

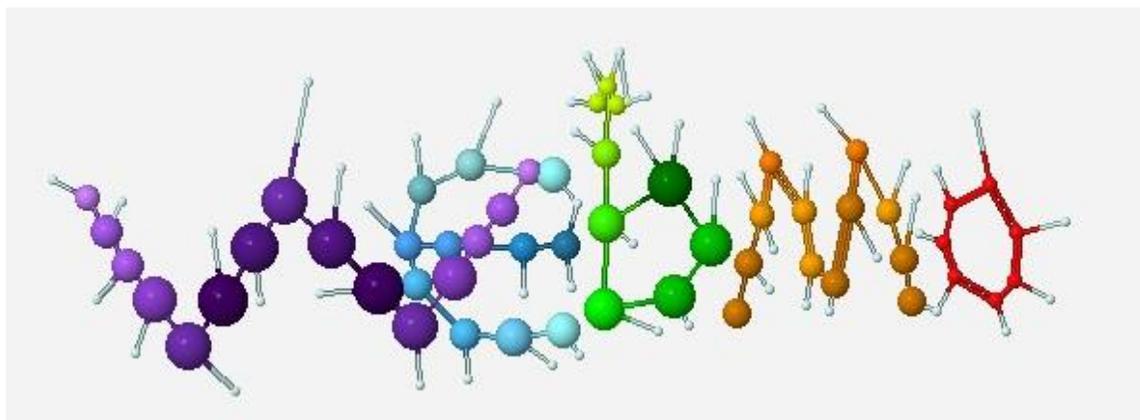
Computational Chemistry

in the High School Classroom

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Abstract

Computational chemistry programs have proven to be powerful research tools and our project aimed to bring this technology to the classroom. We developed a teaching module surrounding the web-based software WebMO to address topics chemistry students typically struggle with. Through implementation of the curriculum at Millbury High School, it was found that the students generally possessed a stronger understanding of the topics addressed after using WebMO and that integration of computational chemistry into the classroom is a worthwhile endeavor.

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Table of Contents

Abstract	ii
Acknowledgements	iii
Table of Contents	iv
1. Introduction	1
2. Background	3
3. Methodology	17
4. Results and Discussion	26
5. Recommendations and Conclusions	48
Literature Cited	53
Appendices	54

1. Introduction

The field of computational chemistry has become an extremely valuable research tool in chemistry, physics, and biology. Computational chemistry began with quantum theory, which is the study of the interaction of atoms with each other and with energy at the subatomic and atomic level. Quantum theory aims to predict the behavior of atoms based on the physics principles that apply at such a small scale. Calculations using quantum mechanics-based equations such as the wave function and Schrödinger equation allow scientists to analyze and predict various characteristics and behaviors of both atoms and molecules. Before computers, this work was very cumbersome and nearly impossible to complete. With the improvement of computer technology, computational chemistry programs were developed and provided an immeasurably easier way to perform these necessary calculations. With this type of computer software, the user gives the computer input of some molecular properties. Based on the software and the given input, the program will perform calculations to model various characteristics of the given molecule, such as geometry, energy, and intermolecular forces. Both chemists and biochemists benefit from the ability of computational software to simulate reactions, particularly those involving substances dangerous to work with or difficult to obtain.

As technology continues to improve, it is the hope of this project group that students can now benefit from such programs as well. Research was done to determine content areas high school chemistry students typically struggle with that fall under the State of Massachusetts chemistry educational standards. A teaching module consisting of a series of chemistry worksheets containing questions addressing some of these topics was then developed. The exercises were designed to be answered using a molecular modeling software found online, known as WebMO. The initial group of questions developed was presented first at Worcester Polytechnic Institute to a small group of volunteers, and then on a somewhat larger scale to volunteers from WPI Chemistry, Biochemistry, and Chemical Engineering majors. After these initial “alpha” and “beta” testing rounds, the worksheets were modified and presented to high school students in a chemistry class at Millbury High School in Worcester, Massachusetts. Over a series of three visits, students

were asked to complete the worksheets using the WebMO molecular modeling software, and then evaluated for their progress.

The overall goal of this teaching module development was to build a bridge between computational chemistry and the use of technology in education. It was determined that many of the abilities of computational chemistry programs could be applied to the State of Massachusetts high school chemistry curriculum standards. Through the implementation of this teaching module and WebMO software, students were provided with concrete visualizations of the chemistry concepts they struggle with. WebMO allowed students to build molecules and examine their properties and behavior on the microscopic level in a way that is otherwise difficult to provide in a classroom. By solidifying molecules and characteristics of them, chemistry concepts should be easier for the students to work with and truly understand. The following report details the analysis of software encountered, the development of a teaching tool to accompany such a program, and the implementation of the developed tool within both a group of college student volunteers and a high school chemistry class.

2. Background

Here we present information pertaining to the goal of the project and the instruments used to attain this end. Molecular modeling is introduced as a key platform for performing modern chemical and physical research and the way in which this powerful tool can be used for teaching students both fundamental and advanced topics in chemistry is also explained. In particular, we discuss the basis for how molecular modeling programs work and the different ways in which they attempt to recreate physical properties of chemicals. From there, we connect how different aspects of this class of software can be applied to chemistry concepts included in the Massachusetts Educational Standards and how they are especially useful for helping students just beginning to grasp such concepts to progress towards more advanced topics.

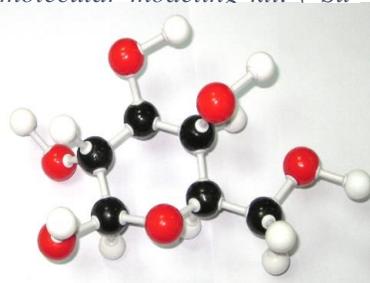
Three following three overarching goals were established at the beginning of this project, and served as the motivation for all that was accomplished:

- To achieve a satisfactory understanding of the theory behind computational chemistry programs in order to understand the modeling system to be incorporated into the high school classroom.
- To build and develop a simple yet effective teaching module to present chemistry concepts in an educational manner which could help students better understand chemistry concepts.
- To measure the extent to which the teaching module was successful and propose improvements that could be made in the future.

2.1. Molecular modeling goals and applications

Models have always been an important part of the scientific method of studying complex systems that require simplification in order to determine their characteristics. When beginning to explore or construct something, approximations are particularly useful because they provide roughly accurate data points in a short amount of time and often are used as an initial

Figure 1 - An example of molecular modeling without computational chemistry. A sucrose molecule built from a molecular modeling kit. ("Su-



guess at the beginning of a larger process that will eventually result in more accurate results down the line. Consider the molecule model at the left. The observer understands that molecules in reality do not actually look like red and black spheres to represent different types of atoms, but by using this model one can estimate the relative polarity of this molecule without performing solubility studies in order to determine this property precisely, based simply on the known electronegativities of the atoms represented and the shape of the model. Molecular modeling programs achieve essentially the same goal as the modeling kit used to build the pictured molecule, but perhaps with a vastly larger array of capabilities. These programs seek to approximate specific properties of molecules by utilizing mathematical equations to describe these properties and are widely used in the beginning stages of modern chemical and biophysical research.

Molecular modeling is just one technique that chemists use to inform the scientific community about the chemical world. Molecular modeling is a particularly useful tool because it is an efficient method of preliminary testing for further research. This modeling system can cut down costs that wet laboratories require as well as return approximate results in a speedy and efficient manner.

This is useful in the research laboratory of course, but what about in a teaching setting? One of the most useful features of any molecular modeling program is the ability to draw a molecule in a 3D context. The whiteboard has become a staple of the classroom and a canvas for instruction, but the ability to compose something quickly in a 3D workspace is something novel, something this project is attempting to bring to the classroom. It is important that students are able to understand that molecules, and generally most compositions of matter, are not planar but are dynamic as three-dimensional structures. Being able to visualize a molecule as it exists in the real world has not been possible up until very recently (except for small molecules with atomic, usually plastic, kits, as shown in Figure 1), so an additional goal of computational chemistry is to model an accurate picture of physical chemistry. Furthermore, computational chemistry allows calculations of properties in a more trivial manner than does wet laboratory work, such as the determination of molecular energy and intermolecular interaction analysis. In short, molecular modeling provides a useful framework of the chemical realm that has uses both in the early and later stages of scientific studies.

2.2. Calculations

Molecular modeling software programs perform mathematical calculations to determine several physical and chemical properties of molecules. In general, computational chemistry programs attempt to find a solution to the Schrödinger equation, as follows:

$$\hat{H}\Psi = E\Psi \quad (1)$$

This function is an eigensystem in which the Hamiltonian operator applied to the wave function (Ψ) of the molecule is equal to an energy term (E) multiplied by the wave function, which is a mathematical expression that describes the system. The energy term in this function adjusts for the relative locations of electrons and the nucleus, and all interactions between them, while the operator is simply a function that is applied to the wave function. Once solved, the wave function can be used to calculate most properties of an atom or molecule's geometry, behavior, or energy. However, because of the complexity of electron interactions within an atom and the increase in this complexity when atoms combine to form molecules, it is impossible to find an exact solution to the Schrödinger equation and therefore varying degrees of approximation must be applied. The computer program performs all the calculations to solve such equations, and gives the important data on the molecular system. While methods that employ greater degrees of approximation give less accurate answers than those with minor approximations, the less accurate methods require much less time and computational power to complete calculations. The types of computational programs studied in this project were based on *ab initio*, semi-empirical, and empirical methods, as discussed below.

2.2.1. *Ab initio*

Ab initio is a Latin term meaning "from first principles". This method of calculation uses pure chemistry and scientific laws to evaluate the Schrödinger equation as accurately and completely as possible. Calculations using methods of this type take more time than other methods and a greater deal of computer power and memory, but give results that are much closer to actual experimental results, i.e. closest to natural phenomena. One method with these calculations begin with the software finding a wave function by using the exact solution for a single electron system (hydrogen atom) and including correction terms in order to extrapolate this to multi-electron systems. This wave function is then

used to solve the Schrödinger equation for the energy term, thus describing the system in a very physically accurate way.

