RUNNING HEAD: Undergraduate Research

A Model for Computational Undergraduate Research Using Molecular Orbital Theory And a Low-Cost Unix Workstation

Submitted by

David R. Dinsmore

In partial fulfillment of the

Requirements for the degree of

Doctor of Education

In

Education Leadership

Acceptance of Dissertation

Submitted to the Graduate Faculty
Of Liberty University in
Partial Fulfillment of
The Requirements for the Degree of

DOCTOR OF EDUCATION

In

EDUCATION LEADERSHIP

____
John Pantana, Ed.D.
Committee Chair

____
Ronald Allen, Ph.D.
Committee Member

____
Kathie Johnson, Ed.D.
Committee Member

____
Terry Spohn, Ph.D.
Committee Member

____
Rebecca Carwile, Ed.D.
Associate Dean, Graduate Studies

____
Karen Parker, Ed.D.
Dean, School of Education

____
Date

Abstract

This research study used current molecular orbital theory and UNIX desktop computer workstations running the PSI suite of programs developed by Dr F. Schaefer group of the Center for Computational Quantum Chemistry at the University of Georgia to investigate the structures and characteristics of several hypothetical hydrogen-lithium compounds. The researcher, a physics professor with no background in computational quantum chemistry, and very limited chemistry background, experienced this project much like an upper-level undergraduate science or mathematics major. Approaching the research experience from the perspective of an undergraduate research student, the researcher was able to gain unique insight into the undergraduate research process. This experience helped define an appropriate framework for computational research that can enhance the academic program for science education at smaller, liberal arts institutions. The use of high-speed, relatively inexpensive, desktop computer systems affords a science faculty with a means to produce an undergraduate research program in theoretical computational research comparable to research done at graduate institutions.

The model described in this study draws from the lessons learned in the preparation for and conduct of the computational research, review of feedback from former researchers doing computational quantum chemistry at the undergraduate level, and examination of current literature on the role of research in undergraduate education.

Computational results of this study verify the optimal structures for Li_3H and Li_3H_2 and identify the vibrational frequencies for both molecules. The research model details the stages of an effective undergraduate research experience, the cognitive skills needed for this type of research, and the benefits of computational research for the

student, academic department and the institution. Finally, the research model describes the key components of an effective undergraduate research program: institutional support, department and faculty support, facilities and equipment, and a well-structured program.

May 13, 2004

© Copyright by

DAVID R. DINSMORE

2004

Dedicated to my friend, Randy Davy,

for his faithful, patient mentorship

and to my wife, Sue Ann,

for her constant, loving support.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER I: INTRODUCTION

Research is recognized as a fundamental component of learning for many masters' level and nearly all doctoral level degree programs in this country. Acknowledging the potential benefits for teaching cognitive skills and enhancing subject knowledge, many academic departments have instituted undergraduate research programs. Major research universities have the necessary resources - equipment, facilities, and graduate assistants - to support undergraduate research programs more readily than liberal arts institutions having few or no graduate programs. Science research in chemistry and physics is even more difficult, because of the requirements for sophisticated laboratories and expensive research equipment. However, the availability of high-speed, relatively inexpensive, desk-top computer systems affords a science faculty with a means to produce an undergraduate research program in theoretical computational research areas that is comparable to research done at most graduate institutions.

This research study used current molecular orbital theory and desktop computer systems to investigate the structures and characteristics of several hypothetical hydrogen-lithium compounds. The researcher, a physics professor with no background in computational quantum chemistry, and very limited chemistry background, experienced this project much like an upper-level undergraduate science or mathematics major. Approaching the research experience from the perspective of an undergraduate research student, the researcher was able to gain unique insight into the undergraduate research process. This experience helped define an appropriate framework for computational research that can enhance the academic program for science education at smaller, liberal arts institutions. The model described in this study draws from the lessons learned in the preparation for and conduct of the computational research, review of feedback from former researchers doing computational quantum chemistry at the undergraduate level, and examination of current literature on the role of research in undergraduate education.

Background

In the September 2003 issue of *Physics Today*, Hilborn and Howes (2003) described the efforts of the National Task Force on Undergraduate Physics to determine what distinguishes a good physics program from a great one. The task force project, known as SPIN-UP (Strategic Programs for Innovations in Undergraduate Physics), visited 21 institutions considered to have thriving undergraduate programs. These physics programs were identified based on their ability to produce numbers of physics majors far above typical nationwide values, or institutions that had significantly increased their number of physics majors in recent years. During each site visit, which normally lasted one and a half days, a team met with physics faculty, physics students, and in most cases, faculty from other science departments and school administrators. Based on the site visit reports, the task force was able to extract a number of common features of these excellent programs. One thing all these programs had in common was an undergraduate research program. The *Physics Today* article states:

> Building a thriving undergraduate program involves more than curricular reform. A flourishing program is challenging, but supportive and encouraging. It includes a well-developed curriculum, advising and mentoring, *an undergraduate research program (emphasis added)*, many opportunities for informal student-faculty interactions, and a strong sense of community that enhances those interactions. In addition, the department emphasizes interactions with students as team members

> in departmental efforts such as outreach to the public and to K-12 schools.
> (Hilborn & Howes, 2003, p. 40)

Not only does an undergraduate program enhance the student's educational development, but also it synergistically produces increased opportunities for student-faculty interaction and faculty mentoring, and incorporates students into departmental team efforts. Hilborn and Howes go on to say that the task force found that the critical academic component for reform is the academic department. This is good news, in that the opportunity exists for a science department faculty to initiate effective reforms of the undergraduate program with minimal outside support.

In recent years, the conduct of undergraduate research in both chemistry and physics has required significant funding for research equipment. Often, the procurement of expensive equipment is particularly difficult for institutions that are primarily undergraduate institutions, such as liberal arts colleges, which often do not offer graduate programs that receive major grant monies to purchase research equipment. However, the development of low cost computer workstations, capable of high-speed computations, provides an area for computational research to flourish at almost any institution. In addition, in the past decade, a significant number of grant sources have been developed to support undergraduate research (Tobochnik, 2001; Osteryoung, 1999; Goodwin & Holmes, 1999).

Less than 20 years ago, the complex quantum mechanical calculations required for the prediction of possible molecular structures could only be done on the largest supercomputers. Today, desktop systems, often costing under $20,000 can perform these lengthy calculations in relatively short times. Computational physicists and chemists can use quantum mechanics to predict new compounds and their associated molecular properties. Using the theoretical results from the calculations, experimental researchers at larger research universities, where the necessary laboratory equipment is available, can then fabricate the theoretical molecular structures. The new molecules may lead to a better understanding of chemical bonding, the creation of new technologies, or they may serve to validate current quantum mechanical theory and modeling techniques.

Problem Statement

Can small liberal arts institutions have undergraduate research programs that produce quality research in physics and chemistry given their typically limited resources? If undergraduate students are capable of, and want to do, original research, can the undergraduate science department at a liberal arts institution provide a meaningful research experience for them? Can low-cost desktop computers provide the opportunity for scientific journal level research at a liberal arts institution?

The researcher set out to answer these questions by becoming a researcher in an unfamiliar research area, much like a physics or chemistry major might in his or her junior or senior year. The computational portion of this research focused on determining the structure and characteristics for two hypothetical lithium-hydrogen compounds, Li_3H and Li_3H_2 molecules. As the computational research progressed, the researcher developed a model based on his experience of the theoretical computational research process, the current literature on undergraduate research, and the experiences of other undergraduate researchers from the University of Georgia.

Computational Research

The goal of the computational research was to discover the bond lengths (the physical distance) between the atoms of the lithium-hydrogen molecules and the energy of each molecule. To do this, the researcher provided a description of the starting geometry of the molecule to the computer. Also needed was a description of the symmetry and occupation of the molecular orbitals using group theory. The program used the initial geometry and electron orbital information to make an initial calculation of the total energy of the molecule. The bond lengths were then changed and the energy calculations repeated until the structure with the lowest possible energy was found.

An unbound molecule has a zero energy value, because it is assumed that the individual atoms are far enough away from each other that they are not attracted to one another. The energy of a bound molecule will be negative, which indicates that energy would have to be added (or work done) to separate the molecule into separate atoms. The more negative the energy, the more stable or tightly bound the molecule will be. Once the lowest (optimum) energy configuration is found, the vibrational frequencies for the molecule must be determined in order to verify the stability of the molecule and to allow laboratory researchers to identify the synthesized molecule. These frequencies are the natural vibrational motions that the atom will undergo when it absorbs small amounts of additional energy, somewhat like the natural vibrational frequencies produced when a guitar string is plucked. Laboratory researchers can use spectroscopy to determine these frequencies. In molecular spectroscopy, the newly created molecule is bombarded with infrared radiation. The vibrational frequencies correspond to the frequencies of infrared radiation that are absorbed or emitted by the molecule.

The computations were done at three levels of theory. Each level involved a more sophisticated and more complex model to describe the wave functions of the electrons, which were used to calculate the molecular bond lengths, the total energy, and the vibrational frequencies. Obtaining similar results by each level of theory provided correlation and afforded the researcher a high level of confidence in the results.

As the computational study progressed, the researcher experienced, first hand, the prerequisite academic background and skills required for this type of research, and gained insight into the proficiency an undergraduate researcher must bring to computational research. In addition, the researcher examined how best to structure the research so that a future student might realize the maximum benefit from a similar research experience.

Molecular Orbitals and Symmetry

The basic tenet of this theoretical approach is that in the process of bonding one atom to another, the atomic orbitals combine to form molecular orbitals (MOs). The electrons that occupy these new orbitals can then be thought of as belonging to the molecule as a whole and not the individual atoms (Whitten, Davis & Peck, 1996). In the application of molecular orbital theory, the symmetry of the molecule is a primary consideration. Molecular orbital theory requires that the atomic orbitals must have exactly the same symmetry in order to combine to form bonding molecular orbitals. The principles of group theory are used to determine the symmetry of the various orbitals. The symmetry is specified by an irreducible representation of a point group. The point group is a designation of the symmetry of the particular molecule under consideration, based on its primary axis of symmetry and the locations of the individual atoms. The irreducible representation is a set of numbers that describe how a structure changes under the various symmetry operations. Thus, in the terminology of group theory, molecular orbital theory states that atomic orbitals on different atoms will only interact (to form bonding orbitals) if they belong to the same irreducible representation of the point group of the molecule (Vincent, 1977). For example, a water molecule has an isosceles triangle shape with an oxygen atom at the peak of the triangle and hydrogen atoms at the other two corners, each the same distance away. This geometric shape has four possible symmetry operations, which may change some of the positions of the atoms, but leave the appearance of the molecule unchanged. In the case of water, which belongs to the C_{2V} point group or has C_{2V} symmetry, these four operations include the identity (in which the molecule remains unchanged-this operation is mathematically necessary to account for all possible operations that leave the molecule unchanged), a 180° rotation on a vertical axis through the oxygen molecule, and two reflections – one through a plane containing all three molecules and the other through a plane containing the oxygen molecule and the vertical axis, and perpendicular to the plane containing the three molecules (See Figure 1). Each of the various orbitals of the atom and molecule can then be described by combinations of the four irreducible representations that describe how that orbital is changed or not changed when a symmetry operation is performed (See Appendix A for the complete C_{2V} symmetry table). An atomic orbital for oxygen and an atomic orbital for hydrogen that belong to the same (irreducible) representation in C_{2V} symmetry (the symmetry of water) will have the possibility of forming a molecular bonding orbital.

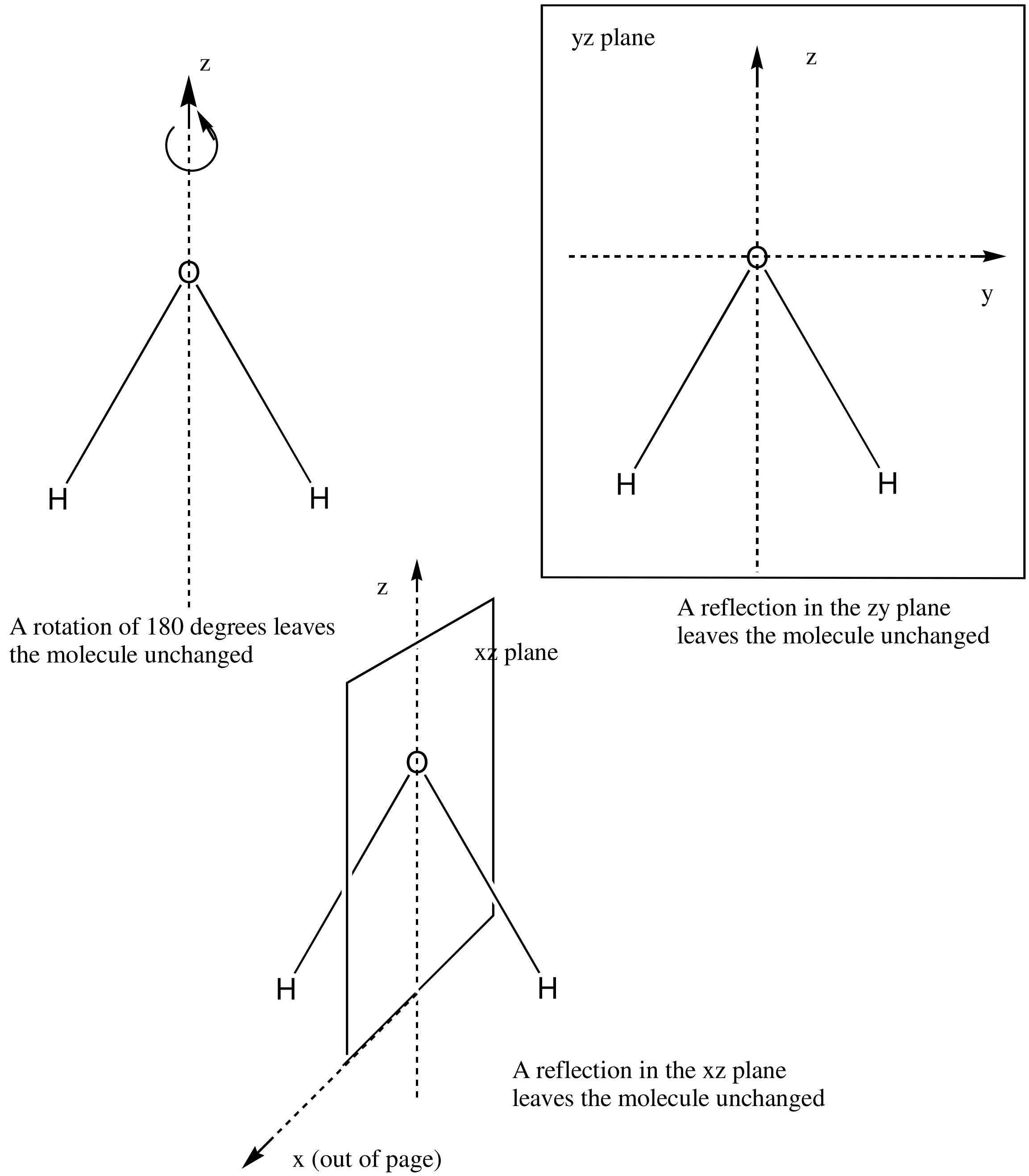

Figure 1. Three of the four symmetry operations that leave the water molecule unchanged (the fourth is the identity operation that changes nothing).

Wave Functions

In quantum mechanics, these molecular orbitals are described by a wave function. Because the mathematical description of the wave function may contain an imaginary part, the wave function only has physical meaning when the wave function is squared. Squaring gives the electron density (a description of where the electron is most likely to be found). Thus, when considering a single atom, the sign of the wave function does not matter; however when orbitals are combined, the signs are important, because when the orbitals overlap, they must be *in phase* (i.e., they must have the same sign). The *in phase* combination of atomic orbitals will result in a bonding orbital (similar to constructive interference with classical waves) and the *out of phase* combination will produce anti-bonding orbitals (as in destructive interference for classical waves). The bonding orbital will result in an energy level for electrons that is lower than either of the two atomic orbitals, thus increasing the potential for formation of a molecule. The anti-bonding orbital will result in an energy level that is higher than the two atomic orbitals and decrease the possibility of forming a molecule.

The electron wave functions are determined by solving the Schrodinger equation, which can only be solved exactly for the hydrogen atom and one-electron ions such as He^+. Before the advent of high-speed computers, approximation techniques for other low proton atoms (with more than one electron) were virtually impossible. Currently, computers enable researchers to use linear combinations of functions to approximate the wave functions for atoms other than hydrogen. Linear combinations of gaussian functions are often used because they yield mathematically simpler solutions than exponential functions. Gaussian functions are also used to approximate the actual hydrogen wave functions. The molecular orbitals, which are formed in the combination of atomic orbitals, can then be constructed by solving for the coefficients of the original (basis set) functions. The PSI suite of programs can use various types of wave functions to perform the calculations and various basis sets to construct the wave functions. In this research, each of the three wave functions techniques utilized used the same basis set – known as 6311PPGSS developed by Pople and coworkers (Davy, Skoumbourdis, & Kompanchenko, 1999).

Computational Methods

The first calculations were performed using the Hartree-Fock self-consistent field wave function (SCF). The SCF wave function method usually provides reliable values for the molecular properties for stable, closed shell molecules. However, when considering unknown molecules, more sophisticated methods must be used to help verify the results obtained from the SCF wave function. Two others are used in this research: the Configuration Interaction wave function model, including all single and double excitations (CISD); and the Coupled Cluster wave function model, including all single and double excitations (CCSD). However, the CCSD wave function can be used only for molecules having no unpaired electrons. Correlating results obtained from the CISD and CCSD wave function calculations validated the results of the SCF wave function, and a high level of confidence can be placed in the theoretical predictions.

Bond Lengths and Energies

The optimal geometry of a molecule is the set of bond lengths and bond angles that result in the lowest possible energy. The energy of the molecule will be a sum of three energies: the electron to nucleus coulomb attraction (given a negative value); the electron-to-electron coulomb repulsion (given a positive value); and the kinetic energy of the electrons (positive value). A bound molecule will have a total energy that is negative, and the more negative the energy, the more stable the compound. Energies are calculated in Hartrees (1 Hartree = 27.2 electron volts).

