepared as powders. Thus, structural characterization of these materials will require high quality powder diffraction data that will enable structure solution and/or refinement of the powder samples.

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

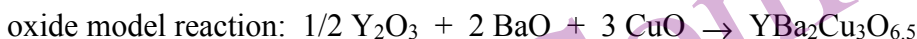


and it is proposed that $\text{CaTi}(\text{NF})_{1.5}$ be prepared analogously:



This reaction scenario is preferred over a direct synthesis approach, in which the precursors are simple compounds or elements that do not need to be pre-synthesized (i.e. they are easily purchased). For example, one could try reacting Ca metal with TiF_4 in N_2 gas. As past experience has shown, however, the problem with this approach is that often undesired intermediate compositions (such as CaF_2 in this case) are preferentially formed. Using a stoichiometric mixture of nitride-fluorides as proposed above should greatly increase the likelihood of obtaining a single-phase product with the desired composition. Undergraduate research students working in my lab have already successfully prepared Ca_2NF powder, and one student is currently working on preparation of TiNF using an ammonolysis route reported in the literature.¹¹ Thus, it is expected that the first trials of the proposed reaction will be completed by summer, 2001. Successful synthesis of the proposed $\text{CaTi}(\text{NF})_{1.5}$ compound would be significant, since no nitride-fluoride analogs of ternary oxides have been previously reported.

A long-term goal of the proposed research involves synthesis of a nitride-fluoride analog to the well-known 1-2-3 high temperature superconductor, $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. The overall reaction typically used for synthesis of the oxide material and the corresponding proposed nitride-fluoride reaction are:



Successful preparation of this phase would be highly significant in terms of comparison of conductivity properties with the analogous oxide material. Whether or not the new material is

superconducting (which also cannot be predicted), valuable insight could be gained as to the role oxygen plays in the superconducting properties of the 1-2-3 oxide phase.

Project Support: This project is currently supported by a grant from Research Corporation (Project #CC4811, \$39,719). Funds have been used to purchase a programmable high temperature (1700°C) tube furnace, pellet press, and supplies to complete the syntheses trials. As mentioned, it will be possible to prepare a few samples as single crystals, although we expect that most of the materials stemming from this work will be synthesized in powder form. While we are well-equipped to characterize single-crystalline samples, we are lacking in capability to perform quantitative characterization of powder samples on-site.

C2.1.b. Synthesis and Crystal Chemistry of Compounds Related to β -Alumina and Magnetoplumbite

Statement of the Problem: Solid-state batteries, high-energy lasers, and memory storage in computer systems are among the many possible applications of the compounds with structures related to those of magnetoplumbite (ideal composition $\text{PbFe}_{12}\text{O}_{19}$) and the well-known β -alumina (ideal composition $\text{NaAl}_{11}\text{O}_{17}$). In addition to the numerous practical applications, many compounds in these systems are fascinating from a purely crystal-chemical perspective. This project will focus on the crystal chemistry of a disordered phase that exists in magnetoplumbite/ β -alumina-related compositions in the $\text{BaO-Al}_2\text{O}_3$ and $\text{BaO-Ga}_2\text{O}_3$ systems. More specifically, the goals of the project are to obtain quantitative structures of the disordered phase from powder diffraction data, and further to study the dependence of the disordered phase on composition.

Background Information and Previous Work: The β -alumina structure consists of slabs of aluminum oxide with the spinel structure ("spinel blocks"), separated by mirror planes ("conduction planes") in which the large cations are located. The magnetoplumbite structure then differs from this only in the arrangement of cations on the conduction planes.

Of particular relevance to the present study is the crystal chemistry of barium hexaaluminate (BHA) and barium hexagallate (BHG). BHA was first reported in 1935¹² as having the ideal magnetoplumbite-type structure with composition $\text{BaO}\cdot 6\text{Al}_2\text{O}_3$, or $\text{BaAl}_{12}\text{O}_{19}$. Several years later it was reported¹³ that this composition does not exist, but rather that BHA actually exists as a two-phase material: so-called Phase I is Ba-poor relative to $\text{BaAl}_{12}\text{O}_{19}$, and Phase II is relatively Ba-rich. Meanwhile, the crystal chemistry of BHG was largely considered to be analogous to BHA, because of the similarity of their powder diffraction patterns.

The Phase I structures in both systems have been subsequently characterized by single crystal X-ray diffraction and shown to have relatively well-ordered structures closely related to that of β -alumina.^{14,15} On the other hand, X-ray and electron diffraction patterns indicate that the Phase II structures in both systems are highly disordered. The structures of the ternary Phase II compositions have never been determined using quantitative methods, although a single crystal study was performed on a Pb-stabilized form of BHA.¹⁶ Also, qualitative models for the Phase II structures have been proposed for both systems using high resolution electron microscopy (HRTEM).^{17,18} All models for the Phase II structures in both systems place the excess Ba atoms *within the spinel blocks* on either side of the conduction planes, although there is disagreement as to exactly how these Ba atoms are positioned.¹⁸ Also, there is some question as to whether the Pb-stabilized form of BHA is truly isostructural with the ternary Phase II BHA composition.¹⁹

Attempts to grow single crystals of BHG in order to quantitatively elucidate the Phase II structure instead only yielded the unexpected and previously unobserved result of a sample with the ideal magnetoplumbite-type structure and ideal $\text{BaGa}_{12}\text{O}_{19}$ composition.¹⁹ No such phase has yet been observed in the Ba-Al-O system, leading one to wonder whether the two systems are actually completely analogous. Clearly, more work is needed before the crystal chemistries of these two systems is completely understood.

Proposed Research: Since the preparation of single crystalline Phase II samples in both the Ba-Al-O and Ba-Ga-O systems appears to be hindered by the disordered nature of the structure, quantitative structural analysis must be completed using powder methods. The present study proposes to utilize the requested powder diffraction system in answering two basic questions pertaining to the crystal chemistry of the Phase II compositions: (1) What is the quantitative structure of both ternary BHA and BHG, and are they isostructural? and (2) Over what range of composition does the disordered Phase II-type structure exist? The positioning of the large Ba atoms in the densely packed spinel blocks is highly unusual for compounds in the magnetoplumbite/ β -alumina system, and in fact BHA and BHG are the only compositions known so far which have it.

Although the Phase II-type structure is complex, adequate trial structures are available so that only structure refinement (and not structure solution) should be necessary, making the analysis more feasible. The compounds proposed for preparation and powder structure characterization have composition $(\text{Ba}_x\text{M}_{1-x})\text{R}_{12}\text{O}_{19}$ ($\text{M} = \text{Sr}, \text{Ca}$ or Pb and $\text{R} = \text{Al}, \text{Ga}, \text{Mg}, \text{Si}, \text{Ge},$ or V). Of the many compositions possible, the following have already been prepared and await characterization: $\text{BaSiAl}_{10}\text{O}_{18}$, $\text{BaSi}_2\text{Al}_9\text{O}_{18.5}$, $\text{BaSi}_3\text{Al}_8\text{O}_{19}$, $\text{BaSi}_4\text{Al}_7\text{O}_{19.5}$, $\text{BaAl}_{12}\text{O}_{19}$, and $\text{BaGa}_{12}\text{O}_{19}$. Note that these materials have or will all be prepared using standard ceramic methods, which are straightforward and easily completed by undergraduate research students.

C2.2. Dr. Allen Hunter

Dr. Hunter is a Full Professor in the Department of Chemistry at Youngstown State University. His research interests are divided between projects involving chemical education initiatives related to X-ray crystallography, and disciplinary research related to organometallic synthesis and materials.

C2.2.a. Chemical Education

Over the past five years, Dr. Hunter has become increasingly active in work devoted to incorporating diffraction methods into the undergraduate chemistry curriculum. A basic premise of the work is that while undergraduate students are taught the importance of structure (particularly molecular structures) early in their chemistry studies, and also learn how liquid-state molecular structures are obtained using NMR methods, they often graduate with little or no background in the important role that diffraction methods play in structure determinations of solids. Due to recent advances in diffraction hardware, theory, and computer software and hardware, diffraction techniques are becoming used more and more by non-crystallographers (e.g. synthetic chemists and geologists) as part of their repertoire of structural tools.^{20,21} Indeed, examination of the literature readily indicates the increasing importance of single crystal X-ray diffraction in organic synthetic chemistry. The significance of these developments is that teaching diffraction methods to undergraduate students is now more feasible and appropriate than

it would have been in past years. Along these lines, Dr. Hunter has developed: (1) an upper-level Solid State Structure Methods course, taught annually at YSU for the past five years; (2) a lecture/computer lab module on single crystal structural methods for courses such as organic analysis and instrumental methods, (3) written an introductory-level 275 page lab manual (available for free in electronic form to anyone who requests it), mainly on using Bruker's SHELXTL programs for single crystal structure analysis; and (4) created other electronic materials designed for student learning of diffraction methods.²² Availability of a dedicated powder diffractometer on-site will enable increased focus on incorporating *quantitative* powder methods into the undergraduate curriculum, as has already been done successfully for single crystal methods. The PI has collaborated with Hunter on several of his Chemical Education projects and would do so on this quantitative powder diffraction course. Indeed, Hunter and Wagner recently attended the Bayreuth Course on Advanced Powder Diffraction Methods (as the only participants from the US) in preparation for this effort.