Density functional theory (DFT)

Density functional theory is an *ab initio* approximation method for the Schrödinger equation that relies on the density or probability of electrons around a particle as a function of the radius from that particle, as opposed to wave functions as other theories employ. This theory calculates the energy of this electron density by evaluating the functional, or mathematical function, of the electron density expressed as another mathematical function, meaning that it returns a number based on the electron density function. The resultant functional is partitioned into a kinetic energy term from the movement of electrons, a potential energy term from the interaction between the electrons and a positively charged nucleus in addition to the interaction between two nuclei, as well as another potential energy term from the repulsive interaction between an electron and other electrons in its vicinity. The final term describes all other electron-electron interactions that may result from various spins of electron pairs and is divided into an energy term for same-spin and mixed-spin interactions. DFT is a popular method for approximation today in the computational chemistry world because it has a high accuracy per unit computer processor (CPU) time ratio in comparison to other methods.

Hartree-Fock (HF)

This method is an older common *ab initio* method and is marked by breaking down the many-electron system that that Schrödinger equation presents into many individual electron system, each of which is defined by an orbital that carries a wave function and an energy level. An approximation of this method is that it takes the average effect of the repulsion of electron-electron interactions and not the explicit interactions, in addition to the fact that the wave function must be described by a mathematical function that approximates it. This is the role of the basis set, which is essentially a set of equations that a method uses in order to approximate the wave function to a certain degree of accuracy. The HF method is the precursor method to DFT.

Moller-Plesset Perturbation Theory

The Moller-Plesset (MP) Perturbation Theory attempts to correct the HF theory, which as mentioned earlier provides an approximation for the repulsion term between electrons and determines the position of an electron solely with respect to the atom's nucleus and the average of other electrons. As this model is not quite accurate, the MP theory uses HF as a starting point and then corrects it for the attraction term between the nucleus and the electron as well as the position of an electron with respect to another electron. The number following MP, such as MP2 or MP3, indicates the number of perturbations, or approximation terms, used in the theory. Generally, the higher this number, the greater the accuracy of the method.

CCSD & CCSD(T)

Called the coupled cluster method, this approach attempts to further approximate the position of the electrons based on occupied and unoccupied orbitals. This method is unique because it takes into account electron energy states, whether at the ground state or excited, which may change depending on the type of bonding or ionization present in the system. The (T) indicates a triple excitation or a perturbation term, much like the number following MP. This method typically costs a great deal of CPU time due to its high level of accuracy.

GVB

The generalized valence bond (GVB) theory is very similar to the CCSD method but further takes into account orbital hybridization in a bond between two atoms (Young, 2001).

2.2.2. Semi-Empirical

Semi-empirical methods, like ab initio methods, are generally based on finding solutions to the Schrödinger equation using accurate chemical and scientific principles. Unlike ab initio methods, semi-empirical calculations use known experimental or theoretical data to apply parameterization/fitting to the Schrödinger equation to make the calculations. These approximations are made based on drawing from a database of known molecules and their properties. These lead to an increase in the speed with which results are obtained, but a decrease in the accuracy of the results, particularly if the molecule be-

ing investigated is not similar to anything in the database of known information to draw from (Ramachandran, 2013). The degree of inaccuracy in semi-empirical methods is based on the approximations made in the calculations.

MNDO

The modified neglect of diatomic overlap (MNDO) method has proven useful mostly for organic molecules and utilizes a very simple basis set that ignores core electrons as well as hybridization effects on electron position. This method seeks to simplify valence shell overlap between atoms to single point charges and only takes into account electrostatic effects between electrons. This results in a poorer prediction of molecular geometry because bond rotation effects and barriers are diminished and some R-groups may come far closer together than physically reasonable.

AM1

The Austin model 1 method has been found to be most effective for calculating heats of formation, more accurately than MNDO, but has been shown to have trouble with this calculation when there are an abundance of polarizable atoms and larger differences in electron density in the system. This is most likely due to the fact that AM1 treats electrons as point charges uninfluenced by polarization due to an external electric field, similar to MNDO.

PM3

The most accurate of the three mentioned semi-empirical methods, parameterization method 3 uses essentially the same set of approximation equations as AM1 but with more accurate parameter sets for atoms and is also the most popular for organic systems. Additionally, this method tends to predict molecular geometries, especially bond lengths and angles, more accurately than AM1 and MNDO. (Young, 2001)

2.2.3. Empirical Methods

Empirical methods are based on assumptions about molecules that are not necessarily based on chemistry principles. These calculations typically are based on treating bonded atoms with simple models, like two balls attached by a spring. The calculations do not incorporate electron-electron or electron-nuclear interactions. These types of cal-

culations require significantly less time and computational power than ab initio and semi-empirical methods, but the results are less accurate due to the simple assumptions.

2.3. Calculation programs

Often in molecular modeling properties are calculated using simulation software. Examples of these programs are GAMESS, Gaussian, TINKER, NWChem, MOPAC, and Firefly. Most of these are available for free download online for educational use, and only require the acquisition of a license to install and use. Gaussian, however, requires the purchase of a license at a cost of several thousand dollars for a single-machine academic use within the US.

2.4. Educational considerations

For reasons to be detailed in section 3 of this report, two separate molecular modeling-based curricula were designed. The first of these was used in the initial alpha and beta rounds of implementation (further detailed in section 3.5) and was designed with two main considerations in mind. First, the Massachusetts High School Standards for chemistry were evaluated. It was important for the content of the teaching module to be relevant to and at the ability level of the typical high school chemistry class. Additionally, research was done to establish which areas of chemistry high school students tend to struggle with. Selection of the topics to be included were made from the overlap of these two critical areas. The second molecular modeling-based curriculum was created to coincide with the lesson plan already being taught by the high school teacher we worked with (explained in section 3.5). The exercises of this second lesson plan were not specifically related to common misconceptions of high school students we researched, but did still address parts of the Massachusetts chemistry standards. The chemistry standards can be found in Appendix A at the end of this report, while both the initial and final sets of exercises can be found in Appendices B and C respectively. These standards, misconceptions, and their relations to our exercises are further explained in the following sections.

2.4.1. Massachusetts chemistry standards

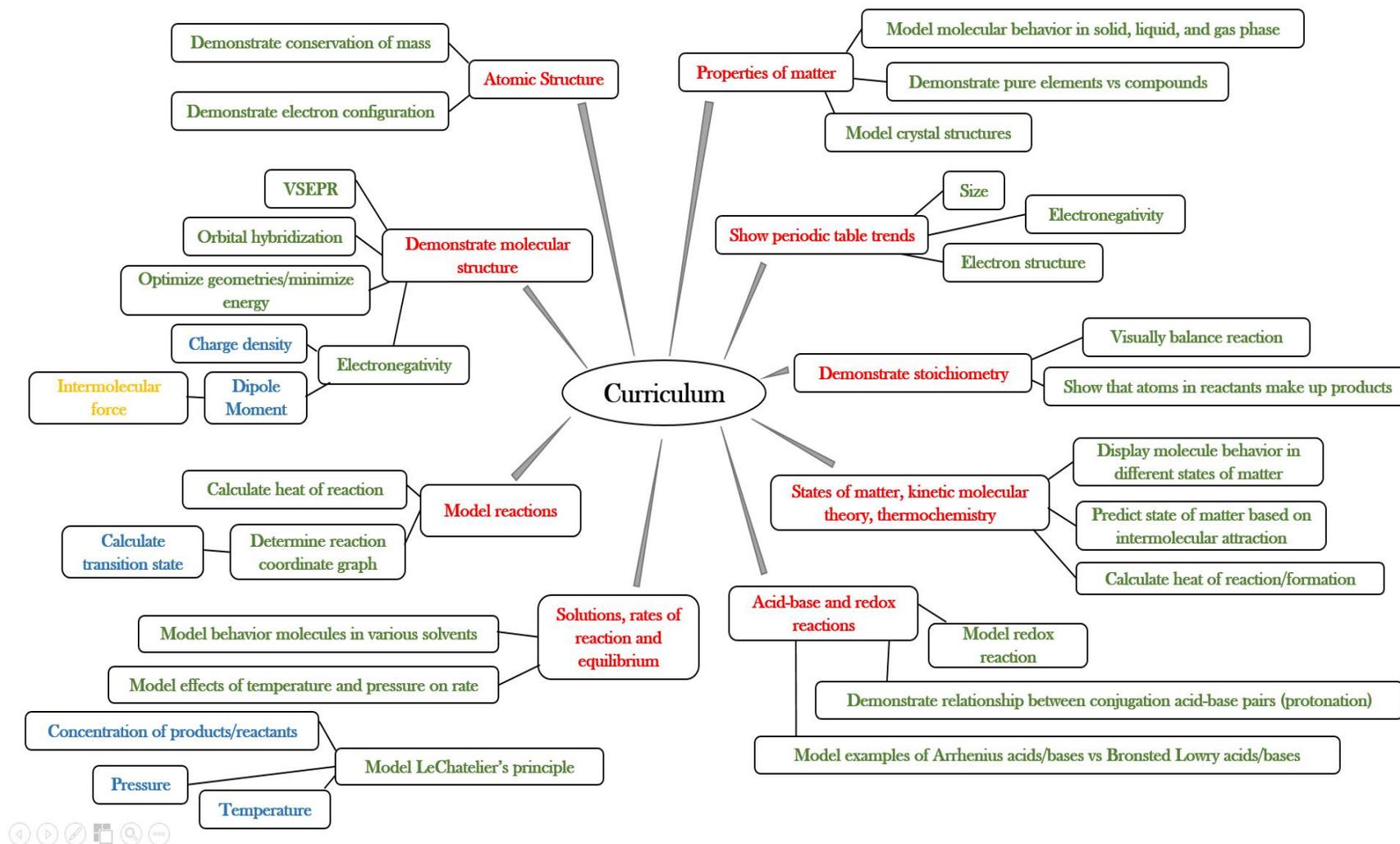
Typically states will set their own individual standards defining what students are expected to learn throughout their education in the public school system. In the state of

Massachusetts, there are a set of these standards governing the required concepts to be learned in high school chemistry classes. The standards are grouped into 8 general topics:

- 1) Properties of Matter
- 2) Atomic Structure and Nuclear Chemistry
- 3) Periodicity
- 4) Chemical Bonding
- 5) Chemical Reactions and Stoichiometry
- 6) States of Matter, Kinetic Molecular Theory, and Thermochemistry
- 7) Solutions, Rates of Reaction, and Equilibrium
- 8) Acids and Bases and Oxidation/Reduction Reactions

(Massachusetts Department of Education, 2006). The set of standards further details the content of each topic and examples of tasks students should be able to complete that fall under each topic. The full outline of these topics and tasks can be found in Appendix A. Our group has consulted these standards in order to design the initial teaching module to augment teaching of the required topics and ensure the material covered would be relevant to the student learning expectations. Figure 2 below shows possible applications of molecular modeling in teaching these standards in the form of a mind map. Each first subcategory of the mind map (in red) defines one of the eight main categories of Massachusetts High School Standards, and the subcategories under them (green, blue, or yellow) define uses of molecular modeling programs that fall into these categories.