Figure 2 is a plot of a one-dimensional representation of the total energy of the hydrogen molecule, H_2, for various atomic separation distances between the two hydrogen atoms. The total energy of the molecule is plotted on the vertical scale against the H-H separation distance (or H-H bond length) on the horizontal scale. When the two hydrogen atoms are too close together, the positive-to-positive repulsion of the two atomic nuclei will push the atoms apart, and give a large positive value for the energy of the molecule. The atoms will continue to move apart until the optimum (minimum energy) position is reached. When the two atoms are too far apart, the attractive force is too weak to produce any interaction and the total energy is represented as zero. As the atoms are brought into close proximity with each other, but still beyond the optimum bond length, the attraction of the nucleus (of one atom) to the electron (of the other atom) will pull the atoms toward each other to a lower and ultimately optimal (lowest) energy state. In this lowest energy state, the H-H bond length will correspond to the point on the energy curve where the slope of the curve is zero (flat). PSI uses the wave functions to calculate the energy and slope (first derivative) in three dimensions for some initial guess at the geometry of a hypothetical molecule. Again using the one-dimensional example of hydrogen in Figure 2, if the slope is positive, then the bond length is too long and the program shortens the bond length and recalculates the energy and slope. If the slope is

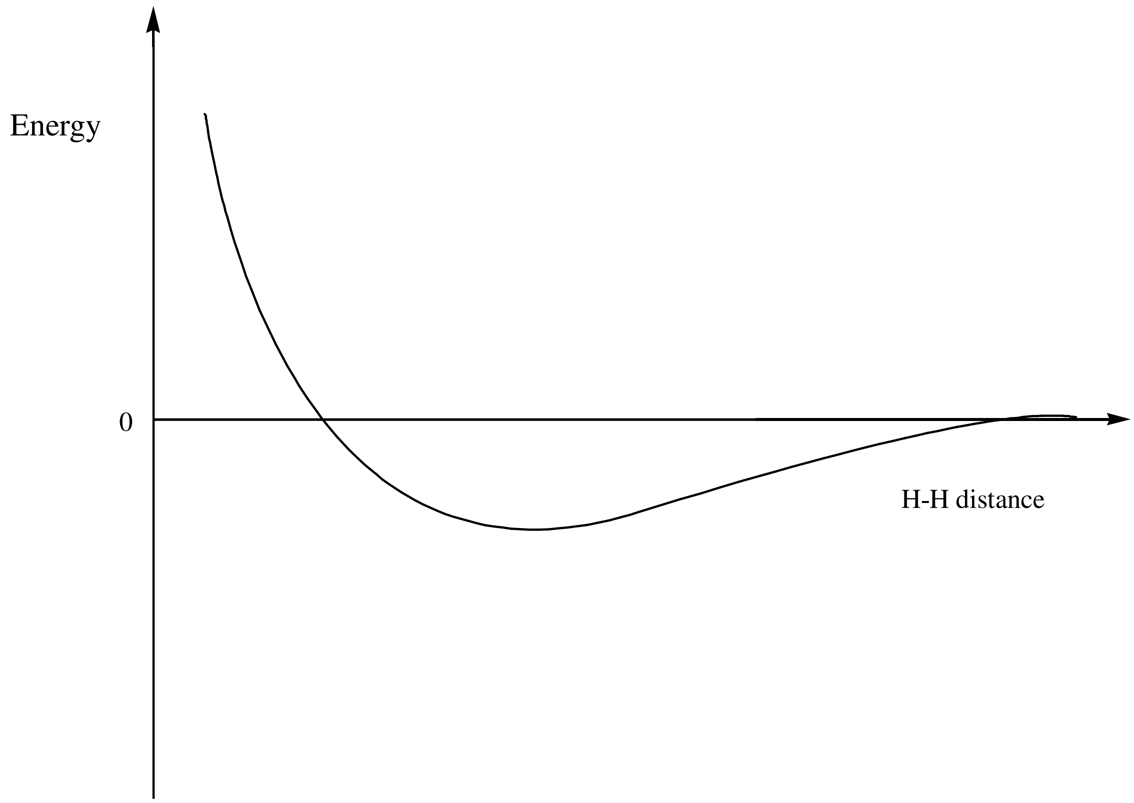

Figure 2. One dimensional energy curve. Total energy of hydrogen molecule vs. atom separation distance.

negative, this indicates an initial guess of the separation distance that is too short, and the program will lengthen the bond length and calculate a new energy. Optimization criteria can be provided as part of the program input, consisting of some minimum value of the first derivative (actually some maximum value for any one of the derivatives and some minimum root mean squared value for all the derivatives) and some maximum change in the energy from the previous step.

Vibrational Frequencies of the Molecule

After the optimal geometry and energy are determined, the next step is to insure that the optimized structure is actually stable. To do this, the vibrational frequencies of the molecule must be calculated. A second derivative calculation is performed, because the frequencies of vibration are proportional to the second derivative. Positive values for the frequencies will indicate that the optimal geometry found in the calculation of the first derivative was actually a minimum point and not an unstable maximum point, since both situations would have a slope of zero. The SFC wave function method produces a function that describes the energy surface, so the second derivative can be calculated by analytical methods (normal differentiation). However, when using the CISD or CCSD method, this is not the case. For the CISD and CCSD levels of theory, second derivatives and frequencies must be calculated by using finite differences of first derivatives.

The actual values of the frequencies are important, because they can be used to verify experimentally the theoretically predicted properties of the molecule. Infrared scattering and absorption experiments can be performed to determine the vibrational frequencies of compounds and thus provide evidence of the validity of the theoretical model for the molecules. The various possible modes of vibration are determined by taking the total number of degrees of freedom (which is the total number of atoms in the molecule times three) minus three translational modes and three rotational modes. For example, for Li_3H_2 one would find a total of nine (15 minus 6) frequencies of vibration. When using CISD or CCSD wave functions, the frequencies are found from two values of the first derivative used for the finite difference calculation. Vibrational frequency is proportional to the force constant, and a large value for the frequency indicates a tightly bound system, just as a large value for the force constant would indicate a high frequency of vibration in a spring-mass system.

The computational results reported for each stable molecule's geometry are the following: the optimized bond lengths (in angstroms), bond angles (in degrees), the energy of the molecule (in Hartrees), and the frequencies of vibration (in cm^{-1}). Calculated values are reported for the SCF, CISD, and CCSD levels of theory with the exception of CCSD results for molecules with an odd number of electrons (open shell), because the PSI suite cannot perform CCSD calculations for open shell molecules.

Professional Significance of the Study

Overwhelmingly, the scientific community has extolled the benefits of research as a key component of graduate education. In the past decade, more and more educators are suggesting that it is equally beneficial at the undergraduate level (Osteryoung, 1999; McIntosh, 2001; Moore, 2001; Seibert, 1988). This research study seeks to contribute to the body of knowledge on the molecular structures of lithium-hydrogen compounds, and in the process propose a low cost model for undergraduate research for mathematics, chemistry, and physics students at undergraduate liberal arts institutions.

CHAPTER II: REVIEW OF THE LITERATURE

Almost fifteen years ago, a report by the National Science Foundation (NSF) stated that the academic community regarded the engagement of undergraduate student majors in meaningful research with faculty members as "one of the most powerful instructional tools" (NSF, 1989, p. 6). At about this same time, Ernest Boyer (1987) published the findings of a Carnegie Foundation study of undergraduate institutions in America. Boyer concluded that research and teaching were constantly in conflict with one another in academia – that faculty members were forced to sacrifice one for the other. However, Boyer emphatically stated that it was essential that, although every professor might not be a publishing researcher, all should be "first-rate *scholars*" (Boyer, 1987, p. 131). Boyer went on to define a first-rate scholar as one who stays current in his or her area of expertise and effectively communicates such information to the students. Robert Gavin, commenting on Boyer's conclusions about the perceived dichotomy between research and teaching, argues that Boyer's study does not make a strong case for undergraduate faculty to concentrate on teaching at the expense of research and publishing (Doyle, 2000). Galvin agrees with Boyer that scholarship is the critical characteristic of the teaching profession and that research and publication are the primary ways scholarship is fostered. Gavin argues that "If research based education is consistently ranked as the best way to educate scientists and it leads to higher completion rates, why not come to the conclusion that research, and the evaluation of that research through publication, should be expected?" (Doyle, 2000, p. 14).

Undergraduate Research Today

Presently, many in the academic community advocate undergraduate research as an essential component of a good undergraduate program, especially in the sciences. However, there seems to be little agreement in the academic community as to what the purpose of research should be or how it should be conducted. In 2000, SRI International reported to the NSF on a study done on the NSF's REU (Research Experience for Undergraduates). The report noted a "lack of consensus on the goals [of undergraduate research] and how to achieve them" (Mervis, 2001, para. 10). The report by SRI, a research and consulting firm, was the result of visits to 12 of more than 500 institutions that have participated in the REU program during the past ten years. The study found significant variation on how the undergraduate research programs were conducted, whom the programs served, and why the schools and students participated (Mervis, 2001).

Nevertheless, scholars continue to advocate research as an indispensable tool for learning at the undergraduate level. Janet Osteryoung (1999), former head of the Chemistry Department at North Carolina State University and now director of the Chemical Division of NSF, states that "research is a powerful tool for learning " because laboratory research compels the student to be "impersonally self-critical and to recognize that standards and procedures are not completely arbitrary but are the basis for insuring accuracy and reliability of experimental results" (p. 43). Gordon McIntosh (2001) believes that the primary goal of undergraduate research should be to promote intellectual development by enabling the student to move from external authority to internal authority. Students move toward internal authority as they begin to make their own interpretations of the evidence, question the results of the research, and move away from the faculty supervisor’s approach and interpretation of the results. John Moore (2001) agrees that the fundamental issue is scholarship, and he argues that teaching and research are not, and should not, be mutually exclusive. Faculty members demonstrate scholarship to the students they mentor and improve their teaching skills as they supervise and participate in research.

For 20 years prior to 1988, an undergraduate research experience was a requirement for the bachelor’s degree at Mt. St. Mary’s College in Los Angles. Surveys and interviews indicated that both faculty and students felt that undergraduate research was worth the time and effort invested (Siebert, 1988). Siebert believes that the primary benefit of the research requirement is student achievement as measured by the quality of the senior thesis produced by each student, and student enthusiasm as demonstrated by the publication of an undergraduate research journal at the college.

Undergraduate Research and Student Learning

According to current models of learning, undergraduate research should provide an excellent opportunity for student intellectual growth. Constructivist educators use the term cognitive apprenticeship model, which is a type of situated cognition model of learning (Kardish, 2000). Those who advocate situated cognition learning argue that knowledge can be seen as a set of conceptual tools that are best learned when used in an authentic learning situation. In a cognitive apprenticeship situation, the student works with a faculty mentor to accomplish an actual research task (an authentic activity), and in the process not only learns to do the task, but also learns to think about the task in the same way as the mentor expert (Brown, Collins, & Duguid, 1989). The underlying assumptions on which cognitive apprenticeship and situated cognition are based are the following: (1) the process of learning takes place as students interact with others (learning is a social process); (2) real competence should be measured in the student's expertise rather than inherent ability; (3) meaningful learning takes place in situations that promote self regulation by the learner, are active, and constructive; and (4) effective learning tasks should be real world assignments rather than contrived academic activities (Kardish, 2000).

Most assessment of undergraduate research has focused on two areas. The first type of assessment is tracking of students after the completion of their research experience, by looking at how many of these students pursue graduate degrees or present papers at conferences. The second primary method of assessing is obtaining information from the student researchers after their research experience (Kardash, 2000). These methods may help predict future success and provide information about student perceptions of the benefits of undergraduate research, but it provides little information about the learning that actually takes place in the research experience. In an effort to identify what makes a good research experience, the NSF has funded a three-year, $650,000 grant to study what students gain from undergraduate research. The study, originally scheduled for completion in 2003, planned to look at four liberal arts colleges with top rated undergraduate research programs. One of the goals of the study is to produce a survey instrument that can be used by other schools to assess their own undergraduate research programs (Mervis, 2001).

A criticism of undergraduate research is that undergraduates do not have the necessary academic background, and thus are not as proficient as graduates in performing research tasks. A study of performance of graduate and undergraduate biology researchers showed no significant difference in the performance of a specific laboratory task (Wray, 2000). As a part of ongoing biology studies, researchers were required to graft prepared tissue from one chicken embryo to another. Wray's study evaluated the grafting procedure proficiency of the researchers by survival of the graft tissue and by rating the stage of the development, after one week, on a scale of 1-10. The study looked at the development of 801 total grafts, 663 done by undergraduate students and 138 done by graduate students. A statistical analysis showed no significant difference between procedures done by undergraduate researchers and graduate researchers in either the percent survival rate of the grafts or the stage of development. It should be noted that these results are for the performance of one specific task; however, they do indicate, in a limited way, that undergraduates can be effective researchers when properly trained and mentored. This same study found that one third of the 63 undergraduate researchers agreed or strongly agreed that their research experience affected their selection of a related undergraduate major. Some 47% of these same students agreed or strongly agreed that the experience influenced their decision to pursue a career or graduate study in a related field. Finally, over 98% of the 63 students felt "participation in undergraduate research helped them understand science and how scientific information is obtained" (Wray, p. 25).

Many others in the academic community support Wray's findings on the positive attitudes of undergraduates about a research experience. The Counsel on Undergraduate Research (CUR) states that undergraduate research can attract the brightest students to an academic discipline and is a major factor in career decisions. The National Task Force on Undergraduate Physics Education examined physical science departments that were highly successful in attracting undergraduate majors to their programs. The department reviews indicated that personal contact with the faculty was a significant factor in the recruiting effort (Wieman, 2001). Other potential benefits for students include increased motivation and the improvement of writing and speaking skills as a result of preparing reports and delivering presentations based on research findings (Goodwin & Holmes, 1999). The preparation of technical reports and papers provides the student important insights into how to document and disseminate research results (Abudayyeh, 2003). In addition to the discipline-specific knowledge, student researchers can acquire many general skills such as word processing, statistical analysis, the design and preparation of graphs and tables, preparation of presentation slides, observation, critical reading, and library research (Lanza & Smith, 1988). Other positive outcomes for the student are freedom in establishing a work schedule and positive interaction with faculty mentors (Abudayyeh, 2003). Garfield concludes that the primary benefit of undergraduate research may be the close working relationship between the student and faculty mentor (Lanza, 1988). Finally, successful student researchers may be more attractive to potential employers if they receive detailed letters of recommendation which describe the nature and scope of the project and the specific skills acquired by the students (Lown, 1993).

Benefits for the Faculty and the Institution

Interaction with talented student researchers can also serve to motivate the faculty member. CUR publications cite improved morale and increased satisfaction of faculty mentors (Goodwin & Holmes, 1999). Other potential benefits for the faculty are stimulation of creative thinking and staying current in the academic discipline. The research process can produce networking contacts which result in increased exposure to new people and ideas, refining of the faculty member's critical thinking skills, learning how to write better proposals, and the creating of contacts with potential funding organizations (Goodwin & Holmes, 1999). A 1999 study of a psychology faculty involved in undergraduate research sought to determine the faculty perceptions on the benefits of research assistantships and the extent to which these benefits were achieved. Although the results were based only on a survey of the faculty's perceptions, the study did suggest that the faculty believed that there were significant benefits to the student in both the acquisition of specific academic skills and the development of interpersonal relationships (Landrum & Nelsen, 2002).

In addition to the benefits for the student researcher and the faculty mentor, undergraduate research programs can enhance institutions that are predominantly undergraduate schools, and those that are smaller liberal arts colleges and universities. Undergraduate research programs help establish or improve the regional and national reputation of a college, which improves recruiting, and retention of students (Goodwin & Holmes, 1999; Lanza, 1988). Funding of research grants can help to upgrade equipment without major expenditures by the school. Finally, undergraduate research programs can provide a measure of excellence in the sciences that might otherwise be impossible at a liberal arts college. Dr. Neal Abraham, Vice President of Academic Affairs and Dean of the Faculty at DePauw University, speaking of liberal arts colleges and universities, states:

> …our science major programs may lack the breath and diversity of those of our university counterparts. However, linking research to the undergraduate curriculum provides a way to achieve a special degree of excellence in science

> within liberal arts limitations. Students come to understand the practice of science by experiencing the ultimate scientific activity in small groups or in one-on-one companionship with the faculty member…[and] they become creators of knowledge. For students this is a frustrating, enlightening and rewarding alternative to pursuing more advanced coursework (which may not be available), and it gives them special skills and perspective. (Goodwin & Holmes, 1999, p. 6).

Thus, undergraduate research provides the potential for a synergistic enhancement of the liberal arts curriculum. Finally, undergraduate research programs can influence the academic environment of a campus, and raise the standards of scholarship and professional activities of the college (Osteryoung, 1999).

Availability of Funding

Since 1986, there have been major federal and private grant programs directed at the predominantly undergraduate institutions and their faculties (Moore, 2001). During this period the faculties of these schools have increased by over 20%; however, the number of proposals and funded grants have not increased, and in the case of NSF programs, the number of grant applications have actually decreased (Research Corporation, 2001; Moore, 2001; Tobochnik, 2001). The suspected decrease in undergraduate research does not seem to be caused by a lack of funds, nor is there any evidence to indicate the undergraduate institutions are not competitive for the funds available. The total amount of funding for undergraduate research increased from 1986 to 2000 with a 30% success rate on proposal approvals (Research Corporation, 2001). Thus, in spite of the perceived benefits and the availability of funding, research at undergraduate institutions could be on a downward trend. This may be due to the prevalent view among faculty that the supervision of undergraduate research is a burden that involves a sacrifice of their own scholarly activities and research (Mervis, 2001). Any efforts to simulate faculty participation in undergraduate research must address faculty concerns about the time intensive nature of mentoring undergraduates and the appropriate compensation for the faculty. A survey of attendees at the 8th National Conference of Undergraduate Research found that crediting time in which the faculty member is involved in mentoring undergraduate researchers would be an effective way to recognize and compensate faculty engaged in undergraduate research (Karukstis, 2000).

The Elements of Successful Undergraduate Research

Fostering success in undergraduate research has at least two major components. The first component is a good undergraduate research program, and the second is a successful undergraduate research experience (URE) for the student. The research program must have support from the institution as a whole, administration and faculty, while the URE primarily depends on the effective planning and execution by the faculty that conduct the program and mentor the undergraduate researchers.

The Undergraduate Research Program

Stevens (1994) lists six characteristics of a good undergraduate research program. First, the program must be based on collaboration between the faculty member and the student. This model differs from that of graduate school. The faculty mentor works closely, often alongside the student, teaching and providing direction as needed yet allowing the student to work independently as appropriate. Second, a good program does not see research and teaching as competing with each other, but complementing one another. The research is done in the teaching environment, often in the same laboratories.

Third, there must be institutional commitment in terms of financial resources for the research. Fourth, the research should be *curiosity-driven*, giving students a chance to explore and discover, thereby challenging and motivating them. Fifth, there must be quality research. Undergraduates, with effective mentorship by the faculty can do first class research, but it will be at a slower pace than in graduate school. Finally, the environment of the institution must be supportive of undergraduate research efforts. This last characteristic refers to the prevailing campus attitude toward the program. Written policy statements that recognize the importance of faculty mentoring and provide appropriate rewards for faculty and students can help to institutionalize the program (Kinkead, 2003).

The Undergraduate Research Experience (URE)

Bentley (1994) proposes seven steps for achieving a successful URE: (1) careful selection of the student, (2) having a peer-reviewed reporting opportunity, (3) having a periodic meeting time between the faculty mentor and student researcher, (4) selection of an appropriate graduate student mentor, (5) carefully defining the tasks and overall objective of the research, (6) conducting the research, and (7) evaluation of the success of the project upon completion. Each of these steps will be discussed below.

Student Selection

West (1994) suggests that the best time to start undergraduate research is either second semester of the sophomore year or first semester of the junior year. Waiting until the middle of junior year will give a chemistry major time for two semesters of basic chemistry, two semesters of organic chemistry and a physical chemistry course containing quantum mechanics and group theory. For other science disciplines, starting after sophomore year can provide the opportunity to take courses beyond the introductory level. For example, a physics student could take a semester of quantum mechanics after completing three semesters of physics. Belliveau (1983) believes that it is critical to make a practical evaluation of the capabilities and the limitations of the student. The research must match the skills of the student (Lown, 1993). The faculty mentor should look for students that have both discipline and initiative, and students who know their own strengths and weaknesses (Wilensky, 2002).

Reporting Opportunity

The reporting of the research can be used as an important part of the reward system. Presentations at a conference, publishing a paper in a peer reviewed journal, or receiving publicity in the school and local paper will provide recognition and motivation for the undergraduate researcher (Belliveau, 1983).

Meeting with the Student Researcher

In addition to regularly scheduled meetings between the student and the faculty mentor, Lanza (1988) uses group meetings with undergraduate researchers. In these meetings, the faculty mentor and the students discuss articles they have read that relate to their research. Initially these meetings help to define terms and clear up confusing concepts. As the students progress, these meetings are used to learn and discuss more sophisticated analytical and statistical issues. The Council on Undergraduate Research has produced a detailed handbook entitled How to Mentor Undergraduate Researchers, describing the elements of mentoring, suggestions on what mentors and students should expect from each other and the research process, and other practical information on the undergraduate research process (Merkel & Baker, 2002).

Graduate Mentors

Small liberal arts colleges may not have graduate students that can serve as mentors for the undergraduate researcher. One method to alleviate some of the supervisory burden of the faculty mentors is to use research supervisory teams. Several faculty members work together in the mentoring of an undergraduate researcher. In addition to allowing a sharing of the duties, this can provide an interdisciplinary research experience for the student (Belliveau, 1983).

Defining Tasks and Objectives

In defining the research project, the student needs to have a clear idea of what the project will entail. The student researcher must know how he or she will be supervised and evaluated, understand the purpose of the research and how the data will be used, and know the goals for the time allotted (Lown, 1993). At Cornell University, Tom Brenna tries to insure that the researchers see the big picture, because most of them begin during the execution phase (Wilensky, 2002). He wants them to know why they are doing the research, when they should expect to get data, and what the data will mean. West (1994) says a good research project should provide more hands on mentoring opportunities for the faculty advisor and the student than graduate research. The project should also be one that the student can leave and return to easily, because of the schedule requirements for undergraduates.

