3. **PROJECT SUMMARY**

NMR has revolutionized the modern study of physico-chemical structure and dynamics. Our chemistry students need to be integrated into and more readily experience its manifold capabilities. Therefore, our educational goal is to increase and diversify the student's exposure to state-of-the-art NMR so they can discover and apply its versatility to challenging problems they will encounter in graduate research or industry. We propose to adapt and implement the excellent and timely curricular model of Davis and Moore [*J. Chem. Ed*. (1999), & NSF DUE #9751056], modifying some of their experiments, and adapting gains from our own research and published sources (mainly *J. Chem. Ed.*).

A 300 MHz FTNMR spectrometer is requested to introduce NMR to students as freshmen, and then to give them progressively more sophisticated experiences as they proceed through advanced courses and undergraduate research. Through four years, NMR will be a central theme in the chemistry/ biochemistry (14 experiments in 9 courses) and physics (3 experiments in 2 courses) programs. Newly adapted nuclear and modern physics lab experiments will expose students to the theory of NMR and its potential for investigating effects of atomic environment.

Over four years students will learn about chemical shifts, spin-spin splitting patterns, quantitation using integrated peak intensities, and simple decoupling. NMR characterization of student-synthesized, organic compounds will be made routine. Precise measurements will be made of isomer ratios, and enantiomeric excess. In advanced organic chemistry they will progress to 2-D COSY and HETCOR techniques. Extension of NMR to solid state and inorganic applications will be part of the analytical chemistry course. A metabolic reaction will be monitored by NMR in the biochemistry course. Thermodynamics of keto-enol equilibria will be studied with NMR in physical chemistry lab, along with a gas phase isotope exchange study. Also the spin-saturation technique will be introduced in an investigation of the kinetics of molecular internal rotation. In physics they will examine free induction decay of nuclei in an external field, Knight shifts, and the coupling of nuclear magnetic moments with their local environments.

4. PROJECT DESCRIPTION AND RESULTS OF PRIOR SUPPORT

4a RESULTS OF PRIOR SUPPORT

Not applicable

4b. PROJECT OVERVIEW

4b.1 The General Context — The College and the Students It Serves.

Westmont is a residential, undergraduate college with 1200 students. Women make up 60% of the student body, and special efforts over the past four years brought ethnic minorities of the entering class from 10% to 16%. Westmont awards B.A. and B.S. degrees in biology, chemistry, computer science, neuroscience, physics, and in conjunction with other universities (e.g., U Cal, Stanford, USC, Cal Tech). This arrangement offers 5 year programs (3 years at Westmont, 2 elsewhere) in chemical engineering and engineering physics, with degrees from both institutions. With a student-faculty ratio of 14 professors have extensive contact with students. Virtually all our majors participate in research. Westmont's science programs have grown especially rapidly since 1986 when a 12,000 sq.ft. building was erected for chemistry and biology. In 1996, the 3000 sq. ft. engineering-physics building was extensively renovated. A capital campaign is underway, and its first priority is a building with an additional 19,050 sq. ft. for science labs. In the 1990's the chemistry + physics faculty grew from 6.5 to 8 FTE, and during the same period, enrollments in courses directly impacted by this proposal grew to exceed 400 (Appendix B). Graduates in chemistry, physics, and biology (who contribute heavily to chemistry courses) increased from 23 to 72 per year. In recent years, 78% of our graduates in chemistry and physics went on to higher studies—34% to professional schools, and 44% to graduate programs such as those at Harvard, Princeton, UCLA, Illinois, and Stanford.

4b.2 General Goals and Objectives.