Figure 2 - Mind map illustrating different applications of molecular modeling that would apply to the Massachusetts Standards for chemistry. The red level corresponds to the general topics listed in section 2.4.1, and the subsequent levels correspond to tasks and concepts molecular modeling can accomplish that fall under these general topics.



2.4.2. Connecting exercises to Massachusetts Standards

Based on the outline of the Massachusetts High School Standards for Chemistry found in Appendix A, our initial set of exercises, which can be found in Appendix B, applied to five of the topics: Chemical Bonding; Periodicity; Chemical Reactions and Stoichiometry; States of Matter, Kinetic Molecular Theory, and Thermochemistry; and Solutions, Rates of Reaction, and Equilibrium, as summarized in Table 1.A below. The Chemical Bonding category of standards covers how atoms share or give electrons to bond together. Periodicity is about the various patterns of atom properties like size and electronegativity that appear across the periodic table. Chemical Reactions and Stoichiometry shows how molecules change through chemical reactions and the conservation of atoms. States of Matter, Kinetic Molecular Theory, and Thermochemistry describes intermolecular interactions and molecular energies in different states of matter. Solutions, Rates of Reaction, and Equilibrium is a topic that describes how solids, liquids, and gases interact with each other when mixing or undergoing chemical reactions. The exercises aimed to be more complex than the tasks listed in the Massachusetts Standards so that students could gain a clear understanding of the underlying basic concepts using the molecular modeling software and apply those concepts to the simpler problems described in the Standards.

Table 1 - Summarizes the purposes of initially designed exercises and how they relate to Massachusetts High School Chemistry Standards. Related topics numbers in parentheses refer to the 8 main categories within the list of Standards found in Appendix A and listed in section 2.4.1.

How Exercises from Initial Curriculum Relate to Mass. High School Standards		
Exercise Type	Purpose of Exercise	Standards
Molecular Energy Calculation	Build reactant and product molecules of a reaction and have the molecular modeling program calculate the molecular energy of each group. Compare the two to determine which reaction direction is more energetically favorable.	4 - Shows energy involved when atoms bond and electron distribution within the bond
		6 - Shows that energy is produced or absorbed in chemical reactions
Balancing Equations	Build reactant molecules then build the products of the reaction using only the atoms in the reactants	5 - Exemplifies how to balance reactions and forces students to apply stoichiometry and atom conservation concepts
Dipole Moments	Build a series of molecules and have the program perform molecular energy calculations to determine the dipole moment of each	3 - Shows how electronegativity of atoms is different across the periodic table and how that difference affects polarity 4 - Shows how electrons are distributed in chemical bonds
Molecular Energy and Electronegativity	Build a series of molecules and perform molecular energy calculations on each to determine strain energy	3 - Shows how electronegativity of atoms is different across the periodic table and how that difference affects polarity 4 - Exemplifies VSEPR theory by showing that shapes where electrons are closer together have higher strain energy involved
Vibrational Frequency	Build given molecules and perform a Vibrational Frequency calculation to see vibrational modes of molecule	6 - Shows that molecules are not static but are constantly in motion

Our second curriculum addressed some of the Mass Standards as well. Specifically, the curriculum brought to Millbury High School related to Periodicity, Chemical Bonding, and Solutions, Rates of Reaction, and Equilibrium. Table 2 describes how each exercise topic relates to applicable Massachusetts.

Table 2 - Summarizes how problems of the second molecular modeling-based curriculum addressed topics from the Massachusetts Standards outlined in section 2.4.1 and in Appendix A.

How Exercises from Second Curriculum Relate to Mass. High School Standards		
Exercise Type	Purpose of Exercise	Standards
Drawing Molecules	Build molecules with given molecular formula in the 3-D workspace of the modeling program	3 - Shows periodic trend in number of valence electrons atoms have 4 - Teaches how atoms bond together and teaches about electron pairs
Dipole Moments	Build assigned molecules and have program calculate their dipole moment	3 - Shows periodic trend in electronegativity of atoms 4 - Demonstrates polarity of bonds and how electrons are shared
Molecular Geometry	Build assigned molecules, then use Geometry Optimization tool to correct molecular 3-D structure	4 - Demonstrates VSEPR theory and how electron pair repulsion determines molecular shapes

2.4.3. Common misconceptions

One of the biggest and most problematic challenges for high school students is the inability to comprehend that matter is particulate in nature (Nakhleh, 1992). The misconception that matter is instead continuous arises from the fact that students can't see particles in everyday life. Without real-life exposure, visualizing and understanding abstract, new ideas becomes difficult. Therefore, it can be challenging for students to understand that a substance such as water, which looks and feels continuous, is actually composed of individual molecules. Studies have revealed many common misconceptions shared by high school chemistry students, some of which are outlined in Table 3 below.

Table 3 - Compilation of some common misconceptions held by high school students or topics that are typically misunderstood at the high school level. From Al-Bualushi (2013), Kind (2013), and Nakhleh (1992).

Common High School Students' Misconceptions	
Misconception or Challenging Concept	Misconception or Challenging Concept
matter is made of discrete particles (Nakhleh, 1992) (Kind, 2013)	misconception that atoms are alive (Nakhleh, 1992)
particles are in constant motion (Nakhleh, 1992) (Kind, 2013)	misconception that molecules expand when heated (Nakhleh, 1992)
there is empty space between particles (Nakhleh, 1992) (Kind, 2013)	misconception that pressure affects the shape of a molecule (Nakhleh, 1992)
misconception that single atoms have properties such as electrical conductance (Nakhleh, 1992)	misconception that atomic size depends on number of protons (Nakhleh, 1992)
size of atoms/molecules relative to macroscopic objects (Nakhleh, 1992)	misconception that interatomic collisions alter atomic sizes (Nakhleh, 1992)
misconception that molecules of the same substance can vary in size (Nakhleh, 1992)	misconception that electrons orbit the nucleus in circular orbits (Nakhleh, 1992) (Al-Bualushi, 2013)
misconception that molecules of the same substance can change shapes in different phases (Nakhleh, 1992)	polarity, molecular shape, molecular polarity, intermolecular forces, octet rule (Nakhleh, 1992)
misconception that molecules have different weights in different phases (Nakhleh, 1992)	applying VSEPR theory to identify molecular structures (Nakhleh, 1992)
misconception that bubbles in boiling water are composed of "air", hydrogen, or oxygen (Nakhleh, 1992)	difference in strength between covalent bonding and intermolecular forces (Nakhleh, 1992)
misconception that gases are weightless (Nakhleh, 1992)	misconception that number of valence electrons equals number of bonds formed (Nakhleh, 1992)
realization that balanced equations represent the rearrangement of atoms (Nakhleh, 1992)	ability to recognize, differentiate between, and describe physical and chemical changes (Nakhleh, 1992) (Kind, 2013)
misconception that chemical equilibria and steady state are static conditions (Nakhleh, 1992) (Kind, 2013)	comprehending differences between coefficients and subscripts in chemical equations (Nakhleh, 1992) (Al-Bualushi, 2013)
identification of redox reactions (Al-Bualushi, 2013)	realization that particles react by breaking and forming bonds (Nakhleh, 1992)

Table 3 Continued	
Misconception or Challenging Concept	Misconception or Challenging Concept
misconception that compounds are formed by combining fragments of molecules (Nakhleh, 1992)	misconception that concentrations of reactants and products are equal at equilibrium (Nakhleh, 1992) (Al-Bualushi, 2013)
misconception that particles can change form by expanding, contracting, burning, exploding (Kind, 2013)	misconception that molecules dissociate when evaporating and reform when condensing (Kind, 2013) (Al-Bualushi, 2013)
differentiation between mass and density (Kind, 2013)	misconception that fuels are destroyed upon burning (Kind, 2013)
misconception that mass becomes energy in combustion reactions (Al-Bualushi, 2013)	understanding how varying concentrations of reactants and products shifts equilibrium (Al-Bualushi, 2013)
misconception that acids burn and destroy materials (Kind, 2013)	misconception that neutralization of an acid is breaking down an acid (Kind, 2013)
misconception that bases don't have corrosive properties (Kind, 2013)	H ⁺ atoms are responsible for acidic behavior (Kind, 2013)
misconception that forward reactions must conclude before reverse reactions can begin (Al-Bualushi, 2013)	the mole as a unit (Kind, 2013)
misconception that ionic materials are composed of individual molecules (Kind, 2013) (Al-Bualushi, 2013)	misconception that there are only two types of bonding (purely ionic or covalent) (Kind, 2013)
ability to realize covalent molecules can be polar, due to electronegativities (Al-Bualushi, 2013)	misconception that energy can be created and used up (Kind, 2013)
ability to identify the type of bonding present in a material (Al-Bualushi, 2013)	difference between reaction rate and equilibria (Kind, 2013)
misconception that Le Châtelier's Principle is always applicable (Kind, 2013)	misconception that a reversible reaction consists of two separate reactions (Kind, 2013)

3. Methodology

The goals of this project were addressed over the course of approximately 20 weeks. The specific details of the work completed in this time are explained in the following sections. First, we completed research into the background theory behind molecular modeling, the various calculations involved and applications, and different software options available for free that could be found online. After this necessary initial research was completed, a lesson plan addressing various high school chemistry topics using one of these molecular modeling programs was developed. This initial lesson plan was used in alpha and beta rounds of initial testing. Then a high school teacher was found, Ms. Pam Graves, who was willing to allow us to work with her students. Upon meeting with this teacher, we determined that our initial lesson plan was inappropriate for this class because it did not fit within our time constraints and because it covered topics that were far too advanced to introduce to the students. Therefore, a new lesson plan was developed to better coincide with Ms. Graves's teaching. Finally, this new lesson plan was brought to a high school chemistry classroom at Millbury High School in Millbury, MA and used to supplement instruction in this class. Results of the molecular modeling teaching were collected via tests and scored on an individual question basis using a four point scale. The results obtained from each of these steps were analyzed and are further described in section 4.