Conducting the Research

Undergraduate research requires a much higher degree of control and monitoring than graduate research. Belliveau (1983) recommends a rigid schedule with reasonable deadlines. He feels the schedule should allow anywhere from 50-70% of the student's time for learning and only 30-50% of the research time for the production of experimental results. The new student researcher will need training. If possible, pairing the novice with an experienced student researcher allows students to teach each other and provides overlap for continuing research activities (Wilensky, 2002; Lanza, 1988). In addition to organizing student researchers into pairs or teams, West (1994) uses regularly scheduled meeting where students can share progress and ideas. He also requires a detailed laboratory notebook in which the student records everything that is done, along with an interpretation of the results. In order to improve research communication skills, West often requires data and conclusions to be transferred to computer storage and submitted to him by the student. He can then react to the data and provide feedback to the researcher. Finally, a good research experience allows the student the freedom to make mistakes (Lanza, 1988).

Evaluating the Success of the Experience

Student presentations, whether formal or informal, provide an effective means of evaluating the research experience. To insure that students have the opportunity to present their findings, West conducts a department level evening seminar each semester. This seminar is devoted to undergraduate research presentations and concludes with an ice cream and cake celebration (West, 1994).

Sources of Funding for Undergraduate Research

Other than talented and motivated faculty, the most critical need for an undergraduate research program is funding. One of the conclusions of the conference participants at “Academic Excellence: Conference on the Role of Research in the Natural Sciences at Undergraduate Institutions” in the summer of 2001, was that “there appears to be a fairly large amount of money available to the faculty at predominantly undergraduate institutions for their research and that these resources may be underutilized at the present" (Tobochnik, 2001, p. 933). Some of the most important funding programs for research at predominantly undergraduate institutions include: the National Science Foundation (NSF), the petroleum Research Fund of the American Chemical Society, the AREA awards from NIH, and regional funding agencies (Tobochnik). Three specific NSF programs are the Research Experience for Undergraduates (REU) program, the Research in Undergraduate Institutions (RUI) program, and the Research Opportunity Awards (ROA) program (Osteryoung, 1999). Other grant programs that focus primarily on the funding of research at predominantly undergraduate institutions are the Research Corporation Cottrell College Science Grants and the ACS/PRF Type B grants (Goodwin & Holmes, 1999). Finally, there are several programs directed at new faculty: the NSF Faculty Early Career Development (CAREER) program, the Camille & Henry Dreyfus Foundation's Faculty Start-up Grant Program for Undergraduate Institutions, and the American Chemical Society/Petroleum Research Fund's Type G grants (Goodwin & Holmes, 1999).

Other Resources

An important resource for faculty engaged in undergraduate research is the Council on Undergraduate Research (CUR). The organization is "dedicated to strengthening science and undergraduate science education." (Halstead, 1997, p. 148) In eight years from 1989-1997, CUR grew from just over 1000 members to over 3500 members divided into seven scientific and mathematical divisions. CUR supports undergraduate research through funding, national conferences, and an abundance of publications and services. Full details on CUR programs can be found in a booklet published by CUR entitled *How to Get Started in Research* (Goodwin & Holmes, 1999).

The lack of sufficient funding, faculty, or equipment at liberal arts colleges and primarily undergraduate institutions can be overcome by collaboration with other colleges or universities. Boyer (1990) encouraged faculty at liberal arts colleges to collaborate with "colleagues at research universities so that resources might be shared" (p. 60). At Liberty University, D. A. DeWitt (personal communication, March 10, 2004) was conducting biological cell research into the causes of Alzheimer's disease through a partnership with researchers at the University of Virginia. Initially having no equipment at his liberal arts institution, Dewitt utilized UVA facilities for his research, which resulted in publication and eventual funding for research equipment at Liberty University. Faculty and students from Bates College and Wellesley College participated in another promising model for undergraduate research at small liberal arts colleges. The summer undergraduate research experience was creatively named *Lumberjack Summer Camp*, because the research involved efforts to optimize computer compiler programs by the *trimming* of logic trees in the programs. The research camp brought together two faculty and six students from each school. Forming a larger research group provided for the fostering of collaborative research efforts in addition to individual research (Johann & Turbak, 2001). The pooling of resources made the research possible, but there were problems. The most significant were the short duration of the experience, the inability to achieve closure on much of the work, and insufficient preparation of the computing environment prior to the beginning of the ten-week experience.

In summary, undergraduate research can enhance the academic experience for students at liberal arts institutions. Students doing research develop the tools and skills of the particular discipline as experienced faculty mentor them. The faculty will be engaged in scholarly activity, which will produce better classroom instruction. In addition, publication of research and presentations at conferences raise the reputation of the institution. Moreover, the school's research facilities are improved by the influx of readily available grants for undergraduate research. Finally, the faculty researcher must recruit the right students and tailor a program that accounts for the abilities, educational background, and time constraints of undergraduates.

Review of Computational Research on Lithium-Hydrogen Molecules

Early ab initio (first principle) computational studies of Li_3H and Li_3H_2 molecular structures were done by Rao, Khanna, and Jena (1991) in a study designed to investigate how metal clusters and crystal structures might differ in their ability to absorb hydrogen. The calculations in the study were performed using Hartree-Fock Self Consistent Field (SCF) level of theory. The optimized geometry was reported for both structures; however, the total energy for each molecule was not. No calculations of the vibrational frequencies were performed, and there were no correlating calculations done at the Configuration Interaction including Single and Double excitations (CISD) or the Coupled Cluster including Single and Double excitations (CCSD) levels of theory. The calculated geometries for the molecules (both planar) are shown in Figure 3.

Rao, Khanna and Jena (1991) found that the Li_nH_m structures were planar when $n \leq 3$ and $m \leq 3$, but the geometry becomes three-dimensional when the molecule contains more than five atoms. Their calculations also showed that the LiH bond distances in all

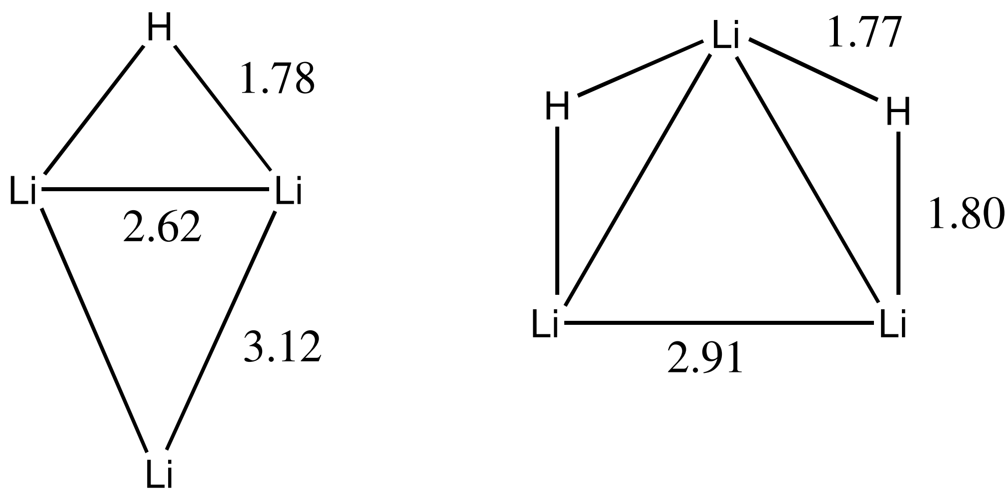

Figure 3. Early SCF calculated structures and bond lengths for Li_3H and Li_3H_2 (All values in Angstroms).

Adapted from "Energetics and electronic structures of hydrogenated metal clusters" by Rao, B. K., Khanna, S.N., & Jena, P.,1991, *Physical Review B, 43*(2), 1416-1421.

the Li_nH_m molecules studied remained about the same at 1.7 ± 0.1 Å (the bond distance in the dimer molecule, LiH, is 1.64 Å).

Bonacic-Koutecky, Gaus, Guest, Cespiva, and Koutecky (1993) examined Li_nH and Li_nH_2 molecular structures and compared them to the structural properties of Li_n molecules. Their work did provide both the molecular structure and the energy of the optimized molecular structures using SCF and CISD level of theory. The results are shown in Table 1.

The optimized molecular structures are shown in Figure 4 (Bonacic-Koutecky et al., 1993 pp. 536 & 531). The bond lengths, also shown in Figure 4, are believed to be those obtained from the SCF optimization calculations. The vibrational frequencies were not reported for any of the structures described in the research. The authors found that in Li_nH structures, the transition from a planar molecule to a three dimensional molecule occurred at n = 6 (Li_5H was planar). Li_nH_2 were found to be planar for $n \leq 4$ (six total molecules). Instead of verifying the stability of the calculated structures by the calculation of the vibrational frequencies, the authors compared their calculated ionization potentials to measured ionization potentials.

The molecular structure and energy results reported by Bonacic-Koutecky et al. in 1993 were again reported in 1996 in a study by Bonacic-Koutecky, Pittner, and Koutecky. It does not appear that any further calculations were performed for the optimal structure, bond lengths, or energies. The results, reported in Table 1 and Figure 4 are exactly the same as those reported in 1996 (Bonacic-Koutecky et al., 1996). This new study examined the optical emissions from excited electron transitions for lithium-

Table 1

Calculated Energy for Optimized Geometries

Molecule	SCF energy (Hartrees)	CI energy (Hartrees)
Li_3H	-22.904624	-22.963138
Li_3H_2	-23.503216	-23.563344

Note. Adapted from "Ab initio CI study of the electronic structure and geometry of neutral and cationic hydrogenated lithium clusters. Predictions and interpretations of measured properties," by V. Bonacic-Koutecky, J. Gaus, M.F. Guest, L. Cespiva, & J. Koutecky, *Chemical Physics Letters, 206*(5,6), 532 & 537.

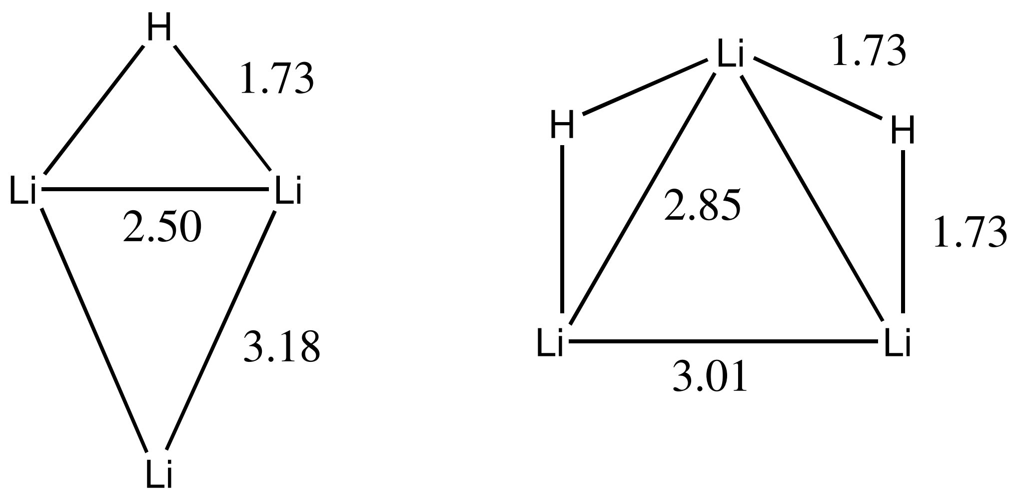

Figure 4. Later CISD calculated structures and bond lengths for Li_3H and Li_3H_2 (All values in Angstroms).

Note. Adapted from "Ab initio CI study of the electronic structure and geometry of neutral and cationic hydrogenated lithium clusters. Predictions and interpretations of measured properties," by Bonacic-Koutecky, V., Gaus, J., Guest, M. F., Cespiva, L., & Koutecky, J., 1993, Chemical Physics Letters, 206(5,6), 528-539.

hydride and sodium-fluoride molecules but again did not provide any information on vibrational frequencies for any structures.

Fuentealba and Reyes (1999) used the results for the optimized structures from Rao, Khanna, and Jena (1991) and Bonacic-Koutecky et al. (1996) in their study of electric dipole polarizabilities. They do not attempt to calculate any of the optimized structures for the molecules but simply use the bond lengths and geometries from the other two studies.

To date, there are no published studies of the predicted vibrational frequencies for Li_3H and Li_3H_2 molecules. This research sought to verify the optimum (lowest energy) geometry of these structures and the associated bond lengths and then to calculate the vibrational frequencies for these molecules.

The literature review suggests that an overwhelming majority of the scientific community agrees that undergraduate research can enhance the educational experience for an undergraduate student. The challenge for the liberal arts science department is to develop an economically feasible undergraduate research program that will foster scholarship in the students and faculty without overburdening the department. The literature review provided a current pedagogical perspective on undergraduate research for the researcher, as he participated in a simulated undergraduate research experience of learning the computational methods and applying these methods to investigate Li_3H and Li_3H_2 molecules. The research experience, combined with the examination of the literature, served as a framework for the proposed model for undergraduate computational research in the sciences at liberal arts institutions.

CHAPTER THREE: EXPERIMENTAL METHOD

The goal of this research was to propose a workable beginning model for conducting relatively low cost computational research employing the UNIX workstations and using the experience gained in conducting the computational investigation of Li_3H and Li_3H_2 structures. The model was based on the research experience of the study researcher, the current body of knowledge concerning undergraduate research, and qualitative data from other undergraduate researchers who have done similar research during a summer Undergraduate Research Experience (URE) or as undergraduate researchers during the school year. It should be noted that this model constitutes only a starting point for a program and not the end state.

The research for the development of this model was a case study in which the researcher is the primary participant. Through a total immersion in the process, the researcher was able to gain important insights into the process. Several specific areas of academic expertise were completely new to the researcher, including symmetry and group theory, quantum calculations of molecular orbitals, and the use of the UNIX operating system. The researcher's initial level of knowledge was much like that of a typical science-major student researcher, although a student with a strong chemistry background would probably have some proficiency in group theory.

Undergraduate Research Model

Potentially, undergraduate research offers the student more than just higher order cognitive learning skills. The real value of the process may lie in the affective values that are observed and learned while the student works in the research environment. The literature indicates that one of the most important components of undergraduate research is the faculty-student mentoring that occurs during the research project (Belliveau, 1983; Lanza, 1988; West, 1994; Wilensky, 2002). The actual skills imparted to the student may be secondary to the mentoring and the socialization that takes place as the student and faculty member work together to acquire new scientific knowledge. Positive affective outcomes for the student could range from simply an appreciation of the challenges and difficulties of doing scientific research, all the way to stimulating a desire to pursue a higher degree in a related field.

In an effort to gain additional insights into the skills and attitudes of student researchers, questionnaires (see Appendix B) were sent via email to former undergraduates who had participated in this type of research in recent years at the University of Georgia. This qualitative data provided triangulation information to reinforce or refute the impressions of the researcher and provided valuable feedback for the recommendations about the final model for undergraduate research. The number of students who participate in this research each year was fairly small, and therefore it was difficult to obtain a large number of responses. The goal was to obtain five or six completed questionnaires. The researcher called the participants in advance, requesting permission to send the questionnaire as an email attachment. The participants returned their completed questionnaires as an attachment to an email message. Particular areas explored by the questionnaire were the academic skills and knowledge that were essential to their success in doing the research; the aspects of the research that they liked and disliked, and why; their recommendations for changes or improvements to the research experience; the most important benefits of the research; and the academic skills that they felt were improved as a result of their work on the research project. Some of the specific academic skills that were addressed included computational proficiency; writing skills; analytic thinking; background research of scientific journals; and mathematics, chemistry, and physics knowledge. Using the questionnaire input to supplement the computational research experience, combined with conclusions drawn from the educational literature on undergraduate research, the researcher was able to evaluate the process and to discern some of the key elements necessary to make a computational, scientific undergraduate research program that is effective, stimulating and rewarding.

Computer Research Method

The theoretical calculations of the characteristics of the hypothetical molecules were performed using the PSI suite of programs developed by Dr. F. Schaefer group at the Center for Computational Quantum Chemistry at the University of Georgia. These programs are designed to run using the UNIX operating system. An IBM RS/6000 workstation was used for the research. At present, two workstations are available to support computational computer research at the university which was the site of the study. The PSI suite of programs use what are known as ab initio (or first principle) theoretical methods to predict the molecular structure and molecular properties using quantum theory.

The Familiarization Phase

The first phase of the research consisted of independent study of background material and initial familiarization on the computer as preparation for the computational research using the quantum calculation programs. This phase consisted of a series of lectures given by the faculty mentor and individual study in the areas of symmetry and group theory, molecular orbital theory, and the UNIX operating system. With this background, the researcher was then introduced to the research using a program that was less sophisticated, in terms of the level of theory used for the quantum mechanical calculations, but was more user friendly. Using this program, named Jaguar (Schrödinger, 1997), the researcher was able to practice setting up the initial geometry with three-dimensional visual representations. Next, the researcher used the actual PSI suite of programs to be used for the research to investigate two well-known structures: water, H_2O; and a lithium ion, Li_3^+. This work helped familiarize the researcher with the general approach to the computational research and enhanced proficiency with the UNIX commands needed to prepare input files, edit input files, interpret output files, and manage the files. During this *train up* phase, the researcher, a physics professor with no graduate courses in chemistry or group theory, and no experience with the UNIX operating system, encountered the research experience much as an undergraduate physics, mathematics, or chemistry student might. This first-hand experience provided a baseline for the development of an effective undergraduate research model for a typical physics, mathematics, or chemistry major at a liberal arts institution.

General Approach

This section describes the general procedure used to perform the theoretical calculations on any given molecule. The particular molecules and structures to be investigated are covered in the following section of this chapter.

The first step is predicting the general geometrical shape of the molecule, which will be the starting configuration for the molecular orbital calculations. Once this is done, then the symmetry of the molecule can be determined. C_{2V} symmetry is used whenever possible because the suite of programs are some what limited in the symmetries for which the calculations can be done, and many molecular structures can be characterized using this symmetry point group. The next step is to prepare the input file for the iterative quantum mechanical calculations of the optimized geometry using the Self Consistent Field (SCF) level of theory. The desired output values when the calculations converge (find the configuration of the molecule where the total energy of the molecule is the lowest possible) are the distances between the atoms and the total energy of the molecule.

Once the optimized geometry was found using the SCF calculations, then the calculation of the vibrational frequencies could be performed. When doing calculations at the SCF level, the program produces a function during the process of finding the location of the minimum for the molecular energy that represents the first derivative. Therefore, the vibrational frequencies, which are proportional to the second derivative, can be found by fairly straightforward differentiation. There was one frequency found for each possible mode of vibration. The number of vibrational modes will always be 3N - 6, where N is the total number of atoms in the molecule, and the number 6 represents three translational (x, y, and z) motions of the molecule and three rotational (x, y, and z axis) motions of the molecule. If all 3N - 6 of the calculated frequencies are positive, then the optimized geometry can, pending the results for higher levels of theory, be considered stable. The determined positive vibrational frequencies are important in terms of stability because they show that small deformations of the molecule will result in attractive restoring forces (the electromagnetic attraction of the positive nuclei for the negative electrons) that will hold the molecule together.

Next, the optimization process must be repeated at the next level of theory, Configuration Interaction, including single and double excitations (CISD). This level of theory uses more wave functions to better approximate the actual molecular orbital wave functions. The computer calculations are more time intensive, but the optimized geometry and energy values from the SCF calculations can be used as a starting point. Once the optimized CISD geometry and total energy have been calculated, then the vibrational frequencies can again be determined. However, the CISD program does not generate a function for the first derivative as the SCF method does. The first derivative values are calculated for every point on the energy surface. This requires that the second derivative must be found by taking a difference of first derivative values. This is done through a series of steps, which require each of the atoms to be displaced slightly, and then have the program calculate the new first derivative of the energy surface (the slope) for the resulting geometry with the atom or atoms slightly displaced. In order to do this, the researcher must first determine a complete set of what are known as symmetry adapted internal coordinates. Each of these internal coordinates corresponds to one of the modes of vibration of the molecule. The difficultly in doing this is that atomic displacements that are asymmetric with respect to the symmetry of the molecule will change the symmetry of the molecule. This requires a change in the type of symmetry used for the calculations. Different displacements require different symmetries to be used to perform the calculations of the first derivatives.

