

Summary of Proposed Work

Berea College proposes to improve its program in chemistry by adding new laboratory experiments involving structural elucidation and molecular dynamics throughout its curriculum. One goal of our laboratory instruction is to have students learn basic experimental techniques and be able to apply these techniques to real world problems. The primary tool we will be using to develop these experiments is a nuclear magnetic resonance (NMR)^{1,2} spectrometer, an ideal tool for adding new structure and dynamic experiments. In the organic course, students are introduced to NMR spectroscopy in the laboratory. They will use ^1H and ^{13}C NMR when they synthesize organic products. In the instrumental analysis and physical chemistry courses, students will be shown how NMR can be used as a tool to determine complicated structures and to probe solution reaction dynamics. In physical chemistry, the students will learn quantum mechanics, where NMR is an ideal system for presenting solvable applied problems. Once they complete their advanced coursework, students will have learned the basics of two-dimensional NMR techniques, including correlation spectroscopy (COSY) and heteronuclear correlation spectroscopy (HETCOR) to solve structural problems.² The last step in the education of our students is a required research experience. NMR will enhance the research interests of the department, while providing a solid foundation for strong student-faculty interactions. Knowledge of NMR, along with Fourier transform infra-red spectroscopy (FTIR), and gas chromatography/mass spectrometry (GC/MS), should prepare our students for a variety of problems they might encounter in a research environment. Implementation of this program will be a model system to be used at other institutions; for example, our affiliation with the Appalachian College Association provides an excellent avenue to bring NMR experiments to an audience that might not otherwise have this wonderful opportunity.

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Previous NSF and ILI Program results

Lee Roecker was the recipient of an ILI award (grant number DUE-9251120) of \$22,008 from 15 July 1992 to 31 December 1994. The project "Laboratory Experiences in Electrochemistry" has supported the development of an inorganic laboratory course and has significantly improved the laboratory component of the instrumental analysis course at Berea College. One fourth of the instrumental analysis course is now devoted to electrochemistry as opposed to less than one sixth of the course before the electrochemical equipment was obtained. In the instrumental course students do polarography and stripping voltammetry- techniques which previously were not accessible to the students. Relating to the general theme of oxidation-state phenomenon, the new inorganic laboratory allows students to perform cyclic voltammetry and make magnetic susceptibility measurements. Dr. Roecker's research students have made extensive use of coulometry and two summers ago began to explore how reaction rates can be measured using electrochemical techniques. The particular reaction they are studying involves the loss of a carbonyl ligand from an electrochemically generated Os(IV) complex. This research effort is still in progress.

Larry Blair directed undergraduate research from 1987 to 1993 with support from NSF under the RUI program (CHEM-8700848 and CHEM-9000576). Students synthesized and characterized a variety of halogen-amine complexes. From his work on these complexes arose the result that the dynamic exchange of amine ligands coordinated to a central Br^+ can be investigated by NMR techniques. In particular, using NMR instrumentation at the University of Kentucky, Blair and his students were able to show that the 2-coordinate complexes of the bis(pyridine) bromine (I) type undergo ligand exchange in the presence of free ligand at rates that can be investigated by NMR line broadening techniques. These studies have not been completed in part because of the difficulty in scheduling research time at the University of Kentucky.

Narrative

1. Current Situation

A. The Chemistry Department at Berea College: Berea College is a unique, four-year liberal arts college with a long tradition of academic excellence. Berea charges no tuition and only admits financially needy students. Berea was founded in 1855 by abolitionists and radical reformers as one of the first southern colleges to have interracial education. Today Berea continues this tradition with a diverse population, including 5% foreign students and 10% African-Americans. All Berea students are required to work a minimum of 10 hours each week in the service of the College. Berea's strongest students are among the finest in the nation, achieving high scores on the MCAT, GRE and other standardized exams and winning awards such as Truman Fellowships, Fulbright Scholarships and Watson Fellowships. Berea is located in central Kentucky and enrolls 1,500 students, 80% of which come from the surrounding Appalachian region. Berea has a wide range of academic programs including the traditional liberal arts, agriculture, technology and industrial arts, nursing, education and business.

The chemistry department has four full-time Ph.D. faculty and is supported by a full-time electronics technician and a chemical hygiene/safety officer. Our chemistry faculty represent the sub-disciplines of physical, inorganic/analytical and organic chemistry. Since 1965, the chemistry department has had an active undergraduate research program and has graduated 225 majors in the last 25 years, of whom more than 70 have gone on to receive M.D. and Ph.D. degrees (See Appendix C for summary of last five years.) All of our majors participate in undergraduate research as a requirement for graduation, either through research courses or summer research programs. During the past 5 years, Berea students have presented more than forty papers at various conferences.

B. Curriculum: By focusing our attention on basic chemical and problem solving skills, our curriculum is designed to prepare our students for a wide range of career choices. Computers and instrumentation enhance these skills and supplement basic wet laboratory skills. Our department has a strong emphasis on hands-on problem solving with a focus on undergraduate research. Additionally, our students are all expected to meet oral and written communication standards established and

learned through their chemistry and general studies courses. Our curriculum is outlined in Appendix B where all relevant courses impacted by this proposal for a chemistry major are indicated.

C. Relevant Resources of the Department: The instrumentation of the chemistry department is described in Appendix A. In terms of doing modern dynamics and structure measurements, the only instrument we lack is a modern FT-NMR spectrometer. With this acquisition, our department will be well equipped to perform and teach almost every important instrumental technique. Our laboratory space is sufficient for expansion to include a new NMR spectrometer. Currently we have two research wet labs, two large teaching labs, two instrumentation rooms and a preparation/stockroom. In preparation for the purchase of a new NMR spectrometer we have recently upgraded the high pressure air facilities in our instrumentation labs so that we can support all current and future instrumentation. The physics department shares computational resources with us on a variety of UNIX operating system computers, where, among other things, our world-wide web pages are maintained. Finally we have a large pool of student labor who help maintain instrumentation, prepare chemicals and laboratories and grade homework. These students are a critical departmental support unit and the jobs provide excellent learning for the students.

Our department has a long history of research funded through individual grants to faculty members from the National Science Foundation, the Petroleum Research Fund, the Camille and Henry Dreyfus Foundation, the Keck Foundation, Research Corporation and the Appalachian Colleges Association. We are supported each year by the college with over \$20,000 for teaching supplies, chemicals and other small equipment. We have an endowment established for chemistry which supports research at the level of \$8,000 each year. In addition, the chemistry department shares an endowment with the biology, physics and geology departments from an endowment established by a grant from the Kresge foundation which is used to maintain instruments and purchase new equipment. This fund generates approximately \$10,000 per year for the department. Another endowment provides \$1,000 per year to support interaction between the Agriculture and Chemistry Departments. Finally the college has long term capital equipment funds which, in com-

bination with the college endowment, can guarantee that we will be supported in our research and teaching needs into the 21st century.

D. Curricular Need: Our curriculum currently lacks sufficient tools to do serious structure determinations. We seek to remedy this situation by adding new NMR spectroscopy experiments to the laboratory portions of our courses starting with organic chemistry II. In recent years, NMR spectroscopy has played a larger role in chemistry as evidenced by the growing body of publications¹⁻⁹ involving this technique as well as the use of NMR in the form of magnetic resonance imaging (MRI) in the medical field. Dr. Baltisberger provides Berea College with a physical chemist who is trained in NMR spectroscopy and is well-versed in both liquid and solid state experiments. He has actively worked to upgrade existing NMR instrumentation and has acquired solid state NMR probes and amplifiers using his research funding. In addition, the research interests of Dr. Roecker and Dr. Blair have been enhanced by NMR spectroscopy; however, they have been forced to carry out their experiments at other institutions. The expertise of Dr. Baltisberger and the growing departmental use of NMR suggest that the time is right for our department to expand the instrumentation to include high field NMR spectroscopy.

