DMR-94 03889

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

APPENDIX

For Consideration by NSF Organization Unit(s)
(Indicate the most specific unit known, i.e. program, division, etc.)

Program Announcement/Solicitation No./Closing Date

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NSF Proposal Number
9403889

Date Received	Number of Copies	Division Assigned	Fund Code	File Location

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☐ A Renewal or
☐ An Accomplishment-Based Renewal

Is This Proposal Being Submitted to Another Federal Agency? YES____ NO____ If YES, List Acronym(s)

Name of Organization to Which Award Should be Made: Youngstown State University

Institutional Code (If known)

Address of Organization, Including Zip Code
410 Wick Avenue
Youngstown, OH 44555

Is Submitting Organization: ☐ For-Profit Organization; ☐ Small Business; ☐ Minority Business; ☐ Woman-Owned Business

Branch/Campus/Other Component (Where work is performed, if different)

Institutional Code (If known)

Title of Proposed Project
Acquisition of a Single Crystal X-ray Diffractometer

Requested Amount $ 71,199 Funded

Proposed Duration (1-60 months) 24 months

Requested Starting Date June 15, 1993

Check Appropriate Box(es) If This Proposal Includes Any of the Items Listed Below:
☐ Vertebrate Animals
☐ Human Subjects
☐ Historical Places
☐ Research Involving Genetically Engineered Organisms
☐ National Environmental Policy Act
☐ Proprietary and Privileged Information
☐ Disclosure of Lobbying Activities
☐ Facilitation for Scientists/Engineers with Disabilities
☐ Research Opportunity Award
☐ International Cooperative Activity: ____________
Country/Countries

PI/PD Department
Chemistry

PI/PD Fax Number

PI/PD Postal Address
Department of Chemistry
Youngstown State University
Youngstown, OH 44555

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Co-PI/PD Raymond E. Beiersdorfer	124-48-5646	Ph.D., '92	216-742-1753	
Co-PI/PD				

NOTE: The FULLY SIGNED Certification Page must be submitted immediately following this Cover Sheet.

*Submission of social security numbers is voluntary and will not affect the organization's eligibility for an award. However, they are an integral part of the NSF information system and assist in processing the proposal. SSN solicited under NSF Act of 1950, as amended.

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PROJECT SUMMARY

This proposal requests funds for the acquisition of a single crystal X-ray diffractometer to support research programs and teaching efforts in the chemistry, geology, physics and materials engineering departments at Youngstown State University. The instrument would also be made available to support similar programs at nearby two and four year colleges, and would be used in collaborative research projects involving YSU faculty and local industry as well. Currently, no single crystal X-ray diffraction facilities are available on campus, nor in local industrial laboratories.

1. INTRODUCTION

Funds are requested towards the purchase of a single-crystal X-ray diffractometer. The instrument is required to support (a) the research programs of faculty in the Chemistry and Geology Departments; (b) collaborative research efforts between YSU faculty and outside industry and research institutions; and (c) teaching efforts in courses in the Chemistry, Physics, Materials Engineering and Geology Departments involving aspects of single crystal X-ray diffraction. At present, no single crystal X-ray diffraction capabilities exist on campus, nor in research labs of local industries.

A single-crystal X-ray diffractometer would enhance current research programs on: microstructure/property relationships in gamma TiAl alloys; bond length and bond valences in oxides related to β-alumina; synthesis and crystallographic analysis of organometallic polymers and rigid rod molecules; chiral phosphonate transition state analogues as inhibitors of HIV-1 protease; and crystal chemistry of pumpellyite. Students at both the M.S. and undergraduate levels will be involved in each of these projects. The lack of single-crystal X-ray equipment on campus currently makes it impossible to train students to conduct research utilizing this technique, which is basic to many areas of materials and chemical research.

The X-ray diffractometer would be placed in the Chemistry Department, where adequate facilities currently exist to house it. In recognition of its commitment to support research programs of faculty and students, and to promote industrial-academic collaborative research projects, Youngstown State University will provide over 50% cost sharing for this equipment.

2. RESEARCH PROGRAMS OF MAJOR USERS

The research programs of the principle investigators is described in detail below. A total of five projects are discussed by the four principle users. The first three projects descibed fall within areas covered by DMR.

2.1 Dr. Timothy R. Wagner

Dr. Wagner is an Assistant Professor in the Department of Chemistry at Youngstown State University. His general research interests involve structure/property relationships in both metallic and ceramic materials, utilizing mainly X-ray diffraction and electron microscopy techniques. Two of his research programs which require single-crystal X-ray diffraction are described below. These projects are: (1) Microstructure/property relations in γ-TiAl alloys; and (2) Bond lengths and valences in β-Alumina and Magnetoplumbite-type oxides.

2.1.1 Quantitative X-Ray Analysis of γ-TiAl Alloys

2.1.1.1 Introduction

Due to increased demand for lightweight high performance and high temperature alloys, an active area of intermetallic alloy research during the past decade has focused on gamma titanium aluminides. The alloys showing greatest promise appear to be those based on the two phase Ti_3Al/TiAl system, having an overall composition of 46-48 atomic percent Al. The two phase microstructure consists of 75-95% TiAl (γ) phase having the $L1_0$ (ordered face-centered tetrahedral) structure, and the remainder consists of the Ti_3Al (α-2) phase with the DO_{19} (ordered hexagonal) structure. These materials have a theoretical density near 3.6 g/cc, and good resistance to oxidation up to temperatures of 850-900 °C. The presence of the α-2 phase improves the room temperature ductility over that of single phase γ-TiAl, although not significantly enough to meet demands for practical applications. Improvements in the properties of the gamma aluminides are steadily being made, however a major problem hindering specific applications is related to inappropriate balance of properties. For example, improvements of fracture toughness or high temperature creep resistance generally reduce both strength and room-temperature ductility. Thus, microstructures composed of α_2 lamellar growth within the γ-TiAl matrix are known to exhibit the best fracture toughness, but relatively poor ductility . In order to achieve an improved combination of strength and ductility, and thus a more rational alloy design, one must control the microstructure in conjunction with the fabrication process. Attainment of this goal requires a single crystal X-ray diffractometer, so that the necessary quantitative microstructural analysis of castings can be performed.

2.1.1.2 Casting of the Samples

This project is a collaborative effort with SensorDek, Inc., which is a local company engaged in intensive research and development in the areas of single crystal semiconductors, alloys, and other applied Materials Science projects. Indeed, SensorDek proposes to fund almost 100 % of the non-capital items, which alone amounts to over 50 % of the total budget requested in this proposal. Currently, SensorDek is engaged in studies of mold wall reactions in the directional solidification of γ-TiAl alloys. This is a Phase I project funded by the Small Business Innovation Research (SBIR) Program of the U.S. Airforce. From the Phase I results, possible mold materials which limit reactions at the liquid TiAl/mold wall interface have been identified[1], and this knowledge will be used by SensorDek for the fabrication of samples in Phase II of the project. The Phase II proposal to be submitted by SensorDek to the Airforce in November 1993 indicates that castings will be prepared using the modified-Bridgeman technique. This technique has not yet been used to successfully grow directionally solidified gamma TiAl alloys as viable engineering materials, and is a technique amenable to industrial production. The primary objective of this collaborative effort centers on the production of complex shape components for possible commercial applications in the aerospace and automotive industries. Before this objective can be attained, quantitative single crystal X-ray analysis of the castings produced by SensorDek is required in order to correlate microstructure and fabrication parameters. This knowledge is necessary to make a more rational design of oriented single crystal fabrication methods possible.

2.1.1.3 Microstructural Analysis

The X-ray analysis of samples provided by SensorDek will reveal: (1) the relative amounts (in volume percent) of TiAl versus Ti_3Al phases; (2) Ti_3Al lamellar spacing within the TiAl matrix; (3) Grain orientations and texturing; and (4) Radial and Longitudinal analysis of the casting. This information is necessary before the reproducible casting of viable engineering materials is possible, due to the strong property/microstructure dependence of gamma titanium alloys. The microstructure of two-phase gamma titanium can be classified into four groups: near gamma, duplex, nearly lamellar and fully lamellar[2]. The fully lamellar structure has the highest fracture toughness, with values ranging from 20 MP$\sqrt{m}$ to 30MPa$\sqrt{m}$[3] depending upon the gamma/lamellar grain volume ratio. The Ti-Al binary phase diagram at the alloy composition of Ti-(46-48 at. %) Al shows two phase reactions: a peritectic ($L + \alpha\text{-Ti(Al)} \rightarrow \gamma\text{-TiAl}$) reaction and a eutectoid ($\alpha\text{-Ti(Al)} \rightarrow \alpha_2\text{-Ti}_3\text{Al} + \gamma\text{-TiAl}$) reaction[3]. When the gamma phase is precipitated out of either the α-Ti matrix or the α_2-Ti_3Al2 matrix, the γ-TiAl/α_2-Ti_3Al lamellar orientation relationship is (111)||(0001) and [110]||[1120]. This is the structure of interest in this work.

X-ray diffraction is the preferred method for non-destructive characterization of oriented single crystals and eutectics, and is required for the microstructural analysis of castings produced under various solidification senarios. The processing parameters will influence the lamellar spacings of the α_2-Ti_3Al phase in the γ-TiAl matrix in a constant composition alloy, and so each casting produced must be evaluated based on the phase distribution, phase orientation, and homogeniety across various cross-sections of the cast product. Castings will be prepared and analyzed until repeatability and performance goals are attained.

The single crystal X-ray analysis will be augmented by transmission and scanning electron microscopy, both of which are available on site. These techniques will be used to analyze structural parameters not amenable to study by bulk-structural X-ray analysis, such as deformation analysis or elucidation of interface structures. Thus, the proposed research should contribute basic knowledge towards increased understanding of microstructure/property relationships in lamellar gamma titanium aluminides, as well as lead to possible practical applications.

References

1. SensorDek, Inc. (Glen A. Schaefer); Air Force SBIR Phase II Proposal, submitted Nov. 1993.
2 Kim, Y-W.; *Acta. Metall. Mater.* **1992**, v. 40, p. 1121.
3. Kim Y-W and Dimiduk M. ; *J. of Metals*. August 1991, p. 40.

2.1.2 Bond Lengths and Valences in β-Alumina and Magnetoplumbite-Type Compounds

2.1.2.1 Introduction

Traditionally, main-group inorganic oxide structures have been described in terms of closest-packing of anions, with the smaller cations dispersed interstitially throughout the anion matrix. Thus cation-cation interactions have often been considered to be a relatively unimportant factor in influencing the structure of these compounds. In recent years, however, evidence has been published which suggests that cation-cation interactions in inorganic oxides are a more important structural parameter than previously believed. One important group of materials for which this appears to be true are β-Alumina and Magnetoplumbite-type compounds. Beta-alumina has ideal composition $NaAl_{11}O_{17}$, while that of magnetoplumbite-type aluminates is $MAl_{12}O_{19}$ where M is typically an alkaline earth element. 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 only in the arrangement of cations on the conduction planes.

The spinel blocks in these structures could be described as the hypothetical spinel $Al_3O_4^+$, so that Al atoms are found in both tetrahedral and octahedral positions. As previously noted by West[1], the bonds from the tetrahedral Al site (i.e. the Al(2) position) are longer than expected for Al^{+3} in tetrahedral coordination. To further investigate the anomaly at the Al(2) position at the spinel blocks, we calculated the apparent valences at the Al positions in several magnetoplumbites and β-aluminas using well established bond length-bond valence correlations. We used the expression proposed by Brown and Altermatt[2], $v = \exp[(R_o - d)/0.37\ \text{Å}]$, where v is the bond valence, R_o is a parameter characteristic of the atom pair forming the bond, and d is the experimental bond distance. The apparent valence of an atom is then obtained by summing the valences of all bonds formed by that atom.

2.1.2.2 Proposed Research

A bond-valence study of several compounds with general formula $MAl_{11}O_{17}$ (M = Group I cation) or $MAl_{12}O_{19}$ (M = group II cation) indicated that the tetrahedral Al sites in the spinel blocks is consistently underbonded, suggesting the possibility that bonds at these sites are elongated due to cation-cation interactions[3]. To further investigate the role of non-bonded interactions in these compounds, we propose to synthesize single crystals of composition $MR_{11}O_{17}$ or $MR_{12}O_{19}$ (where M = Na, K, Sr, Ca, or Ba and R = Al and/or combinations of Mg, Sc, Fe, Ga, or Si). Single crystals will be grown using the flux method, and Na β-alumina obtained in this way will be used to obtain other β-aluminas via ion exchange reactions. The structures of crystals thus prepared will be solved using single crystal X-ray diffraction, from which bond lengths will be obtained. Comparison of experimental bond lengths to bond lengths obtained from bond valence analysis of ideal structures will indicate any deviation from expected parameters, particularly at the tetrahedral cation site of the spinel block. If non-bonded interactions are indeed important in these compounds, we expect that cations larger than Al^{+3} will occupy the tetrahedral site of the spinel block, while smaller cations will preferentially occupy octahedral sites.