After the values of the first derivative had been calculated for all the possible displacements, then a sequence of calculations could be performed to do the necessary coordinate transformations. Once this has been done, the second derivatives and thus the vibrational frequencies could once again be determined. If all the frequencies are positive, and they are relatively close to those obtained by the SCF calculations, then the CISD calculations are complete.

The highest level of theory is the Coupled Cluster with single and double excitations (CCSD). Once the CISD calculations have been completed, the CCSD calculations are fairly straightforward in most cases, because the work of determining the symmetry adapted internal coordinates and the preparing of the new input files for the various symmetries used for the asymmetric displacements has already been done. Following the same general procedure as for CISD, the CCSD geometry, total energy, and vibrational frequencies can be calculated. If the molecule has an odd number of electrons (as in Li_3H_2) the CCSD calculations cannot be performed due to program limitations.

Specific Molecules Investigated

The first lithium-hydrogen compound investigated was Li_3H. Since the molecule has a total of ten electrons (three for each lithium and one for hydrogen), the calculations could be performed at all three levels of theory, SCF, CISD and CCSD. The three most likely configurations of the molecule were examined one at a time. The first was a planar molecule with the hydrogen atom at the center of the three lithium atoms. The second was also planar, but had the lithium atoms forming a triangle and the hydrogen atom bonding with two adjacent lithium atoms. This structure was somewhat diamond shaped. Finally, the third was a three dimensional molecule which has the hydrogen approximately centered above a planar triangle composed of the three lithium atoms (see Figure 5).

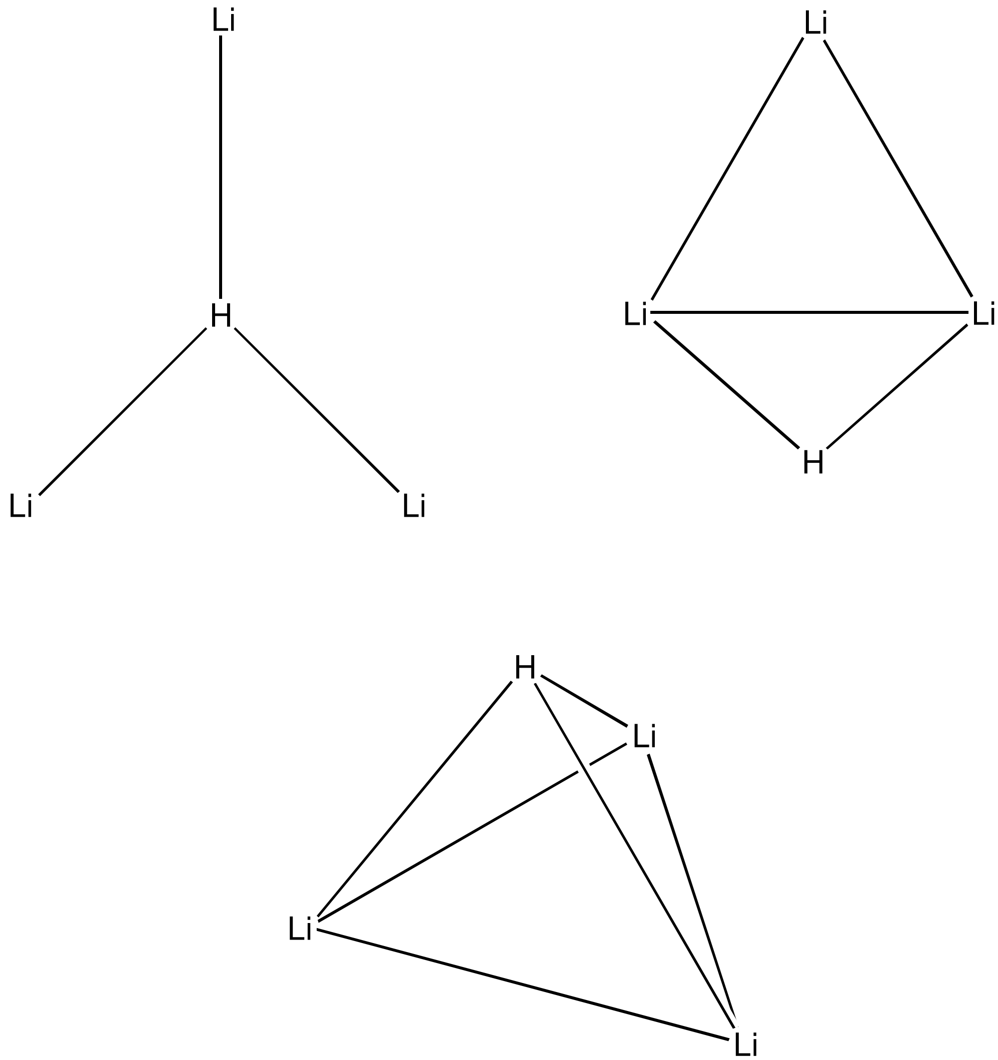

Figure 5. Three hypothetical configurations for Li_3H.

The second lithium-hydrogen molecule on which the calculations were performed was Li_3H_2. The additional hydrogen contributes one more electron, bringing the total for the molecule to eleven. Thus, calculations were performed only at the SCF and CISD levels of theory because of the one unpaired electron. Although there were fewer total calculations to be performed, finding the first derivatives for the asymmetric displacements in the CISD calculations of the vibrational frequencies was complicated by the extra, unpaired, electron. It was more difficult to get the calculations to converge in a reasonable number of iterations. To help the process go more quickly SCF calculations were done assuming the molecule had one additional electron. Once these calculations were optimized, the resulting geometry and energy was used as a starting point for the molecule with only eleven electrons.

For Li_3H_2, there were also three likely configurations of the molecule to be investigated. The first was a planar molecule with the three lithium atoms forming a triangle and two hydrogen atoms, each bound to one of the lithium atoms (with a possible bond between the two hydrogen atoms). The second molecule was also planar, with the same lithium triangle, however, now the two hydrogen atoms are bound so that each is bridging between two lithium atoms. Finally, the third molecule was three-dimensional and was similar to the three-dimensional version of Li_3H described earlier, except that there is another hydrogen below the plane of the lithium triangle, which is a mirror image of the hydrogen above the plane (see Figure 6).

As described earlier, the possible stable geometries were determined by finding those structures that have all positive vibrational frequencies. The following results were reported for all the optimized (lowest energy) molecular structures: all inter-nuclear

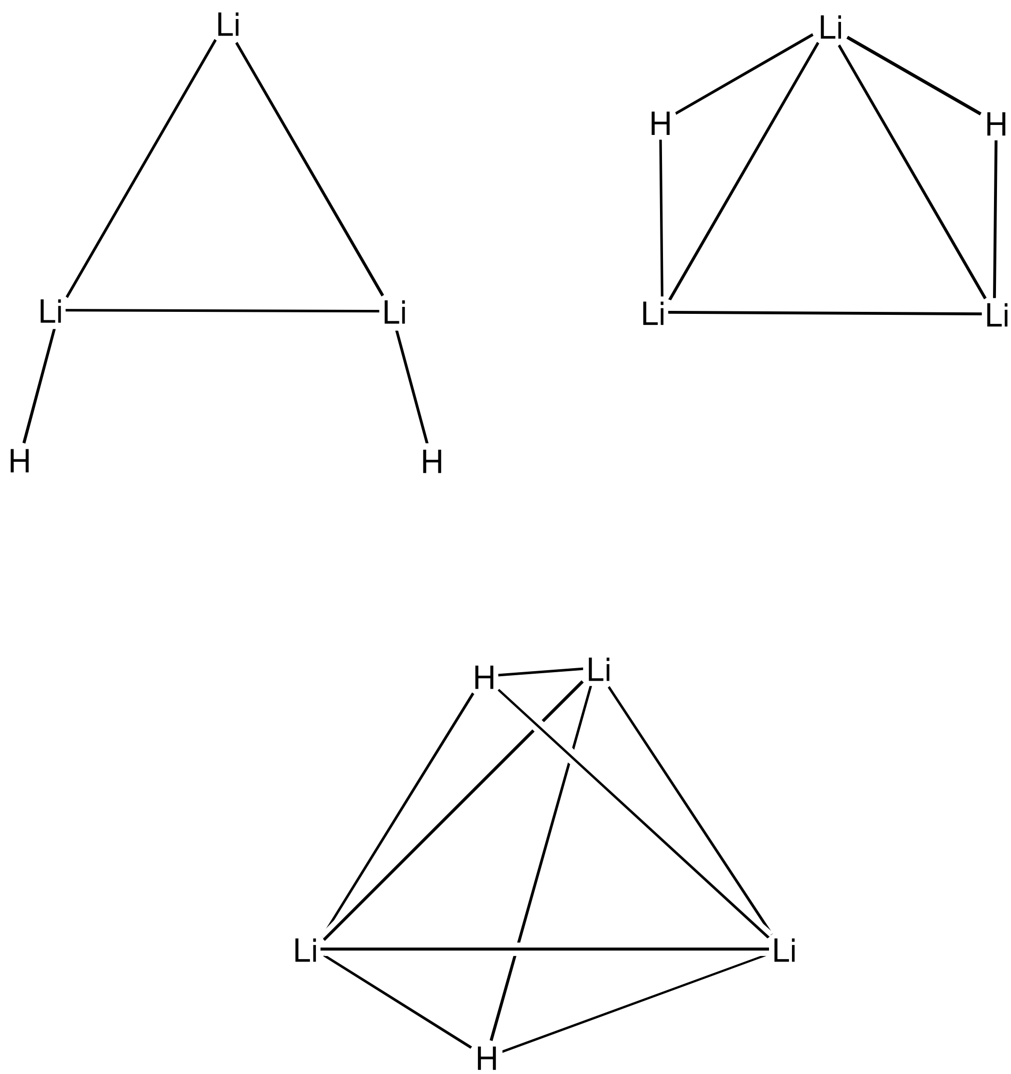

Figure 6. Three hypothetical configurations for Li_3H_2.

distances (bond lengths) in angstroms (Å); the total energy of the molecule in Hartrees (au); and the vibrational frequencies in inverse centimeters (cm^{-1}).

CHAPTER IV: RESULTS AND ANALYSIS

This chapter is divided into two parts. The first part details the computational results obtained from the calculations performed on the three Li_3H structures and the three Li_3H_2 structures. The optimal structure for each of these molecules is identified, and the bond lengths, total energy, and vibrational frequencies are reported for the optimal structures. The second portion of this chapter describes the researcher's analysis of his simulated undergraduate research experience. The questionnaire feedback from former undergraduate researchers in computational quantum chemistry was analyzed and helped to reinforce many of the conclusions about a model for computational undergraduate research in the sciences.

Results of Computations

This study's computations at all three levels of theory confirmed the optimized geometry for Li_3H to be the same as that described by Rao, Khanna, and Jena (1991). The discovery of negative vibrational frequencies for the first planar molecule, with hydrogen at the center (Figure 5), revealed that this structure was unstable. The third geometry, which was three-dimensional and had the hydrogen centered above a planar triangle formed by the three lithium atoms, was stable. However, the total energy of the molecule was higher than the second geometry, the planar diamond shaped molecule with the hydrogen forming a bond with two adjacent lithium atoms. This structure is shown in Figure 7 with the calculated bond lengths. The bond lengths are consistent with those reported by Bonacic-Koutecky et al. (1993). The complete listing of bond lengths, total energy and vibrational frequencies for all three levels of theory are shown in Table 2. The tabulated computational results shown for the CISD and CCSD calculations are highly

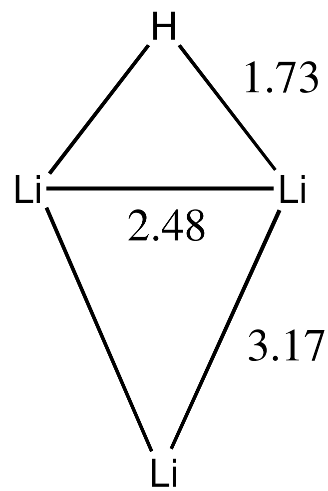

Figure 7. Optimized geometry for Li_3H with bond lengths obtained from SCF calculations (all bond lengths are in Angstroms).

Table 2

Computational results for Li_3H

	SCF	CISD	CCSD
Li-Li Bond (Ang)	3.170	3.034	3.017
Li-Li Bond (Ang)	2.483	2.459	2.477
Li-H Bond (Ang)	1.733	1.717	1.715
Energy (Hartrees)	-22.4060235973	-23.011278015585	-23.01881469
Frequencies (cm^{-1})	1092	1100	1109
	1062	1077	1069
	399	400	540
	384	383	390
	263	286	285
	177	197	198

consistent with the SCF calculations shown and provide a high level of confidence in the computational data.

The study's calculations using the SCF and CISD levels of theory (CCSD level calculations cannot be done for Li_3H_2 because the neutral molecule has an odd number of electrons) confirmed that the optimized geometry for Li_3H_2 was the same as described by Rao, Khanna, and Jena (1991). The first planar configuration investigated (Figure 6) had a hydrogen atom bound to each of two lithium atoms at the corners of a lithium triangle. This structure was found to be unstable. The two hydrogen atoms would begin to bond together to form H_2 and the lithium triangle ring would begin to come apart. The third structure investigated was stable. It was three-dimensional and had a hydrogen atom centered above and below the planar triangle formed by the three lithium atoms. Although it was a stable structure, its total energy was slightly higher than the second structure, which proved to be the optimized geometry. The optimized structure is shown in Figure 8 with the calculated bond lengths. The bond lengths are consistent with those reported by Bonacic-Koutecky et al. (1993). The complete listing of bond lengths, total energy, and vibrational frequencies for the SCF and CISD levels of theory are shown in Table 3. The correlation of the CISD results with the SCF calculations provides a high level of confidence in the computational data.

Undergraduate Research Process Using Computational Methods on UNIX Workstations

The results and analysis presented in this section are based on the computer research experience of the study's author, and the feedback obtained from other former

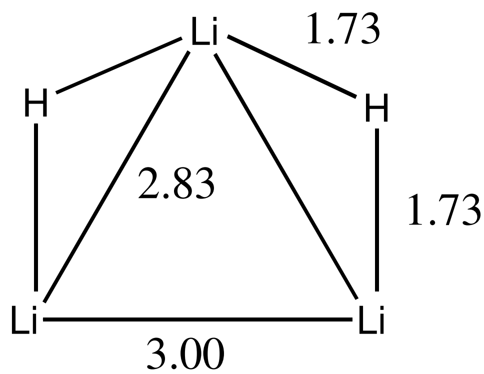

Figure 8. Optimized geometry for LI_3H_2 with bond lengths obtained from SCF calculations (all bond lengths are in Angstroms).

Table 3

Computational results for Li_3H_2

	SCF	CISD
Li-Li Bond length (Ang)	2.834	2.800
Li-Li Bond length (Ang)	2.995	2.965
Li-H Bond length (Ang)	1.733	1.711
Li-H Bond length (Ang)	1.725	1.706
Energy (Hartrees)	-23.50732772370	-23.618322832112
Frequencies (cm^{-1})	1269	1278
	1235	1262
	922	939
	921	929
	436	421
	362	366
	332	321
	246	245
	226	229

undergraduate researchers working on similar research projects in computational quantum chemistry. This section is divided into three parts. The first part describes the three essential stages of the undergraduate research experience: the preparation stage, the computational research work, and the reporting stage. Next is an analysis of the various cognitive skills in which the undergraduate researcher must be competent to use the PSI suite of programs, and understand the computational process and results. Finally, the third part of this section presents the advantages of computer research to a primarily undergraduate institution or liberal arts institution, and the potential benefits of this type of research to the undergraduate researcher, the faculty and the school.

Stages of an effective undergraduate research experience

The first stage, or preparation stage, of the undergraduate research experience consists of academic courses in mathematics, chemistry, and physics and a familiarization phase consisting of self-study and faculty mentor instruction. The initial preparation for an effective undergraduate research experience is a solid academic background in mathematics and science. Consequently, the faculty mentor must insure that the prospective researcher is academically prepared for the research. Based on the integrative nature of the topic, which requires a good foundation in calculus, chemistry, and physics, most undergraduates would not be able to take enough of the necessary courses in less than two years, and many would need three years. A minimum foundation, in preparation for the necessary advanced courses, should consist of three semesters of calculus, three to four semesters of chemistry, and two of physics. In addition to the foundational studies, an a third semester of modern physics or a physical chemistry course would be needed for a basic understanding of quantum mechanics. Additional mathematics, although not essential, would enhance the student's preparation and enrich the research experience.

Assuming the student arrives for the freshman year ready for calculus, three semesters of calculus and a semester of linear algebra would take two years. Of the six former undergraduate researchers, all mentioned the need for calculus or quantum mechanics (which requires calculus) as essential to the research. Four of the six respondents specifically mentioned linear algebra and another stated that he should have had more mathematics beyond three semesters of calculus. See Appendix G for a complete summary of questionnaire responses. A strong mathematics foundation will enhance the research experience. There should be a minimum of three semesters of calculus, and probably four. Linear algebra is not as critical for the computational research; however, an introductory course in linear algebra will give the student a better understanding of how the energy calculations are performed by the UNIX programs. Basic quantum mechanics principles are critical to understanding the concepts of the wavefunction, the formation of bonding and anti-bonding orbitals, and the methods used to find the energy of the molecule. Five of the six questionnaire responses mentioned a course in quantum mechanics, quantum chemistry, or physical chemistry as critical background for this research. The researcher had taken two courses in quantum mechanics at the undergraduate level and taught quantum mechanics as part of a modern physics course. Quantum mechanics is normally covered in a modern physics course, which would be taken as a third semester of physics in the undergraduate's junior year (the first two semesters of physics require a prerequisite of two semesters of calculus). A quantum chemistry course or physical chemistry course might be taken as early as the second year, but not until after two semesters of basic chemistry and at least one semester of organic chemistry. Normally, chemistry majors would take two semesters of organic chemistry during their second year, pushing physical chemistry to the first semester of junior year. Based on the minimum academic courses required, the earliest time to begin computational quantum research would be the summer after sophomore year, and the most likely time would be during the junior year or the summer after junior year. Four of the six respondents began their undergraduate research in the summer after their junior year and two began in the summer after their senior year.

The familiarization phase of the preparation stage can begin before the undergraduate student makes a formal commitment to do undergraduate research and while the prospective student is still taking some of the prerequisite courses, possibly during sophomore year. This phase can be tailored to the academic background of the student and serves not only to get the student prepared for the actual computational research, but also to fill in gaps in the academic background of the specific student. During this phase, the faculty mentor can evaluate the capabilities and limitations of the student as recommended by Belliveau (1983) and provide the necessary instruction to better match the skills of the student to the research as advocated by Lown (1993). The researcher’s academic preparation consisted of a strong undergraduate mathematics background, two semesters of undergraduate chemistry, and nuclear physics at the graduate level. During the preparation stage, the researcher completed independent study assignments in two advanced chemistry topics, symmetry and group theory, and molecular orbital theory. He also completed independent study on the UNIX system operating commands and the use of the UNIX visual editor to prepare input files. A chemistry major might not need much additional instruction in symmetry and group theory, but might need more preparation in quantum mechanics, since this is often covered in detail in an advanced physics course. The researcher's independent study in symmetry and group theory was supplemented by several lectures given by the faculty mentor and individual assistance with assigned exercises. The UNIX commands can be learned by practice on the computer with a known molecule like water. A less sophisticated program called Jaguar was used to allow the researcher to get familiar with the UNIX workstation and management of files in UNIX. One advantage of Jaguar is that it allows the operator to see a three dimensional representation of the molecule (which is not available using the PSI suite of programs), so it is an excellent teaching aide for visualizing the bond lengths and bond angles. The final part of the preparation phase is the use of the PSI suite of programs on the UNIX workstation for a known molecule such as water. The faculty mentor took the researcher through the entire process at all three levels of theory. This first stage took an entire semester – about four months – to complete. The time devoted to work on the familiarization phase was two to six hours per week for about 16 weeks. An undergraduate researcher could complete this phase during the first or second semester of junior year, or it could be incorporated into the first two weeks of an intensive summer research project.