Davis and Moore[1] recently described the incorporation of NMR throughout the chemistry curriculum. This responds to the pervasive growth of NMR in all chemical areas, and it represents a concept that addresses two goals of our department. First, Westmont students need to know state-of-the-art NMR technology. Second, they need to develop a more creative versatility in research. We want to adopt Davis' and Moore's concept, and we propose to adapt their model (hereafter called DM). But we will broaden it substantially by adapting experiments from our own research, and from the literature, and further broaden the approach with NMR experiments in the Physics Department. The educational purpose is to use NMR spectroscopy to develop and exercise student versatility and ingenuity, through structural analysis of an unusually wide range of unknown chemicals and materials, characterization of synthesized intermediates and products, probing of reaction mechanisms, and design of research strategies in chemistry and physics. Modern nuclear magnetic resonance spectrometry has especially great potential for accomplishing this purpose, because this technology has developed in several modes of operation, each with a wide range of applications. Knowledge of its potentials thus gives students a large repertoire of components to build into research strategies. Our present curriculum is too narrow in its NMR applications, being restricted to two kinds of atoms, and one class of material (organic compounds). Since 1983 we have worked with a low field (80MHz) spectrometer, which limited us to qualitative organic applications with semi-quantitative interpretation. A 300MHz FT- NMR spectrometer is therefore requested to teach students high field NMR spectrometry in an extensive array of experimental situations in chemistry, biochemistry, and physics courses, using inquiry-based teaching. Introducing NMR into physics and biological courses will show chemistry students how their chemical training can be adapted to adjacent areas of science, and will acquaint biology and physics students with the synergy between chemical methods and those of their own fields. (The potential of NMR for studying nuclei and their atomic environment is generally overlooked in physics curricula). We expect to broaden student's outlook on the interrelatedness of research approaches. Another outcome will be an enhanced ability of our students to apply "real world," state-of-the-art NMR technology to their undergraduate research, and subsequently to the laboratory problems they will face in graduate studies and industrial lab practice.

4b.3 General Scheme to Accomplish These Purposes.

With a 300MHz FTNMR spectrometer, experiments will be added to our curriculum to demonstrate much of the breadth of NMR's capabilities in biochemistry and chemistry, and to expose physics students to its potentials in nuclear physics, and material science (summarized in AppendixE). In three courses, the chemistry department now offers 5 standard 1-D, liquid phase NMR experiments with organic molecules. With the requested spectrometer we propose to integrate 14 NMR experiments in 9 chemistry courses, adding 2-D studies, work in gas and solid phase, and experiments with inorganic nuclei. In addition to substantial upgrading of 4 of the current 5 NMR experiments, the plan adds 9 new experiments, some standard, some adapted from recent literature and some adapted from our own research. Undergraduate research is expected of all our students, and increased exposure to NMR will broaden and deepen this essential element of our curriculum.

In physics a further 3 experiments with NMR will be added in 2 courses (Modern Physics, Senior Physics Lab), and in research. The aim is to show how the influence of atomic environment on properties of nuclei can be revealed by NMR. To our knowledge the introduction of NMR to an undergraduate physics program is nearly unique**.**

4c.DETAILED PROJECT DESCRIPTION

4c.1 General Chemistry (CHM 5-5H,6-6H—Staff)

A general chemistry experiment will be taken from the DM model directly to study electronegativity using a series of halogenated methanes. This experiment will be done hands-on in CHM 5H (the honors section for which it is easy to schedule NMR time) but the data shared with the regular CHM 5 sections. In CHM 5H about 5 groups of 3 students will each be given a halogenated methane. With help from the instructor and a senior student mentor (from CHM 190), the spectrum of the compound will be observed, and the spectra will be pooled and distributed. The CHM 5 and 5H students will draw conclusions about electronegativity.

Later in the semester as part of the organic chemistry unit, a new discovery based experiment to observe the number of ^{13}C signals and positions of isomeric butanols and pentanols will be done . Again, about 5 groups of 3 CHM 5H students will be given the unknown alcohols, and will assign structures based on the number of carbon signals and chemical shifts. The mentor will demonstrate the NMR procedure to the regular CHM 5 students who will analyze the data identically.

We have incorporated a simple experiment from the DM model for CHM 6 and CHM 6H (honors) that will reinforce the theory of transition metal complexes. Both classes will prepare various transition metal complexes such as $Ni[NH_3]_6Cl_2$, determine the composition titrimetrically, and obtain the UV-vis spectrum. With the instructor's assistance, the CHM 6H (honors) students will also determine magnetic moments by the Evan's NMR method[2], which measures the frequency difference (i.e. chemical shift difference) between a solvent water 1H resonance of an aqueous complex solution of known concentration, and a pure water ^1H resonance contained in a concentric capillary within the standard NMR sample tube. Magnetic susceptibilities are proportional to this difference and allow students to calculate the magnetic moment and infer the number of unpaired electrons in their complexes. Again, the data collected by honors students will be pooled and shared with non-honor students (CHM 6). The results will be discussed in terms of crystal field theory.