Currently evaluation of molecular structure is conducted using basic FTIR, GC/MS and low-field ¹H NMR experiments. Of these techniques, modern FT-NMR is by far the most powerful, but using a EM360 or FX90Q limits the learning options considerably. In addition, NMR experiments are not introduced in the laboratory until late in the second semester of organic chemistry (CHM 222) and then again in physical chemistry (CHM 262) as well as instrumental analysis (CHM 242). Only a small fraction of our majors are currently able to utilize NMR spectroscopy in the laboratory. By adding a new NMR spectrometer and introducing more NMR based laboratories to the various courses described in the next section, we will fill a hole in the educational needs of our student body. With this proposal we anticipate the following benefits: first, students will have opportunity to use NMR spectroscopy to solve structural problems in the second semester of their sophomore year. Second, adding the option of NMR spectroscopy to existing AA, FTIR, GC/MS and electrochemistry experiments will provide students with an array of standard modern instrumental techniques. Finally, the new NMR experiments will be introduced progressively in all

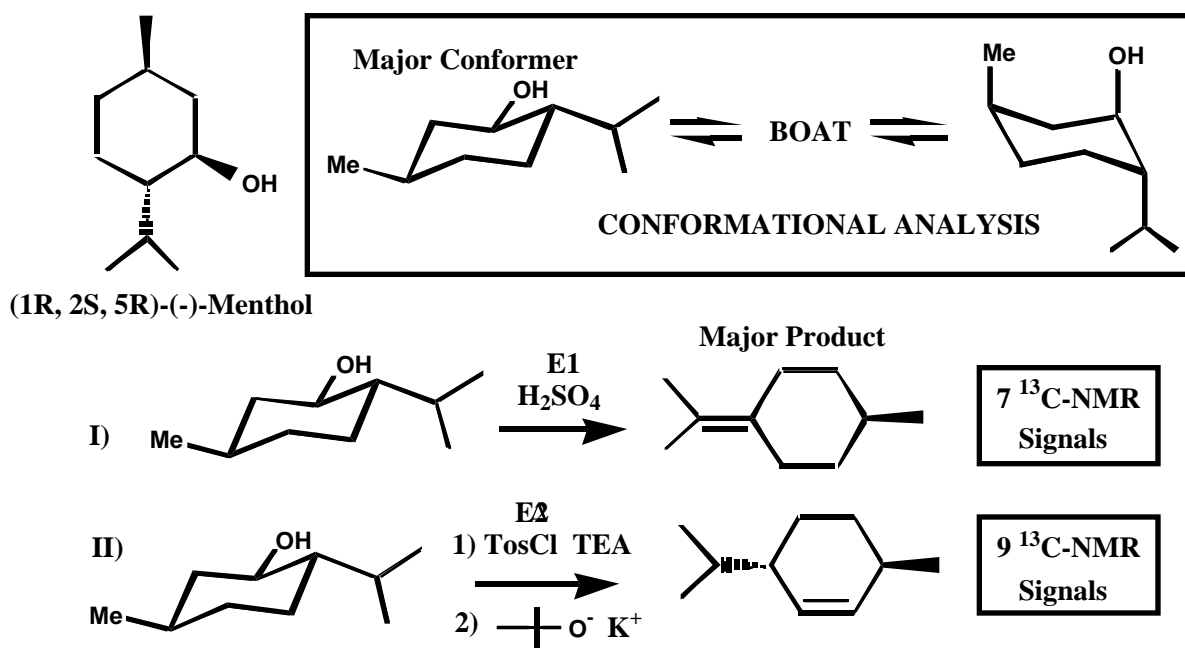
courses beginning with second semester organic chemistry. By building up their understanding of NMR spectroscopy over a series of courses, students will have more time to fully appreciate the technique. The overall goal is to have our students graduate with a high degree of proficiency and knowledge on the theory, function and operation of a high field NMR spectrometer.

2. Development Plan

The basic plan of development is to add at least one new experiment to each of the impacted courses that are possible only with the use of NMR. These experiments have been carefully chosen to introduce the students to various aspects of structure and dynamic determination using NMR spectroscopy. The initial starting point for introduction of these experiments to the curriculum will be in second semester organic chemistry. By the end of first semester organic chemistry, students have been exposed to the theory of ^1H and ^{13}C NMR, and they are ready to see some real applications. The first experiments will illustrate how NMR experiments can elucidate organic structures. In the advanced courses, students will have the opportunity to perform a variety of new experiments that exhibit the multi-nuclear and multi-dimensional nature of the technique. The advanced students will utilize NMR as a tool for measuring dynamics as well as structure. Once students complete the chemistry curriculum, it is hoped that they will have a strong foundation for graduate and professional work in that they will be able to run the NMR spectrometer on their own and interpret results of basic one and two-dimensional experiments.

CHM 222 Organic Chemistry II: Students are introduced to NMR spectroscopy experiments in our organic chemistry laboratory. In the future, this initial contact will be expanded to include NMR spectra of molecules synthesized throughout first and second semester. These molecules, with the aide of chemistry department teaching assistants, would be analyzed on the high field NMR spectrometer. Both the ^{13}C and ^1H raw data (free induction decays) would be placed on our local web server. They would be in a location and format where the students could easily access them. Our students would have the opportunity to process this data off-line and then compare the observed spectra with the structures, thereby increasing their fundamental understanding of the diversity of hydrogen and carbon atoms within organic molecules. This experiment would encourage students to work together with new techniques while learning the importance of NMR in structural analysis.

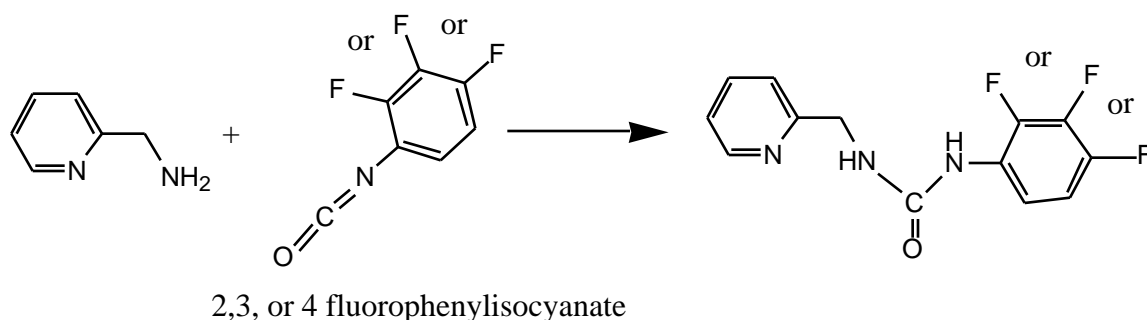
For example, a new laboratory experiment that will be introduced would be the comparison of an E1 and E2 elimination from (1R,2S,5R)-(-)-menthol. As illustrated by the reaction scheme below, students would be exposed to examples of stereochemistry, conformational analysis, rearrangements, symmetry, and NMR spectroscopy. The advantage of this experiment lies in its simplicity and the elegance of the analysis.



In addition, we plan to expand an existing oxidation experiment where students convert cyclohexanol to cyclohexanone. Currently, students use IR and GC to characterize the products and reaction yields.¹⁰ With the new NMR spectrometer, we plan to use ^{13}C NMR to follow the conversion of the $\text{C}_R\text{-OH}$ and $\text{C}_R\text{=O}$ peaks in the cyclohexanol and cyclohexanone respectively.

CHM 242 Instrumental Analysis: Our current Instrumental Analysis course is divided into four units, one of which is NMR spectroscopy. The NMR section of the course uses *NMR Spectroscopy* by Macomber¹¹ as a text. We give students exposure to the kinds of one and two-dimensional experiments they are likely to need once they graduate. While the lecture material is both multinuclear and multidimensional, laboratory work is limited to ^1H . Some experiments (specifically the introduction to processing and data acquisition) proposed by Fuson might be appropriately added with a new NMR spectrometer at Berea.¹² In addition, a new experiment that will dem-

onstrate the utility of multinuclear and 2D NMR involves the characterization of phenylpyridylureas. Performing COSY and nuclear overhauser effect spectroscopy (NOESY) experiments on model systems in CHM 242 is an excellent way to pave the road to doing these experiments in the research environment later. We will expand on a previously reported experiment¹³ and use fluorine substituted phenylisocyanates in the reaction with 2-aminopyridine as shown below.



The recrystallized products will be characterized by ^1H , ^{13}C , and ^{19}F NMR. After examining the 4-fluoro derivative students will discover that assigning protons to specific carbons with the less symmetric 2- and 3- substituted derivatives is more difficult. 2D NMR will then be used to unambiguously complete the assignments of the nonsymmetric 2- and 3- fluoro substituted complexes.