C2.2.b. Disciplinary Research

Overview: Dr. Hunter's current research activities include a new interest in main group heterocyclic ring compounds having SNSN linkages, and a long standing interest in organometallic model complexes, oligomers, and polymers having conjugation down their backbones. His organometallic polymer interests include materials having arylene and fluoroarylene bridges,^{23,24} $(\eta^6\text{-Arene})\text{Cr}(\text{CO})_3$ groups,^{25,26,27} and *trans*- $\text{Mo}(\text{PR}_3)_4(\text{Isonitrile})_2$ centers.^{25,28,29} Following synthesis, these new materials are characterized by a combination of analytical, physical, spectroscopic, electrochemical, and structural methods. Each of these projects heavily utilizes diffraction methods to characterize the new products. While his group uses single crystal (including high resolution charge density) methods where possible, in many cases single crystal samples are not available. In others, qualitative evidence indicates that the bulk material is not identical to the single crystal samples. In each of these cases, quantitative powder methods would provide invaluable structural data on these solid state materials not available from other routes.

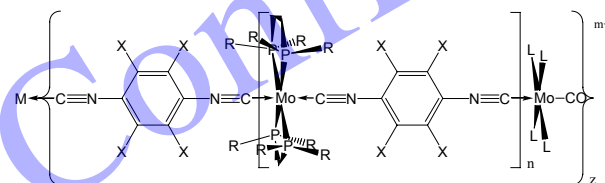
Organic and Organometallic Complexes Having -SNSN- Rings: The heterocycle project was initiated during Hunter's current sabbatical at St. Andrews University in Scotland, and has received NSF-INT support. A series of organic and organometallic heterocyclic species having 5 and 6 membered SNSN rings have been prepared and characterized (e.g., 1,2- $\text{C}_6\text{X}_4(\text{SNSN})$, Y-X(SNSN), Z=X(SNSN), and $\text{L}_n\text{M}(\text{SNSN})$). The bonding in these materials has been analyzed by high level molecular orbital calculations for the gas and solid phases. These results have been compared to those from spectroscopic measurement and conventional and high resolution (charge density) diffraction studies. Elucidating the factors influencing the bonding in the heterocyclic rings, especially the degree of their localization/delocalization as a function of the organic or organometallic fragment structures, is the core of this project. Many of these complexes crystallize in more than one polymorph. It is therefore essential to determine how many polymorphs are observed for each particular sample, and this is best done using powder diffraction methods. Once this has been determined, single crystal structures are determined for as many of the polymorphs as possible. Comparison of the molecular and intermolecular geometries in the different polymorphs allows one to estimate which of the detailed structural and bonding properties found are due to intramolecular and which are due to intermolecular interactions.

Organometallic Crystal Engineering: The use of hydrogen bonds between rigid organic building blocks having aromatic cores is one of the most widely used ways to generate self assembled materials with relatively predictable and tunable geometries. Hunter's work has shown that μ -1,4-C₆F₄ and μ -4,4'-(C₆F₄)₂ bridged Ni, Pd, and Pt phosphine complexes, oligomers, and polymers are remarkably air and thermally stable. These will be used to prepare zero-, one-, two-, and three-dimensional materials for use as organometallic crystal engineering lattice rods. The new organometallic building blocks will have a range of steric and electronic properties at the metal centers and distances and angles between the hydrogen bonding substituents. The specific building blocks to be targeted include:

- X-(μ -fluoroarylene)-[M(PR₃)₂-(μ -fluoroarylene)-]_n-X
- X-(μ -arylene)-[M(PR₃)₂-(μ -fluoroarylene)-]_n-M(PR₃)₂-(μ -arylene)-X
- (NC₅F₄)-[M(PR₃)₂-(μ -fluoroarylene)-]_n-M(PR₃)₂-(C₅F₄N)
- (NC₅H₄)-[M(PR₃)₂-(μ -fluoroarylene)-]_n-M(PR₃)₂-(C₅H₄N)
- where fluoroarylene = C₆F₄, C₆F₃, and (C₆F₄)₂, arylyene = C₆H₄ and (C₆H₄)₂, M = Ni, Pd, and Pt, the metal geometries are *trans*, n = 0 to 5, C₅F₄N = tetrafluoropyridyl and C₅H₄N = pyridyl, X = C(O)OH, C(CH₃)₂OH, C(CF₃)₂OH, OH, NH₂, NR₂, C₅F₄N, and C₅H₄N

Crystallization of these building blocks with one another and co-crystallization with complementary organic building blocks, both in the presence of suitable guests, will result in the self assembly of new hydrogen bonded materials. They will be characterized by chemical, analytical, spectroscopic, thermal, and X-ray crystallographic means. These results will be correlated with the monomer and oligomer properties in solution and the solid state and with the framework structure and guest identity to derive new structure/property relationships. By varying the solubility characteristics of the organometallic building blocks along with their steric and electronic features, we expect to be able to prepare a wide range of self assembled materials having tunable properties including guest selectivities. Clearly, powder diffraction methods will be important for determining structural information on those samples that do not give rise to single crystals and on determining the polymorphism of any that do result in single crystals.

Organometallic Rigid Rods and NanoStars: This project also builds upon the applicant's previous work and involves the synthesis of a series of new rigid rods and star shaped organometallic complexes from 2 to 20 or more nanometers in diameter, i.e.



These nanoscale materials (e.g., n = 0 - 5) will be characterized by analytical, physical, thermal, spectroscopic, electrochemical, and structural methods. They will have a variety of vertex numbers (e.g., Z = 0 - 7 for a range of transition metal ions, M) and geometries and are expected to be sterically crowded near their central cores but to have long inter-fragment distances at their peripheries. The substituents on the isonitrile aromatic rings (e.g., X = CH₃, H, or F), the phosphines on the molybdenum linkers (e.g., R = Alkyl, Fluoroalkyl, 1,4-C₆H₄-X, and Fluoroaryl), and on the molybdenum caps (e.g., L₄ = ((1,4-C₆H₄-OCH₃)₂PCH₂CH₂P(1,4-C₆H₄-OCH₃)₂)₂ or (CO)₄) will be systematically varied to tune molecular solubility, intramolecular steric interactions, and intermetallic electronic conjugation. It is expected that more electron donating phosphine ligands and electron poor isonitrile bridges will produce increased intermetallic conjugation which will be quantitatively evaluated from structural, spectroscopic,

electrochemical, and ESR data. The interactions of these Organometallic NanoStars with surfaces and their potential for electrochemical and material science applications will be qualitatively assessed. It is expected that many of these materials will not be available as single crystals and here powder diffraction methods will be critical.

C2.3. Dr. Raymond Beiersdorfer

Dr. Beiersdorfer is an Associate Professor in the Department of Geology at Youngstown State University. His research interests include geochemical studies of mafic rocks

Crystal Chemistry of Pumpellyite

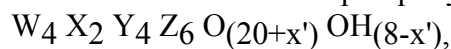
Objective: This work proposes to use the high resolution powder X-ray diffractometer to determine the crystal structure of a suite of specimens of the mineral pumpellyite $((\text{Ca},\text{Mn})_4(\text{Mg},\text{Fe}^{2+},\text{Mn})_{2-x'}(\text{Fe}^{3+},\text{Al})_{x'}(\text{Fe}^{3+},\text{Al})_4\text{Si}_6\text{O}_{(20+x')}\text{OH}_{(8-x')})$. These specimens have been collected from various localities around the world. In addition to the crystal structure determinations, the specimens will be analyzed by electron probe microanalysis (EPMA) to determine their chemical composition. The major goal of this project is to determine the correspondence between changes in the crystal structure of pumpellyite with changes in its composition, particularly the isomorphous exchange of Mg, Fe and Al. Previous attempts to determine the structure of these specimens with a single-crystal X-ray diffractometer were unsuccessful due to problems with grain size. The crystals were too fine-grained to get an adequate data set to analyze.

Background: Pumpellyite forms during the metamorphism of mafic rocks (basalts and andesites) at relatively low pressures (1 - 8 kbar) and temperatures (200° - 350°C). Because mafic rocks are sensitive to physical and chemical changes during metamorphism, they have long been recognized as the foundation of the metamorphic facies concept.^{30,31,32} Although they have been extraordinarily useful as the basis for metamorphic facies, mafic rocks have been less powerful indicators of physical conditions, especially at low and intermediate grades of metamorphism. In large measure, our difficulties stem from the small number of discontinuous reactions in mafic rocks, the complexity of solid solutions in the dominant phases (e.g. pumpellyite, amphibole, and epidote), and the corresponding difficulties of determining thermodynamic properties and experimental stability limits of critical assemblages. The problems of studying low-grade mafic rocks are magnified by the abundance of relict minerals, the small domains of equilibrium, and very fine grain-sizes. As a result, our understanding of low-grade metamorphism of mafic rocks is primitive relative to higher grade equivalents. In recent years combined petrographic and EPMA studies have yielded information about the factors controlling the low grade metamorphism of mafic rocks. However, much of this work is very dependent on assumptions made about the crystal chemistry of pumpellyite. The proposed research will test the validity of some of these assumptions. In addition, it has been proposed³³ that the composition of pumpellyite (coexisting with abrite, epidote, quartz, water, chlorite, \pm actinolite) varies systematically with changes in the intensive conditions of metamorphism, particularly pressure. Fe-rich, Al-poor pumpellyite is characteristic of rocks metamorphosed at hydrothermal systems located at mid-ocean ridges and oceanic volcanic-arc complexes. A comparison of the crystal structure of pumpellyite spanning a wide range of Fe- and Al-contents may reveal changes in the crystal structure that are due to differences in the pressure of

formation.

Chemistry of Pumpellyite

The structural formula of pumpellyite is commonly written as:³⁴



where: W = Ca,Mn; X = (Mg,Fe²⁺,Mn)_{2-x'} (Fe³⁺,Al)_{x'}; Y = Fe³⁺,Al; and Z = Si.