4c.2 Organic Chemistry (CHM 101,102—Marten)

In developing an inquiry-based approach in this class, research problem experiments have long been a part of our courses. Modern NMR technique is essential if solving those research problems is to represent actual practice in graduate schools and industry. The fast data acquisition possible with the requested spectrometer will permit NMR to be introduced in the middle of first term, when typical functional group unknowns will be used, and more advanced applications will be added progressively. The accumulation of experience, and confidence will prepare students for creative applications of NMR in more open-ended research problems. Fast collection of spectra by the requested instrument also makes possible the routine use of NMR to characterize intermediates and products when synthesis experiments are done later in the first term.

As in the DM model, we will study stereochemistry with the reduction of camphor to isoborneol/borneol. Students will be asked to discover what controls the stereochemistry of hydride addition to the carbonyl group in camphor (steric approach or product development control)[3]. Molecular modeling will be used with quantitative NMR measurements. Analogous experiments with other ketones, and other reducing agents will permit students to discover the balance of stereochemical factors in different contexts. The microscale of these experiments necessitates a high field instrument to make them precisely quantitative.

Aldol condensations for the production of substituted chalcones, are the basis for another discovery-based experiment, currently used. Different substituents give different colors, and students use UV-VIS and IR spectroscopy to explore reasons for the color changes. Adding rapid ^{1}H and ^{13}C-NMR analysis, and noting the proton and carbon chemical shift changes, as recently reported,[4] will be used to deepen student understanding of the underlying electronic principles involved in the shifting of the visible absorption bands.

A synthetic research project takes half of the second semester. Having mastered NMR skills by this time, the students will be able to do rapid analyses on starting materials, intermediates and products, thus learning more rapidly about the success of each step of the synthesis. They can then redesign their synthesis protocols as needed.

In addition to chemical shifts, the organic course introduces students to spin-spin splitting patterns, integration of peak intensities, and simple decoupling experiments, as applied to 1D high resolution ^{1}H & ^{13}C spectra and DEPT ^{13}C techniques. With these skills mastered, the students will have the competence to deal with real research problems in organic chemistry. It will also give them enough time on the spectrometer to develop confidence and facility in its operations, before meeting more sophisticated experiments.

4c.3 Advanced Organic Lab (CHM 160—Marten)

The lab component of this course is devoted to modern spectroscopy. Standard texts on NMR spectroscopy are used, supplemented with lectures on more advanced NMR topics. Students examine unknowns with IR, UV-VIS, ^{1}H- and ^{13}C-NMR and mass spectroscopies. Beginning the course with an established competence in NMR operation, students will have more time for more advanced NMR applications that also incorporate molecular modelling. Two new experiments in 2-D NMR will use the COSY technique, and HETCOR for proton-carbon coupling. One of these, adapted from recent literature[5] characterizes an unknown which will be obtained from a natural product isolation such as a terpene. This will be a discovery-based experiment where the student chooses the source of the starting material, and the appropriate techniques for isolation and characterization. NMR will be the major tool used in the characterization. The second new experiment, which we are now designing, includes proton assignments in a hexose glycoside.

4c.4 Biochemistry (BIO/CHM 113-Percival)

NMR can show students a mechanism in a metabolic pathway as they gain experience with *in vitro* monitoring of a biochemical process. In place of the biochemical experiment of the DM model, we will adapt a published experiment[6] where the kinetics of glycolysis can be studied in yeast using ^{13}C NMR spectroscopy under aerobic and anaerobic conditions. Changes in the concentrations of such glycolytic metabolites as the α and β pyranose anomers of glucose are easily measured with the sensitivity provided by ^{13}C-enriched glucose.