3.1. Initial theory and software research

The initial step in this project was to gain a basic understanding of molecular modeling theory and software. Research was conducted into the different calculation methods employed by molecular modeling software, the equations and assumptions used in each method, and the comparative accuracy of each calculation type. Several different programs were found online that could be accessed for free and were tested with the goals of the project in mind. These programs feature different functionalities ranging from simple molecular visualization to in-depth biological and chemical molecular analysis. The ideal program for this project should be extremely user-friendly to first-time users of computational chemistry programs, but still capable of performing calculations that support clarifying common misconceptions among high school chemistry students. Use-

ful calculations gave information such as molecular bond angles and lengths, heats of formation, and polarity, in addition to the ability to show in a 3-D space how molecules appear and behave. Each evaluated program was installed locally and tested to find one that encompassed the most useful functions for this project. Programs were immediately eliminated from consideration if they could not be downloaded and installed for free. Programs were also eliminated if they were too complex to expect high school chemistry students to operate, such as, for example, ones that required the use of coding or overly detailed input. We also eliminated programs if the main function was irrelevant to high school-level chemistry students, such as those that focused on modeling proteins or biological processes. If a program only served as a molecular visualization tool and could not perform any calculations it was also not considered. These brief program assessments are discussed further in section 4.1 below, while a table giving our brief notes from these software evaluations can be found in Appendix D.

3.2. Curriculum planning

Once the ideal modeling software and calculation package combination was determined, a teaching module was developed. We designed our initial teaching module and planned how we would eventually implement it in a high school classroom, but only made it through the testing phase at WPI. This teaching module consisted of several exercises that took advantage of the modeling software capabilities. The questions in the exercises were based on the topics chemistry students are expected to understand by the end of high school as defined in the Massachusetts high school curriculum standards in Appendix A. The initial teaching module was developed to be implemented in a high school class over the course of about a month. The beginning and end of this month-long period would have been marked by a pre- and post-test, respectively, to assess both the effectiveness of the curriculum and the overall progress of the students involved. Between the pre-and post-test sessions, a series of worksheets would have been completed by the participants. . We recorded two different tutorial videos to show to students in the class to provide them with an overview of all of the modeling program functions they would need to use over the course of our program.

During each of the class periods provided to us during that month-long implementation, we planned to briefly review the material from the previous class in order to rein-

force that knowledge and then have the students work on one or two of the exercises that that day's topic. We would then be available to students for help should they need it. About half to three-quarters of the class time would have been given to students to work on the computers, and the rest would be dedicated to a class discussion between the project members and the students. This discussion would focus on asking the students questions about the material just learned to generally ensure that WebMO was used correctly and that students were able to learn from the exercises.

Once this curriculum was fully designed, an initial testing phase plan was developed. The initial testing phase was designed to be a pilot run of the worksheet problems using WebMO that we wrote for this lesson plan. The exercises were to be sent to WPI students along with a survey to collect their feedback on the difficulty of the questions, on the value of the tutorial video, and on the modeling program itself. The execution of this testing phase plan is described in section 3.4.

3.3. Analysis of potential problems and proposed solutions

As part of planning the implementation of this project, it was important to take into consideration the possible issues that could arise along the way. These possible issues could have posed a threat to the completion of the project goals and could result in the need to create a new plan of action. These problems included lack of teacher support due to time, time constraints associated with the WPI term schedule, computer and software-related problems, a lack of student participation or interest, or no need for improvement after students take the pre-test. If possible setbacks could be predicted and examined ahead of time, solutions would be developed and immediately implemented so that progress on the project can continue as soon as possible.

The calculations for this project needed to be performed using specialized computer software and required varying amounts of time depending on the school network, specific calculations being made, and computer capabilities. Teachers would likely be unwilling to sacrifice instruction time in order to test a program that may not even help their students. These concerns about time could be addressed by asking for student volunteers from the selected class to stay after school for program testing. By holding project work sessions outside of school hours, the only class time teachers would be asked to give up would be a short period in which to administer the pre- and post-tests to all stu-

dents in order to have a control with which to compare the results from the students using the teaching module.

Even if time requirements for the proposed work were accepted by the classroom teacher, they may not coincide with the time restraints of the project. This project was allotted 21 weeks (3 WPI terms) to be completed. Based on the initially proposed program, the testing and worksheets involved would require several classroom visits over the course of multiple weeks. It may not be feasible to complete the implementation period within the final seven-week term. One way to address this problem would be to begin the search for prospective high schools early. The overall goals of the project could be explained and software installation could begin during the WPI testing phase, and an explanation of pilot test results and any subsequent improvements would be provided to the teacher before in-class testing. That way, the teacher could offer specific feedback on improvements or features he or she would like to see before the students are ever involved. Another solution to this problem could be to focus only on program improvements, such as editing questions, based on feedback obtained after the WPI testing. This way, everything in the feedback from students could be thoroughly addressed, bringing the program to the optimum level of effectiveness and user-friendliness before bringing it to an outside institution. Future research groups could then carry out the implementation aspect of the project.

When classroom implementation occurs, completion of the designed worksheets requires specialized software to be installed on each computer that students use. Teachers may be unable or unwilling to provide the research group with access to classroom computers to make the necessary installations. In order to avoid this difficulty, teachers and information technology (IT) professionals at the chosen school will have to be made completely aware of the computer access requirements for the project. For this purpose, a list of instructions for the installation of the modeling software and the associated calculation packages needed were developed and can be found in Appendices E, F, and G. From there either necessary permissions could be obtained for installations or installation instructions could be provided to IT professionals in the school for them to complete the installations. A more difficult issue to address may arise with licensing to use the program. It would be impossible to install the software if a license or password request from

the software vendors was denied. In such an event, research would have to continue until a new molecular modeling program could be found that fits the needs of the project.

It is likely that when a teacher is found who agrees to allow program testing within their classroom, he or she may be unwilling to offer students academic credit for the work. Without the offer of class credit, students may not be willing to take the exercises or the pre- and post-tests seriously. If students do not try to do well on the exercises or tests, it will not be possible to determine whether the teaching module was effective. In order to lower the risk of running into this problem, some form of incentive could be offered to participants. This incentive could be in the form of snacks, a raffle for a prize item of some sort, or a small denomination gift card for each participant. Another possible way to lower the risk of disinterested participants would be to target an AP Chemistry class. These students will likely be more interested in participating in a program that could help their understanding of these topics because they had to make the choice to take the advanced level of chemistry, so they are more likely to be interested in the topic itself. These more advanced students also are preparing for the AP exam at the end of the school year, which serves as an incentive for them to learn the material better than the students in a less advanced class who may focus on only remembering parts of topics for shorter periods of time to do well on a particular test.

The purpose of the worksheets and overall goal of the project is to teach students chemistry concepts they struggle with. If students do not struggle with the presented concepts there is nothing to teach. In that situation, it is possible the teacher would request that no more time be spent on project evaluation. If this happens, research efforts could be redirected into either developing another set of worksheets addressing more advanced topics, or finding another group of students to test the program with. If program testing continues, the evaluation can then be focused mostly on the software itself. Students could be asked to provide their opinions on the benefits and shortcomings of the software and of applying it to classroom topics. This information could be helpful in determining whether it would be valuable for schools to incorporate this program or one like it in their chemistry curriculum. If students think the program is too complex or not very informative, they will not benefit from it.

3.4. Alpha & Beta Testing Phase

The first step in implementing the teaching module was a phase of alpha testing. In this stage, a small group of students at WPI were asked to complete one of the questions from the set of exercises written by the group. The volunteers were instructed to watch a video tutorial about using the computational chemistry software (recorded by the group), complete the assigned question (randomly chosen by a project group member from those shown in Appendix B), and then fill out a form online to provide feedback. The feedback form, shown in Appendix H, asked students about their background in chemistry, then for their input on the instructional video, the question provided to them, and the user friendliness of the WebMO software. The results from this feedback form were evaluated and input was considered before continuing testing.

After the alpha testing phase was completed, beta testing commenced. The tutorial video, a random question, and the feedback form were distributed via email to chemistry, biochemistry, and chemical engineering majors. The random question was delivered through use of a randomize Javascript, whose code is available in Appendix I. The question was from the same set used in alpha testing because initial test subjects did not give any negative feedback relating to the questions they were asked. This round of testing was expected to provide a larger test group due to the offer of an incentive. Students were again asked to evaluate the tutorial video, the problems, and using WebMO. This was the final round of testing and evaluation input before the video and questions were presented to high school students. This final round of evaluation allowed for further refinement of the questions and selection of the best written and most helpful ones for high school use. The results from the feedback form administered are further discussed in Results and Discussion below.