The W site consists primarily of Ca in seven-fold coordination with oxygen. However, many pumpellyites exhibit deficiencies in Ca and it has been suggested³⁵ that the W site may contain some iron. The X (M(2)) and Y (M(1)) sites are in octahedral coordination with oxygen. Silica occurs as both isolated tetrahedra (SiO₄) and double tetrahedra (Si₂O₆). The total number of cations per formula unit is 16 and the total number of oxygen per formula unit ranges from 24 to 25 depending on the chosen value of x'. The value of x' is commonly assumed to be 1 so that the X site contains one trivalent and one divalent cation. For example, all recent work concerning the petrogenesis of pumpellyite-bearing rocks^{33,36,37} have assumed that x' is one. Determining the crystal structure of well crystallized pumpellyites exhibiting a wide range of composition will allow one to evaluate whether or not this assumption is reasonable.

Crystal Structure of Pumpellyite

The crystal structure model of pumpellyite was first proposed by Gottardi³⁸ and has been subsequently refined by Galli and Alberti³⁹ and Yoshiasa and Matsumoto.⁴⁰ Each of these studies has been limited to pumpellyite with a restricted range of compositions. For example, the work of Yoshiasa and Matsumoto⁴⁰ was based on a single specimen of Al-rich pumpellyite from the high-pressure Sanbagawa metamorphic belt of Japan. It has been demonstrated that this type of Al-rich pumpellyite, (co-existing with chlorite, actinolite, epidote, albite and quartz) is characteristic of pumpellyite-bearing rocks metamorphosed at relatively high pressure.³³ Aguirre⁴¹ et al. determined unit cell parameters for pumpellyite in a metadolorite from Spain. Artioli⁴² et al. have determined the structure of MgAl-pumpellyites subjected to high pressure in a multianvil device. Gottschalk⁴³ et al. determined that the crystal structure of the synthetic high-pressure phase commonly identified as MgMgAl-pumpellyite to be isostructural with sursassite rather than pumpellyite. Artioli⁴⁴ et al. have studied the Mn crystal chemistry in pumpellyite. It has yet to be determined how the crystal structure of pumpellyite varies with changes in composition, particularly to more iron-rich varieties which are common in rocks that have suffered subseafloor-; high T/P-; hydrothermal-metamorphism.

Proposed New Research: In collaboration with Dr. H. W. Day of the University of California, Davis, I have acquired a suite of 30 pumpellyite specimens, representing diverse metamorphic environments. The specimens come from the collections of the California Academy of Sciences and the National Museum of Natural History, through the courtesy of Dr. Jean DeMouthe and Dr. Pete Dunn, and from various other mineralogists around the world. I have completed microprobe analyses of these specimens. Samples spanning a wide range of composition will be selected for analysis using the XRD.

Summary: Progress in understanding pumpellyite-bearing mafic rocks during the past decade has demonstrated that important insights into low-grade metamorphism can be derived, under favorable circumstances, by using phase-petrological methods rooted in the assumption of chemical equilibrium. However, much of this work is reliant on the validity of assumptions made about the crystal chemistry of pumpellyite. The proposed work on pumpellyite will test the

validity of some of these assumptions and will result in a unique data set that will permit a systematic comparison between crystal structure and composition.

C3. DESCRIPTION AND CAPABILITIES OF PROPOSED INSTRUMENT

The primary requirement of the powder diffractometer system requested is that it provide data of sufficiently high quality for structure determination and refinement of powdered materials. The powder system currently available on-site is a Bruker AXS X1000 multiwire area detector, which is mounted interchangeably with a scintillation detector on a Bruker AXS P4 four circle diffractometer designed mainly for single-crystal work. One problem in using a multiwire area detector for quantitative structure analyses of powders is that the system must always be very well calibrated to prevent errors in parameters such as peak positions, which would be detrimental to obtaining good structural results. In practice, it may be difficult for an operator to achieve or maintain an optimal calibration, and since calibrations must be done frequently, the chance of human error is higher than in conventional systems. Even if the calibrations were always very accurate, however, the multiwire detector has relatively poor resolution and range (i.e. our system collects data only to a maximum of about 95° in 2θ) compared to typical dedicated powder diffractometer systems. Since the multiwire detector is suitable only for long wavelength X-rays (i.e. Cu radiation), the amount of data that can be collected is therefore relatively limited. In addition, due to the configuration of our system, the background signal, particularly at low angles, is quite high. For these reasons, we use our multiwire area detector only for qualitative work – mainly phase identification.

Great strides have been made in recent years in methods for structure determination and refinement of crystal structures from powder diffraction data, and several good software packages are now available to researchers for this purpose, such as SIMPEL, GSAS, FULLPROF and others.⁴⁵ (Note that none of the available powder refinement programs that we are aware of are configured for use with multiwire area detectors.) In order to obtain optimal structural information from any of the available packages, the input data must: (1) be of high enough resolution to minimize peak overlap, thus providing better peak profiles and consequently better structure analysis; (2) consist of peaks of high enough intensity so that they are clearly discernable from background, meaning increased data quality; and (3) be collectable over a large range in 2θ to maximize the number of reflections obtained, thus optimizing the quality of the structure refinement results. The Bruker D8 ADVANCE system requested in this proposal meets all of these criteria, and provides continuity with the Bruker systems (i.e. two P4's and multiwire area detector) already in place.

In order to obtain the highest quality data from the proposed instrument, it will be equipped with a primary beam monochromator. This device eliminates $K\alpha_2$ radiation from the Cu source, so that the sample sees only $K\alpha_1$. Such a highly monochromatic beam will help reduce peak overlap, especially at high diffraction angles, thus increasing the number of resolved peaks for optimal structure analysis. This will be particularly significant for low symmetry structures (such as the disordered oxides studied by Wagner and the organometallic compounds studied by Hunter), because of the larger number of unique reflections observed at high angles for these systems. Of course, by eliminating $K\alpha_2$ radiation, beam intensity is reduced. Göbel mirrors typically are used to increase intensity, but they are not compatible with the primary beam monochromator option, and also result in some loss in resolution and peak shape. Thus, the problem of reduced intensity will

be offset through using a position sensitive detector (PSD) rather than a scintillation detector, which would require larger data collection times to make up for loss of intensity. The PSD offers about the same resolution as a scintillation detector, but can collect four peaks simultaneously, greatly improving the speed of data collection. It also provides better statistics relative to a scintillation detector, due to increased redundancy in data collection.

Other options are requested mainly for specific research and/or educational needs. For example, the capillary mounting stage is needed for analysis of air sensitive nitride-fluoride and organometallic materials produced by TRW's and ADH's groups. Although there are techniques (such as placing a sample between two glass slides) that enable data collection of air sensitive samples on traditional sample stages, we discovered while working with Ca_2NF that the sample decomposed after a few hours exposure to glass, presumably due to interactions with cations in the glass. The problem disappeared when we began using silica capillary tubes, which are much cheaper and more convenient to work with than silica slides would be. Using capillary tubes also enables us to conveniently store samples for later analysis.

The nine-position multiple sample changer is requested mainly to support educational-related uses of the proposed instrument (see next section). The TOPAS software package (as opposed to shareware programs) for structure solution and refinement is requested for several reasons: (1) it can be used as a stand alone Reitveld refinement program, or as a structure solution/refinement package, where the user has the option to input any structure information available to help achieve successful structure determination, (2) the package offers continuity with the data collection software, so that data is easily imported for structure analysis; (3) the software is automatically optimized for the D8 ADVANCE diffractometer; creating correct instrument parameter files for other software packages can be tedious; and (4) the package is much more user-friendly than some shareware programs, such as GSAS, which is an advantage for student users.

C4. EDUCATIONAL IMPACT OF THE PROPOSED INSTRUMENT

Given the already strong emphasis placed on undergraduate research at YSU (seniors must have a capstone, i.e. research, experience in their major to graduate), and the routine utilization of research-grade equipment in upper-level chemistry laboratory courses at YSU, the educational impact of the requested powder X-ray diffractometer system is substantial. To meet the university capstone requirement, all BS chemistry majors are required to take a formal (i.e. classroom) course in research methods, and also to take a laboratory course in undergraduate research, where they work under a professor of their choice on a research project. In keeping with the department's strong hands-on access policy regarding use of research grade instrumentation by undergraduates, these students especially are trained in using the instruments needed for their research projects. The hands on access policy extends to any undergraduate student taking science courses that expresses a desire to learn to use a particular instrument. In fact, the PI has in the past worked with honors students in his freshman chemistry courses, teaching them to use the multiwire detector for routine powder analysis. The proposed instrument would impact mainly students taking upper-level laboratory courses (e.g. inorganic synthesis). Note that by design, these courses all have an independent project component, for which students almost always use advanced instrumentation. In practice, students are trained to use the instruments they need for whatever course they're taking by the faculty member responsible for the instrument. Based on these department requirements and policies, the proposed instrument would undoubtedly be utilized in an educational capacity.

One method for training students to use the current single crystal diffraction facilities, which has proven to be very effective, has been through offering a formal course on Solid State Structural Methods, Chemistry 5832, taught primarily by ADH (and TRW in 2001). Students taking this course gain hands-on experience for the entire process of single crystal structure analysis, from selecting and mounting crystals and collecting data, through final structure refinement. Demand for the course has been high enough to warrant offering it annually (typically 6-10 students take it, mainly chemistry and some geology and engineering students). With the purchase of a dedicated powder diffractometer, two labs involving its use will be integrated into this course.

Still another way that the proposed instrument could have an educational impact is related to the recent REU (i.e. Research Experience for Undergraduates) grant awarded to the department by NSF, as discussed in section C1.f. The new dedicated powder instrument would be available to any of the ten undergraduate researchers supported by the grant that choose a project requiring utilization of the instrument. Since several of these students will be from other universities, the educational impact here goes beyond the YSU campus.