4c.5 Advanced Analytical Laboratory (CHM 122-Anderson, Nishimura, Tro)

In the DM model, inorganic NMR is introduced at the research level, but we feel inorganic NMR ought to reach a broader audience. Moreover, an inorganic NMR experiment can be devised that extends NMR work from liquids to solids. In doing so, students will learn phenomena such as dipolar and quadrupolar interactions, not generally seen in solution chemistry. This serves as an introduction to solid state material science, which has become important in the computer era. Moreover, this extension of NMR study systems will open the door to discussion of the diverse world of inorganic molecular interactions.

In place of the DM experiment on ^{31}P NMR with herbicides, we will extend this model by applying ^{31}P NMR to solids. On the basis of the PI's research, a simple, novel, 6-hour, solid-state experiment has been designed, and will be published[7] using student-obtained results. Students will synthesize a series of Na_2O-P_2O_5 glasses (from 40 to 65 mol% of Na_2O) and analyze the wideline spectra that are obtainable using a standard high field NMR spectrometer. (A solids probe is not needed.) The percentage of each phosphorous environment in the solid is obtained by integration of the components of deconvoluted, ^{31}P powder spectra[8]. Comparing their glass samples to commercially available reference materials, students measure the percentages of different phosphate environments present —tetrahedrally coordinated P, either singly bridged P, or doubly bridged.

4c.6. Physical Chemistry Laboratory (CHM 132/133)

i.*Thermodynamics-CHM 132 (Nishimura).* In the past we have used ^{1}H-NMR to determine approximate keto-enol equilibrium constants for acetylacetone and ethyl acetoacetate in two solvents by simple integration of the proton signals of the equilibrium species. The requested NMR with its variable temperature probe will permit an adaptation of the former experiment with more extensive study of physical chemistry (energetics) in these systems, for example, using the van't Hoff equation to calculate ΔH and ΔS.

In another application, NMR will be adapted to a conventional analysis of liquid-vapor equilibria in binary systems. An example is the construction of temperature-composition diagrams for acetone-chloroform mixtures, for which the mole fractions will be elegantly measured by NMR by signal integration or both pot and distillate samples[9].

An experiment based on DCl-HBr isotopic exchange in the gas phase, using a multinuclear probe to quantify ^{2}D and ^{1}H signals, will be adapted from Shoemaker, et al[10]. This permits determination of the isotopic exchange equilibrium constant, and also shows how NMR can be adapted to gas phase studies. In an additional experiment, relaxation rates of these nuclei will be measured as a function of pressure to gain insight into the relations between molecular dynamics and spin relaxation.

ii. *Kinetics and Quantum mechanics-CHM 133 (Tro)*. We are replacing the DM experiment on cyclohexane with a spectrally simpler kinetics system that gives the same information. NMR will be used to measure kinetics of an internal rotation of a molecule using a spin-saturation transfer technique[11]. One of two N-methyl signals in N,N-dimethylacetamide is saturated using the CW irradiation (spin decoupling) capabilities of the instrument. Over time, as the molecule rotates about the internal carbon-nitrogen bond, the spin saturation is transferred to the other N-methyl group, decreasing its signal from that observed in the absence of spin saturation. Measuring relative areas of the two N-methyl signals at different temperatures, the activation barrier for rotation about the carbon-nitrogen bond is determined. The spin-saturation approach permits examination of a larger range of sample temperatures than is the case for line-shape analysis methods, and avoids curve fitting to obtain kinetic parameters.

4c.7. Modern Physics Lab (PH26—Rogers and Sommermann).

Two classic NMR experiments will be adapted to classroom use. In the first, students will investigate the Knight shift in the NMR spectrum of n-propanol in the presence of paramagnetic Co^{2+} ions at 23^{o} C[12]. The experiment will consist of measuring the shift for the OH group, CH_2 group, and CH_3 group protons as a function of cobalt concentration. A conclusion reached will be that the observed shift is proportional to the fraction of time each alcohol molecule spends attached to the ion. In the second experiment, students will investigate relaxation effects in paramagnetic solutions[12]. As a rule the relaxation rates $1/T_1$ and $1/T_2$ are directly proportional to the concentration of the paramagnetic species, and roughly proportional to μ_{eff}^2, its mean square magnetic moment. Students will study the relaxation effects of protons in water that contains Mn^{2+} ions[13]. From plotting the data, students will observe directly that relaxation rates are proportional to the concentration of paramagnetic ions. Of interest will be the enhanced relaxation experienced by protons in the Mn^{2+} coordination shell due to the unpaired electron.