Achieving a better understanding of the crystal chemistry at the spinel blocks in these materials is an important step towards better understanding their structure/property relationships. For example, β-alumina-type compounds are well known for their relatively high ionic conductivity, which in turn depends upon the composition of the large cations (e.g. Na^+ or K^+) in the conduction layers of the structure. The β-aluminas are well known as being non-stoichiometric, having excess monovalent cations in the conduction planes of the lattice. It is quite possible that the conduction plane composition in these materials is influenced by the anomalous crystal chemistry at the spinel blocks. Thus it has been suggested that the β-aluminas contain excess positive charge in their conduction layers due to the deficiency of local charge at the tetrahedral Al site in the spinel blocks[1]. In general, successful practical applications of crystalline materials, whether related to conductivity, optical, magnetic, catalytic or other properties, depends upon knowledge of the defect chemistry of the system.

References

1. West, A.R.; *Materials Research Bulletin*, **1979**, 14, 441.
2. Brown, I.D. and Altermatt, D.; *Acta Cryst.* **1985**, B41, 244.
3. Wagner, T.R. and O'Keeffe, M.; *J. Solid State Chem.* **1988**, 73, 211.

2.2 Dr. Allen D. Hunter

Dr. Hunter is an Associate Professor in the Department of Chemistry. His research interests include synthesis and characterization of organic and organometallic polymers and rigid rod compounds. Central to the characterization aspect of Dr. Hunter's work is elucidation of the crystal structures of the materials syntesized utilizing single crystal X-ray diffractometry.

2.2.1 Organometallic Polymers and Rigid Rods

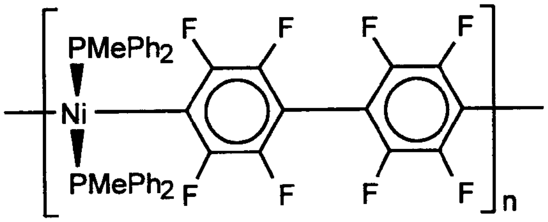
The steric and electronic properties of phosphine ligands (e.g. PR_3 and $R_2PCH_2CH_2PR_2$) in discrete transition metal complexes can be modified independently of one another and can be varied over a wide range by rational changes to the phosphine ligands' structures.[1] In addition, the syntheses of such complexes generally proceeds similarly for all phosphine ligands. The central goal of our research into organometallic polymers is to exploit these characteristics of organometallic phosphine derivatives for materials science applications. Thus, we are interested in novel oligomers and polymers having metal phosphine units as parts of their backbones and/or side chains. By varying the structures of these units in a systematic fashion, we hope to substantially alter these materials' properties and construct detailed structure/property relationships. Analysis of these may allow us to develop a molecular level understanding of the effects that the transition metal centers, ancillary ligands, and repeating unit structures have on polymer properties. Such an understanding may, in turn, eventually allow the rational design of organometallic polymers having superior or unique combinations of properties that are relevant to real world applications. These results will strengthen the fundamental knowledge base of polymer chemistry in general and may contribute to the understanding of structure/property relationships for more conventional polymers.

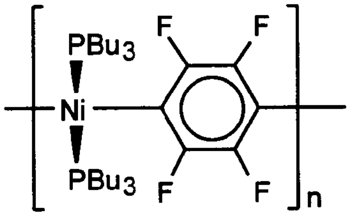
Our work on organic and organometallic polymers has involved several classes of new polymeric materials, including: (1) polyfluoroarylene bridged polymers of square planar transition metal centers (e.g. $-[-Ni(PR_3)_2(\mu-4,4'-C_{12}F_8)-]_n-$, $-[-Ni(PR_3)_2(\mu-1,4-C_6F_4)Pd'(PR'_3)_2(\mu-1,4-C_6F_4)-]_n-$)[2] and polyfluoroarylene bridged polymers of silyl and siloxy centers and copolymers of these with transition metal centers (e.g. $-[-SiR_2-O-SiR_2(\mu-1,4-C_6F_4)-]_n-$, and $-[-SiR_2(\mu-1,4-C_6F_4)Ni(PR'_3)_2(\mu-1,4-C_6F_4)-]_n-$),[3] (2) bifunctional isonitrile bridged polymers of octahedral transition metal centers (e.g. $-[-Mo(R_2PCH_2CH_2PR_2)_2(\mu-CN-C_6H_4-NC)-]_n-$),[4] (3) conventional condensation polymers (e.g. polyesters, polyamides, polyurethanes, polyureas, polycarbonates) having highly fluorinated organic monomers and/or monomers containing organometallic centers (e.g. $-[-O-C(CH_3)_2-C_6F_4-C(CH_3)_2-O-C(O)-]_n-$, $-[-O-C(CF_3)_2-C_6F_4-Ni(PR_3)_2-C_6F_4-C(CF_3)_2-O-C(O)-C_6H_4-C(O)-]_n-$, $-[-NH-C_6H_4-NC-Mo(R_2PCH_2CH_2PR_2)_2-CN-C_6H_4-NH-C(O)-NH-C_6H_3Me-NH-C(O)-]_n-$, and $-[-O-C(CH_3)_2-C_6H_4($_$-Cr(CO)_3)-C(CH_3)_2-O-C(O)-NH-(CH_2)_6-NH-C(O)-]_n-$),[5] and (4) vinyl polymers having highly fluorinated side chains and/or organometallic side chains (e.g. polyacrylates including $-[-CH_2CH(C(O)X)-]_n-$ where $X = O-C(CF_3)_2-C_6F_4H$ and $O-C(CH_3)_2-C_6F_4-Ni(PR_3)_2-C_6F_4H$).[6] This interest also includes their alternating, random, and block copolymers and their blends with conventional organic polymers.

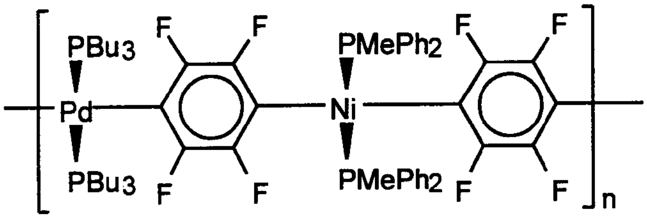
For each new class of organometallic polymers, we begin our studies by preparing and characterizing a series of model compounds[7] and oligomers. This allows us to optimize reaction conditions so that polymers having the required molecular weights can be prepared in the later condensation and addition polymerizations. It also produces new discrete compounds that are often of chemical interest in themselves and whose structures are more readily and completely characterizable by conventional analytical, spectroscopic, and, most importantly, X-ray crystallographic methods than are those of the analogous polymers. Analysis of this data, in combination with molecular modeling/mechanics calculations (also based on the X-ray results), allows the prediction of the steric, electronic, and conformational behavior that is to be expected for the polymers. The polymers are then synthesized using the optimized synthetic methods and their repeating unit structures are established by comparison of their spectroscopic data to that for the discrete compounds. Finally, the materials properties (e.g. their T_g, T_m, solubility, stability, mechanical, chemical, optical, and electronic) of the new polymeric compounds are determined and structure/property relationships are constructed to try to develop a fundamental understanding of the origins of the effects that the mainchain or sidechain organometallic components of these novel polymers have on their materials characteristics. Our research efforts involving each class of novel polymeric materials are outlined below.

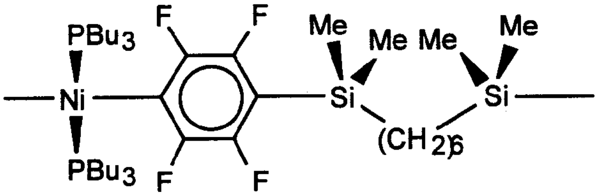
2.2.2 Polyfluoroarylene Bridged Polymers

Our main effort in materials chemistry has involved the synthesis of organometallic species in which square planar metal phosphine centers[2] and/or silyl and siloxy centers[3] alternate with polyfluoroarylene bridging groups, e.g.,









in the backbones of model complexes, oligomers, and polymers. These have been prepared via condensation reactions between organolithium reagents and organometallic monomers, e.g.,[2,3,7]

$$C_6F_4Li_2 + 2\ Fp'I \longrightarrow Fp'\text{-}C_6F_4\text{-}Fp' \tag{1}$$

$$Ni(PMePh_2)_2(C_{12}F_8Li)_2 + 2\ Ni(PMePh_2)_2Br_2 \longrightarrow Br\text{-}Ni(PMePh_2)_2\text{-}C_6F_4\text{-}Ni(PMePh_2)_2\text{-}C_6F_4\text{-}NI(PMePh_2)_2\text{-}Br \tag{2}$$

$$Ni(PBu_3)_2(C_6F_4Li)_2 + Cl\text{-}SiMe_2\text{-}O\text{-}SiMe_2\text{-}Cl \longrightarrow \text{-}[\text{-}Ni(PBu_3)_2\text{-}C_6F_4\text{-}SiMe_2\text{-}O\text{-}SiMe_2\text{-}C_6F_4\text{-}]_n\text{-} \tag{3}$$

$$C_6F_4Li_2 + Ni(PBu_3)_2Br_2 \rightarrow \text{-}[\text{-}Ni(PBu_3)_2\text{-}C_6F_4\text{-}]_n\text{-} \tag{4}$$

$$Pd(PBu_3)_2(C_6F_4Li)_2 + Ni(PMePh_2)_2Br_2 \longrightarrow \text{-}[\text{-}Pd(PBu_3)_2\text{-}C_6F_4\text{-}Ni(PMePh_2)_2\text{-}C_6F_4\text{-}]_n\text{-} \tag{5}$$

(where C_6F_4 and $C_{12}F_8$ are 1,4-C_6F_4 and 4,4'-$C_{12}F_8$, respectively, and Fp' = (η^5-C_5H_4Me)$Fe(CO)_2$). Indeed, we have now prepared a range of such materials including oligomers having from one to four metal centers and representative homopolymers and alternating copolymers for the Ni, Pd, and Si containing compounds and we have found that materials having any of the possible combinations of these structural units can generally be prepared in a rational fashion.[2,3]

These rigid rod materials have been characterized by conventional analytical and spectroscopic (i.e. IR, UV-visible, and especially multinuclear NMR) techniques to determine gross repeating unit structures. However, the most detailed structural information has been obtained by single crystal X-ray diffraction analysis on model compounds and oligomers (see Figures 2.2.2.A and 2.2.2.B, respectively). For these materials, the X-ray crystallographic analyses produced critical information, including: (1) the unambiguous identification of unexpected products and/or products whose isomeric identities were difficult to establish by sporting methods, (2) ligand and backbone conformations, (3) intra- and intermolecular steric and electronic interactions, (4) intermetallic separations as a function of bridging unit (e.g. _ 11.0 Å vs 6.6 Å for 4,4'-$C_{12}F_8$ and 1,4-C_6F_4 complexes of Ni, respectively) and metal center (e.g._ 6.6, 6.8, and 6.5 Å for Ni, Pd, and Si metals in 1,4-$C_6F_4M_2$ complexes, respectively), and (5) bond lengths and angles. This data is then used to: (1) calibrate solid state spectroscopic techniques, such as NMR, so that structural information can be derived for products that are not sufficiently soluble for solution state techniques to be used or that can not be grown as single crystals, (2) form the starting point for molecular modeling/mechanics calculations that are used to predict polymer structures, and (3) rationalize trends in intermetallic conjugation as a function of bridging unit structure.[2,7]

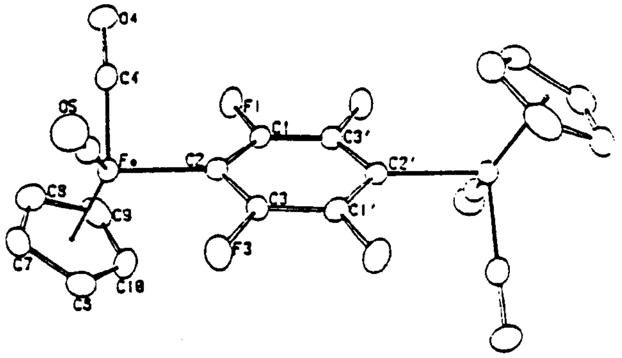
Our synthetic efforts in this area are currently focused on expanding the range of transition metal centers (i.e. Ni, Pd, and/or Pt), silicon containing centers (i.e. SiRR', SiR_2-($(CH_2)_n$-$SiR_2)_n$, SiR_2-(arylene-$SiR_2)_n$, and SiR_2-(O-$SiR_2)_n$), phosphine ligands (i.e. R = $(CH_2)_nCH_3$), $(CH_2)_nPh$, and C_6H_4X where X = H, Me, ^{n}Bu, ^{t}Bu, $SiMe_3$, OMe, and CF_3), and polyfluoroarylene bridging groups (i.e. 1,4-C_6F_4, 1,3-C_6F_4, 4,4'-$C_{12}F_8$, 3,3'-$C_{12}F_8$, 4,4',4'',4'''-$C_{24}F_{16}$, 4,4'-C_6F_4-$SiMe_2$-C_6F_4-, and/or 3,3'-C_6F_4-$SiMe_2$-C_6F_4-) which are present in the backbones of homopolymers and alternating, random, and block copolymers and their oligomers, e.g.