CHM 251 Advanced Inorganic Chemistry: In CHM 251 students will prepare and characterize carboranes as described by Szafram, Pike, and Singh in *Microscale Inorganic Chemistry*.¹⁴ Following their published procedures, potassium dodecahydro-7,8-dicarb-*nido*-undecaborate(1-) and 3-(5-cyclopentadienyl)-1,2-dicarb-3-cobalta-*closo*-dodecaborane(11) will be prepared. Complementing the IR and magnetic moment characterization currently available, students will complete the characterization by ^1H , ^{13}C , and ^{11}B NMR.

CHM 261 Physical Chemistry I: In CHM 261 we will utilize NMR to make kinetics and equilibrium measurements which will replace some of the older gas experiments. In particular, we will study the kinetics of the internal rotation of N,N-dimethylacetamide using a spin-saturation method¹⁵ as an alternative to classical line-broadening techniques. This experiment will be added during the second half of the course when we cover kinetics. This experiment provides a chemically simple system which undergoes hindered rotation about the O=C–N amide bond due to partial resonance of the carbonyl electrons with the nitrogen lone pair electrons. This rotation rate fol-

lows a temperature dependence given by the Arrhenius equation and is an easy example of measuring a temperature dependent rate. The selective saturation of one peak (which we cannot do with our current instrument) will be simple with the proposed instrument. Students will be introduced to the theory of NMR relaxation in this experiment as well. Complete analysis of the data will generate the transition state activation parameters for this molecule, E_a , G^\ddagger , H^\ddagger and S^\ddagger .

CHM 262 Physical Chemistry II: The NMR spectrometer will be used as a tool to teach quantum mechanics in CHM 262 in which students learn the basics of operators and wavefunctions. NMR is a perfect experiment for quantum mechanical demonstrations since it is one of the few physical phenomena well described with low level perturbation theory. Dr. Baltisberger has had students in this course do DQF-COSY and Composite Pulse Inversion Recovery experiments, pushing the limits of existing instrumentation. With the new NMR spectrometer, students would be able to do HETCOR, DEPT, INADEQUATE and other more advanced experiments.

In CHM 262 we will add three experiments. In this course students are given an array of experiments to choose from so not all students would do all three experiments, but they would undoubtedly do at least one and possibly two of these. We have chosen this course as a suitable venue to introduce some exotic experiments which are probably not found in a normal physical chemistry curriculum. Quantum mechanics in general is a substantial challenge to the students and any experiment which can present the observations in a different light may provide the switch which turns on student comprehension. The first new experiment for this course would be a general introduction to the principles of operation of an NMR spectrometer. This would include learning how to set sweep width, pulse widths, filters, frequencies and setting up simple one and two-dimensional experiments. For an unknown sample, students would acquire 1D ^{13}C and ^1H spectra, perform a T_1 determination, and then conduct a 2D DQF-COSY or HETCOR experiment, illustrating how the combination of ^{13}C and ^1H NMR data may be used to identify a compound.

The second will be a simple NMR imaging experiment described by Per-Ola Quist.¹⁶ In this experiment, field gradients are generated across the x-y plane in the probe using the computer controlled course X and Y shims of an instrument. The sample will be a Teflon plug with two holes drilled in it, each filled with water. In the experiment the 1D spectra will be taken under different

gradient settings as the field gradient is rotated in the x-y plane. Using a simple back projection algorithm, students may generate a rough “image” of the two holes in the plug, much the way an MRI instrument would be used to generate the image of a leg, brain or other organ.

The third experiment would be an introduction to nuclear quadrupolar resonance (NQR) spectroscopy and Berry’s phase.^{17,18} The system to be studied is a single crystal of NaClO_3 which is rotated using a magic-angle spinning probe outside of a magnetic field.¹⁹ The ^{35}Cl NQR transition at 29.9 MHz is easily observable with our standard MAS probe. This sharp line splits into a multiplet as the sample undergoes rotation and the wavefunctions acquire a geometric phase due to this rotation. The effect provides a case in which Berry’s phase describes perfectly and simply a problem which would be rather complicated to describe with traditional time dependent quantum mechanics. This lab will be designed for the advanced students in the course who are looking for an unusual challenge.

CHM 290 Chemistry Research: All of our chemistry majors are required to have a research experience. This experience is important in allowing students to expand their boundaries and discover what works and what fails on their own, without a strict lab procedure which has been duplicated repeatedly over the years. An NMR spectrometer aids the research courses considerably in that experiments may now be conducted at Berea which were previously undertaken at other institutions (University of Kentucky, Miami University of Ohio, Indiana University, Ohio State University and Centre College). The amount of time saved will be enormous and more importantly, the students will have a much more hands on experience. Students will be allowed to run the instrument with minimal supervision once they are approved through a short course with Dr. Baltisberger. Combining the NMR with our other instrumentation (see Appendix A) we will have facilities at Berea to do most of the standard analysis that a student might perform in a research environment. In addition, with the solids capabilities under Dr. Baltisberger, the NMR will be utilized for experiments which go beyond the standard experiments. A summary showing how the new NMR spectrometer will be incorporated into the current research projects is given in table 1.

Table 1: Incorporation of NMR into Undergraduate Research at Berea College.

Faculty Member	Probe	Compound	Goal	Experiment	Ref.
Baltisberger, Wempe	^1H , ^{13}C	5-hydroxy-adamantanone and derivatives	Diastereofacial selectivity experiments	2D NOESY NMR	20
Baltisberger	^{31}P , ^{23}Na	NaPO_3 glasses	Evaluate relationship between chain lengths and structure	Liquid NOESY, Solid State MAS	21-24
Blair	^1H , ^{13}C	Bis(amine) halogen (I) complexes	Determine dynamics of ligand exchange. Structural characterization of these complexes.	1D Exchange, Spin Saturation Transfer, and Line Broadening, 2D COSY & NOESY	15
Beebe	^1H , ^{13}C	NIS complexes with tetrabutyl ammonium halides and quinuclidine	Structural elucidation, oxidation selectivity	1D liquids, 2D COSY	25
Roecker	^1H , ^{13}C , ^{31}P	Transition metal surfactants	Intramolecular hydrogen bonding interactions of ligands coordinated to Co(III).	1D liquid state experiments, 2D COSY	

3. Equipment

A. Equipment Request: As outlined in the narrative above, an NMR spectrometer is of highest need at Berea College to add experiments to teach our students this important tool for structure and dynamics determination. Our existing instruments are not capable of doing the kinds of innovative and new experiments proposed. In addition, our undergraduate research program has been hampered by the lack of such an instrument. In short, with current needs and resources at Berea College, now is the time to buy a new NMR spectrometer. The high field NMR spectrometer we are requesting is a Varian Mercury 300. We have also considered Varian Innova, Chemagnetics Infinity, Bruker Avance and JEOL Eclipse instruments. The reason we are looking at a 300 MHz NMR spectrometer is that the cost differential between a 300 MHz instrument and a lower field (250 MHz or below) is not substantial relative to the enormous benefits. Also, a 300 MHz instrument provides a field high enough that we can examine moderately large molecules. This is still probably not large enough to do any serious molecular biology, protein, nucleic acid or carbohydrate work, but it is large enough to study effectively any molecules we use in our laboratory courses. In addition, Dr.

Baltisberger has already purchased a 300 MHz CPMAS probe and high power amplifiers (currently used for his research projects in instruments at Centre College, University of Kentucky and Ohio State University.) We would like to be able to use these resources at Berea both in our classes as well as in research. A higher field instrument would pose difficulties in using this equipment at Berea, so we feel a 300 MHz instrument is most appropriate for our needs.

The reason a Varian Mercury system is being considered is primarily the cost and performance of such a system. The Varian Innova and Bruker Avance systems cost substantially more and have better overall performance than a Varian Mercury (more channels, faster digitizers, pulse shaping capabilities). However, these research grade instruments are equivalent to the Mercury for performing routine experiments (including experiments such as 2D COSY, NOESY, and HETCOR.) For solid state applications, the Mercury sacrifices some sweep width and sampling performance, but all of the basic experiments are again accessible with this instrument. The JEOL eclipse is similar in price and performance with the Mercury, however some of its computer and RF technology is somewhat older and will probably be redesigned in the coming years. The Mercury, on the other hand, is a new instrument (2 years in production) and has been designed to use modern technology from the ground up. The Chemagnetics instrument, while a very strong performer in the area of solid state experiments, lacks some of the essential features to make liquid state experiments convenient and easy.