4c.8. Senior Physics Lab (PH 170—Rogers)

Students will conduct an experiment in measuring free induction decay, in which concepts such as relaxation times, phase, modulation and spin echoes will be highlighted. As an example[14], students will measure the free induction decay of the ^{13}C resonance of $^{13}CH_3I$ (90% enriched). They will obtain an interferogram showing the regular beat pattern, and will determine that the periods of the beats are related reciprocally to the frequency differences in the spectrum. Additionally they will determine J from analysis of the beat envelopes.

4c.9. Opportunities for undergraduate research

(Student research in chemistry and physics involves 20-25 students per year, and averages 2.5 publications each year and 8 presentations per year at meetings.)

i. As part of the studies of Prof. Marten, his students analyze crude organic reaction mixtures and characterize isolated products with NMR, using specialized techniques such as difference NOE, variable temperature rate determinations, and spectral simulations. Work will be extended to products of organometallic reactions such as benzofurans, dichlorocyclopropanes, 1,3-dienes and β-lactams using chiral iron-lactone complexes[15]. Whereas low field instruments are incapable of doing so, it has been shown that high-field NMR instruments permit determination of the optical purity of these compounds using chiral shift reagents. With the proposed NMR spectrometer students can characterize structures and reactions studied in their research projects at a more revealing level than previously possible.

ii. Prof. Anderson and students study glassy lithium electrolyte materials, and find that relaxation times (T_2) of the ^7Li ions as a function of temperature and glass composition are related to ion distributions and mobilities. Mobilities correlate with structural microenvironments, including segregated phases in the solids.[16,17] The requested multinuclear broadband probe, will allow application to other nuclei (e.g., ^{31}P) so that Anderson's students can expand their studies to a larger variety of crystalline and amorphous electro-optical materials [18,19] which are crucial for numerous solid state communication applications (eg. acoustic wave transducers, holographic data processing, etc.). Resistance to radiation damage is enhanced by changing composition with tungsten doping, and NMR spectroscopy is needed to characterize the lithium tantalate phases that form.[18] Preliminary results[19] with tungsten doping suggest a low temperature, short- range "jumping" mechanism and a high temperature, long-range diffusion. A model to explain this can be further developed by students studying the effects of doping with other metals.

iii. The requested NMR will enable Prof. Rogers and his students to test implantation materials for possible use in his off-campus experiments on β-unstable nuclei (see section 4d). Understanding host lattice relaxation effects and electric field gradients is important for determining the nuclear dipole and quadrupole moments of the implanted radioactive nuclei. Students will study various non-cubic crystals to determine suitable hosts for implantation. For example, a non-cubic crystal containing a stable isotope of the element of interest (with non-zero quadrupole moment), will serve as a probe for determination of the crystal electric field gradient at the implantation site, for use in LMR (Level Mixing Resonance) experiments.

4d. EXPERIENCE OF THE PRINCIPAL INVESTIGATORS AND SENIOR PERSONNEL

Stanley Anderson, the project director who will coordinate use of the requested instrument, is an authority[20] on NMR with experience in both teaching and research. He studies structures and properties of complex inorganic materials by observing ion mobilities and local structural microenvironments in glasses, and crystalline and amorphous electro-optical materials.

David Marten is interested in organo-metallics and their use in the synthesis of organic compounds, devising new methods for dienes, lactones, furans, and benzofurans. Recently, optically active β-lactams were synthesized using new chiral iron complexes, and 1,3-dienes were produced by developing a novel fragmentation reaction. He has taught NMR for years, and NMR is important to his studies of reaction mechanisms.

Allan Nishimura, a physical chemist, studies the properties of crystals and molecules adsorbed on surfaces. Many of his publications involve optically detected magnetic resonance. He is also expert in instrumentation and analog and digital electronics, and will direct and participate in the maintenance of the requested instrument.