$$n\ C_6F_4Li_2 + n\ Ni(P(octyl)_3)_2Br_2 \longrightarrow -[-Ni(P(octyl)_3)_2-C_6F_4-]_n- \tag{6}$$

$$2n\ C_6F_4Li_2 + n\ Pt(PMe_3)_2Br_2 + n\ Ni(PEt_3)_2Br_2 \longrightarrow -[-(random\text{-}Pt(PMe_3)_2/Ni(PEt_3)_2)-C_6F_4-]_{2n}- \tag{7}$$

$$n\ Ni(PMe_3)_2(C_{12}F_8Li)_2 + n\ Cl-SiMe_2-O-SiMe_2-O-SiMe_2-O-SiMe_2-Cl \longrightarrow -[-Ni(PMe_3)_2-C_{12}F_8-SiMe_2-O-SiMe_2-O-SiMe_2-O-SiMe_2-C_{12}F_8-]_n- \tag{8}$$

in a controlled fashion. As with their $PMePh_2$ and PBu_3 analogues that have been prepared previously, these new materials will be identified by comparison of their multinuclear solution and solid state NMR spectra to those of representative oligomers that have also been characterized by X-ray diffraction analysis. Again, molecular modeling and mechanics calculations based on these results will be carried out to estimated polymer conformations which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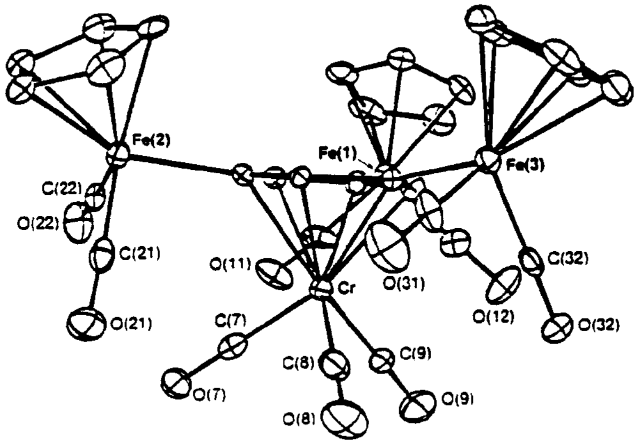
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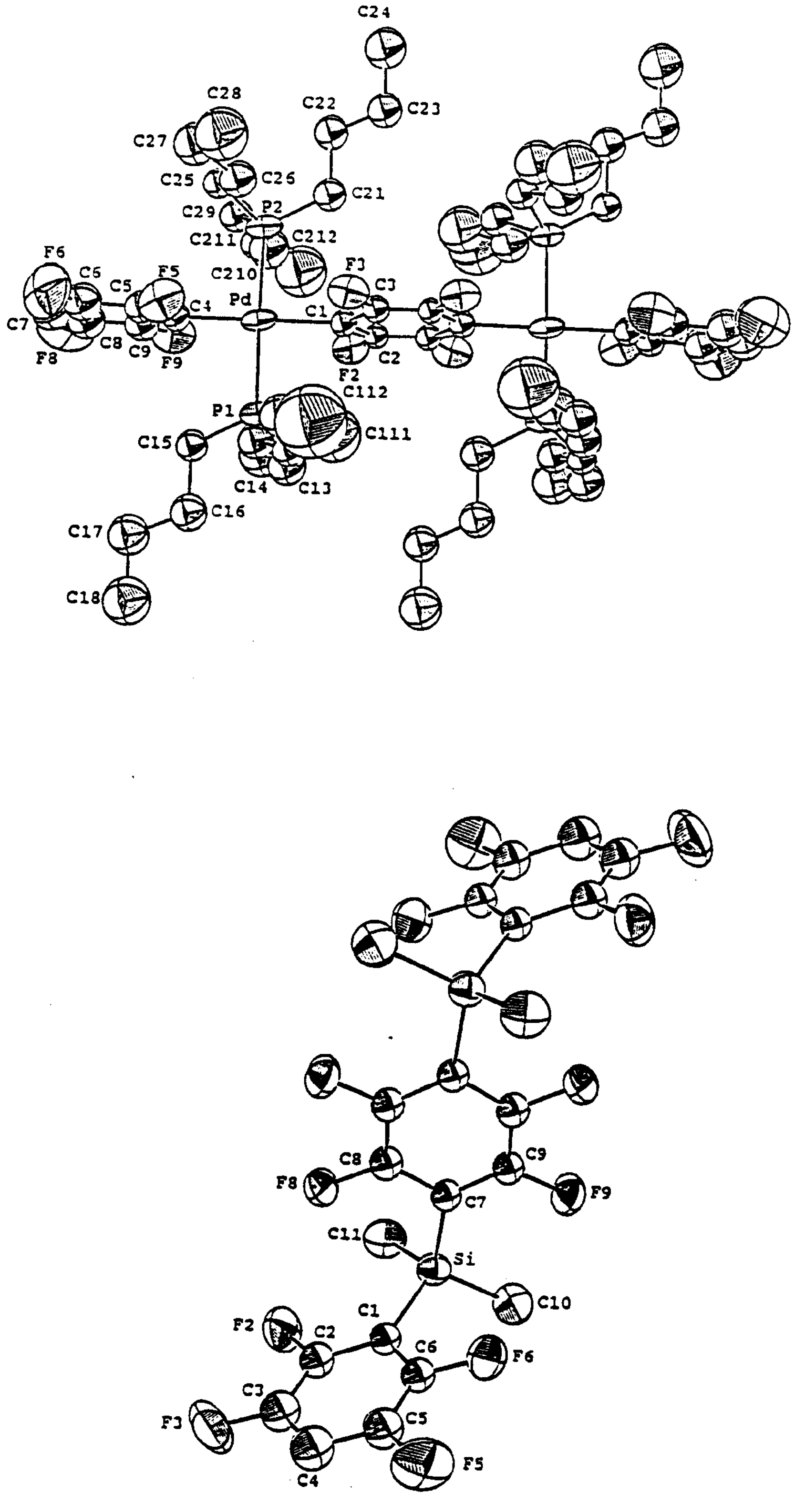
Figure 2.2.2.A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C4

Figure 2.2.2.B

will be experimentally verified by conventional methods. The morphology of the polymers will be evaluated by thermal, optical and electron microscopy, and X-ray diffraction methods.[8] The formation of blends of these organometallic polymers with more conventional organometallic polymers will also be investigated and X-ray diffraction analysis will be carried out, particularly for fibers that have been partially oriented by stretching. Finally, the stabilities and solubilities and mechanical, electrical, and optical properties of these materials will be evaluated. We will then correlate the results of

these various materials properties studies with our structural data from X-ray crystallography to develop structure/property relationships that are as detailed as possible. It is from the study of these that we hope to draw our most fundamental insights into the nature of intermolecular interactions in our organometallic polyfluoroarylene bridged polymers.

2.2.3 Organometallic Materials Having Isonitrile Bridging Groups

We have recently become interested in extending our organometallic polymer studies to materials having bifunctional isonitrile ligands which are neutral in charge and bridge metal centers by the formation of formally dative bonds. We have now completed a pilot study for this project and have made encouraging progress towards demonstrating that the desired rigid rod materials are preparable, characterizable, and sufficiently stable for our desired applications. Thus, the requisite isonitrile ligands and a few representative model compounds, oligomers, and a polymer, have been prepared, e.g.,

$$\mathrm{FpCl} + \mathrm{AgPF_6} + \mathrm{CN\text{-}C_6H_4\text{-}Cl} \longrightarrow [(\mathrm{Fp})(\mathrm{CN\text{-}C_6H_4\text{-}Cl})](\mathrm{PF_6}) \qquad (9)$$

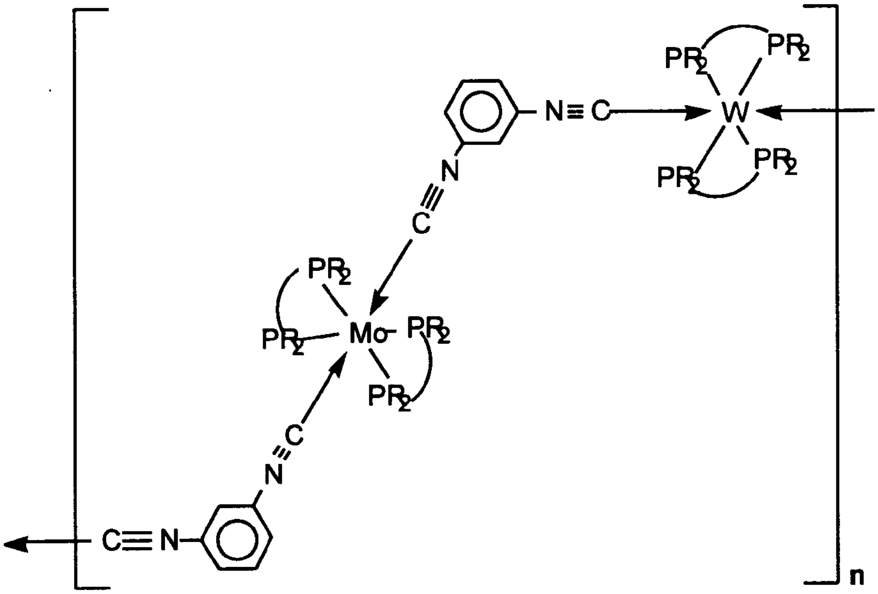
$$2\,[\mathrm{Fp(OCMe_2)}]\mathrm{BF_4} + 1,4\text{-}\mathrm{C_6H_4\text{-}(NC)_2} \longrightarrow [\mathrm{Fp(CN\text{-}1,4\text{-}C_6H_4\text{-}NC)Fp}](\mathrm{BF_4})_2 \qquad (10)$$

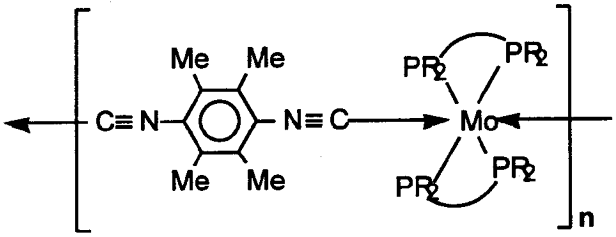
$$\textit{trans}\text{-}\mathrm{M(N_2)_2(dppe)_2} + 2\,\mathrm{CN\text{-}C_6H_4\text{-}Cl} \longrightarrow \textit{trans}\text{-}\mathrm{M(dppe)_2(CN\text{-}C_6H_4\text{-}Cl)_2} \qquad (11)$$

$$\mathrm{n}\ \textit{trans}\text{-}\mathrm{M(N_2)_2(Ph_2PCH_2CH_2PPh_2)_2} + \mathrm{n}\ 1,4\text{-}\mathrm{C_6H_4\text{-}(NC)_2} \longrightarrow$$
$$\text{-}[\text{-}\textit{trans}\text{-}\mathrm{M(Ph_2PCH_2CH_2PPh_2)_2\text{-}(CN\text{-}1,4\text{-}C_6H_4\text{-}NC)\text{-}}]_n\text{-} \qquad (12)$$

(where Fp = $(\eta^5\text{-}C_5H_5)Fe(CO)_2$ and dppe = $Ph_2PCH_2CH_2PPh_2$). These discrete complexes have been fully characterized by conventional analytical, spectroscopic (e.g. IR and multinuclear NMR), and X-ray crystallographic (i.e. for $[(Fp)(CN\text{-}C_6H_4\text{-}Cl)](PF_6)$ and $M(dppe)_2(CN\text{-}C_6H_4\text{-}Cl)_2$) means (see Figure 2.2.3.A).

We are planning to extend these studies to a complete range of isonitrile bridged organometallic model complexes, oligomers, and polymers. These would have a wider range of metal centers in neutral and positive oxidation states (e.g. Cr, Mo, W, Mn^+, Fe^{++}, and Ru^{++}), monodentate (e.g. PR_3 and PAr_3) and bidentate (e.g. $R_2PCH_2CH_2PR_2$, $Ar_2PCH_2CH_2PAr_2$, $Ar_2PCH{=}CHPAr_2$, $1,2\text{-}C_6H_4(PR_2)_2$, and $1,2\text{-}C_6H_4(PAr_2)_2$) phosphine ligands, and rigid and flexible bridging groups (e.g. $1,4\text{-}C_6H_4(\text{-}NC)_2$, $1,3\text{-}C_6H_4(\text{-}NC)_2$, $1,4\text{-}C_6Me_4(\text{-}NC)_2$, $1,3,5\text{-}C_6H_3(\text{-}NC)_3$, and $CN\text{-}C_6H_4\text{-}X\text{-}C_6H_4\text{-}NC$ and where X = SiR_2, CR_2, S, etc.), e.g.