B. Equipment on Hand: As indicated in Appendix A, we have a wide array of instrumentation. Other than a high-field NMR spectrometer, the Department is well-equipped to support its undergraduate program. We will continue to use our EM360 and JEOL FX90Q as instruments for quick ^1H experiments in the introductory courses. We have a DEC workstation for computational modeling and a Macintosh computer lab (sixteen PowerPC 7100/80 computers for student and classroom use) for other data workup.

C. Implementation and Equipment Maintenance: Depending upon delivery times and award notification date, we certainly should be able to implement our program beginning in the Spring semester of 1999 (possibly for CHM 262 in Fall of 1998). One of the PI is already familiar with Varian software and hardware. Other new users will be required to complete a training course offered by

Dr. Baltisberger which will incorporate basic theory as well as operation of the instrument. Successful completion of a practical exam will be required before students are permitted to sign-up for unsupervised instrument time. If need be, blocks of time outside the allotted class period will be reserved for specific class use. The spectrometer will be utilized mornings, evenings, and weekends for undergraduate research purposes.

Spectrometer maintenance will be conducted primarily by Harry Buswell (our instrument repair specialist) and Dr. Baltisberger (who has extensive experience maintaining NMR spectrometers, see next section below.) We plan on purchasing a basic service contract initially until we feel confident in the instrument maintenance. Cryogen costs are expected to be less than \$2500 annually, and the Department will assume this expense with Dr. Baltisberger performing helium and nitrogen fills. He will also be responsible for training other faculty members and Harry Buswell in this procedure.

4. Faculty Expertise

Jay H. Baltisberger is an assistant professor of chemistry and the Principal Investigator. He received his Ph.D. with Professor Alexander Pines at the University of California, Berkeley in 1993, in which his thesis work involved the development of new NMR techniques. He has performed NMR experiments on solids as well as liquids. He has extensive experience in the collection and processing of multi-dimensional NMR spectra as well as a strong theoretical background. He has extensive experience in the operation and maintenance of NMR spectrometers, including building NMR probes, electronics and writing pulse programs on a variety of instruments. While in graduate school he shared responsibility for maintaining seven superconducting NMR spectrometers. These duties included performing routine liquid nitrogen and helium fills. He currently teaches physical chemistry and physical chemistry laboratory and will be responsible for training new users and developing interfaces for students.

Lee E. Roecker, Co-Principal Investigator, is an inorganic chemist who is an associate professor of chemistry at Berea. Lee Roecker teaches advanced inorganic chemistry as well as instrumental analysis where he devotes fully one-fourth of the class to NMR spectroscopy. Lee anticipates that the new high field instrumentation will greatly enhance this portion of the course (as

mentioned earlier). Lee has a good understanding of NMR and in particular its applications to inorganic systems. He has experience using Varian instrumentation at the University of Kentucky where his research interests over the past few years have relied heavily on ^1H and ^{13}C NMR in a project that is examining the reactivity of urea derivatives coordinated to Co(III).

Larry Blair, Co-Principal Investigator, is currently acting dean of the faculty (returning full-time to the department in August 1998) and is a full professor of chemistry, specializing in organic chemistry. Larry actively uses NMR spectroscopy in his research with undergraduates and will bring this expertise in NMR spectroscopy to his organic chemistry courses (CHM 221, CHM 222 and CHM 252) as well.

5. Dissemination and Evaluation

We will use three methods of dissemination. First, we will publish procedures and data from experiments developed with the NMR Spectrometer in the Journal of Chemical Education. Second, we will continue utilizing our world wide web page to publish syllabi and experimental procedures/results from our courses. Third, through our interactions in the Appalachian Colleges Association (of which Berea is a member) we will open our doors for colleagues at these schools to work with us and help them to implement our experiments at their home institutions. Finally, we will publish reports in the CUR Quarterly which is a journal with a somewhat different but distinctly interested readership. As well, we anticipate showing research results at regular conferences in our various disciplines, and reporting educational project results at both the Project Kaleidoscope and the National Council on Undergraduate Research annual conferences.

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- PROFESSIONAL AFFILIATIONS** Project Kaleidoscope Faculty 21 Class of 1995; American Chemical Society; Mineralogical Society of America; Council of Undergraduate Research; American Physical Society; Phi Lambda Upsilon
- SELECTED PUBLICATIONS (10 relevant/current)**
Multiple-Quantum Magic-Angle Spinning and Dynamic-Angle Spinning NMR Spectroscopy for Quadrupolar Nuclei, S. Wang, Z. Xu, J.H. Baltisberger, L.M. Bull, J.F. Stebbins, A. Pines. *Solid State Nuclear Magnetic Resonance*, **8**, 1-16 (1997).
Triple-Quantum Two-Dimensional ²⁷Al Magic-Angle Spinning Nuclear Magnetic Resonance Spectroscopic Study of Aluminosilicate and Aluminate Crystals and Glasses, J.H. Baltisberger, Z. Xu, J.F. Stebbins, S. Wang, A. Pines. *Journal of the American Chemical Society*, **118**, 7209-7214 (1996).

Solid-State ^{17}O Magic-Angle and Dynamic-Angle Spinning NMR Study of the SiO_2 Polymorph Coestie, P.J. Grandinetti, J.H. Baltisberger, I. Farnan, J.F. Stebbins, U. Werner and A. Pines. *Journal of Physical Chemistry*, **99**, 12341-12348 (1995).

Chemical Structure and Oxygen Dynamics in $\text{Ba}_2\text{In}_2\text{O}_5$, S.B. Adler, J.A. Reimer, J.H. Baltisberger and U. Werner, *Journal of the American Chemical Society* **116**, 675-681 (1994).

Cross Polarization Dynamic-Angle Spinning of ^{17}O in L-Alanine, S.L. Gann, J.H. Baltisberger, E. W. Wooten, H. Zimmermann and A. Pines, *Bulletin of Magnetic Resonance* **16**, 68 (1994).

Cross Polarization Under Dynamic-Angle Spinning Conditions, J.H. Baltisberger, S.L. Gann, P.J. Grandinetti and A. Pines, *Molecular Physics* **81**, 1109-1124 (1994)

Pure Absorption-Mode Lineshapes and Sensitivity in Two-Dimensional Dynamic-Angle Spinning NMR, P.J. Grandinetti, J.H. Baltisberger, A. Llor, Y.K. Lee, U. Werner and A. Pines, *Journal of Magnetic Resonance A* **102**, 72-81 (1993).

Dynamic-Angle Spinning Without Sidebands, S.L. Gann, J.H. Baltisberger and A. Pines, *Chemical Physics Letters* **210**, 405-410 (1993).

Identification of the Disorder in Network Modified Silicate Glasses, I. Farnan, P.J. Grandinetti, J.H. Baltisberger, J.F. Stebbins, U. Werner, M.A. Eastman and A. Pines, *Nature* **358**, 31-35 (1992).

^{87}Rb Dynamic-Angle Spinning NMR Spectroscopy of Inorganic Rubidium Salts, J.H. Baltisberger, S.L. Gann, E.W. Wooten, T.H. Chang, K.T. Mueller and A. Pines, *Journal of the American Chemical Society* **114**, 7489-7493 (1992).

SELECTED PRESENTATIONS

“Distributions of Chemical Shift Anisotropy Parameters in Sodium Phosphate Glasses,” 38th Experimental NMR Conference, Orlando, FL, March 1997

“Introduction to Solid-State NMR and Novel Applications to Glasses”, University of Cincinnati Chemistry Department Seminar, Cincinnati, OH, February, 1997

“Novel Applications of Dynamic-Angle Spinning NMR,” Mount Holyoke College Chemistry Department Seminar, South Hadley, MA, January 1993.

“Characterization of Disorder in Network Modified Silicate Glasses Using Dynamic-Angle Spinning NMR,” 26th Congress Ampere on Magnetic Resonance, Athens, Greece, September, 1992.