Finally, there is also a positive educational impact that the instrument will have on the Primarily Undergraduate Institutions (PUIs) which are already affiliated with our single crystal facility. As mentioned previously, interaction with PUIs is a core feature of the successful CCLI grant (see section C1.f.) which will create a WEB-accessible diffraction facility, including purchase of a new CCD single crystal diffractometer. As part of this CCLI project, its PI (Hunter) and the PI of this RUI-MRI have committed to holding a regular summer school directed towards faculty at PUIs on diffraction methods. Although the CCLI proposal emphasizes single crystal methods, plans to incorporate material on powder methods were also outlined in the proposal. With the availability of the dedicated powder diffractometer, this summer school will be able to add a substantial component on powder methods that would otherwise be left out.

The acquisition of the proposed powder diffractometer, especially with its multiple sample changer, will also provide those institutions without their own powder diffraction facilities (the large majority) with the opportunity to integrate powder methods more fully into their teaching and research. In particular, they will be able to pre-arrange a time to send powder samples prepared in their inorganic laboratory courses and research projects by mail/FedEx to YSU. These will be mounted on the sample changer by one of the project applicants or their students, and the resulting data will be returned over the WEB. The PI and one of the Co-PIs (ADH) and their graduate students have routinely run single crystalline samples for external users when their schedules permit. For example, the PI completed four single crystal structures submitted by faculty from colleges in Ohio and California during the Fall 2000 semester. If the current grant is successful, the PI plans to shift some time away from single crystal collaborative work to emphasize powder work.

C5. IMPACT ON EXISTING INFRASTRUCTURE

As indicated in Section H, the YSU chemistry department is well equipped to support the strong emphasis on hands-on undergraduate research, as well as most of the research needs of the faculty and their graduate students. The most significant impact of the proposed instrument on department/university infrastructure, then, is that it adds a capability that does not presently exist on campus, viz., the ability to provide high quality data for *quantitative structure refinement from*

powder data. Our X-ray facility currently consists of two Bruker AXS P4 diffractometers, purchased six years ago in part from NSF funds.⁴⁶ One of these machines uses a Cu X-ray source, and the other a Mo source. The department's powder system consists of a multiwire detector suitable for qualitative work, which is used interchangeably with the scintillation detector on the Cu P4 machine. Since this machine is configured for single crystal work at least 50% of the year, undergraduate research students (i.e. the largest group of users) have had to wait sometimes up to several weeks before single crystal work is done and the area detector can be mounted and calibrated for powder runs. Although it is expected that the new CCD system will decrease some of the single crystal demands on this instrument internally, we also expect to see a greater number of external users requesting access to the single crystal diffractometers when the facility is in place. A dedicated powder instrument would eliminate the problem of "black-out" periods when no powder analysis can be done. Most importantly, it would also provide a new realm of opportunity for research for faculty and their students.

The requested powder diffractometer would be housed in the new ≈ 1200 square foot diffraction facility, along with the two P4's and the new CCD system. The dedicated powder diffractometer would complete this facility, making it a truly comprehensive learning, research, and teaching center for students and faculty across disciplines and institutions.

C6. MAINTENANCE AND OPERATION

The YSU chemistry department is highly dedicated to keeping our instruments well maintained and operating. In fact, our two P4 X-ray diffractometers have had a total down-time of about one month each during the past six years, while the department's 400 MHz NMR has had less than two weeks down time in the past five years, in all cases while waiting for parts. This in-service rate is comparable to that of major research institutions, which is remarkable given the relatively high percentage of instrument operation by undergraduate students at YSU. As further example of the department's commitment in this area, during one usually hot summer we could run only one of our diffractometers at a time, because the city-water cooled dual heat exchanger could not effectively carry the heat away from both instrument tubes. Within a month, the department had purchased a \$6,400 dual water chiller out of its own budget to alleviate the problem.

The chemistry department also has on staff an instrumentation service specialist, Ray Hoff, who is exceptionally skilled at instrument maintenance and troubleshooting. He routinely travels to instrument vendors to take their service training courses when the department acquires a new instrument, and it is expected he would do so if the present proposal is successful. On those rare occasions when outside service technicians are required, we have always been immediately authorized to bring them in. Very recently, the department was informed that we will be able to hire an assistant to help Ray with his increasing workload, resulting from a steady influx of instrument acquisitions in the department in recent years.

The PI will be the principal operator of the diffractometer. He has several years of experience in operating diffraction equipment, including both single crystal and powder X-ray, as well as electron diffraction. For the past six years, he has been the primary operator of and faculty member responsible for the Bruker X-1000 Area Detector currently used for qualitative powder analysis.

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19. Wagner, T.R., "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type BaGa₁₂O₁₉", *J. of Solid State Chem.*, **136**, 120 (1998).
20. Hunter, A.D., "Crystallographic Structure Determination: An Experiment for Organic Analysis and other Non-Traditional Venues," *J. Chem. Educ.*, **75**, 1297-1299 (1998).
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33. Beiersdorfer, R.E. and Day, H.W., "Mineral Paragenesis of Pumpellyite in Low-Grade Mafic Rocks, in Schiffman, P. and Day, H. W., eds., Low-Grade Metamorphism of Mafic Rocks, Geological Society of America Special Paper 296, p. 5 – 27 (1995).
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37. Frey, M., de Capitani, C., and Liou, J. G., "A New Petrogenetic Grid for Low-Grade Metabasites, *J. of Metamorphic Geology*", **9**, 497-509 (1991).

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41. Aguirre, L., Morata, D., Puga, E., Baronnet, A. and Beiersdorfer, R.E., "Chemistry and Crystal Characteristics of Pumpellyite in a Metadolorite from the Archidona region, Subbetic Cordillera, Spain", in Schiffman, P. and Day, H. W., eds., *Low-Grade Metamorphism of Mafic Rocks*, Geological Society of America Special Paper 296, p. 171 – 181, (1995).
42. Artioli, G., Fumagalli, P., Poli, S., "The Crystal Structure of $Mg_8(Mg_2Al_2)Al_8Si_{12}(O,OH)_{56}$ Pumpellyite and its Relevance in Ultramafic Systems at High Pressure", *American Mineralogist*, **84**, 1906-1914 (1999).
43. Gottschalk, M., Fockenberg, T., Grevel, K. D. , Maresch, W. V, Schreyer, W., Wirth, R. and Wunder, B., "Crystal Structure of the High-Pressure Phase $Mg_4(MgAl)Al_4Si_6O_{21}(OH)_7$ an Analogue of Sursassite", *European Journal of Mineralogy*, **12**, 935-945 (2000).
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45. Harris, K.D.M. and Tremayne, M., "Crystal Structure Determination from Powder Diffraction Data", *Chem. Mater.*, **8**, 2554-2570 (1996).
46. "Acquisition of a Single Crystal X-Ray Diffractometer", T.R. Wagner, A.D. Hunter, J.A. Jackson, and R.E. Beiersdorfer, The National Science Foundation Division of Materials Research: Research at Undergraduate Institutions Program and the Ohio board of Regents Action Fund (NSF DMR RUI 9403889 and CAP-098) \$71,199 and \$60,000, respectively, with over \$140,000 in internal match, 1994-96.

SECTION E: BIOGRAPHICAL SKETCHES

Biographical Sketch for Timothy R. Wagner

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

Phone.: 330-742-1960; **e-mail:** trwagner@cc.yosu.edu

website: <http://www.as.yosu.edu/~trwagner/index.html>

a. Professional Preparation:

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

b. Appointments:

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

c. Publications:

i. Five Most Closely Related Publications:

- Nicklow, R; Wagner, T.; and Raymond, C.: "Preparation and Crystal Structure Analysis of Ca_2NF ," *J. Solid State Chemistry*, **submitted, December 2000**.
- Wagner, "Preparation and Crystal Structure Analysis of Magnetoplumbite-Type Barium Hexagallate," *J. Solid State Chemistry*, **1998**, 136, 120-124.
- Wagner T.; O'Keeffe, M.: "Bond Lengths and Valences in Aluminates with the Magnetoplumbite and β -Alumina Structures," *J. Solid State Chemistr.*, **1988**, 73, 211-216.
- Wagner T.; O'Keeffe, M.: "A Structural Model for Barium Hexagallate," *J. Solid State Chemistry*, **1988**, 73, 19-26.
- Wagner, T.; O'Keeffe, M.: "Electron Microscopy of Defects and Disorder in Barium Hexagallate," *Acta Cryst.*, **1985**, B41, 108-112.

ii. Five Other Significant Publications:

- Freeze, S; Norris, P.; and Wagner, T.; "Formation of D-Galactose-derived Ethylene Diamine Ligand and its Complex with Pd(II)," *Carbohydrate Research*, **in press**.
- Norris, P. and Wagner, T.: "Solution and Solid State Structure of the 2,6-anhydro-1,1-bis(ethylsulfonyl)-1-deoxy-D-talitol," *Carbohydrate Research*, **1999**, 322(1-2), 147-150.
- Landis, K.; Hunter, A.; Wagner, T.; Curtin, L.; Filler, F.; Jansen-Varnum, S.: "The Synthesis and Characterization of Ni, Pd, and Pt Maleonitriledithiolate Complexes: X-Ray Crystal Structures of the Isomorphous Ni, Pd, and Pt Congeners", *Inorganica Chimica Acta*, **1998**, 138, 155-162.
- Wagner, T. and Styranec, T.: "Preparation and Crystal Structure Analysis of $\text{Ba}_2\text{BiGa}_{11}\text{O}_{20}$," *J. Solid State Chem.*, **1998**, 138, 313-320.