The goal of these studies is to produce materials that have superior: (1) solubility and stability characteristics, (2) characterizabilities (i.e. due to greater solubilities), (3) processabilities, (4) mechanical properties, and (5) inter- and interchain conjugation properties (i.e. for NLO and electrical applications), e.g.,

$$3\ [\mathrm{Fp'(OCMe_2)}]\mathrm{PF_6} + 1{,}3{,}5\text{-}\mathrm{C_6H_3}\text{-}(\mathrm{NC})_3 \longrightarrow [(\mathrm{Fp})_3(\mu_3\text{-}1{,}3{,}5\text{-}\mathrm{C_6H_3}\text{-}(\mathrm{NC})_3](\mathrm{PF_6})_3 \qquad (13)$$

$$2\ \mathrm{Mo(1{,}2\text{-}C_6H_4(PMe_2)_2)_2(CN\text{-}C_6H_4\text{-}NC)_2} + \mathrm{W(N_2)_2((C_6F_5)_2PCH_2CH_2P(C_6F_5)_2)_2} \longrightarrow$$
$$\mathrm{(CN\text{-}C_6H_4\text{-}NC)(Mo(1{,}2\text{-}C_6H_4(PMe_2)_2)_2)(CN\text{-}C_6H_4\text{-}NC)(W((C_6F_5)_2PCH_2CH_2P(C_6F_5)_2)_2)\text{-}}$$
$$\mathrm{(CN\text{-}C_6H_4\text{-}NC)(Mo(1{,}2\text{-}C_6H_4(PMe_2)_2)_2)(CN\text{-}C_6H_4\text{-}NC)} \qquad (14)$$

$$n\ \mathrm{CN\text{-}C_6H_4\text{-}CMe_2\text{-}C_6H_4\text{-}NC} + n\ \mathrm{Mo(Bu_2PCH_2CH_2PBu_2)_2(N_2)_2} \longrightarrow$$
$$\text{-}[\text{-}(\mathrm{Mo(Bu_2PCH_2CH_2PBu_2)_2})(\mu\text{-}\mathrm{CN\text{-}C_6H_4\text{-}CMe_2\text{-}C_6H_4\text{-}NC})\text{-}]_n\text{-} \qquad (15)$$

The analytical, spectroscopic, and particularly electrochemical data for the discrete complexes will be correlated with the X-ray crystal structures of representative examples to evaluate the repeating unit structures of these materials and the relative electronic bridging abilities of the various isonitrile ligands as a function of molecular structure. The steric restrictions on such isonitrile materials are expected to be less severe than are those for the

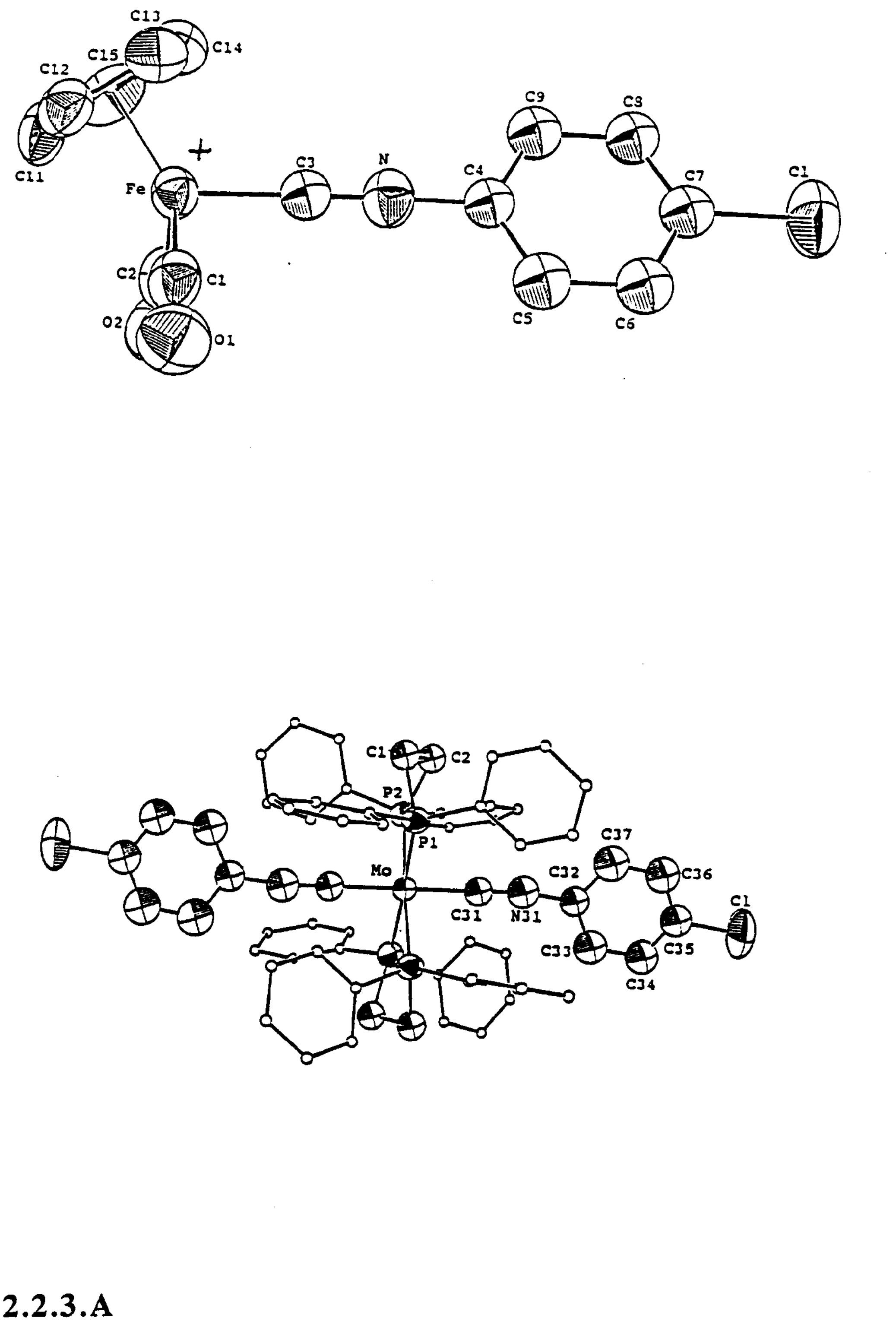

C13
C14
C15
C12
C11
+
Fe
C3
N
C4
C9
C8
C7
Cl
C2
C1
O2
O1
C5
C6
C1
C2
P2
P1
C37
Mo
C32
C36
C31
N31
Cl
C33
C35
C34

Figure 2.2.3.A

phenylene bridged species and the nature of any steric interactions will be evaluated by X-ray crystallography. The effects of bridging group structures on the melting points and solubilities of the model complexes will also be used to estimate relative materials processabilities for the polymers as a function of bridging group. In addition, structure/property correlation studies will be carried out, similar to those described above, to enable a more rational design of the optimum polymeric system and to determine the materials properties and potential utilities of these compounds.

2.2.4 Conventional Condensation Polymers Having Highly Fluorinated Organic Monomers and/or Monomers Containing Organometallic Centers

Conventional condensation polymers are industrially important as both commodity and high performance materials. Although they can be prepared from a wide variety of monomers, the new bonds formed in the condensations are normally either C-O or C-N bonds similar to those in their discrete analogues (e.g. esters, amides, urethanes, ureas, and carbonates, respectively). We are interested in elaborating some of the reactions and organometallic species described above to prepare new organometallic monomers. Thus, new organometallic monomers can generally be prepared by simple extensions of the chemistry used to produce the organometallic model complexes and rigid rod oligomers described above. It is interesting to note that most of these monomers will themselves be rod like in shape. Indeed, monomers having rigid lengths greater than 20 Å will be common. Again, we feel the most important potential advantage of the organometallic materials is that by varying the ancillary ligands on the metals we hope to be able to tune the materials properties of the new organometallic condensation polymers in a rational fashion. Amongst the classes of polymers of interest to us are those derived from the metal arylenes (e.g. $\text{-[-O-C(CH}_3)_2\text{-C}_6\text{F}_4\text{-C(CH}_3)_2\text{-O-C(O)-]}_n\text{-}$, $\text{-[-O-C(CF}_3)_2\text{-C}_6\text{F}_4\text{-Ni(PR}_3)_2\text{-C}_6\text{F}_4\text{-C(CF}_3)_2\text{-O-C(O)-C}_6\text{H}_4\text{-C(O)-]}_n\text{-}$),[3,5] those derived from the isonitrile complexes (e.g. $\text{-[-NH-C}_6\text{H}_4\text{-NC-Mo(R}_2\text{PCH}_2\text{CH}_2\text{PR}_2)_2\text{-CN-C}_6\text{H}_4\text{-NH-C(O)-NH-C}_6\text{H}_3\text{Me-NH-C(O)-]}_n\text{-}$),[4] and those derived from (η^6-Arene)Cr(CO)_3[9] complexes (e.g. $\text{-[-O-C(CH}_3)_2\text{-C}_6\text{H}_4$(_-$\text{Cr(CO)}_3$)$\text{-C(CH}_3)_2\text{-O-C(O)-NH-(CH}_2)_6\text{-NH-C(O)-]}_n\text{-}$). In each case the new organometallic monomer and its closest organic analogue (often itself new) are polymerized under identical conditions. The resulting polymers are then characterized by the conventional methods, including X-ray diffraction, described above and any difference(s) are determined. In addition, this characterization data is compared to that for the unpolymerized organometallic monomers and/or monomer precursors and their model complexes (see Figure 2.2.4.A).[9] Thus, structure/property relationships are developed which can be used to obtain a molecular level understanding of the origin any differences imparted by the metal and its ancillary ligands. During our pilot studies, we have made significant progress in preparing the highly fluorinated organometallic polymers[5] and have begun work on the synthesis of the organometallic monomers required for several classes of these materials.

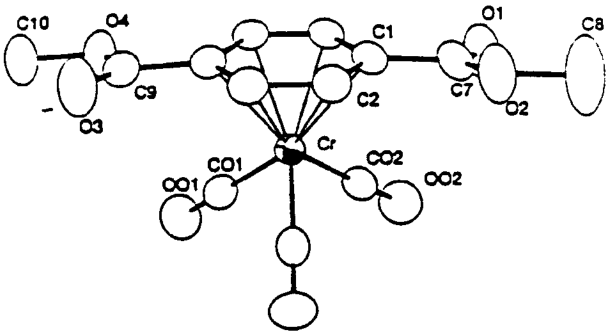


Figure 2.2.4.A

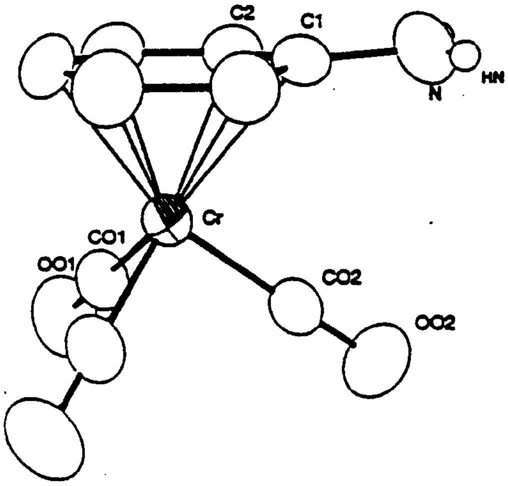


Figure 2.2.5.A

2.2.5 Vinyl Polymers Having Highly Fluorinated Side Chains and/or Organometallic Side Chains

Vinyl polymers are the most commercially important commodity plastics and are also showing increasing potential for high performance applications. We are also interested in elaborating some of the reactions and organometallic species described above to prepare new organometallic vinyl monomers from the reaction of organometallic complexes having reactive functional groups (e.g. OH, NH_2, and CO_2R) on their aromatic ligands (e.g. $(\eta^6\text{-}C_6H_5CO_2H)Cr(CO)_3$, $(\eta^6\text{-}C_6H_5NH_2)Cr(CO)_3$, $(\eta^6\text{-}C_6H_5C(CH_3)_2OH)Cr(CO)_3$, $[(\eta^5\text{-}C_5H_5)Fe(CO)_2(CN\text{-}C_6H_4NH_2)]PF_6$, and $Ni(PR_3)_2(C_6F_5)(C_6F_4(CF_3)_2OH)$ with vinyl reagents having suitable fuctional groups (e.g. $CH_2{=}CHX$ where $X = C(O)Cl$, $(CH_2)_nOH$, $C_6H_4NH_2$, etc). Again, we feel the most important potential advantage of the organometallic materials is that by varying the ancillary ligands on the metals we hope to be able to tune the materials properties of the new organometallic addition polymers in a rational fashion. In addition, such organometallic vinyl polymers almost certainly will be produced in much higher molecular weights than we are likely to be able to do via condensation reactions. Amongst the classes of vinyl polymers of interest to us are those having pendant organometallic or related organofluorine[6] groups attached to conventional addition polymers such as polyacrylates, polyacrylamides, and polyvinylalkanoates. In each case the new organometallic monomer and its closest organic analogue (often itself new) are polymerized under identical conditions. The resulting monomers and polymers are then characterized by the conventional methods, including X-ray diffraction analysis, described above and any difference(s) are determined. Indeed, we have characterized several of the requisite organometallic reagents needed to prepare the new monomers by X-ray crystallography already (see Figure 2.2..5.A).[9] Thus, structure/property relationships are developed which can be used to obtain a molecular level understanding of the origin any differences imparted by the metal and its ancillary ligands. During our pilot studies, we have made significant progress in preparing the organofluorine polymers[6] and the organometallic monomers that are required for several classes of these materials.