3.5. Implementation Phase

After the conclusion of the alpha and beta testing phases, the gamma testing phase began. The subjects used in this testing phase were chemistry students under the instruction of Pam Graves at Millbury High School in Millbury, MA. During the first meeting with Ms. Graves, it was determined that the initial curriculum plan and designed work-

sheet was not actually feasible. This was mainly because of time constraints and the academic level of the class we worked with.

After the testing phase was complete and contact was established with Ms. Graves, there were only six weeks left in the three terms allotted to our project work. The first of these weeks was used to meet Ms. Graves in person to discuss the project specifics and plan class time, the last week was reserved to allow us to analyze data from the class, and the middle week was a school vacation week for Millbury School District. This allowed us only three 1 hour class periods to work with the students, making the original month-long implementation plan impossible.

The next limitation we faced was the academic level of the class we worked with. The original curriculum plan was designed for AP level or similarly advanced chemistry students because some of the topics to be addressed were more advanced than the Massachusetts Standards. Due to scheduling conflicts, we were unable to work with Ms. Graves's honors and AP students. The class we were able to work with was an introductory level class in which the students did not have an adequate background to be able to complete the exercises we had used for alpha and beta testing. Because of these unavoidable problems, new exercises were developed each week for three weeks of class visits to coincide with the topics Ms. Graves taught in class during the week between our visits. The full collection of these new exercises is given in Appendix C.

With the new plan, three classroom visits occurred once per week over the course of 4 weeks, with the students' vacation week in the middle of weeks 2 and 3. Each session focused on material taught in typical classes the week leading up to the visit. Figure 3 below details the adjusted lesson plan and content covered during each visit.

Figure 3 - Visual layout of the revised teaching plan for the three weeks of working with Ms. Graves's students. Each week also included a test at the beginning of the class and a test at the end addressing the topics for that week. The first week started with basic molecule drawing when given the molecular formula. Week 2 reviewed this concept in addition to teaching about determining dipole moments based on relative electronegativity. Week 3 reviewed topics from each of the previous weeks and additionally went over basic VSEPR theory and determination of molecular shape.

Curriculum Plan Implemented at Millbury High School

Week 1	Week 2	Week 3
<ul style="list-style-type: none"> • Introduction to WebMO program • Drawing molecules based on valence electrons given a written formula (ex. CH₄) 	<ul style="list-style-type: none"> • Extra practice with molecule drawing • Determining direction of dipole moment based on differences in electronegativity 	<ul style="list-style-type: none"> • Review of material from weeks 1 and 2 • VSEPR theory and molecule geometry • Feedback form

Each class began with a brief pre-test of three to four questions to gauge students' initial understanding of the topic for that week. Upon completion of the pre-test, students moved to computer workstations and were instructed to build certain molecules and perform calculations or optimizations relevant to the material taught that week. After students had an opportunity to work with the software and see the concepts applied they were given a post-test similar to the pre-test. The pre- and post-tests can be found in Appendix J. The exercises completed between tests using the software can be found in Appendix K.

The pre-test and post-test were graded on a four point scale for each question in order to quantitatively determine whether improvement occurred after working with software. One point meant the student did not show any understanding of the material, two points corresponded to the student showing some understanding but making a major conceptual mistake, three points were awarded if the student showed a good understanding of the material but made a minor mistake, and four points were given if the student got the question completely correct. Examples of graded tests are available in Appendix L.

At the conclusion of the final session, the students were each given a feedback form. This feedback form was redesigned to evaluate their perceptions of the educational value of computational chemistry and the entire curriculum plan using a Likert-type scale in order to obtain quantitative data. The feedback form used can be found in Appendix M.

3.6. Analysis

In order to most accurately analyze the success of this curriculum, the pre- and post-tests were designed to be very similar, but not identical. The reason for this is that we wished to measure the difference in students' understanding of material, so that if they scored higher on the post-test, this would indicate that our teaching bolstered this understanding. For example, both tests may have included a question about the dipole moment of a given molecule, but on the pre-test this may have included some halogen atoms, while on the post-test this may have included some alkaline metals. This forced students to examine the periodic table to determine the differences in electronegativities and how this affected the dipole moment. Exercises were not repeated so as to avoid the potential for students to simply remember the correct answers to problems. The pre- and post-tests contained conceptual questions which related more strongly to students' class work and the Massachusetts Standards, whereas the worksheets contain very specific, calculation-oriented questions which were likely beyond the scope of the material covered in class. By doing this, we based the instruction of subject material solely on the content of the modeling program. In this way, it was possible to determine whether the students' completion of the exercises resulted in greater understanding of chemical concepts.

Quantitative feedback from students was also collected in the form of surveys. Issues such as user friendliness of the software and success in understanding the chemical concepts were addressed by these surveys. The outcome of this feedback is further described in Results and Discussion below.

4. Results and discussion

The results of this project will both help evaluate the current effectiveness of computational chemistry tools for the calculation and visualization of molecules and assist future groups in using these tools to help high school students in chemistry. We discuss our results below (briefly mentioned here).

- **Software review:** Many chemistry related programs were reviewed to determine if they are acceptable for use by high school students.
- **WebMO:** As a compatible software, WebMO was determined to be useful in high school classroom based on its intuitive features and its ease to perform calculation of molecules.
- **Professional Opinion:** Several Professors from Worcester Polytechnic Institute provided advice about the utility of WebMO.
- **Curriculum Standards:** According to Massachusetts' state curriculum standards for high school students, we developed sample problems to address related topics like building 3-D structure and geometry optimization calculation.
- **Implementation:** We performed initial testing at Worcester Polytechnic Institute and a high school classroom in Millbury, MA. The evaluation of WebMO were based on the feedbacks and the performance of the high school students.

4.1. Software review

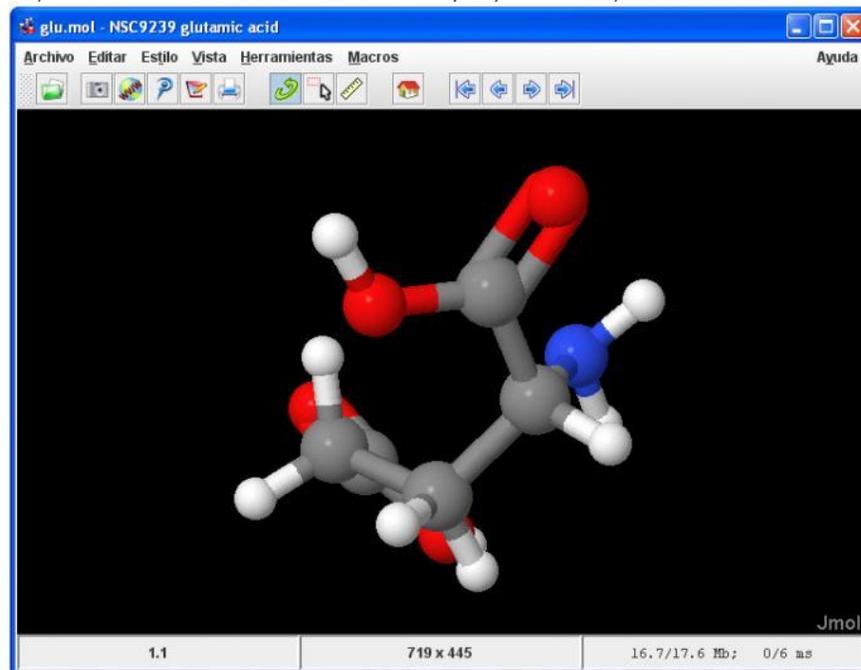
Our first goal of the project was to review several programs to find a platform that could not only allowed the user to build molecules in a 3D virtual workspace but also was able to create the structure of molecules and perform various calculations based on the structure. While many programs are capable of doing this, only few allow the user to click and draw molecules without any type of computer code input. The modeling program that we sought to use needed to fit into this category. The ideal program had to be intuitive so that high school students would not have trouble using it to perform our exercises. Finally, the program needed to be able to display many different types of molecules and calculations of their various properties, not just model biological proteins and systems as some programs are designed to do.

The ideal program was found to be WebMO, a modeling application that translates results from various calculation software packages to three dimensional models of molecules, allowing users to perform a wide variety of calculations and obtain concrete, visible models of the results. For less advanced users, WebMO also provides an intuitive workspace for users to draw and manipulate molecular models without performing calculations. Another advantage of WebMO is that it can be downloaded and installed locally for free, as can the Firefly and MOPAC calculation packages. Other types of programs evaluated are summarized in the following sections based on the reason they were deemed unhelpful. The functionality of WebMO is further discussed in section 4.2.

4.1.1. Visualization programs

Many of the free programs found online that were tested are built solely as visualization platforms, which are essentially just viewing interfaces that allow the user to import a structure and look at the molecule without being able to perform any calculations. These are able to build or upload molecular models, in some cases can calculate basic properties such as bond lengths and angles or molecular weights. Of the programs we tested, Chemitorium (“Chemitorium”, 2013), Jmol (“Jmol”, no date), QMol, RasMol, and VMD+NAMD all fell into this category. Based on the goals of this project, these programs were determined to be of little use to us and were ruled out. As an example, the workspace of Jmol is shown below in Figure 4. There are plenty of tools on this workspace that help the user to view different molecules but the user cannot actually manipulate the molecule or determine properties of the molecule using the software.

Figure 4 - A screenshot of the user interface of Jmol. This program was not chosen because it cannot perform calculations we needed. Image from glu.mol - NSC9239 glutamic acid. N.d. Screenshot. Softonic.com. Web. 12 Feb 2014. <<http://jmol.en.softonic.com/>>.



4.1.2. Biological/drug design programs

One common application of molecular modeling software is the analysis of proteins and various phases of drug design, and there are several programs designed specifically for this purpose. Abalone ("Biomolecular simulations with Abalone", 2013), Ascalaph Designer, Desmond, Fold It, MOIL, and UCSF Chimera are all programs that were tested as potential candidates for this project and determined to fall into this category. The programs were tested by using the software online or downloading the software and inputting basic molecular structure. This project aims to assist in teaching high school-level chemistry concepts more than biology concepts, and therefore these programs were determined to not be useful.