The undergraduate researcher enters the second stage of the research when he or she begins work on a hypothetical molecule or an existing molecule that merits further theoretical study. The faculty mentor will normally propose the molecule based on his or her previous work, or the current research of others in the field of computational quantum chemistry. Another possibility for the student researcher would be to continue work on a structure that the faculty mentor or another student researcher has already started. Having a new student researcher assist another more experienced student researcher can reduce the time commitment of the faculty mentor; however, in small liberal arts institutions there may not be enough undergraduate researchers to allow students to have an experienced undergraduate research partner. The distinguishing feature of this stage of the research is that the undergraduate researcher is now beginning to perform calculations on new structures, or verifying theoretical predictions of other researchers. This what the students usually refer to as *real* research, and it is highly motivating when students feel they are making a contribution to the scientific body of knowledge. Four of the six former researchers indicated that one of the aspects of the research they enjoyed the most was the discovery of something new and making a contribution to the field.

Although this research is totally computational, which allows a record of all computations to be preserved in computer files, the researcher found that it was extremely helpful to keep a traditional laboratory notebook, just as a laboratory researcher would in a chemistry or physics laboratory experiment. Even though all of the essential input files and output files are stored in the computer, it was invaluable to have a record of what was done each day. The laboratory notebook provided a chronological record of the research, problems encountered, instruction and advice from the faculty mentor, tips on how to use UNIX commands more effectively, and symmetry calculations that must be performed for the input files. It also provided a way for the faculty mentor to monitor the progress of the undergraduate researcher. In addition to making notes during the actual computer work, the researcher used the laboratory book to summarize what had been done and to transcribe any notes from discussions with the faculty mentor. An undergraduate researcher can become less dependent on the faculty mentor more quickly, and will be more efficient in subsequent calculations if a detailed laboratory notebook is maintained on a daily basis.

Even after having performed the calculations at all three levels of theory on a known molecule, the undergraduate researcher will need a great deal of assistance when investigating the first new structure. As the number of atom and electrons in the molecule increases, the structure becomes increasingly complex, and the number of possible modes of vibration increases. Certain skills such as knowing reasonable starting values for the bond lengths and the values of the force constant matrix require experience in using the PSI suite of programs. The faculty mentor must work closely with the undergraduate researcher at the start of the independent work so that the input file is correct. A constant frustration at this stage will be errors in the format of the input file. In the beginning, the new researcher will not be able to interpret error messages that indicate format errors and omissions. Thus, early on, the student and faculty mentor must work side by side until the undergraduate gains some experience. As a school's research program grows, faculty members can share the supervisory tasks, or other more experienced undergraduate researchers can assist. The time devoted by the faculty mentor to supervision should not be viewed as a negative issue, however, because it is one of the strengths of undergraduate research. Three of the former researchers responded to the question on what aspect they most enjoyed about the research, stating, "direct interaction with my research mentor," "working in a research group," and "help was available, but I was encouraged to work independently."

Each molecule investigated will normally have several possible geometric configurations to be investigated. As a consequence, the computations at each level of theory will have to be repeated using basically the same steps. During this project, the researcher used a set of instructions for carrying out the second derivative calculations at the CISD and CCSD levels of theory that were prepared by a previous researcher. These instructions were generic but were very helpful. By using the instructions, the new researcher is less likely to skip steps in the process. The instructions helped remind the researcher about which files to save, how to label these files, and which files can be deleted. This step-by-step approach insures that an organized record of all research work is maintained and allows the faculty mentor to be able to recognize the files by their names. A detailed set of standard procedures is an important part of a good undergraduate computational research program.

For most undergraduate researchers, the independent research work will continue until a point is reached where the undergraduate must stop due to time constraints. Sufficient time must be provided in the program for the researcher to do the necessary preparation for the final stage, which is the presentation of the results. Although the results may be presented in a scientific journal as a separate journal article, it is more likely that the computational results will be part of a larger body of results from computations done by the faculty mentor and/or other undergraduate researchers. However, it is important that the undergraduate researcher be given the opportunity to present his or her own results and conclusions. This provides the student researcher an opportunity for improving background research skills, writing skills, and oral presentation skills. It also is a means of recognition of academic achievement.

Two of the former researchers indicated that one of the most important benefits of their research was the publishing of papers based on their research. Even if the research does not progress to the point of publishing results in a scientific journal, the student should present the research in the form of a paper, senior thesis, or oral presentation to the department or a student conference. Merkel and Baker (2002) and West (1994) describe some ideas for student presentations.

Only a few undergraduate researchers will progress to the point of innovative research during their time as undergraduate researchers. However, students may still have an opportunity to try out some of their own ideas in follow-up investigations during additional research prior to graduation or even after graduation. Three of the former researchers indicated that their research was done during the summer after their senior year and one had done research during the previous summer as well. One of the advantages of computational research is that a student can use discretionary time to work on new ideas on the computer, without the need for direct supervision by a faculty member or concerns about laboratory safety.

Cognitive Skills Needed in the Computational Process

The single most important advanced knowledge area for the computational quantum research is symmetry and group theory. It is an important component of several parts of the computational process. Most mathematics majors or physics majors will not have had any instruction in this area and will be at a disadvantage if additional instruction is not provided. Chemistry majors will have had some of the concepts and will probably be able to make up any skill gaps during the initial computer familiarization phase. The researcher, having a physics background, had no experience with molecular symmetry or group theory. However, through independent study of *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications* by Vincent (1977) and assistance from the faculty mentor in working the text exercises, the prerequisite skills were mastered.

Symmetry and group theory is used at the very beginning of the input process when the overall symmetry of the molecular structure must be determined. The symmetry group most often used is C_{2v}. The input file geometry must account for the symmetry of the molecule, because the computer program will generate the left half of the molecular structure based on the input geometry for atoms on the z-axis and the right side, and the fact that C_{2v} molecules are symmetric upon reflection through the x-z plane. The researcher must also understand the significance of the character table for the symmetry used (see Appendix A for the C_{2v} table), and how to take what is known as a reducible representation and convert it to a linear combination of irreducible representations (for the C_{2v} point group there are four irreducible representations labeled A_1, A_2, B_1 and B_2). By doing this, the electrons can be placed in the lowest energy molecular orbitals that match the symmetry of the molecule as a whole. This process is difficult for the new student even with some knowledge of group theory. The guidance of the faculty mentor is essential, but the student needs a foundation in the concepts to understand the principles applied in the process. Finally, symmetry concepts must be used when doing the computations of the vibrational frequencies at the CISD and CCSD levels of theory. These calculations require that the atoms of the molecule be displaced slightly so that a calculation of the energy and first derivative can be made. Some of the displacements are symmetric; for example, the left and right hydrogen atoms together move out from, or in towards, the oxygen. Others are asymmetric; for example, the left hydrogen atom moves out from the hydrogen while the right atom moves in toward the atom. Since the asymmetric displacements destroy the symmetry of the molecule, a new symmetry must be used to allow the calculations to be carried out. This step again requires using group theory to put the electrons in the proper orbitals when the symmetry of the molecule is changed. Three of the six former undergraduate researchers listed a physical chemistry course as one of the courses that was most helpful in preparing for the research, and two of the other three listed it as a course they wished they had taken prior to the beginning of their research. The physical chemistry course provides an introduction to symmetry and group theory in addition to an introduction to quantum mechanics.

Molecular orbital theory is another important cognitive skill that is required for this research. This will not be a problem for chemistry majors, although mathematics and physics majors will need some instruction. Most of what is needed can be found in basic chemistry textbooks, and the faculty mentor can provide the specific details through instruction and practice during the familiarization phase. However, the molecular orbital theory can only be applied when understood in the context of symmetry. This is because the essential part of the theory says that atomic orbitals on different atoms interact to form molecular orbitals that belong to the whole molecule and produce stronger bonding that reduces the total energy of the molecule. But these atomic orbitals will only interact with each other if they have the same type of symmetry, or in the words of group theory, they belong to the same irreducible representation of the point group (Vincent, 1977).

Understanding of quantum mechanics is not as essential to the actual computational process as the two areas described above. The student researcher should have been introduced to quantum theory in a physical chemistry course or a modern physics course. With this background, the undergraduate researcher will have been exposed to wave theory and the solutions to the Schrodinger equation for the hydrogen atom. Probably more important is that the student researcher have some experience with linear algebra, since the computer calculations involve the use of matrix solutions to a system of linear equations. The mathematics major and the physics major might be expected to have had a course in linear algebra, but the chemistry major probably will not have taken this course. Two of the former undergraduate researchers had taken a course in linear algebra and felt it was helpful in preparing them for this research. Two others listed linear algebra skills as essential to the conduct of their research.

In today's college environment, one might expect that all science majors will have basic proficiency with computers; however, many will not know much about computer programming and computational programs. For today's student who has grown up being familiar with the use of computers, though, learning the UNIX operational commands and file system should not be difficult. A course in computer programming would be helpful but is not a prerequisite. The researcher had some experience with Fortran programming and the use of a Fortran program for computer modeling as part of his master's thesis. However, the UNIX commands are very different from Fortran. Some individual study in an introductory text on UNIX and practice during the familiarization phase were sufficient preparation to master the basic skills needed to manage files and use the UNIX screen editor. In order to prepare the input files for the computations, the researcher must know the basic UNIX screen editor commands to properly create and edit lines of input parameters to the input files. Four of the six former undergraduate researchers listed computer programming and/or UNIX skills as essential to their research work, although, none of the six stated that they had taken any courses in programming or the use of UNIX. Two of the six said they wished they had taken a course in programming prior to the start of their research experience.

One of the significant strengths of this type of computational research is that it requires that the researcher integrate knowledge and skills from chemistry, physics, mathematics, and computer science. Even if the student is weak in one or more of these areas, the skill gaps can normally be bridged by individual study and instruction from the faculty mentor in the familiarization phase, and through coaching as the mentor and student work through the actual research. All of the former researchers listed mathematics, chemistry, and physics courses as the most helpful in their preparation, indicating that a solid mathematics and chemistry/physics foundation is essential. However, five of the six said they wish they had taken additional courses in mathematics, chemistry, or computer science. Although none felt fully prepared, they were able to be successful through learning the necessary skills as they participated in the research experience. By tailoring the preparation during the familiarization phase to each individual student, the faculty mentors can insure the undergraduate research experience provides the maximum benefit for the student.

Benefits of Undergraduate Research for the Student, Department, and Institution

The first benefit of undergraduate research is an enhancement of the academic experience of the student. The undergraduate that has the opportunity to participate will have the chance to learn new knowledge and apply the knowledge that he or she brings to the experience. All the higher skills of analysis, synthesis, and evaluation from Bloom's

Taxonomy are used as the researcher progresses through the research process. This computational research is particularly effective because it requires the integration of knowledge from mathematics, physics, chemistry, and computer science. However, any undergraduate computational research program in the sciences will undoubtedly provide integrative learning and a good deal of analysis and synthesis requiring knowledge from several academic disciplines. Research is active learning, which current educational research has recognized as an effective method for improving science teaching at the college level. The six former researchers were asked to score how their computational research experience improved their skills in the following areas: general computer skills, computational skills, writing skills, analytic thinking, research skills, and mathematics/chemistry/physics knowledge. They scored each area on a scale of 1 (no improvement) to 5 (significant improvement). Every area had an average score of 4 or higher, with the exception of writing skills (average score of 3.50), indicating that in all these areas the students felt the research experience had resulted in improvement or significant improvement of their academic skills. Even in the lowest area of writing skills the average score was between some improvement and improvement. See Table 4 for the complete results.

A second important benefit of this undergraduate experience is increased student motivation. Simply stated, it is exciting to discover something new and to have the freedom to experiment on one’s own. In addition, undergraduate students appreciate the one-on-one interaction that only a faculty mentor can provide. Two of the former researchers stated that the aspect of the research they enjoyed the most was doing “real”

Table 4

Summary of responses to question #10 (Completed questionnaires are in Appendix F).

Question #10 reads: Please indicate with a number from 1-5 the degree to which you feel your research experience improved in the following areas: (5 – Significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

Undergraduate researcher:	#1	#2	#3	#4	#5	#6	**Average**
General Computer Skills	4	5	4	4	5	5	**4.5**
Computational Skills	5	5	4	4	5	5	**4.7**
Writing Skills	4	3	2	3	4	5	**3.5**
Analytic Thinking	5+	5	3	4	4	4	**4.2**
Background research of scientific journals	3	5	4	3	5	4	**4.0**
Math/Chemistry/Physics knowledge	3	5	5	4	4	4	**4.2**

research, and two others said "learning something new…and trying out my own ideas" and "figure something out and contribute to the field." Three said a favorite aspect of the research was a social one, that is, working with a faculty mentor, working independently but having the faculty member available for help, or working in a research group. There were only three things mentioned as dislikes by the six researchers. One of these was frustration, but even it was stated in a positive light, in that frustration made the eventual success that much more satisfying. The other two negative comments had to do with the mentoring process. One researcher had difficulty in meeting with his student mentor during the academic day and another felt that some faculty regarded undergraduate researchers as "slave labor." It is interesting that of the six former undergraduate researchers, only two indicated any improvements they would recommend to the undergraduate research experience. One wished that he had taken linear algebra prior to the research, and another felt that more than one student mentor should have been assigned to each student (apparently due to an incompatibility of student schedules which made the student mentor unavailable during the academic day).

The third benefit of the undergraduate research experience is that it opens doors to future academic and career opportunities. Three of the researchers stated that the most important benefit of the research was that it led directly to their current career. Another stated that it helped in knowing how graduate research worked and how to select a graduate department and professor. Another stated that it expanded his "graduate school opportunities and marketability." In addition to these benefits, two of the former researchers said that a most important benefit was publishing a paper based on their research.

Computer computational research has several unique benefits for the academic department. As already mentioned, this research integrates several academic disciplines. Thus, several academic departments can have an undergraduate research program through collaborative efforts of interested faculty from each department. This collaboration allows small departments to share the responsibilities for organizing the research program and mentoring the students. A second benefit is the relatively low cost for scientific research. Modern chemistry or physics research can rarely be financed at educational institutions other than major research universities. Computational theoretical research can be done on very capable high-speed workstations that are available for a fraction of the cost of most pieces of research equipment. The two UNIX workstations used in this research were purchased for about $20,000 each.

The last two benefits of computer research are related to each other. They include flexibility and safety. The undergraduate student researcher, faced with the demands of a full load of undergraduate courses, can schedule time to work alone on the computer that fits into his/her schedule. There are none of the laboratory safety concerns that would require constant supervision in a chemistry or physics laboratory. The student cannot damage the equipment or harm himself or herself by trying something new. A key to the computer room is the only expense for the department in providing a student access to research time. Although having the workstation in the faculty mentor's office sometimes has disadvantages, the student and faculty member may benefit from having the workstation in the mentor's office, as was the case during this study. This situation allowed the researcher to work independently and have access to the mentor as needed. Once the researcher became fairly proficient in using the programs, the faculty mentor was only needed when difficult problems arose. This allowed the faculty member to work on other duties but still be available to assist in the research process when needed.

Finally, undergraduate research offers benefits to the educational institution's faculty, facilities and academic reputation. First, the Goodwin and Holmes (1999) argue that undergraduate research can motivate the faculty. Discovery is often just as exciting for the faculty as it is for the undergraduate. During this research, three members of the faculty spent many professionally fulfilling days during the summer performing computational research. The primary motivation was the challenge of the research and the desire to learn something new. The added benefit was increased scholarship as these faculty members sharpened their analytic skills and broadened their knowledge. There is no doubt that this excitement and newly acquired academic skills carry over into classroom instruction.

Publishing results in scientific journals can improve the ability of the institution to receive research funding. As detailed in chapter two, there are presently many sources of funding available to support undergraduate research. This funding offers the school the opportunity for equipment and facility improvement from outside normal funding sources. As equipment and facilities improve, more students can be accommodated in the undergraduate research program. These elements work together synergistically to improve the reputation of the institution as students and faculty publish papers and make presentations at conferences.

When the reputation of the institution improves, recruiting is enhanced. Good science students, who once were drawn to the big research universities, will be attracted to a smaller liberal arts undergraduate school that can offer them the advantages of undergraduate research with a faculty mentor. Large research universities often place most of their emphasis on graduate research, and if undergraduate research is done, the mentors are likely to be graduate students. Smaller liberal arts institutions and primarily teaching institutions can offer unique educational mentoring opportunities to science majors who want to do undergraduate research. Finally, the institution benefits because undergraduate research programs can improve student retention.

Undergraduate science research has the potential to produce a margin of excellence for the liberal arts institution by enhancing the academic experience of the student, improving the scholarship of the faculty and promoting recruitment and retention. Computational research can provide a relatively low cost, flexible, safe program that provides a challenging multidisciplinary learning experience for mathematics, chemistry, or physics majors.

CHAPTER V: RECOMMENDATIONS

Based on the research of the current study, it is recommended that undergraduate research be part of the academic offerings at all four-year institutions of higher learning, not just those universities with graduate research programs. Smaller liberal arts colleges and universities and other primarily teaching institutions can provide a margin of excellence for their students by making a commitment to fostering undergraduate research programs. The challenge for liberal arts institutions desiring an undergraduate research program in chemistry or physics is to develop a first-rate research program that can be carried out at reasonable cost. This study suggests that computational research using powerful desktop workstations can provide a cost effective approach to scientific research in theoretical chemistry and physics. Because of the mathematics and computer skills that are also demanded by this research, computational undergraduate research will also appeal to students from these disciplines. There are several key components to this undergraduate research model. They include institutional support, department and faculty support, facilities and equipment, and a well structured program. Each of these components is described in this chapter.

Institutional Support

First and foremost, the leadership of the institution must recognize and communicate the desire and support for undergraduate research. The school's president, as the lead administrator, must be an advocate, in addition to the school's leader of academics, the provost or head of academic affairs. This support can take many forms but should, at a minimum, consist of written policy statements and a commitment of institutional resources. Institutional policy statements should make undergraduate research a priority for a quality academic program. Departments should be encouraged to develop undergraduate research programs by providing institutional funding to supplement funding from outside sources, and as necessary, research space. Ideally, existing laboratory space should be utilized in order to keep startup costs to a minimum. Computational research can be done at a workstation in the office of a faculty mentor, or in the corner of an undergraduate chemistry or physics laboratory. The most significant financial commitment that the leadership can make to the support of an undergraduate research program is compensation for faculty time needed to supervise the undergraduate research program and to mentor the student researchers. This could be in the form of additional pay for hours of overload based on the number of students mentored, or it could be in the form of credit in the teaching load. Faculty cannot be expected to mentor students in quality research efforts without recognition by the school leadership of the time involved.

Department and Faculty Support

While institutional leadership can promote an atmosphere that encourages and fosters scholarship through undergraduate research, Hilborn and Howes (2003) have noted, in their report on excellence in undergraduate programs, that the academic department is the critical element in initiating academic reform. Undergraduate research is often seen as taking the faculty away from their teaching responsibilities, research, or other duties (Boyer, 1987, 1990; Doyle, 2000). Thus, it is vitally important that the department chair and the faculty be committed to undergraduate research before an effort is made to establish a program. It may be only a small portion of the department that is actually involved in the mentoring of students, but others in the department will be asked to sacrifice in support of the program by assuming some of the duties of the mentoring faculty, helping to administer the program, sacrificing some of the department budget, or serving as members of committees reviewing student papers or presentations. Motivation to support undergraduate research will increase as faculty members experience some of the benefits of increased scholarly activity on the part of the faculty and the student majors in the department.

When a majority of a department's faculty has bought in to the idea, the department chair must be willing to commit resources to get the program started. In the case of computational research, this could be in the form of sufficient funds to purchase at least one workstation plus any required software. The department may be able to receive funds from the institution or grants from outside sources, but an investment of department resources sends the message that undergraduate research is an endeavor worthy of the use of precious department funds. For computational research, there are minimal additional expenses to get started. As the program grows, additional space and workstations may be required, but a small room and two workstations can easily support five to six student researchers, especially if the research area is configured so that the students can work on the computers at any time.