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2.3 John A. Jackson

Dr. Jackson is an Assistant Professor in the Department of Chemistry. His research interests include organophosphorous chemistry and studies of biologically active molecules.

2.3.1 Chiral Phosphonate transition State Analogues as Inhibitoror of HIV-1 Protease

Single-crystal X-ray analysis would be invaluable in determining the absolute stereochemistry at phosphorus, and other stereocenters, in the proposed synthetic chiral phosphonate transition state analogues.

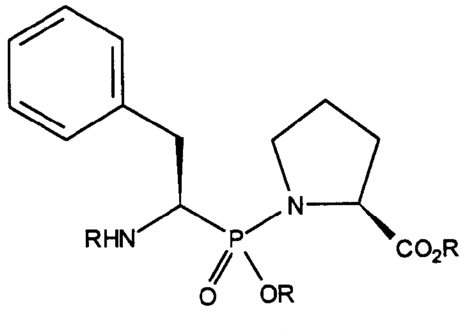


Figure 1

Inhibition of the human immunodeficiency virus 1 (HIV-1) is the subject of considerable attention. The use of transition state analogues as enzyme inhibitors is well documented. One category of enzyme inhibitors of particular interest are phosphonate analogues, which resemble the transition state of a particular substrate undergoing hydrolysis.

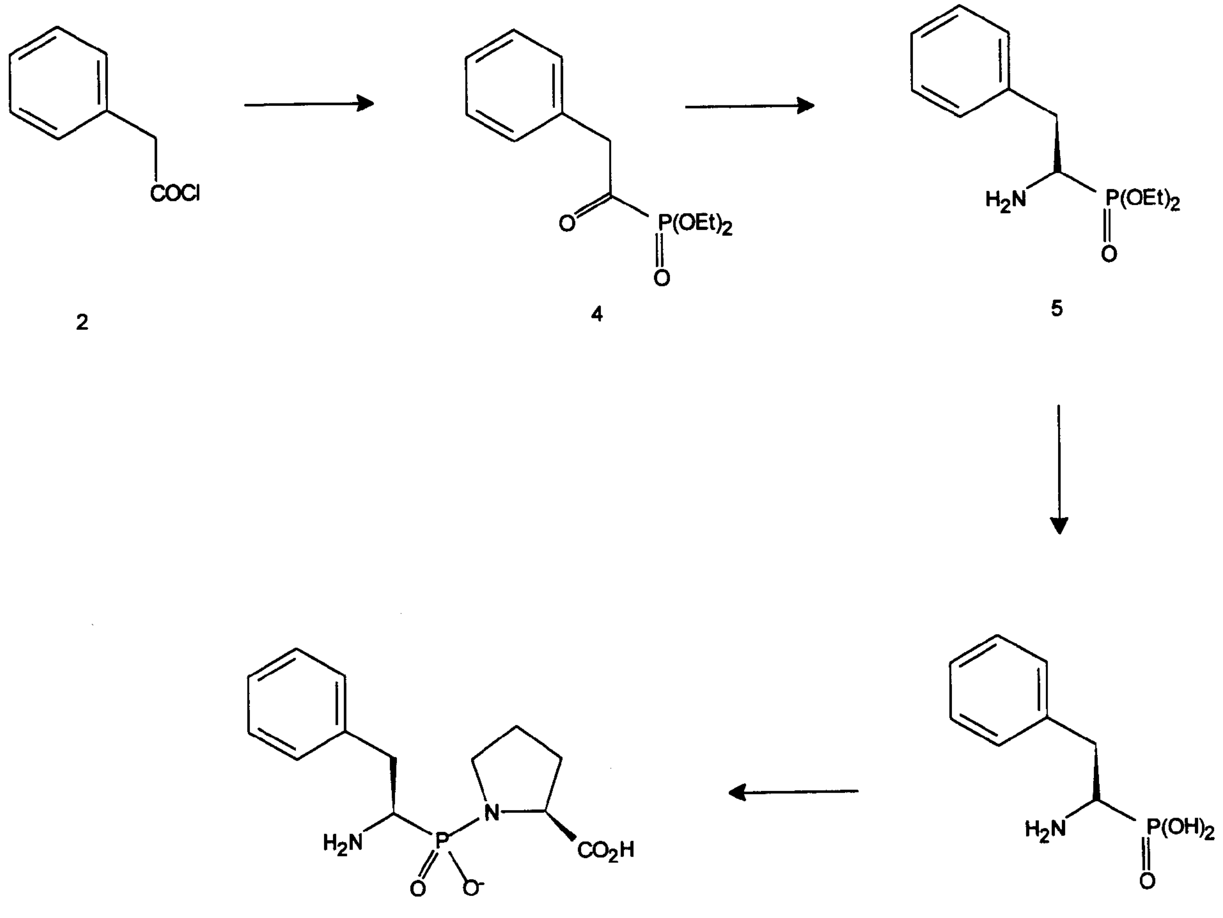
An issue of importance in the rational design of transition state analogues is the effect of stereochemistry on the ability of a proposed inhibitor to fit a particular enzyme active site. In the proposed synthesis of chiral phosphonate transition state analogues of HIV-1 protease, a chiral phosphonopeptide (Figure 1) would be the building block for a series of analogues. Establishing unambiguously the absolute stereochemistry at phosphorus and other stereocenters is imperative in evaluating the efficacy of the proposed inhibitors in future design.

Obtaining suitable crystals for X-ray analysis can be accomplished in several ways. The parent compounds themselves may be crystalline. The use of organometallic derivatives of aromatic compounds and the use of strychnine salts of carboxylic acids are just two of many methods of modification of a substrate to obtain suitable crystalline material for X-ray analysis.

Hydroxyethylamine analogues,[1] and phosphinic acid derivatives[2] of the p17/p27 Tyr-Pro substrate cleavage sites have been sucessfully explored as inhibitors of HIV-1 protease. The use of phosphorus containing peptide analogues as inhibitors of proteases has been well documented.[3] Initial plans for this work center around the synthesis of phosphonate building block **1** (Scheme 1). In place of tyrosine (found in the actual HIV-1 protease cleavage site[4]) is the phosphonate derivative of phenylalanine **5**. Disconnection of phosphonate **1** leads to inexpensive precursors phenylacetyl chloride (**2**) and proline (**3**).

Treatment of phenylacetyl chloride (**1**) with triethyl phosphite affords ketophosphonate **4**.[5] Amination of phosphonate **4** (certain modifications should be possible) produces α-aminophosphonate derivative **5**. Phosphonate ester hydolysis of **5** produces α-aminophosphonic acid **6**. Coupling of α-aminophosphonic acid **6** with a suitably protected proline derivative followed by deprotection would provide target building block **1**. Building block **1** would be available for preparation of suitable derivatives, which in turn would be examined for HIV-1 inhibitory potency.

Scheme 1



2 4 5

1 6

Many modifications of this simple scheme would be possible. Proline provides a chiral handle, which could allow separation of diasteromers of **1** formed as a result of a racemic synthesis of **6**. Alternatly, use of chiral reducing agents in the reductive amination of ketophosphonate **4** could provide α-aminophosphonate **5** in optically active form. Ring modification of suitable phenylacetyl chloride derivatives could drastically alter inhibitory potency of the resulting phosphonopeptides.

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2.4 Raymond E. Beiersdorfer

Dr. Beiersdorfer is an Assistant Professor in the Department of Geology. His current research interests include geochemical studies of mafic rocks.

2.4.1 Crystal Chemistry of Pumpellyite

2.4.1.1 Objective

I propose to use the single crystal X-ray diffractometer to determine the crystal structures of a suite of specimens of the mineral pumpellyite ($((Ca,Mn)_4\ (Mg,Fe^{2+},Mn)_{2-x'}\ (Fe^{3+},Al)_{x'}\ (Fe^{3+},Al)_4\ Si_6\ O_{(20+x')}\ OH_{(8-x')})$. These specimens have been collected from various localities around the world. In addition to the crystal structure determinations, the specimens will be analysed 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 the crystal structure of pumpellyite with changes in its composition, particularly the isomorphous exchange of Mg, Fe and Al.

2.4.1.2 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 (Eskola, 1920, 1939; Turner, 1948). 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 recently been proposed (Beiersdorfer and Day, in press) that the composition of pumpellyite (coexisting with ablite, epiodte, quartz, water, chlorite, ± 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 stucture of pumpellyite spanning a wide range of Fe- and Al-contents may reveal changes in the cyrstal stucture that are due to differences in the pressure of formation.

Chemistry of Pumpellyite

The structural formula of pumpellyite is commonly written as (Coombs et al, 1976):

$W_4 X_2 Y_4 Z_6 O_{(20+x')} OH_{(8-x')}$,

where:

$W = Ca,Mn$

$X = (Mg,Fe^{2+},Mn)_{2-x'}\ (Fe^{3+},Al)_{x'}$

$Y = Fe^{3+},Al$

$Z = Si$

The W site consists primarily of Ca in seven-fold coordination with oxygen. However, many pumpellyites exhibit defeciencies in Ca and it has been suggested (e.g. Springer et al., 1992) 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 (e.g. Liou et al., 1987, Frey et al., 1991, Beiersdorfer and Day, in press) have assumed that x' is one. Determining the crystal structure of well crystalized 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 Gottardi (1965) and has been subsequently refined by Galli and Alberti (1969) and Yoshiasa and Matsumoto (1985). Each of these studies has been limited to pumpellyite with a restricted range of composition. For example, the work of Yoshiasa and Matsumoto (1985) was based on a single specimen of Al-rich pumpellyite from the high-pressure Sanbagawa metamorphic belt of Japan. It has recently been demonstrated that 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 (Beiersdorfer and Day, in press). It has yet to be determined how the crystal structure of pumpellyite varies with changes in composition, particulary to more iron-rich varieties which are common in rocks that have suffered subseafloor-; high T/P-; hydrothermal-metamorphism.

2.4.1.3 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 am presently undertaking complete microprobe analyses of these specimens. Samples spanning a wide range of composition will be selected for analyisis using the the single-crystal XRD.

As an adjunct to the single-crystal XRD and EPMA work, I hope also to carry out Mossbauer spectroscopic determinations of the ferrous/ferric ratios in suitable specimens. I am presently conferring with scientists with such laboratories in an effort to arrange a suitable collaboration.

2.4.1.4 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 compostion.

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Beiersdorfer, R. E., and Day, H. W., in press, Paragenesis of pumpellyite-bearing mafic rocks: in Schiffman, P., and Day, H. W., eds, Geological Society of America Memoir

Coombs, D. S., Nakamura, Y., and Vuagnat, M., 1976, Pumpellyite-actinolite facies schists of the Tayanne Formation near Loeche, Valiais, Switzerland: Journal of Petrology, v. 17, p. 440-471.

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Frey, M., de Capitani, C., and Liou, J. G., 1991, A new petrogenetic grid for low-grade metabasites: Journal of Metamorphic Geology, v. 9, p. 497-509.

Galli, E. and Alberti, A., 1969, On the crystal structure of pumpellyite: Acta Crystallographica, V. B25, p. 2276-2281.

Gottardi, G., 1965, Die kristallstruktur von pumpellyit: Tschermaks mineralogishe und Petrographische Mitteilungen, v. 10, p. 115-119

Liou J. G., Maruyama, S., and Cho, M., 1987, Very low-grade metamorphism of volcanic and volcaniclastic rocks - mineral assemblages and mineral facies, in Frey, M., eds., Low Temperature Metamorphism: Glasgow, Blackie & Sons, p. 59 - 113.