10. Wagner, T.: "HREM of Electron-Beam-Induced Damage in L-Ta₂O₅," *J Solid State Chem.*, **1991**, *91*, 189-203.

d. Synergistic Activities:

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

e. Collaborators & Other Affiliations:

(i) Collaborators:

Casey Raymond, Kent State University

(ii) Graduate and Post Doctoral Advisors:

Michael O'Keeffe (Ph.D), Arizona State University

Lawrence Marks (Post. Doc.), Northwestern University

(iii) Thesis and Postgraduate Scholar Sponsor:

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

Biographical Sketch for Allen D. Hunter

Permanent Address: Department of Chemistry, Youngstown State University, Youngstown, OH, 44555-3663, 330-742-7176, adhunter@cc.yzu.edu

Sabbatical contact information (Aug. 2000 - July 2001): Department of Chemistry, St. Andrews University, St. Andrews, Fife, Scotland, KY16 9ST, 44-1334-467304, adh2@st-andrews.ac.uk

a. Professional Preparation:

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

b. Appointments:

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

c. Publications: Allen has a total of 42 peer reviewed publications (24 since 1992 and 11 since 1996) and has also given 44 oral/poster presentations.

(i) Most Closely Related Publications:

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

(ii) Other Significant Publications:

6. Hunter, A. D. *Journal of Chemical Education*, **1998**, 75, 1424.
7. Hunter, A. D.; Bianconi, L. J.; DiMuzio, S. J.; Braho, D. L. *Journal of Chemical Education*, **1998**, 75, 891-893.
8. Hunter, A. D. *Journal of Chemical Education*, **1998**, 75, 1297-1299.
9. Bennett, M. A.; Ditzel, E. J.; Hunter, A. D.; Khan, K.; Kopp, M. R.; Neumann, H.; Robertson, G. B.; Zeh, H. *Dalton*, **2000**, 1733-1741.
10. Adrian, J. C.; Barkin, J. L.; Fox, R. J.; Chick, J. E.; Hunter, A. D.; Nicklow, R. A. *Journal of Organic Chemistry*, **2000**, 65, 6264-6267.

d. Synergistic Activities:

Allen is very involved in the scholarship of teaching. This has been recognized at YSU by his being designated a Master Teacher in the College of Arts and Sciences, by his receiving substantial Faculty Development Funding for new curriculum innovations, and by his being appointed the Science representative on the General Education Committee during the development of the new Gen. Ed. program last year, at the state level by his being invited to be a founding member of The Ohio Project for Science Education, and at the national level by several NSF Teaching Instrumentation, Education Materials Development, and

Curriculum Innovation grants. He has also published 3 papers in the *Journal of Chemical Education* over the last three year and has released a 275 page student text on diffraction methods via the WEB. He is a founding member and the representative for Ohio's Predominantly Undergraduate Institutions on the Ohio NMR, MS, and X-Ray Crystallography Consortia. He is on the Advisory Board of the W. M. Keck Foundation Center for Molecular Structure (Cal. State. Fullerton). He is also active in the International Center for Diffraction Data, including its Crystallographic Education subcommittee, in the International Union of Crystallography: Committee on Crystallographic Education, and in the Council of Undergraduate Research, and he is the organizer of sessions on crystallographic education at upcoming ACA and ACS national meetings. Finally, Allen is very involved with professional development opportunities for regional science teachers. Indeed, he has spearheaded our efforts to launch a YSU MS program optimized for this group.

e. Collaborators & Other Affiliations:

(i) Collaborators (in last 4 years and in addition to YSU colleagues):

- Alex Slawin, St. Andrews University, Scotland.
- Chase Smith, Holly Cross.
- Cliff Berkman, San Francisco State University.
- Derrick Woollins, St. Andrews University, Scotland.
- Frank Blockhuys and Herman Geise, University of Antwerp, Belgium
- George Richter-Addo, University of Oklahoma.
- Jim Adrian, Union College.
- John Cashman, Seattle Biomedical Institute.
- Pual Kelly, Loughborough University, England
- Philip Coppens, University of Buffalo.
- Simon Coles, UK National Diffraction Facility, Southampton, England
- Viktor Zhdankin, University of Minnesota - Duluth.
- Vyacheslav (Slava) Samoshin, University of the Pacific.

(ii) Graduate and Post Doctoral Advisors:

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

(iii) Thesis and Postgraduate Scholar Sponsor:

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

Biographical Sketch for Raymond E. Beiersdorfer

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

Phone.: 330-742-1753; **e-mail:** ray@cc.yzu.edu

website: <http://www.as.yzu.edu/~geology/>

a. Professional Preparation:

Queens College, CUNY	Geology	BA	1979
Univ. of California - Davis	Geology	MS	1982
Gulf Oil Expl. & Prod. Co.	Exploration Geologist		1983-85
Monash University	Research Fellow		1985-86
Univ. of California - Davis	Geology	PhD	1992
University of Calgary	Geology Post Doc		1993

b. Appointments:

Youngstown State University, Geology	Associate Professor	1996-Present
Youngstown State University, Geology	Assistant Professor	1993-1996

f. Publications:

j. Five Most Closely Related Publications:

1. Beiersdorfer, R.E. and Day, H.W., **1995**, Mineral paragenesis of pumpellyite in low-grade mafic rocks, in Schiffman, P. and Day, H. W., eds., *Low-Grade Metamorphism of Mafic Rocks: Geological Society of America Special Paper 296*, p. 5 - 27
2. Aguirre, L., Morata, D., Puga, E., Baronnet, A. and Beiersdorfer, R.E., **1995**, Chemistry and crystal characteristics of pumpellyite in a metadolorite from the Archidona region, subbetic cordillera, Spain, in Schiffman, P. and Day, H. W., eds., *Low-Grade Metamorphism of Mafic Rocks: Geological Society of America Special Paper 296*, p. 171 - 181
4. Bégin, N. J., Ghent, E. D. and Beiersdorfer, R.E. , **1995**, Low temperature metamorphism of the Crowsnest Volcanic Suite, southwestern Alberta, *Canadian Mineralogist*. v. 33, p. 973 - 983
4. Beiersdorfer, R. E., **1993**, Metamorphism of a late Jurassic volcano-plutonic arc, northern California, U.S.A., *Journal of Metamorphic Geology*, v. 11, p. 415-428
6. Springer, R.K., Day, H.W. and Beiersdorfer, R.E., **1992** Prehnite-pumpellyite to greenschist transition, Smartville complex, near Auburn, California, *Journal of Metamorphic Geology*., v. 10, p. 147 - 170

ii. Five Other Significant Publications:

6. Beiersdorfer, R. E., **1999**, The Effect of Heating on Apatite Solubility and Cation Exchange in Zeoponic Soil, *NASA Contractors Grant NAG9-39 Final Report*. p.1.1 - 1.12
7. Beiersdorfer, R. E., 1999, Calcium Solubility and Cation Exchange Properties in Zeoponic Soil, in Banerot, R.B. and Sickorez, D.G., eds., *NASA/ASEE Summer Faculty Fellowship Program 1998, NASA Contractors Report - 1999-208923*. p.2.1 - 2.13
8. Beiersdorfer, R. E., **1997**, Solubility and cation exchange properties of synthetic apatite and clinoptilolite mixtures, in Hyman, W.A. and Sickorez, D.G., eds., *NASA/ASEE Summer Faculty Fellowship Program 1997, NASA Contractors Grant NAG9-931 Final Report*. p.1.1 - 1.12

9. Peterson, T. D., Currie, K. L., Ghent, E. D., Bégin, N. J., and Beiersdorfer, R.E., **1997**, Petrology and economic geology of the Crowsnest Volcanics, Alberta, *Geological Survey of Canada Geoscience Contributions, Canada-Alberta Agreement on Mineral Development (1992-1995)*, R. W. Macqueen (ed.), *Geological Survey of Canada, Bulletin 500*, p. 163-184
10. Bégin, N. J., Beiersdorfer, R.E. and Ghent, E. D. , **1995**, Mineralogical and geochemical analyses of the Crowsnest Volcanics, southwestern Alberta, *Current Research 1995-E; Geological Survey of Canada* , p. 11-25

g. Synergistic Activities:

Throughout the early stages of his career, the main focus of Ray's research was to increase our understanding of the geochemical processes that occur during the low-temperature fluid-rock interaction of basaltic rocks. He started off studying terrestrial basalts and in 1994 he expanded his research to include the lunar environment. The expectations of his appointment at YSU included a shift in his research focus to environmental science. He has accomplished this by working on research problems in soil geochemistry, specifically on the development of a solid-substrate, slow-release fertilizer for space and terrestrial applications. Ray has worked on X-ray (both powder & single crystal) diffraction projects with undergraduate geology research students. During the past five years he has had a consistent record of externally funded scholarship and publication. He has published six manuscripts (three refereed and three non-refereed) and twelve abstracts (all refereed). In addition to twelve presentations at international-level conferences, he has given sixteen presentations regionally, mostly at universities in Ohio. Additionally, he was awarded a YSU Distinguished Professorship in Scholarship during the 1996-97 academic year. He has played a leadership role in his department in modernizing the department curriculum. He makes an important contribution to the educational mission of the geology department and the environmental studies program, teaching seven different courses per year (on average). He is constantly trying new innovations to improve his classes. He has presented at conferences and published manuscripts on science education. Ray was selected as a Project Kaleidoscope Faculty for the 21st Century. As an Assistant Professor, he won a national science teaching award. As an Associate Professor, he was awarded a YSU Distinguished Professorship in Teaching and the University Scholars Provost Award for Teaching .

h. Collaborators & Other Affiliations:

(i) Collaborators:

Douglas Ming, NASA Johnson Space Center

(ii) Graduate and Post Doctoral Advisors:

Howard W. Day (Ph.D), University of California - Davis
Edward D. Ghent (Post. Doc.), University of Calgary

(iii) Thesis and Postgraduate Scholar Sponsor:

The geology department does not offer a graduate program. I have supervised undergraduate research by seven YSU Geology majors since 1996.