“ ^{17}O Dynamic-Angle Spinning NMR Studies of Silicate Glasses,” 1991 American Geophysical Union Fall Meeting, San Francisco, CA, December 9-13, 1991.

Larry Blair
BEREA COLLEGE

- EDUCATION** *Ph.D. in Chemistry*, Stanford University, CA, 1970. Thesis work: Gas Phase Acidities by Ion Cyclotron Resonance Spectroscopy.
B.A. in Chemistry, Berea College, KY, 1966.
- EXPERIENCE** *Dean of the Faculty*, Berea College, 1996-present
William J. Hutchins Alumni Professor of Chemistry, Berea College, 1992-present.
Chair, Natural Science, General Studies Core Course, Berea College, 1987-1994.
Professor of Chemistry, Berea College, 1984-1992.
Associate Professor of Chemistry, Berea College, 1977-1981.
Assistant Professor of Chemistry, Berea College, 1971-1977.
- DOCTORAL ADVISORS** John Brauman, Professor of Chemistry, Stanford University and
and John Baldeschwieler, Professor of Chemistry, California Institute
of Technology.
- COLLABORATORS** Carolyn P. Brock, Professor, University of Kentucky
- RESEARCH STUDENTS** Peter Willis (Berea College Class of 1994), Aaron Bailey (Biology,
BC '94), Brian Napier (BC '94), Tianpei Xin (BC '96), additional 37
other research students since 1990.
- AWARDS AND HONORS** Fellow, American Association for the Advancement of Science, 1995;
National Science Foundation RUI Grant, 1987-90; NSF RUI Renewal
Grant, 1990-93; The Camille and Henry Dreyfus Teaching/Research
Postdoctoral Program, 1990-91; Seabury Award for Excellence in
Teaching, Berea College, 1983; Various research grants from Research
Corporation, Tennessee Eastman Company, National Science Founda-
tion, and The Camille and Henry Dreyfus Foundation, 1971-1990.
- PROFESSIONAL AFFILIATIONS** Council on Undergraduate Research; American Chemical Society;
American Association for the Advancement of Science
- SELECTED PUBLICATIONS (10 relevant/current)**
Selective Oxidation of Secondary Alcohols by Bis(quinuclidine)bromine(I) Bromide, L. Blair, R.
Bledsoe, K. Burberry, and J. Struss. *J. Org. Chem.*, in preparation.
A New Positive Halogen Reagent. Oxidation of Secondary Alcohols to Ketones by
Bis(quinuclidine) bromine(I) Bromide in the Presence of Pyridinium Catalyst. L. Blair, S. Hobbs,
N. Bagnoli, L. Husband, N. Badika. *J. Org. Chem.*, **57**, 1600-1603 (1992).
Structure of Bis(quinuclidine)iodine(I) Tetrafluoroborate. L. Blair, C. Brock, Y. Fu, P. Chen, and
M. Lovell. *Acta. Cryst. C.*, **44**, 1582 (1988).
A New Br⁺ Reagent. Oxidation of Alcohols to Carbonyl Compounds by Bis(quinuclidine) bro-
mine(I) Tetrafluoroborate. L. Blair, K. Parris, O. Lee, K. Jenkins, R. Feese, T. Belcher, D. Badger,
D. Morris, and C. Kuhn. *J. Org. Chem.*, **51**, 5454 (1986).
A Stable Br⁺ Complex. A Twisted Bicyclo[2.2.2]octane Derivative. Synthesis and Structure of
Bis(quinuclidine)bromine(I) Tetrafluoroborate. L.K. Blair, K.D. Parris, P.S. Hii, C.P. Brock. *J.*
Am. Chem. Soc., **105**, 3649-3653 (1983).

Halogen-Amine Complexes in Chemical Synthesis. I. The Oxidation of Alcohols by 1,4-Diazabicyclo[2.2.2]octane-2Br₂ Complex. L.K. Blair, J. Baldwin, W.C. Smith, Jr. *J. Org. Chem.*, **42**, 1816 (1977).

Tetrahedral Intermediates in Gas-Phase Ionic Displacement Reactions at Carbonyl Carbon. O.I. Asubiojo, L.K. Blair, J.I. Bauman. *J. Am. Chem. Soc.*, **97**, 6685 (1975).

Formation, Reactivity, and Relative Stability of Clustered Alkoxide Ions by Ion Cyclotron Resonance Spectroscopy. L.K. Blair, P.C. Isolani, J.M. Riveros. *J. Am. Chem. Soc.*, **95**, 1057 (1973).

Ion Cyclotron Resonance Spectroscopy. J.I. Brauman, L.K. Blair. *Determination of Organic Structures by Physical Methods*, **5**, F.C. Nachod, J.J. Zuckerman, Eds., Academic Press, New York, 151 (1973).

Gas-Phase Acidities of Alcohols. J.I. Brauman, L.K. Blair. *J. Am. Chem. Soc.*, **92**, 5986 (1970).

Lee E. Roecker
BEREA COLLEGE

- EDUCATION** *Ph.D. in Chemistry*, University of North Carolina, Chapel Hill, 1985.
M.S. in Chemistry, University of Cincinnati, Cincinnati, OH, 1982, *Summa Cum Laude*. (Edward Deutsch)
B.S. in Chemistry, University of Cincinnati, Cincinnati, OH, 1981, *Magna Cum Laude*. (Edward Deutsch)
- EXPERIENCE** *Associate Professor of Chemistry*, Berea College, 1996-present
Assistant Professor of Chemistry, Berea College, 1989-1996.
Assistant Professor of Chemistry, University of Dayton, 1988-1989.
Postdoctoral Fellow, Ohio State University (D. H. Busch), 1987-1988.
Postdoctoral Fellow, Australian National University (A. M. Sargeson), 1985-1987
- DOCTORAL ADVISOR** Thomas J. Meyer, Professor of Chemistry, University of North Carolina
- COLLABORATORS** Jeanette Krause-Bauer, Staff Crystallographer, University of Cincinnati;
W. Greg Jackson, Professor, University of New South Wales, Australian Defence Force Academy, Canberra, Australia
- RESEARCH STUDENTS (last 5 years)** Liwen Liu (Berea College Class of 1996), Angie Carrier (Agriculture, BC '94), Jun Xu (BC '98), L. Nelson Elam (BC '96), Anastasia Coots (BC '97), Anne Kinton (BC '97), Janet Akande (BC '97), Irina Gagau (BC '98), Hershel Jude (BC '98), Denny Marshall (BC '97), Joni Norris (BC '98), Pele Okullo (BC '96), Laura Bertram (BC '96), Robert Little (BC '96), Tianpei Xin (BC '96), Li Jing Sun (BC '95), Joseph Bogale (BC '96), Jason Swango (BC '95), Sisay Gebrekidan (BC '96), Mike Clark (BC '96), Charlotte Mundy (Agriculture, BC '96), Shing Mirn Lee (Mathematics, BC '96), Miranda Prewitt (BC '96), Regina Hicks (BC '94), Bereket Berhane (Physics/Mathematics, BC '94), Thomas Demond (Agriculture, BC '94)
- AWARDS** Appalachian Colleges Association Mellon Research Grant 1995, 1996;
National Science Foundation-ILI Grant, 1992
- PROFESSIONAL AFFILIATIONS** Council on Undergraduate Research; American Chemical Society;
Kentucky Academy of Sciences, Board of Directors
- SELECTED PUBLICATIONS (10 relevant/current)**
Space Exploration and Instrumental Analysis: An Internet Experience, L. Roecker. *Council on Undergraduate Research Quarterly*. March (1997).
Analysis Of First-Order Kinetic Data By A Differential Technique. L. Roecker, S.M. Lee, L. Liu, L.J. Sun, K. Zaerpoor. *International Journal of Chemical Kinetics*, **29**, 333-338 (1997).
Synthesis and Base Hydrolysis of the Pentaammine(dimethyl sulfide)cobalt(III) Ion, A. Ellis, A. Fultz, R. Hicks, T. Morgan, L. Parsons, M.J. Saderholm, L.A. Smith, M. Stabb, J.K. Starnes, L.J. Sun, L. Roecker. *Australian Journal Chemistry*, **45**, 2049-2055 (1992).
Oxidation of Hydroquinones by [(bpy)₂(py)Ru^{IV}(O)]²⁺ and [(bpy)₂(py)Ru^{III}(OH)]²⁺. Proton-Coupled Electron Transfer, R.A. Binstead, M.E. McQuire, A. Doveloglou, W.K. Seok, L. Roecker, T.J. Meyer, *Journal of the American Chemical Society*, **114**, 173 (1992).