Springer, R. K., Day, H. W., and Beiersdorfer, R. E., 1992, Prehnite-pumpellyite to greenschist facies transition, Smartville Complex, near Auburn, California: Journal of Metamorphic Geology, v. 10, p. 147-170.

Turner, F. J., 1948, Mineralogical and structural evolution of the metamorphic rocks: Geological Society of America Memoir, v. 30

Yoshiasa, A. and Matsumoto, T., 1985, Crystal structure refinement and crystal chemistry of Pumpellyite: American Minearologiist, v. 70, p.1011-1019.

3. DESCRIPTION OF PROPOSED EQUIPMENT

The Rigaku AFC7S model single crystal X-ray diffractometer was chosen for the following reasons: (1) the instrument meets the basic requirements of all proposed users; (2) the quotation (see attached quotation) for the basic instrument is competitive with quotations obtained from other manufacturers; and (3) the software for this system, teXsan, is a particularly user friendly package which is advantageous for both teaching and research purposes.

The AFC7S diffractometer is a sealed tube system, and the basic package requested consists of a 3kW generator, one Cu X-Ray tube, a DECpc 433 dxLP computer to control the instrument, and a 50MHz, 32 MB Silicon Graphics Iris Indigo system with a 540 MB system disk for structure analysis using the teXsan comprehensive crystallographic software package. The requested system also has low temperature analysis capabilities, to minimize decomposition of molecules in the X-ray beam and reduce vibrational motions.

4. JUSTIFICATION OF NEED

During the past two years, YSU has recuited four new faculty members (i.e. the applicants of this proposal), all of whom are actively involved in research projects requiring single crystal X-ray diffraction facilities. In addition, other faculty on campus have also expressed interest in utilizing the proposed instrument for their research projects: Drs. James Mike, Daryl Mincey, Fred Koknat, and Cynthia Bearer of the Chemistry Department, and Dr. Jeff Dick, Geology. YSU is dedicated to fostering research (especially projects involving undergraduates) within the university and between university faculty and outside industrial and research institutions. This dedication is reflected by the matching funds made available to us from the university, which amount to about 65 % of the capital funds requested. YSU's effort to establish faculty-industrial collaborative research is demonstrated by SensorDek's involvement in this proposal, as well as by the interest expressed in collaborative projects involving the requested diffractometer by the NASA Research Center (Cleveland, OH) and also Packard Electric, a large local manufacturer, (see atached supporting letters). YSU is also committed to high quality teaching, and has for example established an equipment replacement policy to ensure that courses have access to state-of-art equipment as much as possible. Local two- and four-year colleges would also be welcome to utilize the proposed intrument for teaching or research projects of interest to them. The acquisition of a single crystal X-ray diffractometer at YSU would thus provide many benefits to YSU faculty and students as well as to the surrounding community in general.

5. MAINTENANCE AND OPERATION

The repair and maintenance of the X-ray diffractometer will be the responsibility of the YSU chemistry department. The 1993-94 supply budget of $86,000 is sufficient to provide the routine materials neeeded to operate the diffractometer. The on-campus "Electronics Maintenance Services" (four full-time staff) is equipped and staffed to handle routine maintenance and repair tasks. There is no charge to the department for these services. Past experience has shown that this staff is well qualified to maintain complex scientific instrumentation, including a wide range of state-of-the art spectrophotometers, chromatography apparatuses, electrochemical equipment, and an automated powder X-ray diffractometer. In addition, the chemistry department has an annual maintenance budget of $25,000 for major repairs requiring outside assistance. However, repairs necessary during the first two years of operation will be covered under the service contract which is to be funded by the SensorDek Phase II Air Force SBIR grant.

The University has in place a radiation control officer to handle governmentally mandated safety programs due to the X-ray generator. One of the applicants, A.D. Hunter, will be designated the X-ray coordinator with released time to enable him to maintain the instrument and teach prospective users in its operation. He will also perform a service crystallography function for minor users as required.

The diffractometer will be made available to non-YSU academic researchers for teaching purposes (i.e. for the local two- and four-year colleges or other universities) and to conduct research. Access to the instrument will be open to essentially all qualified academic users with a small service fee (projected at $20-$100 per day) being levied on outside users to offset maintenance costs (e.g. X-ray tube replacement, computer hardware replacement, software updates, etc.). A list of submitted samples will be maintained so that should a backlog develop, access can be allocated to those who have not recently utilized the system or have less stable samples. YSU actively supports the science and technology needs of local industry, as evidenced through the existence of the campus-based Technology Development Center, as well through collaborative research agreements with industrial concerns such as SensorDek (see Sec. 2). Such industrial users pay for access to university facilities and faculty expertise, either through collaborative grant-funded research (e.g. as in the contributions from SensorDek to this proposal's budget) or through direct charges on a full cost recovery basis. Indeed, Packard Electric is a major local manufacturer (20,000 employees) which has already expressed an interest in utilizing the proposed diffractometer facility to aid in their manufacturing and design processes, as indicated by the attached supporting letter. The combination of collaborative grants, charges to industrial users, and nominal fees to academic users are expected to make the proposed facilities fully self operating. This, combined with YSU's equipment replacement policy, will ensure the proposed X-ray diffractometer will be functional for years to come.

6. EXISTING SUPPORT FACILITIES

No single Crystal X-ray diffraction facilities currently exist at Youngstown State University, nor are such facilities available at local industrial research and development laboratories. The nearest such facility is at the University of Akron, which is a 1 hour drive from Youngstown. Note however that the NASA Research Center of Cleveland has expressed strong interest (supporting letters to be forwarded) in acquiring time on the requested YSU instrument (meaning additional travel time for them), because the demands on the Akron instrument are so great that outside users have difficulty gaining access.

An automated Rigaku powder X-ray diffractometer is available in the geology department, and the chemistry department has an Enraf-Nonius X-ray machine with a Debye-Scherrer powder camera. Powder X-ray diffraction, while useful as an adjunct technique in our work, is insufficient for the projects described in this proposal, since these all require detailed knowledge of bond lengths, bond angles, phase orientation relationships and other data not available from powder systems.

Electron microscopy (EM) facilities are available on campus. These consist of a Hitachi Model S-450 Scanning EM in the biology department, and a Siemens 102 Transmission EM in the chemistry department. While electron microscopy techniques are useful to elucidate some information of use in the projects of TRW and ADH, such as phase relationships and morphology, these techniques are best used to supplement single Crystal X-ray data.

Particularly in the case of TEM studies, it may be tempting to use the 2-dimensional images as accurate descriptions of the 3-dimensional bulk structures. Since samples studied by TEM are typically less than 100 Å thick, there is some controversy as to whether or not these samples accurately represent the bulk structure. For this reason, many electron microscopists use single-crystal X-ray diffraction as a complementary technique to their TEM studies in order to obtain a reliable average bulk structure of the material of interest.

The chemistry department is well equipped with the necessary facilities to carry out the synthesis of all materials proposed for study, as described in section 2, with the exception of the gamma TiAl alloys to be studied by TRW. These are to be prepared by SensorDek as discussed earlier.

The requested single Crystal X-ray diffractometer will be housed in the chemistry department, which consists of over 32,000 sq. ft. of recently (i.e. late 1980's) remodeled space. Currently, the chemistry department's 30 year old Enraf powder X-ray machine is located in a laboratory with an adjoining darkroom and electrical, plumbing and safety features designed especially for X-ray equipment. The Enraf powder system will be removed and relocated to make room for the new diffractometer.

7. CONTRIBUTION FROM INDUSTRY

SensorDek, Inc. , a small Materials Research & Development Company based in Niles, Ohio, agrees to contribute $227,358 in the form of funds requested in their Phase II Air Force SBIR Proposal entitled "The Structure-Property Relationships in Directionally Solidified gamma TiAl Alloys", which was submitted in November, 1993. This proposal describes work (see section 2.1) which will be conducted in collaboration with Dr. Wagner , Dept. of Chemistry , Youngstown State University. The amount of $227,358 comprises nearly 100% of the total non-capital costs of our overall budget, and 53 % of our total requested budget for two years of $428,525.

8. CONTRIBUTION FROM PROPOSING INSTITUTION

Youngstown State University agrees to contribute $120,000 towards the cost of the proposed instrument. This comprises 62% of the capital funds requested. In addition, the university agrees to contribute $9,968 to the non-capital costs in the form of a tuition match.

9.0 BIOGRAPHICAL SKETCHES

Biographical Sketch for Timothy R. Wagner

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

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

In the spring of 1988, Dr. Wagner joined Professor Lawrence Marks' group in the Department of Materials Science at Northwestern University, Evanston, Illinois, as a postdoctoral fellow. At Nortwestern University, Dr. Wagner conducted HREM studies of electron and ion-stimulated surface reactions & damage in oxides. He spent the summer of 1990 as a supporting laboratory scientist at the Pharmaceutical Products Division, Abbott Labs, North Chicago, Illinois. This project involved programming and documentation of robotics software for chemical analysis. In the Fall of 1990, Dr. Wagner then joined the faculty of the Chemistry Department at the Illinois Institute of Technology, Chicago, Illinois, at a Visiting Assistant Professor. He remained at IIT for two years, and began his current position as Assistant Professor of Chemistry at Youngstown State University in the Fall of 1992.

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

B. Refereed Journal Publications.

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

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

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

(4) M.I. Buckett, S.R. Singh, H. Fan, T. Wagner and L.D. Marks, "Electron-Stimulated Damage Processes in Oxides Under Ultra High Vacuum (UHV) Conditions", Proc. 47th Ann. Mtng. of the Electron Mic. Soc. of America, (1989) 636-7.

(5) T. Wagner, "HREM of Electron-Beam-Induced Damage in L-Ta_2O_5", J. Solid State Chem., 91, (1991) 189-203.

C. List of other Collaborators.

(1) Dr. Glen Schaefer, SensorDek, Inc.

(2) Dr. Steven Hues, Naval Research Labs

D. Names of Mentors.

(1) Ph.D. Advisor: Michael O'Keeffe, Department of Chemistry, Arizona State University, Tempe, Arizona 85287.

(2) Postdoctoral Advisor: Lawrence Marks, Department of Materials Science, Northwestern University, Evanston, Illinois 60208.

Biographical Sketch for Allen D. Hunter.

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

A. **Vitae.** Allen Hunter received his Honors B.Sc. in Chemistry in 1981 from the University of British Columbia in Canada with a graduating thesis under Dr. E.E. Burnell entitled "A NMR Structural Determination of Azulene Oriented in a Nematic Liquid Crystal". He obtained his Ph.D. degree from the University of British Columbia in 1985 under Dr. P. Legzdins with a thesis entitled "Aspects of the Organometallic Nitrosyl Chemistry of Cr, Mo and W". He worked as a postdoctoral fellow with Dr. M. Bennett of the Research School of Chemistry at the Australian National University in Canberra, Australia, doing metal phosphine chemistry (1985-86) and with Dr. M. Cowie at the University of Alberta in Canada doing single crystal X-ray diffraction studies for Dr. D. Seyferth of M.I.T. (1987). From 1987 to 1992 he was an Assistant Professor of Chemistry at the Chemistry Department of the University of Alberta where he currently holds an Adjunct appointment. On September 15th of 1992 he joined Youngstown State University as an Associate Professor of Chemistry and he currently holds a Research Professorship there. He is a member of the American Chemical Society and the American Association for the Advancement of Science.

Allen received a Izaak Walton Killam Memorial Postdoctoral Fellowship and a NSERC Postdoctoral Fellowship for 1985-87 and he held a Natural Sciences and Engineering Research Council of Canada, NSERC, Graduate Scholarship for 1981-85. He received the Governor General's Gold Medal in Arts and Sciences, the Lefevre Medal and Prize in Honors Chemistry, and the Society of Chemical Industry Merit Award in 1981. He held an NSERC Undergraduate Summer Research Award in 1980 and 1981. He was awarded the Chemical Institute of Canada Prize in 1980 and a Charles A. and Jane C.A. Banks Foundation Scholarship for 1978-80.

During the 1990-93 period Allen received over $400,000 (US), excluding overhead, in external funding at the University of Alberta from the Canadian NSERC granting agency and US and Canadian Industry for his work on organometallic polymers and biologically active organometallics.

B. **Refereed Journal Publications,** Five Most Relevant (1 - 5) and Five Other Significant Publications (6 - 10). A series of eight other manuscripts describing our work on organometallic polymers are currently submitted for publication or are in preparation.

(1) Sturge, K.C.; Hunter, A.D.; McDonald, R.; Santarsiero, B.D.: "Organometallic Polymer and Linear Mono-, Bi-, and Trimetallic Octafluoro-p,p'-biphenylene-Bridged Complexes of Bis(methyldiphenylphosphine)nickel: X-ray Crystal Structures of $Ni(PMePh_2)_2(4,4'-C_{12}F_8H)Br$ and $Ni(PMePh_2)_2(4,4'-C_{12}F_8H)_2$," *Organometallics* **1992**, *11*, 3056-3062.