**SUMMARY
PROPOSAL BUDGET** YEAR **1**

ORGANIZATION Youngstown State University					FOR NSF USE ONLY				
					PROPOSAL NO.	DURATION (months)			
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Timothy R Wagner					AWARD NO.				
					Proposed	Granted			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)					NSF Funded Person-mos.		Funds Requested By proposer	Funds granted by NSF (if different)	
	CAL	ACAD	SUMR						
1. Timothy R Wagner - PI-PD	0.00	0.00	0.00	\$ 0		0	\$		
2. Raymond E Beiersdorfer - Co-PI	0.00	0.00	0.00			0			
3. Allen D Hunter - Co-PI	0.00	0.00	0.00			0			
4.									
5.									
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00			0			
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00			0			
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)									
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00			0			
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00			0			
3. (0) GRADUATE STUDENTS						0			
4. (0) UNDERGRADUATE STUDENTS						0			
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						0			
6. (0) OTHER						0			
TOTAL SALARIES AND WAGES (A + B)						0			
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)									
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						0			
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)									
Bruker D8 ADVANCE Powder Diffractometer				\$ 200,450					
Less YSU Cash Match				-30,140					
TOTAL EQUIPMENT						170,310			
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)									
						0			
						0			
F. PARTICIPANT SUPPORT COSTS									
1. STIPENDS \$ _____						0			
2. TRAVEL _____						0			
3. SUBSISTENCE _____						0			
4. OTHER _____						0			
TOTAL NUMBER OF PARTICIPANTS (0)									
TOTAL PARTICIPANT COSTS						0			
G. OTHER DIRECT COSTS									
1. MATERIALS AND SUPPLIES						0			
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						0			
3. CONSULTANT SERVICES						0			
4. COMPUTER SERVICES						0			
5. SUBAWARDS						0			
6. OTHER						0			
TOTAL OTHER DIRECT COSTS						0			
H. TOTAL DIRECT COSTS (A THROUGH G)						170,310			
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)									
TOTAL INDIRECT COSTS (F&A)						0			
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						170,310			
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)						0			
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						\$ 170,310	\$		
M. COST SHARING PROPOSED LEVEL \$ 30,140				AGREED LEVEL IF DIFFERENT \$					
PI / PD TYPED NAME & SIGNATURE* Timothy R Wagner					DATE			FOR NSF USE ONLY	
ORG. REP. TYPED NAME & SIGNATURE*					DATE			INDIRECT COST RATE VERIFICATION	
								Date Checked	Date Of Rate Sheet

SUMMARY PROPOSAL BUDGET Cumulative

ORGANIZATION Youngstown State University				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Timothy R Wagner				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-mos.		Funds Requested By proposer	Funds granted by NSF (if different)
	CAL	ACAD	SUMR				
1. Timothy R Wagner - PI-PD	0.00	0.00	0.00	\$	0	\$	
2. Raymond E Beiersdorfer - Co-PI	0.00	0.00	0.00		0		
3. Allen D Hunter - Co-PI	0.00	0.00	0.00		0		
4.							
5.							
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	0.00	0.00	0.00		0		
7. (3) TOTAL SENIOR PERSONNEL (1 - 6)	0.00	0.00	0.00		0		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (0) POST DOCTORAL ASSOCIATES	0.00	0.00	0.00		0		
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.00	0.00	0.00		0		
3. (0) GRADUATE STUDENTS					0		
4. (0) UNDERGRADUATE STUDENTS					0		
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0		
6. (0) OTHER					0		
TOTAL SALARIES AND WAGES (A + B)					0		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0		
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
			\$ 170,310				
TOTAL EQUIPMENT					170,310		
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)					0		
2. FOREIGN					0		
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____			0				
2. TRAVEL _____			0				
3. SUBSISTENCE _____			0				
4. OTHER _____			0				
TOTAL NUMBER OF PARTICIPANTS (0)				TOTAL PARTICIPANT COSTS	0		
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES					0		
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					0		
3. CONSULTANT SERVICES					0		
4. COMPUTER SERVICES					0		
5. SUBAWARDS					0		
6. OTHER					0		
TOTAL OTHER DIRECT COSTS					0		
H. TOTAL DIRECT COSTS (A THROUGH G)					170,310		
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)					0		
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					170,310		
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)					0		
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					\$ 170,310	\$	
M. COST SHARING PROPOSED LEVEL \$ 30,140				AGREED LEVEL IF DIFFERENT \$			
PI / PD TYPED NAME & SIGNATURE*			DATE	FOR NSF USE ONLY			
Timothy R Wagner				INDIRECT COST RATE VERIFICATION			
ORG. REP. TYPED NAME & SIGNATURE*			DATE	Date Checked	Date Of Rate Sheet	Initials - ORG	

SECTION F: BUDGET JUSTIFICATION

Bruker D8 ADVANCE X-Ray Powder Diffractometer System: **\$200,450**

Quote Includes (see Appendix):

- Complete System Optimized for Quantitative Structure Analysis
- Shipping and Installation
- System Maintenance Training Course (4 days) for Chem. Dept. Instrumentation Specialist

Total Budget: **\$200,450**

YSU Cash Match (30% of Total Budget Over \$100,000): **\$ 30,140**

TOTAL AMOUNT REQUESTED FROM NSF: **\$170,310**

Current and Pending Support**See GPG Section II.D.8 for guidance on information to include on this form.)**

The following information should be provided for each investigator and other senior personnel. Failure to provide this			
Investigator: Timothy R. Wagner, PI	Other agencies (including NSF) to which this proposal has been/will		
Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support	Project/Proposal Title: Integration of Computer Technology into the General Chemistry Curriculum		
Source of Support: NSF-DUE-CCLI-A&I			
Total Award Amount: \$94,945		Total Award Period Covered: 07/01/2000 - 06/30/2002	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the proj.	Cal:	Acad: 1.5	Sumr:
Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support	Project/Proposal Title: Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment		
Source of Support: NSF-DUE-ILI #9851107			
Total Award Amount: \$44,600		Total Award Period Covered: 06/01/1998 – 05/31/2001	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal:	Acad: 0.5	Sumr:
Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support	Project/Proposal Title: Synthesis and X-Ray Structure Characterizations of Nitride-Fluoride Analogs to Metal Oxides		
Source of Support: Research Corporation Cottrell Grant			
Total Award Amount: \$39,719		Total Award Period Covered: 05/15/1999 - 12/31/2001	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the	Cal:	Acad: 3	Sumr: 2
Support: <input checked="" type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support	Project/Proposal Title: REU-Research experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities		
Source of Support: NSF-CHEM-REU #0097682			
Total Award Amount: \$180,000		Total Award Period Covered: 06/01/2001 – 05/31/2004	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal: 1	Acad:	Sumr: 1
Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support	Project/Proposal Title: WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions		
Source of Support: NSF-DUE-CCLI-A&I			
Total Award Amount: \$260,000		Total Award Period Covered: 01/01/2000 - 12/31/2003	
Location of Project: Youngstown State University and a Consortium of 22 other Predominantly Undergraduate Institutions			
Person-Months Per Year Committed to the	Cal: 2.0	Acad:	Sumr:
*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.			

Current and Pending Support**See GPG Section II.D.8 for guidance on information to include on this form.)**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information			
Investigator: Allen D. Hunter, Co-PI		Other agencies (including NSF) to which this proposal has been/will be	
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: X-Ray Diffraction Analysis Throughout the Curriculum: a Powerful Tool for Understanding Molecular Structure and Bonding			
Source of Support: NSF-DUE-CCLI-EMD-POC # 9980921			
Total Award Amount: \$74,707		Total Award Period Covered: 05/01/2000 – 04/30/2002	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal:	Acad: 3	Sumr: 1.5, 1.5
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: The Ohio Project for Science Teaching			
Source of Support: Ohio Board of Regents			
Total Award Amount: \$4,000 to YSU		Total Award Period Covered: 07/01/1999 – 06/30/2000	
Location of Project: Youngstown State University and other Ohio Universities			
Person-Months Per Year Committed to the Project.	Cal: 0.5	Acad:	Sumr:
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: A Proposal to Establish a State-of-the-Art Ohio Mass Spectrometry Consortium			
Source of Support: Ohio Board of Regents Investment Fund			
Total Award Amount: \$88,900 to YSU		Total Award Period Covered: 06/01/1999 – 05/31/2000	
Location of Project: Youngstown State University and other Ohio Universities			
Person-Months Per Year Committed to the Project.	Cal: 0.5	Acad:	Sumr:
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: Investigative Approaches in the Natural Sciences			
Source of Support: NSF-DUE-IWR #9850079			
Total Award Amount: \$183,579		Total Award Period Covered: 06/01/1998 – 05/31/2001	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal: 0.1	Acad:	Sumr:
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: Integration of Materials Characterization Throughout the Chemistry and Physics Curricula: Purchase of Thermal Analysis, Viscometry, and Gel Permeation/Size Exclusion Chromatography Equipment			
Source of Support: NSF-DUE-ILI #9851107			
Total Award Amount: \$44,600		Total Award Period Covered: 06/01/1998 – 05/31/2001	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal: 3	Acad:	Sumr:
*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.			