4.1.3. Advanced user programs

In addition to the above programs, initial program research also included Xeo, VegaZZ, Raster3D, and ACD/3D Viewer ("ACD/ChemSketch Freeware", 2013). These programs relied on coding or technical information inputs in the form of coordinates in

order to perform calculations, which puts them beyond the skill of the high school students because they require knowledge of coding and scripting. While this type of program may allow for more fine-tuning and manipulation of calculations and the accuracy of results, the complexity of such user-interfaces is far beyond the scope of this project. This is because few high school students are exposed to coding, and this project's goal is developing a program that is accessible and usable in high school students. For that reason, these programs were also eliminated from considerations for classroom use.

4.2. WebMO

WebMO was found to be the best choice for our project needs. While this program does not do any of the calculations itself it instead serves as a visual interface for other simulation programs, such as Firefly, Gaussian, TINKER, and NWChem. WebMO is useful because it takes an input structure from what the user has built in graphical user interface and sends the input to simulation programs for calculation. Then the program takes the output file and converts it back into something that can be displayed in the workspace. This is very useful because the user does not have to bother with coding an input file or with all the various theory and basis set options and then running the simulation program from the command-line. This makes WebMO ideal for casual computer users and maintains the same level of accuracy and computational power without advanced user knowledge. WebMO is easy to use and comes naturally to most users. Our first experience with this program was straightforward: all of the commands were apparent and it felt like just like a point-and-click kind of application. We did not require a manual to get started, with the exception of the installation, and running jobs was a simple task because of the drop down menus and easy-to-use job manager.

4.2.1. Features explored

In order to become familiar with the interface and features of WebMO, several introductory tutorials found under the WebMO Help Menu were followed. Figure 5 shows how WebMO was used for a simple dipole moment calculation.

Figure 5 - The following sequence of screenshots provides a basic understanding of WebMO's setup and interface. The example shown is a dipole moment calculation on a molecule of HF.

WebMO Job Manager **A**

B

Choose Computational Engine **C**

Configure Gamess Job Options **D**

WebMO Job Manager **E**

Number	Name	Description	Date	Status	Time	Actions
153091	HF - Example	Molecular Energy - Gamess	3/7/2014 15:44	Complete	0.0 sec	
153090	H2O pm3 LS MO KR	Geometry Optimization - Mopac	3/7/2014 15:44	Complete	0.0 sec	

Calculated Quantities **F**

Quantity	Value
Route	\$CONTRL SCFTYP=RHF RUNTYP=ENERGY
Symmetry	C1
Basis	6-31G(d)
RHF Energy	-99.9875477394 Hartree
Dipole Moment	2.191429 Debye
Partial Charges	

View Job 153091: HF - Example, Molecular Energy - Gamess **G**

After logging into WebMO, the user was automatically taken to the “Job Manager” page (A). In WebMO, “jobs” are created and calculations are performed on each job to provide

the user with useful results. After a job is created, the molecule(s) are built and the calculations to be performed are selected. Following this, WebMO runs the job (completes the calculations) and displays its results. A new job was created by clicking on the “New Job” button. This brought the user to the “Build Molecule” screen (B). In this example, a molecule of hydrogen fluoride was built. A hydrogen atom was selected from the periodic table menu located at the left of the screen. A single click in the workspace created a hydrogen atom. A fluorine atom was created in a similar way. The bond was created by clicking on one atom and dragging to the other. Clicking the right arrow button at the bottom of the screen took the user to the “Choose Computational Engine” screen (C). For this exercise, Gamess was selected and the next button was clicked. On the “Configure Gamess Job Options” screen (D), a name for the job was entered and the “Molecular Energy” calculation was selected. a molecular energy calculation calculates the potential energy of the molecule, which is a result of intermolecular interactions. Descriptions of the other types of calculations that can be run are found in section 4.2.3. Hitting the next button brought the user back to the “Job Manager” (E). As soon as the status of the job changed from “Running” to “Complete” (clicking the “Refresh” button will update this), the magnifying glass symbol was clicked. Once brought back to the “Build Molecule” space, the user scrolled down to the “Calculated Quantities” section (F). This is where the results of the job calculations are displayed. The user clicked the magnifying glass next to “Dipole Moment” to display a dipole moment arrow on the HF molecule in the “Build Molecule” window (G) at the top of the page.

It was found that the WebMO interface was very straightforward when seen for the first time. Additionally, WebMO displayed tips and comments at the bottom of the screen which were found to be helpful. The only confusion arose when selecting a computational engine, basis set, and theory for the job. There were no explanations as to how to pick one, or which methods are best for which purposes. However, a student using WebMO would not necessarily need to know anything about selecting these parameters if they were told which to use.

The three-dimensional viewing capabilities of WebMO were found to be quite desirable, especially considering that the purpose of using an interface such as this is to aid students in visualizing matter at the molecular level. It was also found that WebMO has

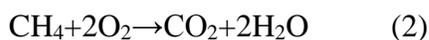
some excellent shortcut abilities for building complex molecules. First, the Clean-Up command will add H atoms that are missing and correct molecular structure. This is all accomplished by clicking a single button. Secondly, the Fragment feature can be used to quickly add parts of or entire molecules, rather than build them up one atom at a time. Additionally, after completing a calculation with a given molecule, a new job can be created with the same molecule by simply clicking the “New Job Using This Geometry” button.

When logged in as an administrator, several useful things can be accomplished apart from the standard addition, deletion, and viewing of users and jobs. In the “Interface Manager”, different computational engines can be enabled or disabled. Student confusion surrounding which computational engine to select can be eliminated by only allowing the necessary engine to be available. In the “Fragment Manager”, new fragments or molecules can be created and accessed by any user. This is particularly useful in the case that students must run a calculation on a complex molecule that would require significant time to build manually.

Following this initial testing of WebMO, a comprehensive “cheat sheet” was created, visually depicting each of the buttons and providing brief descriptions. This visual aid was designed as a visual aid for students trying WebMO for the first time. The WebMO Cheat Sheet can be found in Appendix N. Additionally, a WebMO tutorial video was created and is referenced in Appendix O.

4.2.2. Test calculation in WebMO

The heat of reaction for the combustion of methane was calculated in WebMO. The reaction is given by equation 2 below.



This was done by running Geometry Optimization (discussed in the next section) jobs (using Gaussian, Hartree-Fock, and Routine: 6-31G(d)) on a single molecule of each of the reactants and products separately. The heat of reaction was calculated as follows:

$$\Delta E = nE_{(\text{products})} - mE_{(\text{reactants})},$$

where $n = \text{product coefficient}$ and

$m = \text{reactant coefficient}.$

The theoretical value obtained was then compared to an experimental value. The results of these calculations are summarized in Table 2. The theoretical results agreed well with experimental results indicating the usefulness of computational chemistry methods.

Table 4 - Table showing values obtained in the calculation of the heat of reaction for the combustion of methane. All values (except for the Experimental heat of reaction) were calculated by building the tabulated molecules on WebMO and performing Geometry Optimization calculations.

Heat of Reaction of the Combustion of Methane as Calculated Using WebMO			
Reactants	Calculated Energy [kJ/mol]	Products	Calculated Energy [kJ/mol]
CH₄	-105532	CO₂	-492634
2O₂	-785198	2H₂O	-399132
Total Reactant Energy:	-890730	Total Product Energy:	-891766
<u>Experimental Heat of Reaction</u> (Damalski):	-891 kJ/mol	<u>Calculated Heat of Reaction:</u>	-1036 kJ/mol

4.2.3. Calculation capabilities

Several types of calculations can be performed with WebMO. The following are explanations of each of these features:

- **Molecular Energy:** Calculates the potential energy of the molecule. This energy value is a result of intermolecular and intramolecular interactions
- **Geometry Optimization:** Finds the molecular structure that minimizes the potential energy of the molecule
- **Vibrational Frequencies:** Calculates the different vibrations a molecule undergoes due to interactions between electrons
- **Transition State Optimization:** Calculates the transition state energy, which is the maximum point on a plot of potential energy vs time for a molecule or molecules undergoing a reaction

- **PM3 Heat of formation:** Calculates the amount of heat that is produced when one mole of a compound is formed from its basic atoms.
- **Dipole Moment:** Shows which part of an atom is most electronegative.
- **Partial Charges:** Shows the charge on individual atoms within a molecule caused by unequal electron distribution.

4.3. Discussion with WPI professors

As part of our planning to determine a reasonable format for the WPI testing, we spoke with two different professors from the Chemistry & Biochemistry department at WPI. We consulted Professors Heilman and Brodeur to obtain their insight into the educational value of the initially designed exercises (given in Appendix B), and whether said exercises were appropriate for our target high school audience, and whether it would be possible to perform our alpha and beta testing within a WPI chemistry class. Both professors were extremely helpful with their feedback relating to our questions and how to adjust our plan to the audience we wanted to reach (chemistry students), but unfortunately because of time constraints and already planned coursework, we were not able to work with either of their first year chemistry classes for this project.

4.3.1. Professor Destin Heilman

Professor Destin Heilman of the Chemistry & Biochemistry department at Worcester Polytechnic Institute noted that in his experience in general chemistry, students most often misunderstand the concept of the mole and have difficulty grasping its importance in reaction quantities. This is in parallel to what Professor Brodeur, of the Chemistry & Biochemistry department, has mentioned concerning the misconception of stoichiometry. Students seem to have difficulty with the fact that a certain number of moles of a chemical reacts with a number of moles of another chemical to produce a product(s). Professor Heilman particularly emphasized the idea that chemistry is collisional and that matter is transformed with the same constituents rather than destroyed and created again. Additionally, he mentioned this concept's importance in equilibrium of a reaction and that it is the equal rates of forward and reverse reactions, governed by these collisions, not the equal concentrations of reactants and products that determines equilibrium. Finally, Professor Heilman suggested that, based on the complexity of the computer

modeling program as well as the depth of the questions of our proposed curriculum, the average high school will probably not be a good place for our program's introduction. He recommended looking either to more advanced students or high schools.