(2) McDonald, R.; Sturge, K.C.; Hunter, A.D.; Shilliday, L.: "Synthesis and Spectroscopic Characterization of Linear Mono-, Bi- and Trimetallic Bis(methyldiphenylphosphine)nickel Complexes having 1,4-Tetrafluorophenylene Bridges," *Organometallics*, **1992**, *11*, 893.

(3) Macdonald, P.M.; Hunter, A.D.; Lesley, G.; Li, J.: "Solid State Distortions of Linear Mono-, Bi-, and Trimetallic Bis(Tri-n-ButylPhosphine) Nickel and Palladium Complexes Having 1,4-Tetrafluorophenylene Bridges as Observed Via ^{31}P CP/MAS NMR Spectroscopy," *Solid State Nuclear Magnetic Resonance*, **1993**, *2*, 47-55.

(4) Guo, X.A.; Hunter, A.D.: "Polyesters, Polycarbonate, and Polyurethanes from a Novel Monomer: a,a,a',a'-Tetramethyl-1,4-tetrafluorobenzenedimethanol," *J. Polym. Sci., Part A*, **1993**, *31*, 1431-1439.

(5) Guo, X.A.; Hunter, A.D.; Chem, J.: "Preparation and Characterization of Acrylates and Polyacrylates Having Variable Fluorine Contents and Distributions," *J. Polym. Sci., Part A*, 24 pages, **in press**.

(6) Chukwu, R.; Hunter, A.D., Santarsiero, B.D.; Bott, S.G.; Atwood, J.L.; Chassaignac, J.; "Electrochemical, Spectroscopic and Structural Studies of Mono- and Bimetallic Complexes of Iron: X-ray Crystal Structures of $CpFe(CO)_2\text{-}C_6F_5$, $4\text{-}CpFe(CO)_2\text{-}C_5F_4N$ and $1,4\text{-}C_6F_4(CpFe(CO)_2)_2$," *Organometallics*, **1992**, *11*, 589-597.

(7) Hunter, A.D.; McLernon, J.L.: "Arene-Bridged Polymetallic Clusters: s,p Complexes of $CpFe(CO)_2$ or $Cp'Fe(CO)_2$ and $Cr(CO)_3$, $Mo(CO)_3$ or $W(CO)_3$," *Organometallics*, **1989**, *8*, 2679-2688.

(8) Hunter, A.D.; Szigety, A.B.: "Phenylene-Bridged Organometallic Complexes of Iron and Manganese," *Organometallics*, **1989**, *8*, 2670-2679.

(9) Hunter, A.D.; Shilliday, L.; Furey, W.S.; Zaworotko, M.J.: "A Systematic X-ray Crystallographic Study of the Structural Manifestations of the _-Donor and _-Acceptor Substituent Effects in Substituted $(h^6\text{-Arene})Cr(CO)_3$ Complexes," *Organometallics*, **1992**, *11*, 1550-1560.

(10) Hunter A.D.; Ristic-Petrovic, D.; McLernon, J.L.: "Biphenyl-, Terphenyl-, Naphthalene-, and Anthracene-Bridged Bimetallic Complexes of Iron and Chromium," *Organometallics*, **1992**, *11*, 864-871.

C. List of Other Collaborators.

(1) M. Williams, Department of Chemical Engineering, University of Alberta, Edmonton, Alberta, Canada

D. Names of Mentors.

(1) B.Sc. Honors Thesis Advisor. Dr. E.E. Burnell, Department of Chemistry, University of British Columbia, Canada.

(2) Ph.D. Advisor. Dr. P. Legzdins, Department of Chemistry, University of British Columbia, Canada.

(3) Postdoctoral Advisors. Dr. M. Bennett, Research School of Chemistry, Australian National University, Canberra, Australia. Dr. M. Cowie, Department of Chemistry, University of Alberta, Canada.

Biographical Sketch for John A. Jackson

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

A. **Vitae**. John Anthony Jackson is currently an Assistant Professor at in the Department of Chemistry at Youngstown State University. He received a B. A. in Chemistry at the University of Minnesota in 1982. From 1982 until 1984, he continued his studies in chemistry at the University of Minnesota as a part time student. He attended the University of Iowa from 1984 to 1990, and received his Ph. D. in Organic Chemistry in 1990 under the supervision of Professor David F. Wiemer. He performed postdoctoral research in the Department of Chemistry at Loyola University Chicago from 1990 until 1992 with Professor Charles M. Thompson. In 1992, he assumed a 9-month sabbatical replacement position teaching Organic Chemistry at Mansfield State University of Pennsylvania. During the summer of 1993, he returned to Loyola University Chicago as a Visiting Research Associate in the Department of Chemistry, working again with Professor Charles M. Thompson. He began a tenure track position in the Department of Chemistry at Youngstown State University in the fall of 1993.

He is a member of the American Chemical Society, (Organic Division, Agrochemicals Division and Pennsylvania Ohio Border Section). He has been elected to serve on the Executive Committee at Large in 1994 in the Pennsylvania Ohio Border Section of the American Chemical Society.

B. **Refereed Journal Publications**:

(1) Synthesis of α-Phosphono Lactones and Esters Via Phosphate-Phosphonate Rearrangement. Jackson, J. A.; Hammond, G. B.; Wiemer, D. F. *J. Org. Chem.* **1989**, *54*, 4 750.

(2) Regiochemistry of the Rearrangement of Cyclohexenyl and Cyclohexadienyl Phosphates to β-Keto Phosphonates. Gloer, K. B.; Calogeropoulou, T.; Jackson, J. A.; Wiemer, D. F. *J. Org. Chem.* **1990**, *55*, 2842.

(3) Methanolysis of Phosphoramidates with Boron Trifluoride-Methanol Complex. Ryu, S.; Jackson, J. A.; Thompson, C. M. *J. Org. Chem.* **1991**, *56*, 4999.

(4) Stereoselective and Chemoselective Oxidation of Phosphorothionates using MMPP. Jackson, J. A.; Berkman, C. E.; Thompson, C. M. *Tetrahedron Lett.* **1992**, *33*, 6061.

(5) Synthesis of Chiral Phosphorus Mustards Derived From Serine. Jackson, J. A.; Frick, J. A.; Thompson, C. M. *BioMed. Chem. Lett.* **1992**, *2*, 1547.

(6) Stereochemical Aspects of Phosphorothiolate Toxicity. Thompson, C. M.; Berkman, C. E.; Ryu, S.; Jackson, J. A.; Quinn, D. A.; Larsen, A. In *Rev. Pestic. Toxicol* (Roe, R. M. and Kuhr, R. J. Eds.) Toxicology Communications Inc., **1993**, *2*, 131-146.

(7) Synthesis of Phosphorylated Tripeptides Representing Poisoned Acetylcholinesterase. Thompson, C, M,; Suarez, A. I.; Lin, J.; Jackson, J. A. *Tetrahedron Lett.* **1993**, *34*, 6529.

(8) Stereocontrol in Horner-Wadsworth-Emmons Condensations of α-Phosphono Lactones with Aldehydes: A Synthesis of Intergerrinecic Acid and Senecic Acid Lactones. Lee, K.; Jackson, J. A.; Wiemer, D. F. *J. Org. Chem.* **1993**, (In Press).

C. List of Other Collaborators.

None

D. Names Of Mentors.

(1) Ph.D. Advisor: David F. Wiemer, Department of Chemistry, University of Iowa Iowa City Iowa 52242

(2) Postdoctoral Advisor: Charles M. Thompson, Department of Chemistry, Loyola University, Chicago, Illinois 60626

Biographical Sketch for Raymond E. Beiersdorfer

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

A. **Vitae**. Raymond Emil Beiersdorfer is currently an Assistant Professor in the Department of Geology at Youngstown State University. He received a B.A. in geology from Queens College, City University of New York in 1979 and an M.S. in Geology from the University of California at Davis in 1982. From 1982 until 1985 he worked as a petroleum geologist for the Gulf Oil Exploration and Production Co in Bakersfield, California where he was responsible for Gulf's exploration efforts in Nevada, Oregon and Washington. In 1985 and 1986 he was the Esso Research Scholar at Monash University, Melbourne, Australia, where he worked on the diagenesis of the Gippsland Basin, offshore Victoria, Australia. In 1987 he returned to the University of California at Davis, where he received his Ph.D. in 1992. His dissertation research was on the metamorphism of the Smartville complex and contiguous rocks, northern Sierra Nevada and Klamath Mountains, California. While working on his Ph.D. he also received the Certificate in College Teaching from the Teaching Resources Center and Graduate Division at the University of California at Davis. After receiving his Ph.D. he was a Post Doctoral Research Fellow at the Department of Geology & Geophysics, University of Calgary, Alberta, Canada working on the metamorphic petrology and mineral potential of the Crowsnest Volcanics, Southern Alberta, Canada.

He has received a Post Doctoral Research Fellowship Award from the Univ. of Calgary (1992), the Harold T. Stearns Award from the Geological Society of America (1991); two Research Travel Awards from the Intl. Geol. Cor. Proj. 294 (1990; 1991); the Van Couvering Award from the Amer. Assoc. Petr. Geol(1990) and a New York State Regents Scholarship (1974-1977).

He is a member of the American Association of Petroleum Geologists, the American Geophysical Union, the Geological Society of America, the Mineralogical Society of America, the National Association of Geology Teachers, Sigma Xi, and the Society of Professional Well Log Analysts.

B. **Refereed Journal Publications.**

(1) 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.

(2) Beiersdorfer, R.E. and Haynes, J., 1991, An integrated approach to geologic writing for non-science majors based on study of a California river. Journal of Geological Education, v. 39, p. 196 - 198.

(3) 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.

(4) Beiersdorfer, R.E. and Day, H.W., 1992, Metamorphic features of the Smartville complex, northern Sierra Nevada, California, in Schiffman, P. and Wagner, D.L., eds., Field Guide to the Geology and Metamorphism of the Franciscan Complex and Western Metamorphic Belt of Northern California, California Division of Mines and Geology Special Publication 114, p. 29 - 47 (refereed).

(5) Beiersdorfer, R.E. and Davis, W., (in press), Suggestions for planning a class field trip, Accepted by the Journal of College Science Teaching. (accepted).

(6) Beiersdorfer, R.E. and Day, H.W., (in press), Mineral paragenesis of pumpellyite in low-grade mafic rocks, Accepted by the Geological Society of America Memoir on Metamorphism of Basalt.

(7) Aguirre, L., Morata, D., Puga, E., Baronnet, A. and Beiersdorfer, R.E. (in press), Chemistry and crystal characteristics of pumpellyite in a metadolorite from the Archidona region, subbetic cordillera, Spain, Accepted by the Geological Society of America Memoir on Metamorphism of Basalt (accepted).

C. **List of Other Collaborators.**

(1) Dr. D.B. Alves, Petrobras, Rio de Janerio, Brazil

(2) Dr. M. Darby, Departments of Geology & Astonomy, West Chester University.

(3) Dr. J.C. Shervais, Department of Geological Science, University of South Carolina.

D. **Names of Mentors.**

(1) Ph.D. Advisor: Howard W. Day, Department of Geology, University of California - Davis, Davis, California 95616.

(2) Postdoctoral Advisor: Ed Ghent, Department of Geology & Geophysics, University of Calgary, Calgary, Alberta, Canada T2N 1N4

10. BUDGET EXPLANATION

	ITEM	1994-95	1995-96
1.	AFC7S Single Crystal Diffractometer	146,000	
2.	Computer for teXsan	2,300	
3.	HP7550 8 Pen Plotter	3,000	
4.	DeClaser 1152 PS Laser Printer	1,199	
5.	2.4 kW Mo X-ray Tube (normal focus)	3,000	
6.	Upgrade to 3 kW Generator	5,000	
7.	XL45 Liquid Nitrogen Dewar	2,700	
8.	Roller Cart for XL45 Dewar Tank	450	
9.	Polarizing Optical Scope	3,000	
10.	Polaroid Cassette	1,000	
11.	Goinometer Heads (5 @ $710 each)	3,550	
12.	Service contract	7,000	7,000
13.	Spare Cu X-ray tubes	3,500	3,500
14.	Consumables	1,000	1,000
15.	CCDB on line access	2,000	2,000
16.	Books: International Tables for Crystallography	500	
17.	Salaries:		
	Two Faculty	32,054	33,633
	Two Graduate Assistants	24,000	24,000
	Two Unergraduate Research Assistant	6,240	6,240
	Fringe Benefits	8,262	8,654
	Faculty: 30% Term, 16% Summer		
	Students: 1%		
18.	Indirect Costs (45% of Salaries)	28,032	28,743
19.	YSU Tuition Match	4,968	5,000
	Yearly Totals:	308,755	119,770

TOTAL PROJECT COSTS	428,525	(Proposed budget for two years)
LESS UNIVERSITY CONTRIBUTION	129,968	
LESS SENSORDEK CONTRIBUTION	227,358	(Items 12 through 18)
REQUESTED FROM NSF	**71,199**	

First Year: 1994

APPENDIX

SUMMARY PROPOSAL BUDGET

FOR NSF USE ONLY			
ORGANIZATION Youngstown State University	PROPOSAL NO.	DURATION (MONTHS)	
		Proposed	Grantec
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Timothy R. Wagner, Ph.D.	AWARD NO.		