Current and Pending Support**See GPG Section II.D.8 for guidance on information to include on this form.)**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information			
Investigator: Allen D. Hunter (continued)		Other agencies (including NSF) to which this proposal has been/will be	
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
			<input type="checkbox"/> *Transfer of Support
Project/Proposal Title: A Proposal for Fulfilling the Goals of the Ohio Mass Spectrometry Consortium			
Source of Support: Ohio Board of Regents Investment Fund			
Total Award Amount: \$500,000		Total Award Period Covered: 06/01/2000 – 05/31/2001	
Location of Project: A Consortium of Ohio Universities including Youngstown State University			
Person-Months Per Year Committed to the Project.		Cal:	Acad: 0.1
			Sumr:
Support:	<input checked="" type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
			<input type="checkbox"/> *Transfer of Support
Project/Proposal Title: REU - Research Experiences for Chemistry at Youngstown State University: A Bridge Between Four-Year Colleges and Ph.D. Research Universities			
* This grant proposal has been recommended for funding by the NSF program officer			
Source of Support: NSF-CHEM-REU #0097682			
Total Award Amount: \$180,000		Total Award Period Covered: 06/01/2001 - 05/31/2004	
Location of Project: YSU			
Person-Months Per Year Committed to the Project.		Cal: 0.1	Acad:
			Sumr:
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
			<input type="checkbox"/> *Transfer of Support
Project/Proposal Title: WEB Accessible Single Crystal X-Ray Diffractometer for a Consortium of Predominantly Undergraduate Institutions			
Source of Support: NSF-DUE-CCLI-A&I and the Ohio Board of Regents Investment Fund			
Total Award Amount: \$200,000 + \$75,000		Total Award Period Covered: 01/15/2001 - 12/31/2003	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.		Cal:	Acad:
			Sumr: 0.50, 0.25, & 0
Support:	<input checked="" type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
			<input type="checkbox"/> *Transfer of Support
Project/Proposal Title: Structural Investigations of Main Group Heterocyclic Rings and Cages			
* This grant proposal has been recommended for funding by the NSF program officer			
Source of Support: NSF: Int Div (Western Europe), Collaborative Projects #0086313			
Total Award Amount: \$13,200		Total Award Period Covered: 02/01/2001 - 08/31/2001	
Location of Project:			
Person-Months Per Year Committed to the Project.		Cal:	Acad: 5
			Sumr:
Support:	<input type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
			<input type="checkbox"/> *Transfer of Support
Project/Proposal Title: Charge Density and Photocrystallography Studies of Ruthenium Nitrosyl and Related Complexes			
Source of Support: Research Corporation - Cottrell College Science Award for Established Faculty			
Total Award Amount: \$ 43,500		Total Award Period Covered: 06/01/2001- 05/31/2003	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.		Cal:	Acad: 2
			Sumr: 1.5
*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.			

Current and Pending Support**See GPG Section II.D.8 for guidance on information to include on this form.)**

The following information should be provided for each investigator and other senior personnel. Failure to provide this information			
Investigator: Allen D. Hunter (continued)		Other agencies (including NSF) to which this proposal has been/will be	
Support:	<input type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: RUI - Crystal Engineering Using Organometallic FluoroArylene Bridged Building Blocks of Ni, Pd, and Pt			
Source of Support: NSF-CHEM/DMR-RUI			
Total Award Amount: \$367,466		Total Award Period Covered: 08/15/2001 - 08/14/2004	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal:	Acad: 3	Sumr: 2
Support:	<input type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: RUI - Organometallic NanoStars			
Source of Support: NSF-DMR/CHEM-RUI			
Total Award Amount: \$368,915		Total Award Period Covered: 08/15/2001 - 08/14/2004	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal:	Acad: 3	Sumr: 1
Support:	<input type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: Electroactive Organometallic NanoStars			
Source of Support: ACS-PRF Type B			
Total Award Amount: \$30,000		Total Award Period Covered: 08/01/2001 - 08/31/2003	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal:	Acad: 3	Sumr: 1
Support:	<input type="checkbox"/> Current	<input type="checkbox"/> Pending	<input checked="" type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: RUI - Acquisition of Electrochemical, Light Scattering, and Inert Atmosphere Systems for Materials Chemistry Research and Education			
Source of Support: NSF-CHEM-MRI			
Total Award Amount: ≈ \$200,000		Total Award Period Covered: 08/01/2001 - 07/31/2004	
Location of Project: Youngstown State University			
Person-Months Per Year Committed to the Project.	Cal: 0.1	Acad:	Sumr:
Support:	<input type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title:			
Source of Support:			
Total Award Amount: \$		Total Award Period Covered:	
Location of Project:			
Person-Months Per Year Committed to the Project.	Cal:	Acad:	Sumr:
*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.			

Current and Pending Support**See GPG Section II.D.8 for guidance on information to include on this form.)**

The following information should be provided for each investigator and other senior personnel. Failure to provide this			
Investigator: Raymond E Beiersdorfer, Co-PI	Other agencies (including NSF) to which this proposal has been/will		
Support: Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/>	<input type="checkbox"/> Submission Planned in Near Future	<input type="checkbox"/> *Transfer of Support	
Project/Proposal Title: Equilibrium Aqueous Chemistry of Zeoponic Substrates			
Source of Support: NRC			
Total Award Amount: \$50,000		Total Award Period Covered: 07/01/2001 - 06/30/2002	
Location of Project: NASA Johnson Space Center			
Person-Months Per Year Committed to the proj.		Cal: 1	Acad: Sumr:
Support: Current <input type="checkbox"/> Pending <input type="checkbox"/>	<input type="checkbox"/> Submission Planned in Near Future	<input type="checkbox"/> *Transfer of Support	
Project/Proposal Title:			
Source of Support:			
Total Award Amount:		Total Award Period Covered:	
Location of Project:			
Person-Months Per Year Committed to the Project.		Cal:	Acad: Sumr:
Support: Current <input type="checkbox"/> Pending <input type="checkbox"/>	<input type="checkbox"/> Submission Planned in Near Future	<input type="checkbox"/> *Transfer of Support	
Project/Proposal Title:			
Source of Support:			
Total Award Amount:		Total Award Period Covered:	
Location of Project:			
Person-Months Per Year Committed to the		Cal:	Acad: Sumr: 2
Support: Current <input type="checkbox"/> Pending <input checked="" type="checkbox"/>	<input type="checkbox"/> Submission Planned in Near Future	<input type="checkbox"/> *Transfer of Support	
Project/Proposal Title:			
Source of Support:			
Total Award Amount:		Total Award Period Covered:	
Location of Project:			
Person-Months Per Year Committed to the Project.		Cal:	Acad: Sumr: 1
Support: Current <input type="checkbox"/> Pending <input type="checkbox"/>	<input type="checkbox"/> Submission Planned in Near Future	<input type="checkbox"/> *Transfer of Support	
Project/Proposal Title:			
Source of Support:			
Total Award Amount:		Total Award Period Covered:	
Location of Project:			
Person-Months Per Year Committed to the		Cal:	Acad: Sumr:

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

SECTION H: FACILITIES, EQUIPMENT, AND OTHER RESOURCES

H1. Laboratory Facilities

The Youngstown State University Chemistry Department is located on the 5th and 6th floors of the Ward Beecher Science Hall. It was originally built in the mid-1960s, was extensively upgraded in the mid-1980s, and plans are currently in place for the building of a substantial extension starting in 2005. The main labs and instrumentation rooms to be used by PI's and students in this project include:

- A dedicated chemistry major/research student computer lab having twelve Windows NT workstations loaded with conventional software, including:
 - SHELX-TL, etc., for diffraction analysis software,
 - Word processing,
 - NMR prediction and analysis software,
 - PC Spartan Pro and other molecular modeling/orbital software,
 - Data analysis software for the FT-IR, DSC/TGA, NMR, etc.,
 - Online access to the holdings of OhioLink (i.e., the Ohio universities shared card catalogue and internet access to almost all chemistry journals),
 - Remote software to operate the university's LC-MS and X-ray diffractometer (summer of 2001) instruments.
- A solid state synthesis lab containing a programmable Thermolyne High Temperature Tube Furnace (1700°C), two non-programmable tube furnaces, and a hydraulic press.
- An organometallic synthesis research lab suitable for two to three students, which directly opens onto the adjacent Advanced Synthesis Lab.
- The Advanced Synthesis Lab which has bench space and one and a half fume cupboards for each of 24 students. At least 6 student positions are dedicated to student research full time during the Fall and Winter semesters and all are available for student research during the summer. One bench in this lab is dedicated to high temperature solid-state reactions, using a programmable Lindberg Heviduty Tube Furnace.
- The Small Instruments Annexes having the following small instrumentation purchased by the PI from previous ILI/CCLI grants:
 - a TA Instruments 2910 DSC and a 2050 TGA,
 - a Cannon CT-518 constant temperature bath for viscometry measurements,
 - a GBC Instruments/Polymer Labs GPC-SEC-HPLC system (i.e., autosampler, isocratic/gradient pump, column oven, RI and diode array UV-visible detectors, and data system),
 - a Jasco 410 FT-IR (0.9 cm⁻¹ resolution), and
 - a basic Vacuum Atmospheres HE-43-2 inert atmosphere glove box.

H2. Youngstown State University Instrumentation Facilities

Youngstown State University has an assortment of research-grade equipment, located in two closely related instrumentation centers. These are nominally: The Center for Biomedical and Environmental Research, which is housed on the 4th floor of the Ward Beecher science hall and specializes in instrumentation for the characterization of biological materials, and The Structure & Chemical Instrumentation Center, S&CIC,

which is housed on the 5th floor of the Ward Beecher science hall and specializes in the characterization of non-biological materials. The two centers work closely together, sharing both staff, faculty participants, and instrumentation funding. Both centers were established to serve the teaching and research needs of faculty and students from YSU and other PUIs and to help meet the needs of users from local governmental organizations and industry (in that priority). They have a full time Ph.D. Scientist, Bruce Levison (with a Ph.D. in chemistry and nearly 15 years of post-graduate experience with analytical instrumentation), to assist with data collection and analysis, 0.75 of a full time Instrumentation Service Specialist, Ray Hoff (with a BS in Physics and a dozen years university instrumentation service experience), trained undergraduate and MS student assistants to run the instruments and collect data, and faculty advisors to assist with instrumentation operation and experiment development (10 individuals). The major instruments in these centers are all research grade and were purchased with a combination of NSF, Foundation, State, and internal funds. In addition to the smaller chromatographic, spectroscopic, physical, and analytical instruments expected at any MS level institution (some of which are described above), the centers are equipped with the following modern instrumentation, in addition to the diffraction facility described in the next section:

- a 400 MHz multinuclear NMR with four probes, Variable Temperature, VT, and Pulsed Field Gradient, PFG, accessories, and several work stations.
- a LC-MS instrument with an autosampler and a Solid Phase Micro Extraction, SPME, interface and both Electro-Spray, ESI, and Atmospheric Pressure Chemical Ionization, APCI, inlets.
- two automated GC-MS systems (both with autosamplers and one with a solids probe and one with an SPME interface). One of these is optimized for synthetic samples and one for trace environmental samples.
- several electrochemical systems.