Nivaldo Tro has specialized in surface chemistry, focusing on sorption and desorption of inorganic and organic molecules, and also in energy transfer.

Warren Rogers does research at accelerator labs in Chicago, Michigan St. Univ. and the GANIL facility (France) on the determination of ground-state nuclear magnetic and electric quadrupole moments of short-lived β-unstable nuclei. He collaborates with physicists from Rutgers, Michigan St. Univ., Univ. of Leuven (Belgium), and the Weizmann Inst. (Israel) working with β-radiation detected by NMR and LMR.

Frank Percival is a plant physiologist with interests in metabolism. His recent emphasis has been on production of anthocyanins in *Arabidopsis.*

Michael Sommermann does theoretical nuclear physics, including research on nuclear structure and collective phenomena in heavy nuclei, and also studies on skyrmion models of nuclear interactions.

4e. EVALUATION

In the graduating classes of 1996 through 2000, 23% of chemistry graduates had co-authored publications. The most direct observation of improved student learning will be made during student's undergraduate research, and in the resulting publications. By comparing NMR future projects to past ones we will score for the frequency of NMR use, and look for more sophisticated and creative applications of NMR in student projects. In addition, as part of a program on documenting academic outcomes, recently funded by the Irvine Foundation, our department is committed to routinely surveying students two years after graduation, asking how technology, and NMR in particular, proved useful in graduate studies or employment, and how our program might be improved. We will also write to research supervisors of our graduates who have gone on to graduate schools, or to industrial and government positions to ask how our students compare with others in their knowledge of instrumentation and methodologies, and in their ability to design research strategies. Responses should show a difference before, and after revisions of the chemistry and physics programs are completed.

4f. DISSEMINATION OF RESULTS

4f.1 Publications.

Results will be shared within the wider chemical education community using all means at our disposal, especially publication, professional meetings, and the Internet.

The experiment described for CHM 122 is being submitted for publication. Further teaching experience (e.g. the 2-D experiment devised for CHM 160) will be submitted to journals such as *J. Chem. Ed.*, and presented on our chemistry and physics department Internet homepages. Faculty web pages will incorporate the proposed experiments into their posted course syllabi. Journal reprints will be available for any who request them.

4f.2 Professional Meetings.

The chemistry department has been active (hosting workshops and meetings as well as participating) in the California Association of Chemistry Teachers, (teachers from high school to university), and this provides a good opportunity to report on our teaching experiences there. In addition, we will report our experience in presented papers and poster sessions to the Education Division in national and regional meetings of the American Chemical Society.

One of the present Co-PIs, Prof. Warren Rogers, was the designer and organizer of the “Conference Experience for Undergraduates”(CEU), which was held in conjunction with the national meeting of the Division of Nuclear Physics. The CEU enables undergraduate students from all over the country to present their research to the professional community. With 60 students accepted for each of the conferences in 1998 and1999, the response from students and established researchers has been enthusiastic. The CEU provides a venue for publicizing the usefulness of NMR in physics curricula. The funds supporting this conference, were two supplements attached to an RUI grant that has been renewed for three years.

Research students and faculty will continue to report their scientific research in professional meetings as well as in journals (Appendices C, and D). Over the past several years, student research has been presented in an average of 2.5 publications per year, and 8 reports per year in professional meetings. Especially in conferences for undergraduate researchers, the value of teaching NMR across the curriculum will be increasingly obvious. Westmont students are frequent contributors in annual research conferences for undergraduates sponsored by the American Chemical Society in southern California, and in annual meetings of the Western Spectroscopy Association.

4g. EQUIPMENT REQUEST

4g.1 300 MHz FTNMR Spectrometer and Accessories.