Faculty members should be encouraged to seek out interdisciplinary partnerships with other departments. Computational research offers the possibility of creating an undergraduate research team by drawing interested faculty from the chemistry, physics, mathematics, and computer science departments. The primary researcher is now part of a three-person team consisting of faculty from the Mathematics Department and the Department of Biology and Chemistry.

Finally, the department can commit to faculty development in undergraduate research by sending interested faculty to professional development opportunities like the annual conference held by the Council for Undergraduate Research (CUR). Now in its tenth year, the conference provides sessions on all facets of the undergraduate research process. Appendix C details topics to be covered at one such national conference.

The Essential Features of a Computational Undergraduate Research Program

The undergraduate research program will take many forms based on the type of research, the resources available, and the personalities involved. However, because the ultimate goal is to provide the best possible experience for the undergraduate researcher, there are several essential elements that should be present in every undergraduate research program. First, there must be a process to recruit and screen potential undergraduate students. Second, there must be a formalized process that insures timely completion of the research, what is often referred to as the URE – undergraduate research experience. Finally, there must be assessment of the program, including assessment of the individual students and the program as a whole. One of the greatest dangers is to have a program that looks like undergraduate research, but in reality is just undergraduates helping faculty do the faculty member's research. If this happens, the student researcher may become nothing more than a laboratory assistant, or what one of the former questionnaire respondents referred to as slave labor.

The recruiting process will, most likely, be informal at first. Contacts made with promising students in the classroom or current laboratory assistants will help the faculty to identify potential candidates. However, once the program begins to grow and has several students involved, the department may want to schedule an orientation meeting once or twice per year where students are invited to see what is being done in the undergraduate research program. Student researchers rather than the faculty should be used to give the briefings. Screening applicants should be a formalized process, and every good undergraduate research experience will require that the student have a good foundational academic preparation. For computational quantum chemistry research, this will take most students at least two years of mathematics, chemistry, and physics. When a student is identified as a prospective candidate, the faculty mentor should meet with the student to determine the student's qualifications and interests. A written checklist should be used to assist in determining if and when the student might be ready to begin and what type of undergraduate research program he or she may desire – summer research, research during the academic year, or performing the research for a senior thesis. This screening can identify what prerequisite courses are still needed and the type of familiarization training the student will need. The checklist can be kept on file and updated each semester. See Appendix D for a sample checklist for screening applicants.

The second essential feature of an undergraduate program is a formalized undergraduate research experience. The best way to do this is through the creation and signing of a contract between the student and the department or the faculty mentor. In this way, the expectations of the department can be clearly communicated to the student so that the student knows what is expected in terms of time commitment and the final product. It is important that this contract be one that is based on the desires of the student as well as the department. It must be somewhat flexible in terms of research outcomes, because the undergraduate student can only be expected to commit some maximum number of hours to research. The primary expectation for the student's work is that it should be of high quality. This may mean doing much less than what a graduate researcher would do, but nevertheless, doing it well. On the other hand, the student knows that by a certain time, a product is required. This product may be a formal paper or an oral presentation, but there should be a specified end to the research. Contracts will vary, but at a minimum, the following topics should be included in the contract: (1) a brief description of the research to be done; (2) the schedule for the URE; (3) the minimum research hours per week (in the case of computational research, it may be necessary to schedule certain hours that are dedicated to each student researcher); (4) requirements for regular meetings with or informal written progress reports to the faculty mentor; (5) requirements for record keeping, such as the use of a laboratory notebook detailing a chronological record of all computational work; and (6) the final formal report to be produced by the student at the conclusion of the research. See Appendix E for a sample research contract outline. In preparing the schedule, the faculty member must insure that ample time is built into the schedule for familiarization and for the preparation of the final product. As noted by Belliveau (1983) as little as 30-50% of the total student time will be devoted to the gathering of actual research data.

The contract is the vehicle to promote a quality undergraduate research experience, but it is the faculty mentor who must carefully drive the process. Undergraduate research must be seen more as a partnership between the faculty mentor and the student researcher, rather than as a corporation with the faculty member as supervisor and the student as subordinate. This will require a significant commitment of time and energy on the part of the faculty mentor, but time that is well spent in the scholarly development of both student and faculty member. As the research progresses, it is important that the faculty member allow the research to be driven, whenever possible, by the curiosity of the student. This may mean that the research does not progress as far as the faculty member had hoped, but it may progress much further in terms of sparking the intellectual development of the student. Computational research allows the student to try out new ideas, even when the faculty member is not present. The only consequence of a bad idea is the construction of a molecular structure that the theory says will not hold together. When the student does try new ideas, it is important that the faculty mentor and student exchange ideas on both successes and failures, as just as much or more of the learning may take place discussing an unstable structure or why a computation failed. Finally, the mentor must insure that the final product is professional and is presented in a forum that provides recognition for the efforts of the student. If merited, the student should be allowed to make a presentation at a conference outside the school. No only does this provide additional experience for the student and an opportunity to learn from other students and faculty, but also it motivates the student and enhances the reputation of the undergraduate research program within the school and the reputation of the institution outside the school.

The final essential feature for an undergraduate research program is assessment. An important part of the assessment will be the final products produced by the student researchers. The reports and papers will provide the department one way of evaluating the program and the URE of the students. Student presentations can be videotaped as a means of preserving oral reports. In addition, the department should use an assessment instrument such a questionnaire to provide student feedback. This questionnaire should be tailored to the research program and be designed to improve the URE for the student.

It should seek to determine, from the standpoint of the student, if the experience has been a valuable one and in what way it has contributed to the student's academic, social, and personal development. Determining if actual academic subject matter learning or improvement of research skills has taken place is more difficult and might require some form of pre- and post-assessment tools. However, even in the absence of such instruments, the student feedback instrument should not be neglected. The questionnaire used for the former student researchers (Appendix B) would provide a good starting point for a department assessment instrument on computational research and many other types of undergraduate research. One of the expected outcomes of the National Science Foundation three-year study on undergraduate research is the production of an instrument that can be used to evaluate an undergraduate research program (Mervis, 2001). Finally, the department should establish a system for tracking its student researchers after graduation. Many departments already have formal or informal systems for keeping in touch with their academic majors after graduation. If so, the undergraduate researchers, if not department majors, could be added to the list of those to be tracked. If there is no system to track majors, the department sponsoring the research should establish a system. The system could be as simple as maintaining an email distribution list and a list of contact phone numbers and addresses. Addresses are important, because mail can be forwarded if email addresses and phone numbers change. If contact is maintained, the department can follow the careers of the graduated researchers, and if desired, send them follow-up questionnaires to examine the impact of the research experience later in their academic or professional careers. As noted in chapter 4, the feedback from the six former undergraduate researchers (Appendix F) was obtained through the use of email. The most difficult part of communicating with the respondents was finding their current email addresses.

Limitations of the Study

The most critical limitation of this study is that the researcher was not an undergraduate student. The researcher is a college physics teacher with over fourteen years of teaching experience at the undergraduate level. His graduate work was in nuclear engineering and had little direct application to quantum chemistry research, other than the study and research skills acquired in the process of master's level work. The goal of the research study was to construct a framework based on learning the process, theory and tasks necessary to perform computational chemistry research by becoming a first-time participant, just as an undergraduate student would. The knowledge and skills required for the researcher are exactly the same as for an undergraduate, only the time needed to become proficient will vary based on the ability and background of the particular researcher. A student who has taken a physical chemistry course might learn some of the symmetry and group theory knowledge more quickly. Thus, the time and effort required to gain the necessary skills would vary, but the academic background and research skills, such as using UNIX, which must be learned will be generally the same for all participants.

The study is also limited in that the computational research process examined was very specific – the use of the PSI suite of programs to perform quantum chemistry calculations for only two molecules. However, although many of the results and recommendations are based on the research experience of the researcher, and biased by his perceptions, they are well supported by the responses of the other six undergraduate researchers and by most of the current literature on undergraduate research.

Finally, the six questionnaires received from former researchers do not represent a random sample of former undergraduate researchers doing computational quantum chemistry research. Due to a fairly limited number of former undergraduate researchers in this field and a lack of tracking information on many of the participants, the six who responded were all undergraduate researchers who had been successful in completing the research process. Nevertheless, no attempt was made in advance to find former researchers who had a favorable experience, even though all six were very positive about their research experience.

Recommendations for Further Study

The next step in this research field would be to study and evaluate this model in a pilot program. This would require the active recruiting of several students interested in doing computational research. In all likelihood, candidates will be drawn from physics majors or minors, or chemistry majors or minors. Mathematics majors should also be considered after they have completed two semesters of physics. A formal program should be established using instruments similar to the checklist for recruiting (Appendix D) and the contract (Appendix E). Faculty mentors should be responsible for supervising the familiarization phase based on the students' academic backgrounds. Pre- and post-test instruments could be administered to the student participants to evaluate knowledge and skills acquired. Feedback in the form of questionnaire responses using the questionnaire from this research (Appendix B) would provide good comparison data to the responses in this study. An evaluation of the program could be done using the survey instrument expected from the National Science Foundation Study on undergraduate research when it becomes available.

A high-quality undergraduate research program can be the difference between a good science program and an excellent one. Liberal arts institutions and primarily undergraduate institutions can develop an undergraduate research program at minimal cost using computational research. The cost of high-speed powerful workstations continues to drop. Virginia Tech has built a supercomputer that is listed in the top ten fastest supercomputers at a fraction of the cost of a typical supercomputer by combining 1,100 desktop Apple computers (Nystrom, 2004). Computational research offers a relatively low cost, interdisciplinary approach to scientific research. Small institutions will normally have fewer numbers of science faculty interested in mentoring undergraduate research, but the ability of this research to draw faculty from at least four different disciplines allows the small liberal arts school to form a team of faculty mentors to support a viable undergraduate research program. Based on the experience gained by the researcher, he is now capable of serving as a mentor for undergraduate research and his research team at this University has grown to three members. The research computers are two aging UNIX workstations currently located in the office of one of the team members. The challenge ahead for this research team is to seek funding to purchase a new workstation, to obtain a small area dedicated to research work that provides security of the workstations, and to recruit undergraduate researchers. With the support of the institution, the department, and the faculty, an undergraduate research program in computational quantum chemistry can become a reality at this liberal arts institution.

REFERENCES

Abudayyeh, O. (2003). Undergraduate research mentoring model in constuction engineering and management. *Journal of Construction Engineering and Management, 129*(1), 65-69.

Belliveau, J. F. (1983). Establishing an undergraduate research program: Some problems and suggested solutions. *Journal of Chemical Education, 60* (8), 670-671.

Bentley, W. E. (1994). Undergraduate researchers within a biochemical engineering research program: Factors influencing quality and learning experience. *Proceedings of the American Society for Engineering Education,* Washington, DC, 1461-1464.

Bonacic-Koutecky, V., Gaus, J., Guest, M. F., Cespiva, L., & Koutecky, J. (1993). Ab initio CI study of the electronic structure and geometry of neutral and cationic hydrogenated lithium clusters. Predictions and interpretations of measured properties. *Chemical Physics Letters, 206*(5,6), 528-539.

Bonacic-Koutecky, V., Pittner, J., & Koutecky, J. (1996). Ab initio study of structural and optical response properties of excess-electron lithium-hydride and sodium-fluoride clusters. *Chemical Physics, 210*, 313-341.

Boyer, E. L. (1987). *College: The undergraduate experience in America*. New York: Harper & Row.

Boyer, E.L. (1990). *Scholarship Reconsidered: Priorities of the Professoriate*. Princeton, NJ: The Carnegie Foundation for the Advancement of Teaching.

Brown, J. S., Collins, A., & Duguid, P. (1989). Situated cognition and the culture of learning. *Educational Researcher, 18*, 32-42.

Davy, R., Skoumbourdis, E. & Kompanchenko, T. (1999). Complexation of hydrogen by lithium: Structures, energies and vibrational spectra of $Li^{+}(H_2)_n$ (n=1-4), Li-$H(H_2)_m$ and Li-$H^{+}(H_2)_m$ (m=1-3). *Molecular Physics, 97*(12), 1263-1271.

Doyle, M. P. (Ed.) (2000). *Academic excellence: The role of research in the physical sciences at undergraduate institutions.* Tucson, AZ: Research Corporation.

Fuentealba, P. & Reyes, O. (1999). Density functional study of Li_nH_m clusters. Electric Dipole Polarizabilities. *Journal of Physical Chemistry A, 103,* 1376-1380.

Goodwin, T. & Holmes, B. (1999). *How to get started in research* (2nd ed.). Washington, DC: Council on Undergraduate Research.

Halstead, J.A. (1997). Council on Undergraduate Research: A resource (and a community) for science educators. *Journal of Chemical Education, 75*(11), 148-149.

Hilborn, R. C. & Howes, R. H. (2003). Why many undergraduate physics programs are good but few are great. *Physics Today,56*(9), 38-44.

Johann, P. & Turbak, F. A. (2001). Lumberjack summer camp: A cross-institutional undergraduate research experience in computer science. *Computer Science Education, 11*(4), 279-304.

Kardash, C. M. (2000). Evaluation of an undergraduate research experience: Perceptions of undergraduate interns and their faculty mentors. *Journal of Educational Psychology, 92*(1), 191-200.

Karukstis, K. K. (2000). A report on CUR 2000: The many facets of undergraduate research. *Journal of Chemical Education, 77*(1), 1388-1389.

Kinkead, J. (2003). Learning through inquiry: An overview of undergraduate research. *New Directions for Teaching and Learning, 93*, 5-17.

Landrum, R. E. & Nelsen, L. R. (2002). The undergraduate research assistantship: An analysis of the benefits. *Teaching of Psychology, 29*(1), 15-19.

Lanza, J. (1988). Education: The whys and hows of undergraduate research. *BioScience, 18*(2), 110-112.

Lanza, J. & Smith, G. C. (1988). Undergraduate research: A little experience goes a long way. *Journal of College Science Teaching, 18*(2), 118-120.

Lown, J. M. (1993). Involving undergraduates in faculty research. *Advancing the Consumer Interest, 5*(3), 29-31.

McIntosh, G. (2001). Intellectual development and undergraduate research in physics. *Journal of College Science Teaching, 30*(6), 412-413.

Merkel, C. A. & Baker, S. M. (2002). *How to Mentor Undergraduate Researchers.* Washington, DC: Council on Undergraduate Research.

Mervis, J. (2001). Student Research: What is it good for? *Science* [Online], *293*(5535). Available: Ebscohost/Academic Search Premier [2003, May 23].

Moore, J. W. (2001). Research, Discovery, and Education. *Journal of Chemical Education, 78*(4), 431.

National Science Foundation. (1989, April). *Report on the National Science Foundation workshops on undergraduate education*. Washington, DC: Author.

Nystrom, L. (2004). Great X-pectaions. *Virginia Tech Magazine, 26*(2), 8-10.

Osteryoung, J. (1999). Integrating research and education. *Chemtech*, *29*(7), 42-44.

Rao, B. K., Khanna, S.N., & Jena, P. (1991). Energetics and electronic structures of hydrogenated metal clusters. *Physical Review B, 43*(2), 1416-1421.

Research Corporation. (2001). *Academic excellence, the sourcebook: A study of the role of research in the natural sciences at undergraduate institutions*. Tucson, AZ: Author.

Schrödinger, Inc. (1997). Jaguar v 3.0 [Computer Software and manual]. Portland, OR.

Siebert, E. D. (1988). Undergraduate research: Is it really worth it? *Journal of College Science Teaching, 18*(2), 92-97.

Stevens, J. G. (1994). Why should my institution be interested in undergraduate research? Unergraduate research in perspective. *Council on Undergraduate Research Quarterly,138-142*.

Tobochnik, J. (2001). The importance of undergraduate research. *American Journal of Physics, 69*(9), 933-934.

Vincent, A. (1977). *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications.* London: John Wiley & Sons Ltd.

West, D. X. (1994, March). A voice of experience: Characteristics of a successful research program for undergraduates. *Council on Undergraduate Research Quarterly, 146-149*.

Whitten, K. W., Davis, R.E. & Peck, M.L. (1996). *General Chemistry with Qualitative Analysis* (5^{th} ed.). New York: Saunders College Publishing.

Wieman, C. (2001, May). A modest proposal: Recruit undergraduate majors. *APS News,* p. 5.

Wilensky, J. (2002). Undergraduate research in human nutrition and health. *Human Ecology, 30* (2), 4-6.

Wray, D.D. (2000). The effectiveness of undergraduate researchers and the effect of undergraduate research on the student (Doctoral dissertation, Idaho State University, 2000). *Dissertation Abstracts International, 61*, 2244.

APPENDIX A: CHARACTER TABLE FOR THE C_{2V} POINT GROUP

Table A1

C_{2V} Character Table Showing the Four Irreducible Representations (A_1, A_2, B_1, B_2).

C_{2V}	I (Identity)	C_2(180˚rotation)	σ_v (xz reflection)	σ_v (yz reflection)
A_1	+1	+1	+1	+1
A_2	+1	+1	-1	-1
B_1	+1	-1	+1	-1
B_2	+1	-1	-1	+1

APPENDIX B: QUESTIONNAIRE SENT TO FORMER UNDERGRADUATE RESEARCHERS

Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1. Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

2. Briefly describe the nature of your first undergraduate research project.

3. What college courses were most helpful in preparing you for this research?

4. What specific academic skills/knowledge (if any) do you feel was essential to your research work?

5. Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

6. Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

7. What were the most important benefits to you of your research experience?

8. What changes or improvements would you recommend to your experience?

9. Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

10. Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills:

Computational skills:

Writing Skills:

Analytic Thinking:

Background research of scientific journals:

Math/Chemistry/Physics knowledge:

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

APPENDIX C: CUR 10TH NATIONAL CONFERENCE AGENDA

Crossing Boundaries
Innovations in Undergraduate Research

CUR 10th National Conference

Conference Program

Key: ♣ Repeated Session
(\$) Funding Session

Wednesday, June 23rd		
5:00 pm - 9:00 pm	**Workshop Leader/Speakers Bureau Prep Room Open**	
6:30 pm - 8:30 pm	**Line Dinner for arriving National Conference Participants**	
8:00 pm - 10:00 pm	**Welcoming reception**	
Thursday, June 24th		
7:00 am - 8:00 am	**Line Breakfast**	
8:00 am - 9:50 am	**Opening Plenary Session:** **Undergraduate Research: Current and Future Challenges** Cora Marrett, University of Wisconsin System Carlos Gutierrez, California State University, Los Angeles	
10:00 am - 11:00 am	**Workshop Session I**	
	The Research Laboratory as Context for Minority Student Success: Continuing the Conversation Carlos Gutierrez, California State University, Los Angeles	
	How to Get Started in Research with Undergraduates Merlyn Schuh, Davidson College Michael Castellani, Marshall University	
	Incorporating Environmental Themes and Problems into Undergraduate Research and Teaching Rebecca Roberts, Ursinus College Catherine Roberts, College of the Holy Cross Alison Draper, Trinity College	
	Engaging Undergraduates in the Research Process in Psychology: From Inception to Publication Mukul Bhalla, Loyola University New Orleans Steven Kass, University of West Florida	
	Integrating Research into an Undergraduate Laboratory Quinn Vega, Montclair State University	
	Incorporating Scientific Communication into Summer Research Mary Walczak, Paul Jackson, Charles Umbanhowar, Jr.David Van Wylen St. Olaf College	
	Getting the Biggest Bang for the Buck: Integration of Research into Undergraduate Science Education Charlotte Hammond, Dennis Opheim, Allan Smits Quinnipiac University	
	Promoting Undergraduate Research through Running Undergraduate Research Conferences Kathleen Morgan and Meg Blasberg, Wheaton College	