Intramolecular Hydrolysis of Coordinated Acetonitrile in a Binuclear Complex of Cobalt(III). X-Ray Crystallographic Analysis of Salts of $[(\text{tren})\text{Co}(\mu\text{-NH}_2, \mu\text{-L})\text{Co}(\text{tren})]^{4+}$ (L = OH, $\text{CH}_3\text{C}(\text{O})\text{NH}$), N.W. Alcock, I.I. Creaser, N.J. Curtis, L. Roecker, A.M. Sargeson, A.C. Willis, *Australian Journal Chemistry*, **43**, 643-54 (1990).

Intramolecular Quadridentate Synthesis: X-Ray Crystallographic Analysis of $[(\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2)\text{Co}(\text{NH}_2(\text{CH}_2)_2\text{N}=\text{C}(\text{NH}_2)\text{CH}_2\text{S}(\text{CH}_2)_2\text{NH}_2)](\text{CF}_3\text{SO}_3)_3 \cdot \text{H}_2\text{O}$, E. Deutsch, J. Lydon, L. Roecker, *Australian Journal Chemistry*, **42**, 339-47 (1989).

Intramolecular Condensation of Coordinated Acetonitrile with an Amido Ion in a Binuclear Complex of Cobalt(III). X-ray Crystallographic Analysis of $\text{Na}[(\text{NH}_3)_3\text{Co}(\mu\text{-OH}, \mu\text{-NH}_2, \mu\text{-CH}_3\text{C}(\text{NH}_2)_2)\text{Co}(\text{NH}_3)_3](\text{S}_2\text{O}_6)_2 \cdot \text{H}_2\text{O}$, L. Roecker, A.M. Sargeson, A.C. Willis, *Journal of the Chemical Society Chemical Communications*, 119-121 (1988).

Hydrogen Atom Transfer in the Oxidation of Hydrogen Peroxide by $[(\text{bpy})_2(\text{py})\text{Ru}^{\text{IV}}=\text{O}]^{2+}$ and $[(\text{bpy})_2(\text{py})\text{Ru}^{\text{III}}\text{OH}]^{2+}$, J. Gilbert, L. Roecker, T.J. Meyer, *Inorganic Chemistry*, **26**, 1126-1132 (1987).

Oxygen Atom Transfer in the Oxidations of Dimethyl Sulfide and Dimethyl Sulfoxide by $[(\text{bpy})_2(\text{py})\text{Ru}(\text{O})]^{2+}$, L. Roecker, J.C. Dobson, W.J. Vining, T. J. Meyer, *Inorganic Chemistry*, **26**, 779-781 (1987).

Hydride Transfer in the Oxidation of Alcohols by $[(\text{bpy})_2(\text{py})\text{Ru}(\text{O})]^{2+}$. A $k_{\text{H}}/k_{\text{D}}$ Kinetic Isotope Effect of 50, L. Roecker, T.J. Meyer, *Journal of the American Chemical Society*, **109**, 746-754 (1987).

SELECTED PRESENTATIONS

“A Quantitative use of ^{57}Fe Mössbauer Spectroscopy- The Determination of Amorphous and Crystalline Ferric Phosphate in Commercial Samples.” Kentucky Academy of Sciences, Frankfort, KY, November, 1996.

“Analysis of First-order Kinetic Data by a Differential Technique.” Kentucky Academy of Sciences, Frankfort, KY, November, 1996.

“Synthesis, Characterization, and Reactivity of a bis(ethylenediamine)cobalt(III) Complex of *N*-(2-pyridylmethyl)urea.” Western Kentucky University, Departmental Chemistry Seminar, 1996.

“Synthesis and Reactivity of Cobalt(III) Complexes Coordinated by Monodentate and Bidentate Thioether Ligands- Observation of a Large Chelate Effect.” Kentucky Academy of Sciences, Bowling Green, KY, November, 1995.

“Collaborative Writing With Undergraduate Students.” 1994 Conference on College Composition and Communication, Nashville, TN. March, 1994.

“The Kinetics and Mechanisms of Carbon/Sulfur Cleavage in a Thioether Ligand Coordinated to Cobalt(III).” ACS Southeastern Regional Meeting, Johnson City, TN, October 19, 1993.

ILI DETAILED BUDGET (EQUIPMENT LIST)

Item	Number	Unit Price (list)	Unit Price (discounted)	Total Price (discounted)
1. JEOL Ecliplse+300 MHz Broadband NMR Spectrometer				
Magnet/Shim System :				
7.05 T superconducting magnet with 54 mm bore, 14 channel shims and lock, L-He transfer tube				
RF Section: Broadband transmitter, ¹ H and X Decouplers, ² H Internal Lock and frequency synthesizers				
Digital Acquisition control system				
Host Workstation: SGI Indigo ² with DELTA FT-NMR Software package, 4.0 GB DAT				
Probes and Accessories: 2 Channel Broadband VT Probe with ¹ H/ ¹⁹ F and ¹⁵ N to ³¹ P channels.				
	1	\$215,730		
2. High power duplexer and cables for detection using high power amplifiers	1	\$15,990		
3. Anti-vibration legs	1	\$8,060		
4. Liquid He for installation	1	\$2,000		
5. JEOL Educational Discount	1		-\$41,730	
		\$241,780	\$200,050	\$200,050
		Total Project Cost:		\$200,050
		Non-NSF Contribution:		\$100,050
		NSF Request:		\$100,000

Appendix A: Major Equipment

Type	Brand	Model Number	Year Acquired/Cost
AA Spectrometer	Unicam	929	1995/\$25,000
GC (x2)	Varian	3400	1990/\$20,000
DEC Alpha Workstation	Data Systems	500	1997/\$15,000
GAUSSIAN94	Gaussian	G94	1997/\$2,000
GC	Varian	3700	1986/\$8,000
GC	Hewlett-Packard	5890	1993/\$12,000
GC/MS	Hewlett-Packard	5890/5972	1996/\$65,000
FT-NMR (90 MHz)	JEOL	FX90Q	1992/Donation
NMR Data-system	Tecmag	Leo-J	1993/\$15,000
High Power RF Amp	AMT	M3446	1996/\$13,100
MAS NMR Probe	Varian	VT	1996/\$35,100
		CPMAS/300NB	
CW-NMR (60 MHz)	Varian	EM360	1979/Donation
FTIR	Mattson	RS1000	1994/\$30,000
UV/Vis Spectrometer	Perkin-Elmer	Lambda 3B	1990/\$10,000
UV/Vis Spectrometer	Varian	Cary 219	Donation
CW-IR (x2)	Perkin-Elmer	710 B	Donation
Polarographic Analyzer/ Stripping Voltmeter	EG&G	264A	1992/\$20,000
Potentiostat/Galvanostat	EG&G	273A	1992/\$20,000
SMDE	EG&G	303A	1992/\$5,000
Polarimeter			
pH Meters (x4)	Fisher		
Rotary Evaporator (x2)	Brinkmann	RE111	
VIS Spectrometer (x10)	Milton Roy	Spectronic 20D	1985-1996
HPLC	*	*	1997/\$24,000

*we have recently been approved \$24,000 by Berea College to purchase a new HPLC. The bids are just going out (so we have no firm instrument manufacturer or model specifications), but we anticipate this will be in place by mid-spring.

Appendix B: Description of Courses Impacted Substantially by Project

***CHM 222. ORGANIC CHEMISTRY II.** A continuation of CHM 221. The study of the chemistry of aldehydes, ketones, amines, carboxylic acids, carbohydrates, and benzene derivatives. The course will include multi-step organic synthesis, reaction mechanisms, and mass spectroscopy. Prerequisite: CHM 221. Three lectures and one 3-hour laboratory period each week. Annual Enrollment†: 30.