We request funds for a 300MHz pulsed NMR spectrometer such as a Bruker DPX AVANCE-300 series, with variable temperature, multinuclear broadband accessory with probe, and software for off-line calculations. With the relatively small cost differential between 200 and 300 MHz the latter is a better buy because the higher field provides higher resolution (important for solid state studies we hope to add in the future), and speedier data acquisition (important as future student enrollments increase). This modular spectrometer will be upgradable to state-of the art for many years, and are easy to service. Although we also considered the Varian Mercury 300, and JEOL Eclipse+300 spectrometers, the Bruker system which we are currently leasing, seems best for our particular situation. It will allow for easy addition of other options at reasonable cost (see item v, below). Moreover, it is known for its high quality and ease of maintenance, making it the least expensive in the long run, considering repairs and parts. The justification for the items requested follows:

i. High field strength (300MHz) is needed to obtain the high resolution that is critical for studying protons in complicated organic molecules (CHM 102 & 160), and for the quantitative measurements in most of the experiments outlined above. The higher sensitivity that comes with higher field strength will also facilitate heteronuclear observations and 2D experiments.

ii. The computer software requested (e.g.Bruker's WINNMR) is necessary to enable large numbers of students to use the NMR instrument. Shortening the time needed for each experiment will allow more kinds of experiments to be assigned. With computer network access, some students can analyze data while others use the spectrometer. Westmont has an X-Windows license to interface the NMR with the campus computer network so that students can process data in their dorms. (Connections are available in every room.) Software like Bruker's WINNMR is needed to make this possible, even though a basic communication control unit (e.g., Bruker's CCU) and software (XWIN-NMR) is included with the general spectrometer package.

iii. A multinuclear broadband option with probe (e.g., Bruker VT CPMAS) is needed for kinetic and thermodynamic measurements and it will allow study of a wide range of compounds containing various elements. This will allow the NMR experiments described for the advanced (inorganic) analytical lab (CHM 122) as well as the organic lab.

iv. Variable temperature thermostatting is needed for all the proposed experiments. Thermostatting is mandatory for all high field NMR work to give stable signals and reproducible spectra. The variation in temperature settings is necessary for the thermodynamic and kinetic measurements in the CHM 132 & 133 courses. Prof. Anderson's research students study structural changes in inorganic glasses over a wide temperature range, and Prof. Rogers' students will be studying prospective host materials over a range of temperatures also.

v. Future upgrades are planned with the suggested instruments, including the following. a) A gradient accessory is required for gradient spectroscopy that has been developed in recent years for doing 2D experiments rapidly. As upper division classes grow it will become necessary to add a gradient system (e.g. Bruker Grasp II plus inverse probe). We should be able to handle a limited number of 2D experiments with the requested instrument for a few years. b) The DPX AVANCE-300 is compatible with Bruker's LEVEL I SOLIDS ACCESSORY, which we hope to add in the future so that routine high resolution studies could be done on a wider range of solid state materials than is possible using only the wideline mode. An auto-sampler will be added when enrollments require it, and additional experiments are introduced.

4g.2 Supporting Equipment

The section on “Facilities, Equipment & other Resources” lists general major equipment available. The labs are fully equipped with standard, minor equipment and supplies. In particular, they are well supplied with equipment for chemical synthesis, natural product isolations, and UV-visible-IR spectrophotometry. There are computer work stations in the labs, and shop facilities in nearby rooms. The 80MHz FTNMR spectrometer used since 1983 is incapable of most experiments outlined above, and it broke down beyond repair in late 1997 (parts are now unavailable). Early in 1998 Westmont negotiated the short-term lease of a Bruker DPX AVANCE-300 spectrometer until funds become available for purchase of a new instrument. The availability of this instrument is enabling us to smooth out the design of several of the experiments mentioned above.

4g.3 Installation, Maintenance, and Operation

Bruker has certified our site as suitable for the 300 MHz instrument (Appendix F). An annual budget of $2000 for routine maintenance service has been set after consulting with NMR users at U. Calif., Santa Barbara, who have similar instrumentation. A service contract (parts only, quoted at $5238, see Appendix G) will be purchased after the initial warranty expires. Finally, we have institutional commitment (Appendix H) from our provost to provide funds to keep the NMR running. The Chemistry Department’s monthly budget allows for cryogenics at $ 500 for liquid helium and liquid nitrogen. Our experience with the leased spectrometer will allow us to refine these cost estimates if necessary.

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