	Mentoring Undergraduate Research Experiences at Remote Locations Gubbi Sudhakaran and Mike Jackson, University of Wisconsin-La Crosse Wm. Christopher Hughes and Amelia Cohen, James Madison University	
	An Overseas Sabbatical, C'est Magnifique! Thomas Wilson, Marshall University Rexford E. Adelberger, Guilford College Stuart B. Crampton, Williams College	
	Changing Institutions: A Revolution One Step at a Time Marcus Webster, St John's University Chris Rohlman, Albion College	
	Working at the National Science Foundation: Life as an NSF Rotator Jeff Ryan and Theodore Hodapp, National Science Foundation Jill Singer, Buffalo State College	
	Curricular Elements that Enhance Undergraduate Research Diane Husic, East Stroudsburg University Tim Elgren, Hamilton College Tom Wenzel, Bates College	
	What Deans Can Do To Support Undergraduate Research: Deans' Roundtable Michael Nelson, University of Wisconsin - La Crosse Mike Nelson, University of Wisconsin - La Crosse Norine Noonan, College of Charleston Mike Tannenbaum, Marist College David Brakke, James Madison University Beth Cunningham, Bucknell University Neal Abraham, DePauw University	
11:00 am - 11:20 am	**Break**	
11:20 am - 12:20 pm	**Workshop Session II -- FUNDING SESSIONS**	
	$ ♣ Ten Ways to Blow a Grant Proposal **(repeated see Workshop VI)** Naomi Amos, Randolph-Macon Woman's College	
	$ E-Grants Charlie Havekost, Grants.gov	
	$ The Bucks Start Here! Ron Siatkowski, Lawrence Funke, ACS Petroleum Research Fund	
	$ NSF Programs Relevant for Mathematics and Computer Science Faculty at PUIs Zsuzsanna Szaniszlo, Valparaiso University Lee Zia, NSF DUE Janet Andersen, Hope College	
	$ Research Corporation Programs in Chemistry, Physics and Astronomy Silvia Ronco, Research Corporation	
	♣ Assessment of Undergraduate Research Experiences **(repeated see Workshop II)** Patricia Soochan, Howard Hughes Medical Institute David Van Wylen, Saint Olaf College	
	$ ♣ NSF DUE CCLI Program Overview **(repeated see Workshop IX)** Theodore Hodapp, Duncan McBride & Jeff Ryan, National Science Foundation Jill Singer, Buffalo State College	
	$ Opportunities for Students and Faculty at NASA James Gorman & Warfield Teague, NASA, Office of Education	
	$ ♣ NIH Academic Research Enhancement Awards (AREA) **(repeated see Workshop III)** Jean Chin, National Institutes of Health	
12:20 pm - 2:00 pm	**Line lunch with special topic discussion tables** **1. Merck/AAAS funded programs** Susan Painter, Merck Michael Tannenbaum, Marist College	

	2. Student Learning Outcomes of Undergraduate Research Keith Miller, University of Wisconsin - Oshkosh Maureen McCarthy, American Psychological Association **3. Interdisciplinary Undergraduate Research** Andrei Ludu, Northwestern State University Steve Deckelman, University of Wisconsin-Stout **4. Scholar Communities** Glenn Acree, Belmont University **5. Integrating Research into First Year Courses** Vickie Geisler, State University of West Georgia **6. Undergraduate Research Abroad** Isai Urasa, Hampton University	
2:00 pm - 3:00 pm	**Workshop Session III -- FUNDING SESSIONS**	
	Writing Excellent Research Proposals - The ACS PRF View Ron Siatkowski, Lawrence Funke, ACS Petroleum Research Fund	
	♣ Assessment of Undergraduate Research Experiences **(repeated see Workshop II)** Patricia Soochan, Howard Hughes Medical Institute David Van Wylen, Saint Olaf College	
	♣ NIH Academic Research Enhancement Awards (AREA) **(repeated see Workshop II)** Jean Chin, National Institutes of Health	
	The Camille & Henry Dreyfus Foundation: An Overview of Support for Undergraduate Institutions Mark Cardillo, The Camille & Henry Dreyfus Foundation, Inc.	
	NSF Physics Lawrence Brown, National Science Foundation Physics	
	Funding Opportunities at NIMH Nancy Desmond, National Institute of Mental Health	
	Research Funding Opportunities in the Geosciences Jeffrey Ryan, National Science Foundation/Division of Undergraduate Education	
	New Multidisciplinary Programs from NSF Chemistry Katharine Covert, National Science Foundation Chemistry	
	Funding Opportunities in Social Sciences at the National Science Foundation Gregory Chu, National Science Foundation, SBE/BCS	
3:10 pm - 4:10 pm	**Workshop Session IV -- DISCIPLINARY: FUTURE CHALLENGES**	
	Administrators Mentoring Faculty Towards Externally Funded Research Naomi Amos, Randolph-Macon Woman's College	
	Teaching Research Integrity and Bioethics to Science Undergraduates Julio F. Turrens, University of South Alabama Elizabeth Davidson, Arizona State University	
	Overcoming Historical Barriers to Research in HBCU Settings Adeleri Onisegun, Morris College	
	Creating a Safe Lab Environment in Geosciences Research Kirsten Menking, Vassar College Gregory Hancock, College of William Mary, Brannon Anderson, Furman University	
	Getting a Tenure-Track Faculty Position at a Primarily Undergraduate Institution Mark Biermann, U. S. Naval Academy David McGee, Drew University Kevin Riggs, Stetson University Karen Kolehmainen, California State University, San Bernardino	
	Sneaking Research Into Your Teaching: Challenges for Generalists at PUIs Brenda Wilhelm, Mesa State College	
	Outcomes from the Undergraduate Research Summit on Chemistry Thomas Wenzel, Bates College Other CUR Chemistry Councilors	

	Defining Undergraduate Research Experiences in the Social Sciences Julia Wallace and B. Keith Crew, University of Northern Iowa John Pollock, The College of New Jersey
	Faculty Perceptions of the Benefits of Undergraduate Research David Lopatto, Grinnell College Anne-Barre, Hunter Center to Advance Research and Teaching in the Social Science Jim Swartz, Grinnell College
	Future Challenges in Undergraduate Research in Biology Larry Wimmers, Towson University
	Mathematical Biology--Linking Mathematicians and Biologists through Student Research Tom Sibley, St. John's University Charles Rodell, College of St. Benedict Gordon Brown, St. John's University
	Raising the Bar in Student Research in Psychology: Beyond 'Mood and Music' Mark Zrull, Appalachian State University Joanne Altman, Washburn University
4:20 pm - 6:30 pm	**Funding Fair & Poster Session with Reception**
6:30 pm - 8:00 pm	**Reception & Banquet (adults only)**
8:00 pm - 10:00 pm	**Open Houses & Discussion Groups** ***Posters may still be viewed***
Friday, June 25th	
7:00 am - 8:30 am	**Line Breakfast with special topic discussion tables** **1. Academic Women's Negotiating Styles** Susan Matts, Mary Washington College **2. Undergraduate Research Committees** Ed House, Idaho State University **3. Redesigning General Chemistry Curricula** Girija Subramaniam, Penn State **4. Student Research Journals** Robin Harris, Georgia College & State University **5. Networking with Science and Humanities Faculty On Campus** Maria Bohorquez, Drake University **6. Attracting/Retaining Underrepresented Groups in STEM** Mary Crowe, Coastal Carolina University **7. Animal care and IACUCs** Jill Manske,University of St. Thomas Marcus Webster, Saint John's University
8:30 am - 9:40 am	**Plenary II:** **Models of Multidisciplinary Research** Jill Schneiderman, Vassar College Mark R. Weaver, The College of Wooster
9:40 am - 10:00 am	**Break**
10:00 am - 11:00 am	**Workshops V**
	Summer in Paris: Undergraduate Research Program at Pennsylvania State University-Delaware and the University of Paris Elizabeth Dudkin and Robert C. Black, Penn State University
	National Science Foundation Funding Opportunities in Biology Sally O'Connor, National Science Foundation
	Latino Community Research through an Interdisciplinary Approach Julie R. Alexandrin, Lorrie Gardella & Wayne Steely, Saint Joseph College
	National Science Foundation Major Research Instrumentation (MRI) Program Angela Klaus, National Science Foundation

	Crossing Disciplinary Boundaries: Creating an Interdisciplinary Research Program for Undergraduates Susan Eve, University of North Texas Keith Whitworth, Texas Christian University	
	Merck/AAAS Undergraduate Science Research Program: Interdisciplinary Focus on Funding Undergraduate Research Susan Painter, Merck Research Laboratories Linda Akli, American Association for the Advancement of Science	
	Research at Comprehensive Colleges (I) - An Administrative Perspective John Mateja, Murray State University David F. Brakke, James Madison University William Campbell, University of Wisconsin - River Falls Lawrence Panek, Widener University	
	Justice as a Motivation for Multidisciplinary Research: Continuing the Conversation Jill Schneiderman, Vassar College	
	So I've Got Tenure: Now What? Samuel Abrash, University of Richmond Tim Elgren, Hamilton College Roger Rowlett, Colgate University Rosemary Marusak, Kenyon College	
	Ongoing Challenges Faced by Research-Active Faculty at Primarily Undergraduate Institutions: Generating New Ideas and Sustaining Research Productivity Diane Husic, East Stroudsburg University Julio dePaula, Haverford College Kerry Karukstis, Harvey Mudd College	
	Interdisciplinary Materials Science at a Small Liberal Arts College: Integration of Curriculum and Research Sasha Dukan and Scott Sibley, Goucher College	
	♣ National Science Foundation Proposal-Writing Workshop **(repeated see Workshop VI)** Theodore Hodapp, Duncan McBride, Jeff Ryan National Science Foundation Jill Singer, Buffalo State College	
	Integrating Research, Teaching and Community Participation: The Collaborative Effort to Improve Water Quality in a Local Watershed: Continuing the Conversation Mark Weaver, The College of Wooster	
	Best Practices for Undergraduate Research in Sociology Carla Howery, American Sociological Association Diane Pike, Augsburg College	
11:10 am - 12:10 pm	**Workshop Session VI**	
	♣ National Science Foundation Proposal-Writing Workshop **(repeated see Workshop V)** Theodore Hodapp, Duncan McBride & Jeff Ryan, National Science Foundation	
	♣ Ten Ways to Blow a Grant Proposal **(repeated see Workshop II)** Naomi Amos, Randolph-Macon Woman's College	
	CUR Review of a Science Division Carl Salter, Moravian College Michael Tannenbaum, Marist College	
	Administrative Support of Research Responsibilities Barbara J. Byrne, University of the Sciences in Philadelphia Maria Moyer, Richard Stockton College of New Jersey Sally Mateja, Murray State University	
	Creating and Implementing an Undergraduate Interdisciplinary Integrated Research Methods/Statistics Two-Course Sequence at William Paterson University Kathy Silgailis and Martin Williams, William Paterson University	
	A Fork in the Road - Multiple Societies Michael Nelson, University of Wisconsin - La Crosse Timothy B. Holst, University of Minnesota-Duluth Jill Singer, Buffalo State College Jim Gentile, Hope College	

	Organizing Society for Undergraduate Research, Scholarly and Creative Activities (SURSCA): A student organization to support undergraduate research Tim Lyden, Bill Campbell and Ginny Coombs, University of Wisconsin-River Falls	
	Research Opportunities at the Interface of Science and Art Richard R. Hark, Juniata College Patricia S. Hill, Millersville University Michael Henchman, Brandeis University	
	Expanding a Summer Research Program across Disciplines Andrea Chapdelaine and Frieda Texter, Albright College	
	Research at Comprehensive Universities II: A Faculty Perspective Michael P. Castellani, Marshall University Charlotte Otto, University of Michigan - Dearborn Lydia K. Fox, University of the Pacific Luis Martinez, University of Texas, El Paso	
	The NCUR/Lancy Program and Interdisciplinary Studies Martin Ramirez, Loyola Marymount University Marcus Webster, St. John's University	
	Conducting Behavioral Research Following IRB and HIPAA Regulations Vincent Prohaska, Lehman College Linda Rueckert, Northeastern Illinois University Tara Kuther, Western Connecticut State University	
	NSF National Ecological Observatory Network (NEON) Funding Interdisciplinary Science Liz Blood, National Science Foundation Jeffrey Goldman, American Institute of Biological Sciences	
12:10 pm - 1:30 pm	**Line Lunch with special topic discussion tables---CUR Affinity Groups** 1. Arts & Humanities Issues -- Andrew Harris 2. Biochemistry -- Roger Rowlett 3. Canadian Issues -- Katherine Darvesh 4. College & University Administration Issues -- Neal Abraham 5. Environmental Research -- Christine MacTaylor 6. Issues for Directors of Undergraduate Research Programs -- Janet Stocks & Sandra Gregerman	
1:30 pm - 2:30 pm	**Workshop Session VII**	
	On-line Grant-seeking Resources Frances Vinal Farnsworth, Middlebury College Linda Freed, University of Wisconsin-Oshkosh	
	Educating State Legislatures About the Importance of Undergraduate Research -- A Discussion on the Why and How to Organize an Undergraduate Research Poster Session at Your State Capitol John Mateja, Murray State University Elizabeth Ann Nalley, Cameron University Kathleen Cargill, The College of St. Scholastica Patricia Pukkila, University of North Carolina, Chapel Hill	
	Research Issues at Small (fewer than 1500 undergraduates) Undergraduate colleges Naomi Amos, Randolph-Macon Woman's College	
	Collaborative Student Research Involving Handheld Computers Laura Guertin and Deb LaBelle Penn State University Delaware County	
	SURE/SEED: A Chemistry Collaboration at Stonehill College Bonnie L. Troupe, Louis Liotta, Craig Almeida & Ellen Sletten, Stonehill College	
	Conducting Interdisciplinary Research Abroad Daniel Wubah, David Owusu Ansah, Judith A. Wubah James Madison University	
	The Benefits of Challenging Pre-Medical Students to Conduct Research in Non-Traditional Areas Kerry Cheesman, Capital University	
	Interdisciplinary Research: How to Get Started and Make It Work Anne M.F. Moore, The University of the Pacific Barbara A. Lawrence, Eastern Illinois University	

	Working with Public and Private Institutions as Collaborative Adventures Donald Linn, Indiana U-Purdue U Fort Wayne Wingfield V. Glassey, The College of Wooster Ruth E. Nalliah, Huntington College John M. Farrar, Indiana U-Purdue U Fort Wayne	
	Bio 2010--- A Proposed Interdisciplinary Undergraduate Biology Curriculum: Implications for PUIs Elaine Hoagland, Council on Undergraduate Research James Gentile, Hope College Jason Taylor, Ecological Society of America	
	 Developing Campus-wide Interdisciplinary Undergraduate Research Programs: The NCUR/Lancy Initiative Silvia Ronco, Research Corporation Thomas Werner, Union College Jill Singer, Buffalo State College	
	Evaluation for Dummies and Everyone Else: Seven Ways to Evaluate Success in Undergraduate Research John Pollock, The College of New Jersey Julia Wallace and Paul Wiener, University of Northern Iowa Herb Childress, Duke University	
	What Research on Learning Can Tell Us about Undergraduate Research Samuel Abrash, University of Richmond David Lopatto, Grinnell College	
	Commuting, Jobs, Culture, and Undergraduate Research Participation Debra Zellner, Montclair State University Nancy Oley, Medgar Evers College, City University of New York Vincent Prohaska, Lehman College, City University of New York	
	Crossing Disciplinary Boundaries in Undergraduate Research John Falconer, University of Nebraska at Kearney Mike Tannenbaum, Marist College Royce Engstrom, University of South Dakota Susan Painter, Merck Research Laboratories	
	Models of Successful Research in PUIs Vijendra Agarwal, The College of Staten Island/City University of New York Mark Biermann, United States Naval Academy Paul De Young, Hope College Shila Garg, The College of Wooster	
2:40 pm - 3:40 pm	**Workshop Session VIII -- DISCIPLINARY: CROSSING BOUNDARIES**	
	The Polio Project: Remembering an Epidemic across Disciplinary Boundaries Stephen Kercher, Susan McFadden, Cheryl Lapp, Ralph Beliveau, University of Wisconsin Oshkosh	
	Inter-society Collaboration: CUR and the American Physiological Society Jeff Demarest, Juniata College Dee Silverthorn, University of Texas	
	Sponsored Programs Administration - The Basics Frances Vinal Farnsworth, Middlebury College Linda Freed, University of Wisconsin-Oshkosh Lori Bettison-Varga, The College of Wooster Naomi Amos, Randolph-Macon Woman's College	
	Assessment of Undergraduate Research: Where Do We Go from Here? Linda Rueckert, Northeastern Illinois University Kathleen Morgan, Wheaton College	
	Mainstreaming Student-conducted Research in Every Course in the Social Sciences Paul Wienir, Western Michigan University John Pollock, The College of New Jersey	

	Undergraduate Research in Chemistry Involving Partnerships Thomas Wenzel, Bates College Other CUR Chemistry Councilors	
	Undergraduate Research in Mathematics: How to Engage More Students and Faculty at All Levels Zsuzsanna Szaniszlo, Valparaiso University Joseph Gallian, University of Minnesota-Duluth Robert Hoar, University of Wisconsin-La Crosse	
	Opportunities and Challenges in Applied Research and Service Learning: Nurturing the Academy-Agency Interaction Jonathan Vaughan, Hamilton College Joanne Altman, Washburn University Susan Larson, Concordia College	
	Varieties and Pitfalls of Mentoring Andrew Harris, Ann Brunjes and Kevin Curry & Sandra Neargarder Bridgewater State College	
	Dissemination of the CUR Message through Discipline-Specific Meetings: A Panel Discussion with Four Biology Councilors Marcia O'Connell, The College of New Jersey Kelly McConnaughay, Bradley University Jeffrey Osborn, Truman State College Gisele Muller-Parker, Western Washington University	
	Scholar Communities: Undergraduate Research in the Arts & Sciences Glenn Acree, Belmont University	
	Crossing Disciplinary Boundaries- Bioinformatics, Computational Ecology, and Mathematics Paula Dehn, Debra Burhans & David Sheets Canisius College Janet Andersen, Hope College	
	Breaking Free: Collaborating Outside The Department Brannon Andersen, Furman University Edward Hansen, Hope College	
3:40 pm - 4:10 pm	**Break**	
4:10 pm - 5:40 pm	**Plenary III:** **CUR Fellows** Speakers to be announced	
5:40 pm - 6:00 pm	**Free time - assemble for trip to dinner on Riverfront**	
6:00 pm - 9:00 pm	**Dinner on the Riverfront with entertainment**	
Saturday, June 26th		
7:00 am - 8:15 am	**Line Breakfast with informally arranged discussions**	
8:15 am - 9:40 am	**Plenary IV:** **Community-Based Research** Alanah Fitch, Loyola University of Chicago Ray Turner, Roxbury Community College	
9:40 am - 10:00 am	**Break**	
10:00 am - 11:00 am	**Workshop Session IX**	
	Roxbury Community College and Harvard University School of Public Health Team Up to Support Community-Based Undergraduate Research: Continuing the Conversation Ray Turner, Roxbury Community College	
	Establishing Interdisciplinary Undergraduate Research in Computational Studies: Connections with Industry Ignatios Vakalis, Terry Lahm, Andrea Karkowski Capital University	
	Successful NSF - REU, ROLE, Undergraduate Research Centers, and MRI proposals: Reviewers' Perspectives Kerry Karukstis, Harvey Mudd College	

	Julio De Paula, Haverford College Rosemary Marusak, Kenyon College	
	Fostering Undergraduate Research through Rhetorically-Based Library Instruction Rebecca Donlan & Kathleen Hoeth Florida Gulf Coast University	
	International Partnership for Technical Assistance to Smallholder Coffee Farmers of Nicaragua Susan Jackels, Seattle University	
	Learning is Local: Using the At-Hand Landscape in Undergraduate Research Herb Childress, Duke University Julio Rivera, Carthage College	
	How to Get Involved in CUR Samuel Abrash, University of Richmond	
	Research Collaborations Nancy Oley, Medgar Evers College, City University of New York Susan Larson, Concordia College-Moorhead	
	Using Colleges and Universities to Forge Community Confluence of Interests Garon Smith, The University of Montana	
	Research across the Curriculum Sherri Morris, Kelly McConnaughay & Keith Johnson Bradley University	
	NSF DUE CCLI Program Overview **(repeated see Workshop II)** Duncan McBride, Theodore Hodapp & Jeff Ryan National Science Foundation Jill Singer, Buffalo State College	
	The Urban Floodplain: An Interdisciplinary Laboratory Carol Ekstrom, Robert Strandburg & Mike Kirby Rhodes College	
11:10 am - 12:10 pm	**Workshop Session X**	
	Community-Based Research: Continuing the Conversation Alanah Fitch, Loyola University of Chicago	
	Successful NSF-CCLI and CAREER proposals: Reviewer's perspectives Lori Bettison-Varga, The College of Wooster Gerald Van Hecke, Harvey Mudd College Thomas J. Wenzel, Bates College	
	Preparing Students To Do Research on Emotionally-Challenging Topics Michael Bassman & Susan McCammon East Carolina University	
	Crossing the Boundary from Service-Learning to Community-Based Research Jo Paoletti, University of Maryland	
	Crossing Boundaries with Brown v. Board Jocelyn Payne, Melissa Roberts Becker, Renee Cambiano & Linda Moss Northeastern State University	
	Signature Laboratories as a Tool for Integrating Research and Education Jeffrey Collett, John Brandenberger & David Cook Lawrence University	
	International Research Internships for Students Bridget Gourley, DePauw University Tim Elgren, Hamilton College	
	Mentoring Writers: Strategies for Incorporating Writing in Undergraduate Research Herb Childress, Duke University	
	Linking Undergraduate Research to the Job Market Brenda Wilhelm, Mesa State College	
	The Use of GIS in Interdisciplinary Research/Service Learning Projects Stephen Van Horn, James Dooley, Walter Huber Muskingum College	

	Research as Service to the Community: Giving the People What They Want Stephanie Golski, Erin McGrath, Hope Corman Rider University Ken Reardon, Cornell University	
	Community-Based Research and Research Policy: Connecting the Dots Richard Worthington, Loka Institute	
12:20 pm - 12:45 pm	**Closing Plenary**	
12:45 pm - 2:00 pm	**Line lunch**	
2:00 pm - 6:00 pm	**Afternoon Field trips** **Dinner on your own**	
Sunday, June 27th		
7:00 am - 8:30 am	**Line Breakfast**	
5:00 am - 11:00 am	**Check out**	

APPENDIX D: SAMPLE CHECKLIST FOR SCREENING CANDIDATES FOR UNDERGRADUATE RESEARCH.