CHM 242. INSTRUMENTAL ANALYSIS. An advanced course that explores how various analytical instruments work and how our understanding of chemistry is enhanced by the use of instrumental techniques. The course is divided into four units- analytical separations, UV/Vis and infrared spectroscopy, NMR spectroscopy, and electrochemistry. In laboratory, students will have the opportunity to use state of the art UV/Vis, infrared, nuclear magnetic resonance, and atomic absorption spectrometers in addition to several gas chromatographs, a mass spectrometer, and a variety of electrochemical equipment. There will be 3 hours of lecture and 3 hours of laboratory work each week. Prerequisite CHM 241. Offered in the spring each year. Annual Enrollment†: 10.

CHM 251. ADVANCED INORGANIC CHEMISTRY. An advanced course that investigates modern concepts in inorganic chemistry including atomic and molecular orbital theory, molecular symmetry, periodicity, ligand field theory, and coordination chemistry. There will be 3 hours of lecture and 3 hours of laboratory work each week. Prerequisite CHM 222, CHM 241, MAT 130, PHY 116 or PHY 215. Offered in the spring of alternate years. Annual Enrollment†: 5.

***CHM 261. THERMOCHEMISTRY.** An advanced study of classical thermodynamics and chemical kinetics. Topics include a detailed study of energy, entropy and enthalpy, multi-component phase diagrams, real gases, electrochemical systems, reaction kinetics and transport processes. The fundamental goal is to achieve a physical description of general chemical phenomena with a strong emphasis on mathematical models. There will be 3 hours of lecture and 3 hours of laboratory work each week. Prerequisites: CHM 241; PHY 116; MAT 130. Three lectures and one 3-hour laboratory periods each week. Annual Enrollment†: 15.

CHM 262. QUANTUM CHEMISTRY. An advanced study of quantum mechanics and statistical mechanics. Topics include in-depth treatment of various fundamental problems in quantum mechanics (particle in a box, rigid rotor, harmonic oscillator), applications of these problems to chemical systems, atomic and molecular orbital theory and structure, spectroscopy, lasers and statistical mechanics. The fundamental goal is to achieve a physical description of the quantum nature of matter and how this manifests itself in chemical problems. This course relies heavily on mathematical approximations to difficult differential equations and interpretation of these answers in terms of probabilities. There will be 3 hours of lecture and 3 hours of laboratory work each week. Prerequisites CHM 241, MAT 130, PHY 116. Annual Enrollment†: 5.

***CHM 290. INDEPENDENT STUDY.** A program of directed research that involves laboratory experiments and literature study. A laboratory experience in CHM290 is required of all chemistry majors unless the requirement is waived in lieu of an equivalent experience approved by the Chemistry Department. Prerequisite by permission of the instructor. Offered as requested and as faculty time allows. Annual Enrollment†: 2-4 (varies with offerings).

Total number of students affected over next 5 years: 700 (Many of these students will use the spectrometer in 5 or 6 courses)

† Enrollments indicate yearly average enrollment over 5 year period for all sections of a course.

* Course required of all majors.

Appendix C: Chemistry Majors

Year	Chemistry Graduates	Graduate School	Medical and Allied Health	Industry	Teaching and Others
1997	13	6	2	4	1
1996	9	5	2	1	1
1995	4	2	1	0	1
1994	10	3	4	3	0
1993	8	5	2	0	1
Totals	44	21	11	8	4

Graduate Schools

Harvard University
 Johns Hopkins University
 University of Kentucky
 University of Cincinnati
 University of North Carolina
 Montana State University
 Rochester University
 Drexel University
 Stanford University
 University of California, Davis
 University of Tennessee, Knoxville
 University of Virginia
 Wake Forest University
 Purdue University

Medical Schools

University of Kentucky
 University of Louisville
 Johns Hopkins University
 Tufts University
 University of Virginia

Industry

Ashland Oil
 USDA
 FDA
 Proctor and Gamble
 Other local
 chemical companies

Appendix D: Presentations and Papers Involving Berea College Undergraduates (since 1993)***denotes undergraduate, underscore denotes presenter**

Lee Roecker, Shing Mirn Lee*, Liwen Liu*, Li Jing Sun*, and Koorosh Zaerpoor*. "Analysis of First-order Kinetic Data by a Differential Technique." *International Journal of Chemical Kinetics*. **1997**, 29, 333-338.

Irina Gagua*, Janet Akande*, Jun Xu*, Nelson Elam*, Tianpei Xin*, Lee Roecker. "Synthesis And Reactivity Of Phenylurea Derivatives Coordinated To Cobalt(III)." Kentucky Academy of Sciences, Frankfort, KY, November, 1996.

Joseph Bogale*, Laura Dicken Bertram*, Lee Roecker. "Synthesis Of Transition-Metal Surfactants." Tenth National Conference on Undergraduate Research, UNC-Asheville, April 1996.

Bereket Berhane*, Liwen Liu*, Lee Roecker. "The Kinetics and Mechanisms of Carbon/Sulfur Cleavage & Formation Reactions of Thioether Ligands Coordinated to Cobalt(III)." Tenth National Conference on Undergraduate Research, UNC-Asheville, April 1996.

L.Nelson Elam*, Billy Helton*, Miranda Prewitt*, Tianpei Xin*, Jun Xu*, Lee Roecker. "Synthesis, Characterization, And Reactivity Of Phenylurea Derivatives Coordinated To Cobalt(III)." Tenth National Conference on Undergraduate Research, UNC-Asheville, April 1996.

Larry Nelson Elam*, Billy Helton*, Miranda Prewitt*, Lee Roecker, Anthony C. Willis, Alan M. Sargeson, Tianpei Xin*, and Jun Xu*. "Synthesis, Characterization, and Reactivity of Phenylurea Derivatives Coordinated to Cobalt(III)." ACS Southeastern Regional Meeting, Memphis, TN, November, 1995.

Anastasia S. Coots*, Angie Carrier*, and Lee Roecker. "Determination of the Alleopathic Molecule(s) in the "Tree of Heaven" (*Ailanthus Altissima*) by GC/MS." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Amer Lahamer, Lee Roecker, Chris Langley*, Li Jing Sun*, Scott Taber*, and Christy Hensley*. "Determination of the Amounts of Crystalline and Amorphous Ferric Phosphate using Mössbauer Spectroscopy." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Joni Lynn Norris* and Lee Roecker. "Wood Stuck—Investigations into the Reactivity of Superglue with Wood." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Jun Xu*, Nelson Elam*, Tianpei Xin*, and Lee Roecker. "Reactivity of Phenylurea Derivatives Coordinated to Cobalt(III)." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Nelson Elam*, Jun Xu*, Tianpei Xin*, and Lee Roecker. "Synthesis, Characterization, and Reactivity of Phenylurea Derivatives Coordinated to Cobalt(III)." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Pele Okullo* and Lee Roecker. "Reevaluation of the Activation Parameters for the Base Hydrolysis of a Cobalt(III) Complex Coordinated by Dithiahexane." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Amer Lahamer, Lee Roecker, Chris Langley*, Li Jing Sun*, Scott Taber*, and Christy Hensley*. "A Quantitative Use of ^{57}Fe Mössbauer Spectroscopy." Kentucky Academy of Sciences, Bowling Green, KY, November 16-18, 1995.

Larry K. Blair, Randy K. Bledsoe*, Kieth Burberry*, and John Struss*. "Selective Oxidation of Secondary Alcohols by Bis(quinuclidine)bromine(I) Bromide. A 2-Coordinate Bromine(I) Positive Halogen Reagent." *J. Org. Chem.*, submitted July 1995.

Thomas R. Beebe, Leslie Boyd*, Steve B. Fonkeng*, Jamie Horn*, Teresa M. Mooney*, Matt J. Saderholm*, and Mike V. Skidmore*. "Selective Oxidation of Alcohols Using the 1:1 Complex of N-Bromosuccinimide and Tetrabutylammonium Iodide." *J. Org. Chem.* **1995**, *60*, 6602-6603.

Nelson Elam*, Jun Xu*, Tianpei Xin*, and Lee Roecker. "Synthesis, Characterization, and Reactivity of Phenylurea Derivatives Coordinated to Cobalt(III)." CHEMIST Workshop, Berea College, August 1, 1995.

Jun Xu*, Nelson Elam*, Tianpei Xin*, and Lee Roecker. "Reactivity of Phenylurea Derivatives Coordinated to Cobalt(III)." CHEMIST Workshop, Berea College, August 1, 1995.