The department also has available a Medium Resolution Transmission Electron Microscope (Siemens 102), which the PI uses to obtain diffraction patterns of disordered oxides.

H3. Youngstown State University Diffraction Facilities

The YSU Structure Center Diffraction Facility is currently located in a 400 square foot lab with adjacent dark room. This lab contains two 6 year old Bruker-AXS P4 diffractometers. One has a X-1000 multiwire area detector and a Cu tube and is used primarily for powder studies. The other has a serial detector, a LT2 low temperature system, and a Mo tube and is used for the large majority of single crystal samples.

The YSU Diffraction Facility has two 6 year old Bruker-AXS P4 single crystal diffractometers, located in a 400 square foot lab with an adjacent sample preparation room. One of the diffractometers has a X-1000 multiwire area detector and a Cu tube and is used primarily for studies of organic molecules and for qualitative powder studies. The other has a serial detector, a LT2 low temperature system, and a Mo tube and is used for

the large majority of single crystal samples. As mentioned in Section C, the NSF (i.e., DUE-CCLI-A&I 0087210) and the Ohio Board of Regents Action Fund (i.e., OBoR-AF #491) has funded our proposal “WEB Accessible Single Crystal X-Ray Diffractometer for Undergraduate Instruction at a Consortium of Predominantly Undergraduate Institutions”) and these funds will be used to purchase a Bruker-AXS APEX CCD diffractometer (or equivalent for June 2001 installation). This will be used by faculty and students from the two dozen PUI institutions who are members of the **YSU-PUI Undergraduate Diffraction Consortium**. It will be housed in a new diffraction lab to be built in the chemistry department, consisting of more than twice the space of the current facility. In addition to the CCD system and two P4 diffractometers, space will be reserved in the facility for possible future addition of a dedicated powder diffractometer.

H4. External Powder Diffractometer Availability

There is one powder X-ray diffraction instrument comparable to the one requested herein located at the Kent State University Chemistry Department (about a 45 minute drive from YSU), although it is not as optimized (and is not currently used for) quantitative structural work. This instrument is a Bruker D5000, equipped with a standard reflection sample stage and scintillation detector. Because it does not have a capillary stage, this instrument cannot be used for the PI's major research area, for reasons mentioned in section C3. Also, the PI has been informed several times (by Kent State Faculty Users) that the instrument is heavily used, so that at best only limited time is available for external users. This means it would be impossible for our undergraduate research students to gain hands-on experience with the instrument. In fact, the PI was recently informed that Kent State plans to submit a proposal in the future to acquire a second system to meet their high internal demands for powder diffractometer time. Since Kent State's diffractometer cannot adequately meet their own internal needs, clearly it cannot be expected to meet our growing research and educational needs as well.

SECTION I: SPECIAL INFORMATION AND SUPPLEMENTARY DOCUMENTATION

II. RUIIMPACT STATEMENT

IIa. The Situation at Predominantly Undergraduate Institutions, PUIs

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

IIb. Youngstown State University as a PUI

Youngstown State University is an urban PUI situated in the heart of downtown Youngstown. It has approximately 12,000 undergraduates enrolled in 1 and 2 year associate degree programs (more commonly found at community colleges) and in 4 year bachelors degree programs from our Colleges of Arts & Sciences, Business, Education, Engineering, Fine & Performing Arts, and Health & Human Services. We also have a variety of MS-level programs totaling approximately 1,200 students (primarily in the college of education), but offer no Ph.D.s in NSF supported fields. YSU is an *open enrollment commuter institution* (more than 90% of our students live off campus). Reflecting our region's blue collar roots, the typical YSU student is in the first generation of their family to attend college and works an average of 30 hours per week to support their studies. Our students are a relatively hard working and motivated group, but this combination of factors significantly impacts our ability to get them involved in research.

IIc. Encouraging Undergraduates to Participate in Research

To encourage a greater research participation by all students, the University's new General Education program has been restructured and was implemented in the Fall 2000 semester. One aspect of this change has been to very strongly encourage all lab (and to the extent possible, lecture) courses to follow a *discovery oriented collaborative research model*. This is facilitated by the small size of our upper level labs and courses (i.e., 5 to 25 students). In addition, many science labs are being restructured to integrate research like (or even real

research) projects with the more skills oriented exercises. In addition, all bachelors students are now required to complete a capstone course which integrates research, written and oral communication, and critical thinking components. In the sciences, this course will typically be an undergraduate research project coupled to a course that gives formal training in research methods.

IId. The Research Situation in the YSU Chemistry Department

Our department is considered to be one of the strongest on campus, and the administration often holds us up as the model of how to integrate scholarship, teaching, and service in a synergic fashion. We have 15 full time faculty positions divided between our traditional Analytical, Biochemistry, Inorganic, Organic, and Physical Chemistry Divisions, and our new Chemical Education Division. Each division is similar in size with many interdisciplinary faculty being associated with more than one division. For example, one of the Co-PIs (ADH) teaches largely in the Organic Division but also covers some Biochemistry and Inorganic Courses, and his research interests span the range of organometallic and polymer chemistry, diffraction methods, and Chemical Education.

IIf. Recent Changes in the YSU Chemistry Department

Ten of our fifteen faculty have been at YSU for less than nine years. This, coupled with the strong support of the senior and retired faculty and a total replacement of the administration, has enabled a dramatic change in our department's activities and profile. A decade ago, the scale of externally funded research in our department was limited (largely due to administrative impediments) and was concentrated in the Analytical and Physical Divisions. With our rejuvenation, almost all faculty are now involved in research. Both our publication rates and our success at raising external funding to support this effort have increased dramatically (e.g., by more than an order of magnitude for external grants). Department faculty have been particularly successful in funding state-of-the-art instrumentation for use in our courses and student research projects.

IIf. The Chemistry Program at YSU

Our department graduates approximately 30–40 BA and BS majors in Chemistry and 5–10 MS students each year. Our students have developed an *extremely strong regional and growing national reputation* for the quality of their preparation for either graduate school or industry. As part of our new General Education program, and reflecting the simultaneous change from quarters to semesters as of Fall 2000, we have fundamentally revised our undergraduate and MS course sequence. For example, one major change is that we now offer more flexibility in the upper-level chemistry courses that a student may take. The curriculum is now structured such that our BA and ACS approved BS students will now complete all of their required courses in their first three years. This will leave their Senior year free for focusing on research like laboratory courses, undergraduate research projects, and possibly internship experiences. This should significantly enhance the integration of their teaching and research experiences and the extent of their involvement in research. In our graduate program, we have decreased the formal course load which our MS students are required to take, and rearranged our offerings so that the

students will be able to complete them in their first year (rather than the 5 quarters typical previously). We have also instituted more formal training in chemical safety, research, writing, and presentations. Again, this combination should significantly enhance their research productivity. Finally, we have historically had few formal programs to support the professional development needs of regional teachers. We are now instituting more formal programs, including: a new College of Arts and Sciences/College of Education program for pre-service teachers and new master's level programs for in-service teachers. The master's programs will include an MS in Chemistry with a Chemical Education Emphasis (Fall 2000 start) and an MA in Science Education. The MS in Chemistry will require the same core chemistry courses as our other MS programs but will differ in that the research project will be in the area of Chemical Education.

11g. The Research Facilities at YSU

In the early 1990's, the administration began to support faculty research initiatives much more aggressively than in previous years. At this time, while there was strong encouragement to pursue research activities involving students, there was almost no appropriate equipment or instrumentation to do so in practice, particularly for projects needing major instrumentation. Since that time, the PIs and other collaborators, either from various departments at YSU or from regional colleges, have worked diligently to build the infrastructure at YSU so as to be able to do competitive research. This infrastructure is now largely in place. For example, YSU now has the following modern instrumentation: a 400 MHz multinuclear NMR spectrometer equipped with PFG and VT, an LC-MS and two GC-MS systems, Thermal Analysis and GPC instrumentation for Polymers, a variety of other chromatography, analytical, and spectroscopic instrumentation, and the X-ray facility discussed in detail previously. The department is now helping plan a new science building for 2007.

11h. Benefits from the Proposed Project

Acquisition of the proposed state-of-the-art powder diffractometer benefits our program not only by providing new research capabilities currently unavailable to us, but also in a dynamic sense in that a successful research program overall depends upon the availability of a critical mass of state-of-the-art instrumentation. Many synthetic projects for example depend upon access to both NMR and diffraction instruments. Given our already excellent single crystal X-ray diffraction equipment, purchase of the requested powder diffractometer would complete our X-ray diffraction facilities, providing a comprehensive facility for research, teaching, and learning. Because of our strong "hands-on" access policy regarding undergraduate access to *all* research-grade equipment in our department, our students are perhaps the primary beneficiaries of this acquisition. Although one-on-one training of students to use major instrumentation is time consuming and inefficient from a research productivity point-of-view, it has an amazing positive impact on our student's professional lives. This is reflected in their evident rising levels of confidence as they interview for jobs and realize the competitive edge that this hands-on training has given them. Indeed, many of our students have gone on to do very well in major industrial positions (e.g. at Pfizer, DOW, and many others), and top Ph.D. graduate schools (University of Wisconsin and University of Pennsylvania are recent examples).