Checklist for URE
(Maintain on file in the department)

1. Student academic background:
2. Other experience:
3. Academic major or proposed major:
4. Planning to do research during the academic year or during the summer?
5. Familiarization requirements:
6. Faculty mentor:
7. Senior thesis? Y N
8. Proposed start date:
9. Contract signed? Y N

APPENDIX E: SAMPLE RESEARCH CONTRACT

Note: To be completed and signed prior to the start of undergraduate research project.

Undergraduate Research Contract

1. Proposed research topic:

2. Research schedule: (attach schedule documents as necessary)

3. Minimum hours per week for research during the academic year. Indicate times and workstation scheduled exclusively for this student.

4. Regular meeting requirements between the faculty mentor and student. (Indicate any requirements for progress reports)

5. Laboratory notebook requirements:

6. Final product (Senior Thesis/Conference Presentation/Department Presentation)

APPENDIX F: SIX RESPONSE QUESTIONNAIRES FROM FORMER UNDERGRADUATE RESEARCHERS IN COMPUTATIONAL RESEARCH

#1

Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1.Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

In the summer between by sophomore and junior years.

2.Briefly describe the nature of your first undergraduate research project.

Analysis of the efficacy of plane wave (Fourier) basis functions for quantum chemical calculations using the Morse oscillator as a model system.

3.What college courses were most helpful in preparing you for this research?

Nearly all my chemistry, physics, and mathematics courses.

4.What specific academic skills/knowledge (if any) do you feel was essential to your research work?

Linear algebra, quantum mechanics, numerical analysis, and computer programming skills.

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

Perhaps a physical chemistry course.

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

The computer programming and the direct interaction with my research mentor, from whom I learned a tremendous amount.

7.What were the most important benefits to you of your research experience?

I published two papers as a result of my undergraduate research experience, which greatly expanded my graduate-school opportunities and marketability.

8.What changes or improvements would you recommend to your experience?

None.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

I learned all my fundamental quantum mechanics from my mentor, an assistant professor.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills: 5

Computational skills: 5

Writing Skills: 3

Analytic Thinking: 5

Background research of scientific journals: 5

Math/Chemistry/Physics knowledge: 5

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

The undergraduate research experience exposed me to the true graduate-student experience and thus prepared me well for my Ph.D. resesearch. Many students arrive in graduate school with the incorrect notion that life as a Ph.D. student will be much like that of a college student: do well in your classes, work reasonably hard, and everything else will fall into place. They are often surprised by the level of commitment and creative thought expected of them. I consider undergraduate research vital to preparation for any higher level research.

#2
Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1.Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

Summer after junior year.

2.Briefly describe the nature of your first undergraduate research project.

QC investigation of a complex potential energy surface. Could it exist, if so, what properties would it exhibit.

3.What college courses were most helpful in preparing you for this research?

Calculus (with theory), P. Chem, O. Chem, InO Chem.

4.What specific academic skills/knowledge (if any) do you feel was essential to your research work?

QM basics, Bonding Theories, Calculus

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

No

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

Most important: Feeling like I was doing "real" research. I knew we would publish the results.

Also important: The expectation that I would be the driving force of the investigation. Help was available, but I was encouraged to work independently.

7.What were the most important benefits to you of your research experience?

Understanding the purpose of education.

8.What changes or improvements would you recommend to your experience?

None.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

Special Q.C. classes given by post-docs and grad students. My mentor was a post-doc.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills: 4

Computational skills: 5

Writing Skills: 4

Analytic Thinking: 5+

Background research of scientific journals: 3

Math/Chemistry/Physics knowledge: 3

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

#3

Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1.Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

I did some summer research after my Junior year in Chemical Oceanography at U. Washington, but did not start Comp. Chem. until the summer after my senior year.

2.Briefly describe the nature of your first undergraduate research project.

Though not officially "first" this is a survey about Comp. Chem. So I will tell you about my first comp chem. project at U. Georgia (if you want to know about Oceanography let me know.) I worked on determining the structure of the ClF2 radical. Through high-level theoretical calculations we settled some discrepancies in the experimental IR spectrum and the geometric structure.

3.What college courses were most helpful in preparing you for this research?

Inorganic Chemistry, Physical Chemistry.

4.What specific academic skills/knowledge (if any) do you feel was essential to your research work?

Specific knowledge that came in handy was MO theory (from Inorganic Chem) and spectroscopy (from P-chem). The spectroscopy was essential for this particular project. MO theory was useful, but I think that I put more of an MO spin on the project than was absolutely necessary just because I took to that way of thinking from the start.

More generally, my undergraduate education was based more on figuring out chemical problems rather than knowing chemical facts. This helped research a lot. Also, the ability to look up, find, read, and understand literature references came in very handy. I certainly had not mastered these skills going into my first project, but I knew what was necessary to get started and which direction to go.

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

More math. I only took 1 math class in College (tested out of Calc I, took Calc II and was not required to do Calc III). Comp . Chem. is pretty Math intensive and so I had to pick up a lot of it on the fly.

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

The answer to both of these questions is the same: the frustration! It is very discouraging when you work and work on something but cannot figure it out. Seeing the extent of knowledge in this one small area is very overwhelming. However, because of that frustration and hard work it is a HUGE feeling of accomplishment when you finally do figure something out and contribute to the field.

7.What were the most important benefits to you of your research experience?

If I trace it forward enough, I could say my current job is the most important benefit. It all started with that first project. I was pretty clear about what I wanted to do with my life career-wise from a pretty early age (not just chemistry, but theoretical chemistry) so research just confirmed that.

At the time I think the biggest benefit was to show me that I could do this sort of thing. There is an idea among beginning chemistry students that everything has already been figured out. Even when you get beyond that, it is still hard to believe that you with your small bit of knowledge can actually contribute.

8.What changes or improvements would you recommend to your experience?

None. I had a great experience and would not change a thing.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

Each undergraduate was assigned to a senior level graduate student to learn the basics, but it was a large group and everyone helped out. From beginning graduate students to long term postdocs to the leading faculty member.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills:	5
Computational skills:	5
Writing Skills:	4
Analytic Thinking:	4
Background research of scientific journals:	5
Math/Chemistry/Physics knowledge:	4

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

I was always interested in chemical bonding theory so I took to this type of research right away. I was lucky to find the Schaefer group because I never really liked experimental work all that much. However, I was more interested in the qualitative visual aspects of MO diagrams. In a Math intensive group like Georgia, I had to pick up a lot of on the fly, I always felt a little behind until I realized that I had strengths where others were weak. This is a problem that I see now with my own students feeling intimidated by the extent of the field. They just do not think they compete in such a “lofty” field. I have always thought that computational chemistry was ideal for undergraduates because they do not have to know all the details of the research to do calculations and interpret the data. All you need is a PC, and not a very large one either. I am finding that it is more difficult than I thought. There is a lot of jargon in the field and when things do not go according to plan (the truly interesting cases) there are many computational “tricks” picked up over the years that are difficult to teach to a newcomer. I have had students who have really taken to this type of work and others who have not. Those who have not were not poor students, just more hands on experimental types. I am trying to get to a point where I can have senior research students work with new students to teach them the basics so that I do not have to go through it every time. Also trying to work out some collaborations within the department so that people can do both expt. And comp. work.

I would very much like to see the results of this survey as I am also in the position of building an undergraduate computational chemistry research program.

#4
Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1.Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).
summer after my junior year

2.Briefly describe the nature of your first undergraduate research project.
ab initio study of ground-state isomers of a silicon organic compound

3.What college courses were most helpful in preparing you for this research?
Calculus, Linear Algebra, Complex Functions

4.What specific academic skills/knowledge (if any) do you feel was essential to your research work?
elementary computer programming skills, basic UNIX skills, linear algebra, Quantum Chemistry

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?
C programming, Quantum Chemistry (or Physical Chemistry II)

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.
I enjoyed learning something new that no one in the world new. I enjoyed getting on a computer and trying out my own ideas. I enjoyed working in a research group with lots of other students to talk and learn from. My graduate-student mentor spent a lot of time with me, but I disliked the fact that he was often not around during normal daylight hours.

7.What were the most important benefits to you of your research experience?
I discovered the field of computational quantum chemistry, which would allow me to use computer science, mathematics, chemistry and physics all at once. I chose this career path. More specifically, I returned to the same location for my graduate work. I began many friendships and scientific collaborations that continue.

8.What changes or improvements would you recommend to your experience? Perhaps having more than one mentor assigned to each undergraduate project would produce more creative thinking (with better conversations) and provide more support to the student.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

My primary mentoring was from a graduate student. He spent considerable time with me, but was often sleeping during the day, which occasionally made contact difficult. He was very hands-on and made sure that we made good progress, particularly in the first few weeks.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills: 4

Computational skills: 4

Writing Skills: 2

Analytic Thinking: 3

Background research of scientific journals: 4

Math/Chemistry/Physics knowledge: 5

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

#5

Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1. Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.). The summer after my sophomore year in college I did research in the area of theoretical/computational chemistry at the University of Kansas. The summer after my junior year I did research in the same area, but at the Center for Computational Quantum Chemistry at the University of Georgia.

2. Briefly describe the nature of your first undergraduate research project. At Kansas my research project involved the study of chaotic motion in intensive laser fields. At CCQC I carried out computer simulations/computations on high energy density all nitrogen compounds.

3. What college courses were most helpful in preparing you for this research? Physical Chemistry, Quantum Chemistry, Modern Physics, Linear Algebra, Diff. Eqns., as well as my earlier chem/physics/math courses.

4. What specific academic skills/knowledge (if any) do you feel was essential to your research work? The quantum chemistry and linear algebra were key components to understand my research. My background in computers was very useful.

5. Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience? A computer science course in C and Unix would have been useful. I already had the chem/physics/math courses coverged.

6. Briefly describe the aspects of the research you enjoyed the most, and any you disliked.
   I enjoyed (and still do) the interdisciplinary element to computational chemistry and other fields. Integrating my knowledge of computers, physics, math, and chemistry was a skill my undergraduate program focused on. The only aspect to my summer research that I disliked was the vast difference in research group working environments and treatment by professors. Some professors see students as collaborator, while other see students as slave labor.

7. What were the most important benefits to you of your research experience?
   The most important benefits was publishing a paper, seeing how the graduate research process worked, and understanding that the group work environments was central to choosing a department and professor for my graduate research.

8. What changes or improvements would you recommend to your experience?

9. Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)
   The primary mentoring I received was from graduate students.

10. Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills: 5

Computational skills: 5

Writing Skills: 5

Analytic Thinking: 4

Background research of scientific journals: 4

Math/Chemistry/Physics knowledge: 4

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.
    Undergraduate research is an excellent opportunity to explore different research interests. My undergraduate research provided a real world example of how I could apply the knowledge I learned in my undergraduate courses. The research also influenced my choice of college courses during my junior and senior years.

#6
Questionnaire on your undergraduate research experience

Note: By completing this questionnaire I give consent to allow the information to be used for the evaluation of undergraduate research in computational chemistry. I understand that the information in this questionnaire may be reported in David Dinsmore's doctoral dissertation, as well as various educational journals. I understand that my participation in this project is voluntary and that I may choose not to respond to the questionnaire or any question therein. I also understand that no reference to my identity will be given in any reports or publications.

1.Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

Summer after junior year

2.Briefly describe the nature of your first undergraduate research project.

I carried out two projects: (1) Compute high-accuracy estimates of the singlet-triplet gap in acetylene to help interpret recent experimental results, and (2) Carry out a study of the potential energy surface of a diradical.

3.What college courses were most helpful in preparing you for this research?

I had an unusually good (i.e., challenging) undergraduate course in quantum chemistry, which actually covered the material that one supposes should be covered in such a course (variational methods, perturbation theory, term symbols, spectroscopy). This was immensely helpful.

4.What specific academic skills/knowledge (if any) do you feel was essential to your research work?

1. Basic understanding of quantum chemistry; 2. Familiarity with computers in general and UNIX in particular; 3. Ability to write well and put together research reports and, ultimately, drafts of papers.

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

A course (or independent study) in linear algebra would have been very beneficial.

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

It was most fun doing work on systems that other researchers (experimentalists) were actually pursuing; this made it feel more significant and part of a team effort. It was also fun learning about the theories and how they worked. Writing some computer code was part of the research experience, and this was valuable in appreciating how the quantum programs worked.

7.What were the most important benefits to you of your research experience?

I gained exposure to quantum chemistry, which would not have happened otherwise for me at the undergraduate level. I went on to make a career in this area.

8.What changes or improvements would you recommend to your experience?

The training I received over the summer was first rate. It would only have been improved if I had taken linear algebra beforehand.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)

One graduate student mentor met with me daily. One postdoc instructed us once a week. The program lasted about 10 weeks.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills: 4

Computational skills:4

Writing Skills:3

Analytic Thinking:4

Background research of scientific journals:3

Math/Chemistry/Physics knowledge:4

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

It was one of the most enjoyable research experiences I’ve ever had.

APPENDIX G: SUMMARY OF QUESTIONNAIRE RESPONSES.

Responses to each question are numbered to correspond to questionnaires 1-6. (Appendix F); a final response, labeled R, is that of the researcher, when appropriate.)

1. Describe when you began your undergraduate research work (ex: summer after my junior year, during my sophomore year, etc.).

   1- Summer after junior year.
   2- Summer after senior year.
   3- Summer after junior year.
   4- Summer after junior year.
   5- After senior year.
   6- After junior year and after senior year.

2. Briefly describe the nature of your first undergraduate research project.

   1- Quantum computation investigation of a complex potential energy surface.
   2- Analysis of the efficacy of phase wave basis functions for quantum chemical calculations.
   3- Ab initio study of ground state isomers of a silicon organic compound.
   4- Computing high-accuracy estimates of the singlet-triplet gap in acetylene and studying the potential energy surface of a diradical.
   5- Determining the structures of the ClF_2 radical.
   6- Computer simulations/computations on high energy density compounds of nitrogen.
   R- Optimal structures, energies and vibrational frequencies for Li_3H and Li_3H_2.

3. What college courses were most helpful in preparing you for this research?

   1-Calculus, Physical Chemistry, Organic Chemistry, Inorganic Chemistry.
   2-All my chemistry, physics and mathematics courses.
   3-Calculus, Linear Algebra, Complex Functions.
   4-Quantum Chemistry.
   5-Calculus, Physical Chemistry, Inorganic Chemistry
   6-Linear Algebra, Differential Equations, Modern Physics, Physical Chemistry, Quantum Chemistry
   R- Calculus, Modern Physics,

4. What specific academic skills/knowledge (if any) do you feel was essential to your research work?

   1-Quantum basics, bonding theories, calculus
   2-Linear algebra, quantum mechanics, numerical analysis, computer programming skills.
   3-Elementary computer programming skills, UNIX, linear algebra, quantum chemistry.

4-Basic quantum chemistry, familiarization with computers and UNIX, writing ability and preparing reports.
5-Molecular orbital theory, inorganic chemistry, literature research skills.
6-Quantum chemistry, linear algebra, computer background.
R- Symmetry and group theory (a physical chemistry or quantum chemistry course would cover this)

5.Looking back, were there any courses you wish you had taken prior to beginning your undergraduate research experience?

1-No.
2-Physical Chemistry.
3-C Programming, Quantum Chemistry.
4-Linear Algebra.
5-More mathematics.
6-Computer science covering C programming and UNIX.
R- N/A

6.Briefly describe the aspects of the research you enjoyed the most, and any you disliked.

1-Doing real research. Working independently and knowing help was available.
2-Computer programming and direct interaction with professor mentor.
3-Learning something new. Trying new ideas. Being in a research group. Dislike - Hard meeting with the graduate mentor during the day.
4-Doing real research. Learning the theory and how the programs worked.
5-Figuring something out and making a contribution. Dislike – frustration.
6-Integration of math, chemistry and physics. Dislike – Being viewed as slave labor by some professors.
R- Doing real research. The excitement of figuring out the molecule and getting results. Working as a team.

7.What were the most important benefits to you of your research experience?

1-Understanding the purpose of education.
2-Publishing two papers, which led to future opportunity.
3-Integrating four disciplines and having the work lead to a career path.
4-It became a career area.
5-Current job and career.
6-Published a paper. Understanding how graduate research works and how to select a department and a professor.
R- N/A.

8.What changes or improvements would you recommend to your experience?

1-None.
2-None.
3-Maybe have more than one mentor for each undergraduate project.

4-None, except taking Linear Algebra first.
5-None.
6-None.
R- N/A.

9.Describe briefly the primary mentoring your received during the research (ex: a faculty member, a graduate student, a more experienced undergraduate student)
1-Post-doctoral student.
2-Assistant professor.
3-Graduate student.
4-Graduate student, daily. Post-doctoral student, weekly.
5-Graduate student, also Post-doctoral student and a faculty member.
6-Graduate students.
R- Assistant professor.

10.Please indicate with a number from 5-1 the degree to which you feel your research experience improved the following areas: (5 – significant improvement, 4 – Improvement, 3 – Some improvement, 2 – Little improvement, 1 – No improvement)

General computer skills:

Computational skills:

Writing Skills:

Analytic Thinking:

Background research of scientific journals:

Math/Chemistry/Physics knowledge:

(See Table 4 in chapter 4 for a complete summary of response to question 10)

11. Please provide any other comments you have about your undergraduate research experience in computational chemistry.

1- None.
2- This experience exposed me to the true graduate student experience…the level of commitment and creative thought expected. I consider undergraduate research vital to preparation for any higher-level research.
3- None.
4- It was one of the most enjoyable research experiences I've ever had.
5- Idea for undergraduates because the student does not have to understand all the details of the research to do the calculations and interpret the data. Some students really do well in this type of research, but others, who are not poor students, but more hands on do not take to it.

6- Undergraduate research is an excellent opportunity to explore different research interests. My research provided a real world example of how I could apply the knowledge I learned in my undergraduate courses. It also influenced my choice of college courses during junior and senior year.

R – N/A