Angie Carrier*, Anastasia S. Coots*, and Lee Roecker. "The Alleopathic Effects of the Tree of Heaven on Germination and Growth of Lettuce Seeds." CHEMIST Workshop, Berea College, August 1, 1995.

Joni Lynn Norris* and Lee Roecker. "Wood Stuck- Investigations into the Reactivity of Superglue with Wood." CHEMIST Workshop, Berea College, August 1, 1995.

Amer Lahamer, Lee Roecker, Chris Langley*, Li Jing Sun*, Scott Taber*, and Christy Hensley*. "Determination of the Amounts of Crystalline and Amorphous Ferric Phosphate using Mössbauer Spectroscopy." CHEMIST Workshop, Berea College, August 1, 1995.

Anastasia S. Coots*, Angie Carrier*, and Lee Roecker. "Determination of the Alleopathic Molecule(s) in the "Tree of Heaven" (*Ailanthus Altissima*) by GC/MS." CHEMIST Workshop, Berea College, August 1, 1995.

Pele Okullo* and Lee Roecker. "Reevaluation of the Activation Parameters for the Base Hydrolysis of a Cobalt(III) Complex Coordinated by Dithiahexane." CHEMIST Workshop, Berea College, August 1, 1995.

Jason H. Swango* and Lee Roecker. "Reactivity of Cobalt(III) Complexes Coordinated by Monodentate and Bidentate Thioether Ligands." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 8 April 1995.

Tianpei Xin* and Lee Roecker. Synthesis, Characterization, and Reactivity of a Urea Derivative Coordinated to Cobalt(III). Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 8 April 1995.

Li Jing Sun*, Chris Langley, Lee Roecker, and Amer Lahamer. Measurement of Amorphous and Crystalline Ferric Phosphate by Mossbauer Spectroscopy. Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 8 April 1995. *Li Jingwon honorable mention.*

Joseph Bogale*, Laura Dicken Bertram* and Lee Roecker. "Synthesis of Transition-Metal Surfactants." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 8 April 1995.

Jason H. Swango*, Brian Napier* and Lee Roecker. "Reactivity of Cobalt(III) Complexes Coordinated by Monodentate Thioether Ligands." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 16 April 1994.

Shing Mirn Lee*, Li Jing Sun*, Koorosh Zaerpoor*, and Lee Roecker. "Analysis of First-Order Kinetic Data by a Differential Technique." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 16 April 1994. *Shing Mirn won honorable mention.*

Joseph Bogale*, Laura Dicken Bertram* and Lee Roecker. "Synthesis of Transition-Metal Surfactants." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 16 April 1994.

Liwen Liu*, Paul Harder* and Lee Roecker. "An Unexpected Cyclization Reaction of a Bidentate Thioether Ligand to Form a Tetradentate Ligand." Regional Undergraduate Chemistry Poster Competition, University of Kentucky, Lexington, KY, 16 April 1994.

Liwen Liu*, Paul Harder* and Lee Roecker. "An Unexpected Cyclization Reaction of a Bidentate Thioether Ligand to Form a Tetradentate Ligand." Eighth National Conference on Undergraduate Research, Western Michigan University, April 1994.

Regina Hicks* and Lee Roecker. "Azide Trapping During the Base Hydrolysis of the Pentaamine(dimethyl sulfide)cobalt(III) Ion- Evidence for a Dissociative Mechanism." Eighth National Conference on Undergraduate Research, Western Michigan University, April 1994.

Etta Boss-Cole* and Larry K. Blair. "Halogen-Amine Complexes as New Positive Halogen Reagents." Eighth National Conference on Undergraduate Research, Western Michigan University, April 1994.

Peter Willis* and Larry K. Blair. "Oxidation of Alcohols by Halogen-Amine Complexes. New Positive Halogen Reagents." Eighth National Conference on Undergraduate Research, Western Michigan University, April 1994.

Shing Mirn Lee*, Li Jing Sun*, Koorosh Zaerpoor* and Lee Roecker. "Analysis of First-Order Kinetic Data by a Differential Technique." Kentucky Academy of Sciences, Georgetown, KY, October 21-23, 1993.

Bereket Berhane*, Liwen Liu* and Lee Roecker. "The Kinetics and Mechanisms of Carbon/Sulfur Cleavage in a Thioether Ligand Coordinated to Cobalt(III)." Kentucky Academy of Sciences, Georgetown, KY, October 21-23, 1993. *Liwen won the prize as the outstanding undergraduate presenter in the chemistry division.*

Li Jing Sun*, Koorosh Zaerpoor* and Lee Roecker. "Analysis of First-Order Kinetic Data by a Differential Technique." ACS Southeastern Regional Meeting, Johnson City, TN, October 19, 1993.

Tom Beebe, Leslie Boyd*, Steve Fonkeng*, Jamie Horn*, Teresa Mooney*, Matt Saderholm* and Mike Skidmore*. "Simple and Competative Oxidations of Alcohols With the Complex Formed When N-Bromosuccinimide is Mixed With Tetrabutylammonium Iodide." University of Kentucky Poster Competition, April 24, 1993.

Regina Hicks* and Lee Roecker. "Azide Trapping During the Base Hydrolysis of the Pentaamine(Dimethyl Sulfide)Cobalt(III) Ion- Evidence for a Dissociative Mechanism." University of Kentucky Poster Competition, April 24, 1993.

Li Jing Sun* and Lee Roecker. "Analysis of First-Order Kinetic Data by a Differential Technique." University of Kentucky Poster Competition, April 24, 1993.

Billy Helton* and Lee Roecker. "Synthesis, Characterization, and Reactivity of a Urea Derivative Coordinated to Cobalt(III)." University of Kentucky Poster Competition, April 24, 1993.

Bereket Berhane* and Lee Roecker. "The Kinetics and Mechanisms of Carbon/Sulfur Cleavage in a Thioether Ligand Coordinated to Cobalt(III)." University of Kentucky Poster Competition, April 24, 1993. *Bereket won honorable mention.*

Appendix E: Brief Vitae of Other Berea College Chemistry Faculty**Thomas Beebe**
BEREA COLLEGE

- EDUCATION** *Ph.D. in Chemistry*, University of Wisconsin, Madison, 1960.
A.B and B.S. in Chemistry, Ohio University, Athens, OH, 1954.
- EXPERIENCE** *Nathaniel Southgate Shaler Memorial Professor of Chemistry*, Berea College, 1987-present.
Chairman, Department of Chemistry, Berea College, 1986-present.
Visiting Professor - Cornell University, 1983-1984 & 1991-1992.
Professor of Chemistry, Berea College, 1966-present.
Associate Professor of Chemistry, Berea College, 1963-1966.
Assistant Professor of Chemistry, Berea College, 1959-1962.
- AWARDS AND HONORS** Pew Outstanding Teacher-Scientist in the Appalachian Region, 1987; Kentucky Academy of Science College Teacher of the Year, 1986; Seabury Award for Excellence in Teaching, 1968; Phi Beta Kappa, 1953
- RESEARCH** Has recieved 29 research and teaching grants totalling \$311,700 to work with 152 students over 35 years from funding sources such as PRF, NSF, Research Corporation and Dreyfus Foundation.
- PUBLICATIONS** Fourteen papers in refereed scientific journals on the chemistry of positive iodine compounds, specifically N-iodosuccinimide and acetyl hypoidodite

Michael Wempe
BEREA COLLEGE

- EDUCATION** *Ph.D. in Chemistry*, Miami University of Ohio, Oxford, OH, 1996.
M.S. in Chemistry, Miami University of Ohio, Oxford, OH, 1993.
B.A. in Chemistry, Hanover College, Hanover, IN, 1991.
- EXPERIENCE** *Visiting Assistant Professor of Chemistry*, Berea College, 1996 to present.
Graduate Research and Teaching Assistant, Chemistry Department, Miami University of Ohio, Oxford, OH, 1991 to 1996.
Laboratory Assistant, Chemistry Department, Hanover College, 1991.
- RESEARCH** Supervised 4 summer research students, 1 independent study and 4 short term research students in 1997.
- PUBLICATIONS** Four papers published or submitted to refereed scientific journals on rearrangement of ^{13}C sites in bicyclo-ring systems.