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds Granted By NSF (If Different)
1. Timothy R. Wagner, PI		3	1.5	$ 18,698	$
2. Allen D. Hunter, co - PI					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1 - 6)				32,054	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				24,000	
4. (2) UNDERGRADUATE STUDENTS				6,240	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A + B)				62,294	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				8,262	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				70,556	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $1,000.) PLEASE SEE BUDGET EXPLANATION PAGE FOR ITEMIZED LIST					
TOTAL PERMANENT EQUIPMENT				191,199	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 2. TRAVEL 3. SUBSISTENCE 4. OTHER 4,968 (YSU tuition)					
( ) TOTAL PARTICIPANT COSTS				4,968	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				4,500	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER CCDB On-Line Access, Books, Service Contract				9,500	
TOTAL OTHER DIRECT COSTS				14,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				280,723	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 45% of salaries					
TOTAL INDIRECT COSTS				28,032	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				308,755	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPM 252 AND 253)					
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$308,755	$

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY		
		INDIRECT COST RATE VERIFICATON		
INST. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Of Rate Sheet	Initials - DGC

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*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPM 233

Second Year: [illegible]

APPENDIX

SUMMARY PROPOSAL BUDGET

ORGANIZATION Youngstown State University	FOR NSF USE ONLY PROPOSAL NO.	DURATION (MONTHS Proposed	Grante
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Timothy R. Wagner, Ph.D.	AWARD NO.		

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds Granted By NS (If Different)
1. Timothy R. Wagner, PI		3	1.5	$ 19,631	$
2. Allen D. Hunter, co - PI		2	1	14,0C2	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1 - 6)				33,633	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				24,000	
4. (2) UNDERGRADUATE STUDENTS				6,240	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A + B)				63,873	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				8,654	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				72,527	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $1,000.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 2. TRAVEL 3. SUBSISTENCE 4. OTHER 5,000 (YSU tuition)					
( ) TOTAL PARTICIPANT COSTS				5,000	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				4,500	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER CCDB On-line access, Service Contract				9,000	
TOTAL OTHER DIRECT COSTS				13,500	
H. TOTAL DIRECT COSTS (A THROUGH G)				91,027	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) (45% of salaries)					
TOTAL INDIRECT COSTS				28,743	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				119,770	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPM 252 AND 253)					
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$119,770	$

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY INDIRECT COST RATE VERIFICATON		
INST. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked	Date Of Rate Sheet	Initials - DGC

NSF Form 1030 (8/90) Supersedes All Previous Editions

*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPM 23

Cumulative Budget

APPENDIX

SUMMARY PROPOSAL BUDGET

ORGANIZATION Youngstown State University	FOR NSF USE ONLY PROPOSAL NO.	DURATION (MONTHS) Proposed / Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Timothy R. Wagner, Ph.D.	AWARD NO.	

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds Granted By NSF (If Different)
1. Timothy R. Wagner, PI		6	3	$ 38,329	$
2. Allen D. Hunter, co - PI		4	2	27,358	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1 - 6)				65,687	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				48,000	
4. (2) UNDERGRADUATE STUDENTS				12,480	
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A + B)				126,167	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				16,916	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				143,083	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $1,000.) PLEASE SEE BUDGET EXPLANATION PAGE FOR ITEMIZED LIST					
TOTAL PERMANENT EQUIPMENT				191,199	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
F. PARTICIPANT SUPPORT COSTS 1. STIPENDS $ 2. TRAVEL 3. SUBSISTENCE 4. OTHER 9,968					
( ) TOTAL PARTICIPANT COSTS				9,968	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				9,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				18,500	
TOTAL OTHER DIRECT COSTS				27,500	
H. TOTAL DIRECT COSTS (A THROUGH G)				371,750	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				56,775	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				428,525	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPM 252 AND 253)					
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ 428,525	$

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY INDIRECT COST RATE VERIFICATON
INST. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked / Date Of Rate Sheet / Initials - DGC

NSF Form 1030 (8/90) Supersedes All Previous Editions

*SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPM 233

CURRENT AND PENDING SUPPORT

APPENDIX VII

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

Investigator: Timothy R. Wagner

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

Support ___Current ___Pending _x_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: 400 MHz NMR Spectrometer (co-applicant; A. Hunter, PI)

Source of Support: NSF, Chemistry Division

Award Amount (or Annual Rate): $ 250,000 Period Covered: 1994

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending _x_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: Polyfluoroarylene Bridged Organometallic Polymers of Ni, Pd, and Pt (co-applicant; A. Hunter, PI)

Source of Support: NSF, Materials Division

Award Amount (or Annual Rate): $ approx. 350,000 Period Covered: May 1994-August 1997

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

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

NSF Form 1239 (8/92)

USE ADDITIONAL SHEETS AS NECESSAR

CURRENT AND PENDING SUPPORT

APPENDIX VII

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

Investigator: Allen D. Hunter

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

Support ___Current _X_Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: Polyfluorarylene Bridged Organometallic Polymers of Nickel: Rigid Rod Materials

Source of Support: American Chemical Society, Petroleum Research Fund

Award Amount (or Annual Rate): $ 25,000 Period Covered: May 1994-August, 1996

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: 25% Acad: Summ:

Support ___Current ___Pending _X_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: Isonitrile Bridged Organometallic Polymers

Source of Support: Research Corporation

Award Amount (or Annual Rate): $ 38,500 Period Covered: May 1994-August, 1996

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: 35% Acad: Summ:

Support ___Current ___Pending _X_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: Polyfluorarylene Bridged Organometallic Polymers of Ni, Pd, and Pt. (J. Mike & T. Wagner, co-applicants)

Source of Support: NSF, Materials Division

Award Amount (or Annual Rate): $ ≈350,000 Period Covered: May 1994-August, 1997

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: 50% Acad: Summ:

Support ___Current ___Pending _X_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: 400 MHz NMR Spectrometer (with J. Mike, T. Wagner, D. Phillips, J. Jackson, & T. Dobbelstein as co-applicants)

Source of Support: NSF, Chemistry Division

Award Amount (or Annual Rate): $ 250,000 Period Covered: 1994

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

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

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CURRENT AND PENDING SUPPORT

APPENDIX VII

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

Investigator: John A. Jackson

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

Support ___Current ___Pending _x_Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title: 400 MHz NMR Spectrometer (co-applicant; A. Hunter , PI)

Source of Support: NSF, Chemistry Division

Award Amount (or Annual Rate): $ approx. 350,000 Period Covered: May 1994-August 1997

Location of Research: Youngstown State University

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

Support ___Current ___Pending ___Submission Planned in Near Future ___*Transfer of support

Project/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): $ Period Covered:

Location of Research:

Person-Months or % of Effort Committed to the Project. Cal: Acad: Summ:

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

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USE ADDITIONAL SHEETS AS NECESSAR

PACKARD ELECTRIC
Paul Shiller, MS-93G

Division of General Motors Corporation P.O. Box 431 Warren, Ohio 44486

November 3, 1993

Youngstown State University
Department of Chemistry
Youngstown, Ohio 44555

Re: NSF funding for equipment purchase; X-ray diffractometer

Dear Dr. Wagner:

I have received a letter indicating your intention to purchase an X-ray diffractometer. Packard Electric is very interested in having access to such equipment. We would use this equipment to investigate the crystal structure of polymers now in use as well as in the development of newer engineered materials. This type of equipment will be central to our research efforts in about two major projects a year. If the equipment is purchased I look forward to working with you on these projects.

Sincerely,

Paul Shiller

Paul Shiller, PhD
Laboratory Manager

MSC MOLECULAR STRUCTURE
CORPORATION
3200 Research Forest Drive The Woodlands, Texas 77381-4238
Tel 713/363-1033 800/543-2379 FAX 713/364-3628

QUOTATION NO: 4837

October 12, 1993

Dr. Tim Wagner
Youngstown State University
Dept. of Chemistry
Youngstown, OH 44555-0001

Dear Dr. Wagner:

Molecular Structure Corporation is pleased to quote the following offer as shown below. This quotation is valid for 60 days.

Item No.	Quantity	Part No.	Description	Unit Price	Total Price
1.	1		AFC7S single crystal diffractometer including: goniometer, collimator diameters 0.3, 0.5 and 1.0mm, four sided radiation enclosure, AFC controller and interface, MSC/AFC diffractometer control software, two arcless goniometer heads, 3kW sealed tube generator, tube shield and X-ray tube (2.4kW Mo), table-top computer terminal		
2.	1		Extra Huber goniometer head		
3.	2		X-ray tubes: 2.0kW Cu (normal focus)		
4.	1		Polaroid cassette and bracket for diffractometer photography		

Item No.	Quantity	Part No.	Description	Unit Price	Total Price
5.	1		Fixed Tube LN_2 Based Low Temperature System: New design fixed tube liquid nitrogen based low temperature system includes temperature controller with digital temperature readout and thermocouple, stainless steel transfer tubes with concentric warm nozzle, and 100 liter heat exchange Dewar; uses gas boil-off from 100 liter Dewar and is circulated through system via air pump; LN_2 consumption is decreased to 0.95 liters/hour @ -170°C and .56 liters/hour @ -45°C. (No storage Dewar or nitrogen source tank)		
6.	1	XL45	Liquid Nitrogen Storage Dewar: 180 liter capacity, all stainless steel construction, gas and liquid, vent and pressure building valves		
7.	1		Roller Carts for XL45 Dewar Tanks: steel construction, 4 heavy duty casters, low profile for easy loading and unloading		
8.	1	R100W	Haskris R100 refrigerated water cooled heat exchanger for 2kW or 3kW generator		
9 A.		FR-PC743-W3	**Computer to control AFC7S:** DECpc 433 dxLP 33MHz 486 DX based system with SVGA controller 4MB RAM 3.5" 1.44MB floppy 3.5" 127MB IDE hard disk drive Preloaded MS-DOS 5.0 and Windows 3.1 101 keyboard: 2 button mouse		
B.		FR-PC7XV-DE	14" SVGA color monitor		
C.		FR-DE100-AA	EtherWorks LC		
D.		FR-LA95-CA	DECwriter 95 - 24 pin printer		
E.		QL-OTLA9-AA QA-OTLAA-HB	PATHWORKS license PATHWORKS documentation and media floppies *OR* PC/TCP for DOS; FTP Software Inc.		

Item No.	Quantity	Part No.	Description	Unit Price	Total Price
			Computer for teXsan:		
10 A.	1	WB-R50-4016 D3-M62A SD7-S50-4.0.5 DK-P5-001 SC4-W4D-4.0.5D	Silicon Graphics Iris Indigo, 50MHz (R4000) 16" dual scan color monitor 540MB SCSI system disk Power cord destination kit System software/manuals		
B.	1	MO5-CD	CD-ROM update media option for ESD		
C.	1	P-CDR-2A	External CD ROM SCSI drive		
D.	1	P3-T13D	4mm digital audio SCSI tape drive		
E.	1	SC4-FTN-3.5	FORTRAN 77 compiler		
F.	1	SC4-IDO-4.1	Iris development option		
G.	1		Full extended warranty		
11.	1	FR-LN07C-CA	DEClaser 1152 PS laser printer		
12.	1		HP7550 8 pen plotter		
13.	1		teXsan: comprehensive crystallgraphic software package; VMS, UNIX or DOS version available. The direct methods packages SAPI, SIR,and DIRDIF are supplied with teXsan. Optional direct methods programs are available or supported		
14.	1		Extra two (2) years service contract for AFC7S; includes 2 service calls per year; additional calls extra		
15.	1		Microscope:		
		BL 31-27-40 BL 31-26-84-88 BL 31-15-64-02 BL 31-33-05-28	Stereo Zoom 5 0.8x - 4x (power pods) Stand with arm Wide-field eye pieces Nicholas Illuminator		
				TOTAL PRICE FOR ITEMS 1 - 15	$197,000

TERMS

PAYMENT: 50% on order and 50% on delivery. Prices do not include taxes of any kind. Interest at the rate of 12% annually will be charged for any unreasonable delays in payment.

WARRANTY: One year parts and labor warranty contract on equipment; excluding consumables such as X-ray tubes for the sealed tube generator.