4.3.2. Professor Drew Brodeur

Professor Drew Brodeur is a member of the Chemistry & Biochemistry department faculty at WPI. He has experience teaching different levels of chemistry classes and is familiar with all levels of the general chemistry sequence. He was consulted for his experience with topics students often struggle with in the general chemistry and advice on getting a project like this implemented as a pilot or test run within the general chemistry sequence at WPI. The most prominent topic Professor Brodeur emphasized that students often misunderstand was stoichiometry. He further explained that students have the most trouble understanding that in reactions the atoms of reactants split apart and recombine to form products and that nothing new is added. Professor Brodeur also mentioned that to a lesser extent the topics of buffers in acid-base chemistry and basic thermodynamic properties are covered in the general chemistry sequence and are frequently misunderstood by students.

A draft of the worksheet for this project, which can be found in Appendix B, was presented to Professor Brodeur for his analysis of how well it lined up with topics addressed at the general chemistry level. This draft included questions that addressed prediction of molecular shapes and molecular energy, polarity, transition state, energy and heat of reaction, and vibrational frequencies and utilized WebMO in order to confirm predictions or reach conclusions. Professor Brodeur determined that based on the current sequence curriculum, most of the topics addressed would be well-suited for students in the second general chemistry course. The only topics on the worksheet that were beyond the scope of that course were the vibrational frequencies (which he said is addressed in the fourth course of the sequence) and transition states. He also pointed out, however, that the current school year (2013-2014) would be difficult to incorporate such an exercise into the general chemistry sequence because another chemistry education assistance program, known as Sapling, will be in use ("Sapling Learning", 2013). Lastly, Professor Brodeur recommended a couple of other options to consider for implementing this project within the general chemistry sequence. He suggested proposing the program to professors

now in order to be used during E-term or the 2014-15 academic year, but these suggestions extended beyond the timeframe and scope of this project.

4.4. Teaching module implementation

The teaching module was developed in two distinct phases. The first consisted of the alpha and beta testing, which was carried out at WPI over the course of a few weeks. Alpha testing was done with a small group of test students, while beta testing was done with a larger group of students with majors in chemistry, biochemistry and chemical engineering. The second phase included the implementation of the revised teaching module into a high school chemistry class of 16 juniors at Millbury High School in Millbury, Massachusetts.

4.4.1. Pilot run at WPI

Alpha and beta testing were performed with students at WPI with more background in chemistry in order to ensure that the test subjects would be able to understand our questions and the results from the software so they could give us more thorough feedback. The students we targeted were those whose majors included Chemical Engineering, Chemistry and Biochemistry. These students were given a tutorial video (submitted with this report), the WebMO program itself, and a random problem to complete as a sort of test run so that they could become familiar with the program. Once they completed the problem, they were asked to fill out a survey inquiring about their experience and asking for their feedback on the program, the tutorial video, and how they thought the modeling program informed about the topic. Additionally, they were asked if they would use WebMO in the future for their chemistry studies. Below are the specific questions asked of them:

1. What is the highest level of chemistry class you have taken thus far?
2. What comments can you provide about the instructional video provided?
3. Which question did you work on?
4. Was the question asking about material you have learned previously?
5. What feedback can you provide about the question itself?
6. How effective do you think the modeling program was in completing the task?

Student results

The results of the alpha and beta testing phase questionnaire as well as the questionnaire itself are given in Appendix H. While for the most part the participants believed that the instructional video was helpful, some found it difficult to navigate and felt that an outline of the video would be more informative. With respect to the familiarity of the subject matter covered in the sample problem, none of the participants were new to the material, as expected considering that the sample body had chemistry backgrounds. There was a great deal of input about the problems given. Table 5 summarizes the feedback based on which of the questions from Appendix B they completed.

Table 5 - Summary of feedback obtained from alpha and beta testing subjects. In total there were 13 responses to the survey and all feedback was considered in forming the summaries below.

Summarized Feedback from Alpha and Beta Testing at WPI	
Question Number and Topic	Feedback
1. Molecular Energy	All of the subjects believed that the question was well formulated and that the goal of the task was clear and they were therefore able to complete the question in a timely manner. Some brought up the idea that this topic might be too difficult for students at the high school level.
2. Balancing Reactions	All of the testers thought this question was straightforward and easy to understand. The original equation was not difficult to balance, and the material was already well-understood by college-level students.
3. Dipole Moment	Subjects thought this question was clear and easy to understand. One participant mentioned technical difficulties with drawing the molecules and noted that the tutorial did not sufficiently cover this.
4. Molecular Energy	Some testers commented that this question was too technical and wordy, and was made confusing by terms like “strain energy”. Otherwise, testers noted that the task itself was not overly difficult.
5. Vibrational Frequency	All of the test subjects for this question indicated the question was well-written and easy to understand. Testers also stated that the software was helpful on this question as it allowed them to actually see the molecular vibration.

In summary, it appears that the questions themselves were easy to understand but participants had difficulty applying them to the program without proper instruction. An in-class or personal demonstration of WebMO could clear up this confusion. In general, we hoped to have time for the students to familiarize themselves with the program so that they were comfortable with it when they started to work on problems.

As for the efficacy of the modeling program, we received mixed responses. Some thought the program was easy to use and that queuing up results from the job manager made locating former results, and comparing them simple. Additionally, it seemed as though the presentation of data, whether it be geometric or numeric in nature, was clear and informative. On the other hand, some believed that WebMO did not improve learning, but merely saved the user time. Additionally, some could not even use the program due to the browser they were using and it was also brought to our attention that it did not work on a tablet, which may be a more useful platform to consider since manipulation of the model molecule could be performed with the user's hands instead of a mouse device. A hotkey was also advised as a useful tool for adjusting molecule geometries instead of clicking on buttons in the interface, which might make these adjustments tedious. Generally, however, participants believed that once knowledge of the program's use was established, completing the questions was a trivial task. Finally, the majority of participants stated they would use WebMO again if they were forced to. Performance results for the problems the WPI students worked on were not collected because the group was interested in determining how these students felt about the modeling program and associated exercises in general.

With the above feedback in consideration, we adjusted our high school implementation by clarifying how to use WebMO as clearly as possible so that assignments can be completed without problems, rather than students getting stuck on technical issues with the program. We also devised some simpler assignments to complete, such as building a small molecule in the workspace and then running a simple job, in order to get the students as comfortable with the program as possible.

4.4.2. High school classroom use

The molecular modeling program was implemented at Millbury High School every week starting the week of February 3rd and ending the week of February 24th, with

the exception of the week of February 17th due to the school's vacation period during that time. This allowed for three one-hour sessions with the high school students. Because of this time restriction, pre-tests had to be given out at the beginning of each lesson and a post-test at the end of each lesson so as to measure knowledge gained during the session.

4.4.2.1. Classroom Choices

Teacher Ms. Graves gave us the option to and urged the team to work with her college preparation class. As opposed to the honors class, this class was focused on making sure that students were knowledgeable of concepts they will encounter in college and preparing them for the rigorous courses that they may encounter. With the help of this program and the fact that the team members had already spent several years at a university, Ms. Graves hoped that the team could inspire the college prep students to be excited about and interested in chemistry as well as higher education. The students in this class generally lacked interest in more advanced chemistry topics and appeared to be more easily distracted and sociable than higher level classes.

4.4.2.2. Program use

The guest server, available on the WebMO website through common web browsers, was used in the high school classroom, which avoided any technical difficulties with local installation as well as conflicts with the IT department at the school. Additionally, this approach only required internet access and was easy for the students to start up and use. Initially, Java was not updated on the computers at the school so calculation jobs could not be performed but full use of the 3-D molecular drawing space was available for the students to start getting used to building molecules and understanding how many bonds each element can make. This feature was only used for week 1 of the implementation phase.

Java was updated by the IT department on the classroom computers in time for the second lesson and brief use of the calculation capability of the program was included in the curriculum for that lesson. However, due to the large volume of computer users (roughly twenty students in total), access to the WebMO server was slow. This severely

curtailed the curriculum for that lesson and only one molecular energy job could be performed during that day. Rendering of dipole moments for the molecule in question failed as well as the graphics interface crashed on numerous machines during the process. Goals were set for the next lesson so as to avoid this server access issue and make time provided for the class as efficient as possible.

For the third session, the class was split into groups to lessen the demand on the WebMO server. The class was split into pairs so that only ten computers total were in use. The class was further split so that for the first half of the class five of those ten computers were only using the drawing functions of WebMO and no calculations, meaning no server use. The other five computers worked on reviewing the material from week two using molecular energy calculations. Because of the drastically reduced workload for the server, all five groups were able to successfully complete their calculations in a timely manner. Once all students had finished the task they were assigned, the roles switched and the five pairs that had been doing calculations switched to drawing while the five that had been drawing switched to calculations.

4.4.2.3. Class Narrative

The first lesson involved a brief introduction by the IQP team to the students, including the team members' majors, hometown, and reasons for entering their major field of study (chemistry and chemical engineering). The students were receptive and seemed to be genuinely interested in working with the team. After the pre-test was given, for which five minutes were allotted, the students logged on to the computers and then on to the WebMO guest server. Instruction of how to use the tools in the drawing space were given by members of the team while the students played with some of the features provided there. These instructions were followed well and the students seemed to grasp how to use the program fairly easily, a testament to the familiarity with technology on the part of the students and the ease of use of the program itself. Once accustomed to how the program worked, some students began to draw random sets of atoms and connect them at random. However, once given some molecules to work on such as H_2O and BF_3 , the students attempted to connect these atoms correctly and were able to explain to us that they were connecting them according to the number of valence electrons each atom had. One issue with the program perhaps is that it does not account for the number of bonds an at-

om needs to form in order to have a full valence electron shell, and therefore cannot correct a user if they create too many or too few bonds. However, if one were to attempt to say, draw two bonds on a hydrogen atom and perform a calculation, the calculation job would fail because this bonding scheme would be unrealistic. This became a problem in some cases where students would draw water molecules with the correct bent geometry but then connect the two hydrogen atoms as well without considering that these atoms cannot form multiple bonds. Hydrogen atoms have only one valence electron, meaning that they only have one available electron to pair with another atom's electron. Therefore, hydrogen atoms cannot form more than one bond. At any rate, the students worked through some of the problems that were put on the board; a couple of students that had stronger grasps of the subject material were given harder molecules to build, such as methanol and formaldehyde. Post-tests were then given out and collected. Many of the students expressed to our IQP team that they had fun with the program and looked forward to our next visit.

The second lesson reviewed some of the molecule building material that was covered in the previous session and introduced new material based on the relative electronegativities of atoms. This background information had been covered by Ms. Graves during the week between the two sessions so the students had a good understanding of electronegativity trends across the periodic table. The students had learned that electronegativity is a measure of how strongly an atom attracts electrons. However, the concept of a dipole moment of a molecule based on the atoms within the molecule was new to them and had to be briefly discussed before the pre-test was given out. The students were taught that the more electronegative atoms in a molecule bear a partial negative charge, while the less electronegative ones bear a partial positive charge. This creates negative and positive ends of a molecule, which can be represented by an arrow drawn from the positive end to the negative end. This arrow is called the dipole moment. The students seemed to benefit from the short lecture on dipole moments, however, during the computer session, moving past the "Build Molecule" page was very slow due to the large volume of computers trying to access the WebMO server. Ultimately, only a few students were able to get the dipole moment visualization to work. Because of this problem, the

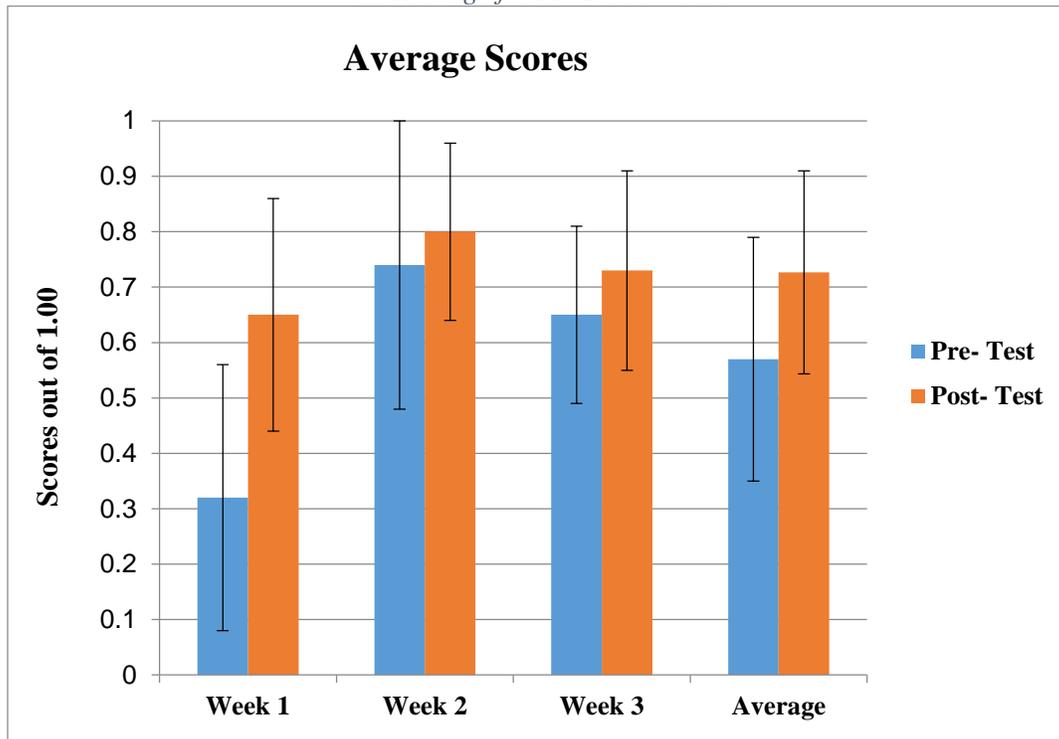
team reviewed the dipole moment concept with the students on the whiteboard before the post-tests were given out.

The third and final lesson turned out to be the most efficient lesson of the three. In this session, the approach was to divide the students into two groups: one that would work solely on drawing molecules with differing geometries and optimizing them in order to visualize each geometry in the 3D workspace, and the other group to work on calculating dipole moments of a series of tetrahedral molecules that differed in the type of substituent only. Additionally, each computer was used by two students. This resulted in four to five computers accessing the calculation WebMO server and ultimately resolved the issue encountered in the previous session where too many people were accessing the server at once. Calculations were performed at an unhindered pace and all dipole moments were calculated within seconds without the server crashing. Additionally, this system forced students to work together in a team and understand why dipole moments were changing due to substituent changes. The students appeared to enjoy the program a great deal more since it was working more smoothly and communicated to the group at the end of this session that they appreciated being able to play around with molecules in 3D and also believed they better understood the molecular geometries and the interaction of electron pairs that influences them due to this capability.

4.4.2.4. Student results and analysis

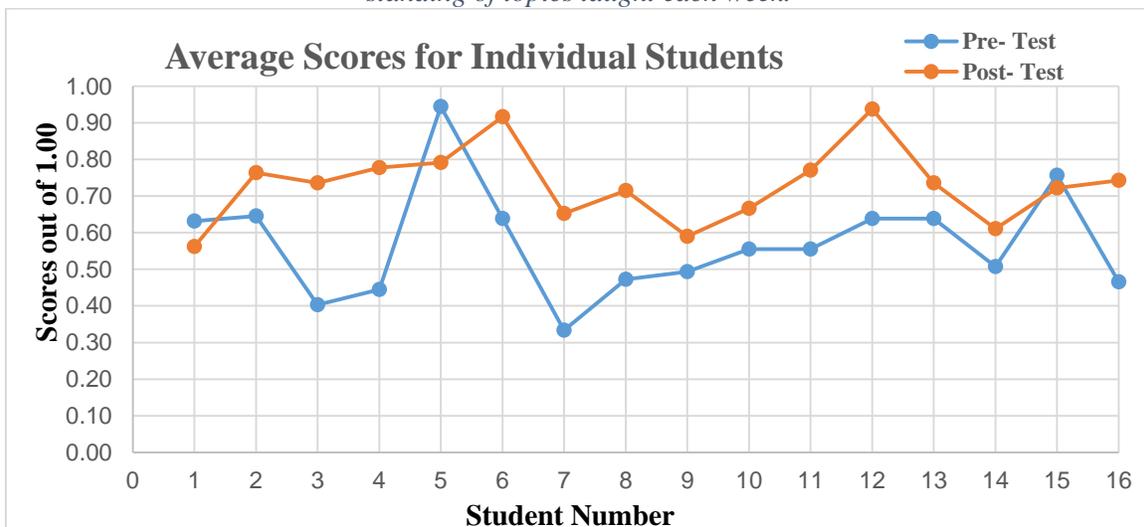
Each week, the students completed a pre-test before working with WebMO and a post-test afterward. These six tests are provided in Appendix J. All the pre- and post-tests were graded and scored on a scale of 1 to 4 points per question. As described in section 3.5, a score of one indicated that the student did not show understanding of the materials the question asked about, and a score of four indicated that the student got the question completely correct. The average pre-test scores each week for the entire class are represented below by the blue bars in Figure 6. The average pre-test score for week 1 was 0.32, for week 2 was 0.74, for week 3 was 0.65, and for the average for all 3 weeks was 0.57. Also, the average post-test score each week for the entire class is shown below as the red bar in Figure 6. The average Post-test for week 1 is 0.65, for week 2 is 0.80, for week 3 is 0.73, and for the average of 3 weeks is 0.73.

Figure 6 - The Average Scores for the Entire Class: First Week, Second Week, Third Week, and the Average for All Three Weeks



The average scores on pre- and post-tests over the course of all three weeks for each individual student are plotted in Figure 6.

Figure 7 - Graph of individual students' average pre- and post-test scores throughout all three weeks. Most showed a trend of improvement, suggesting WebMO did in fact improve their understanding of topics taught each week.



This plot shows that on average, the majority of the students in the class did show an improvement from the pre-tests to the post-tests. This suggests that working with

WebMO and having a visual representation of the concepts being taught each week did help to improve the students' understanding.

Appendix K provides sample pre- and post- tests for a selected student each week. Student #12's pre- and post-tests are shown for Week 1. The topic of the first week was drawing molecules, and this week boasted the biggest improvement between pre- and post- tests. However, this is likely because most students were initially confused by the task and attempted to draw electron orbitals rather than bonds between atoms. This confusion explains why the pre-test scores for Week 1 were so low in comparison with the other two weeks. However, after the WebMO exercises, Student #12 was able correctly indicate single and triple bonds to fill the octets of the atoms in each molecule, answering all of the questions correctly. (Note that the first question on the post-test was not included in calculating the grades. Its complexity was beyond the level taught in the class period.) This trend was true of most students. Following the instruction period, they possessed a better understanding of what the questions were asking and how to answer them.

In Week 2, some students had problems with drawing dipole moments on the pre-test, as demonstrated by Student #3's work presented in Appendix K. The student was confused as to which atoms in a molecule were more or less electronegative, and therefore drew an incorrect dipole moment. However, by the end of the class period, the student was able to correctly identify which regions of a molecule contain partial positive and negative charges, as shown by the post-test. The student's only mistakes in questions 3 & 4 were failure to actually draw the dipole moment. Otherwise, the positive and negative regions were identified correctly.

Week 3 focused on molecular geometry, and Student #9's pre- and post-tests can be found in Appendix K. It is clear that this student, like many others in the class, did not know how to correctly name the geometry of a molecule at the beginning of the class period. However, by the post-test, this student, like many others, had the ability to answer all geometry questions correctly.

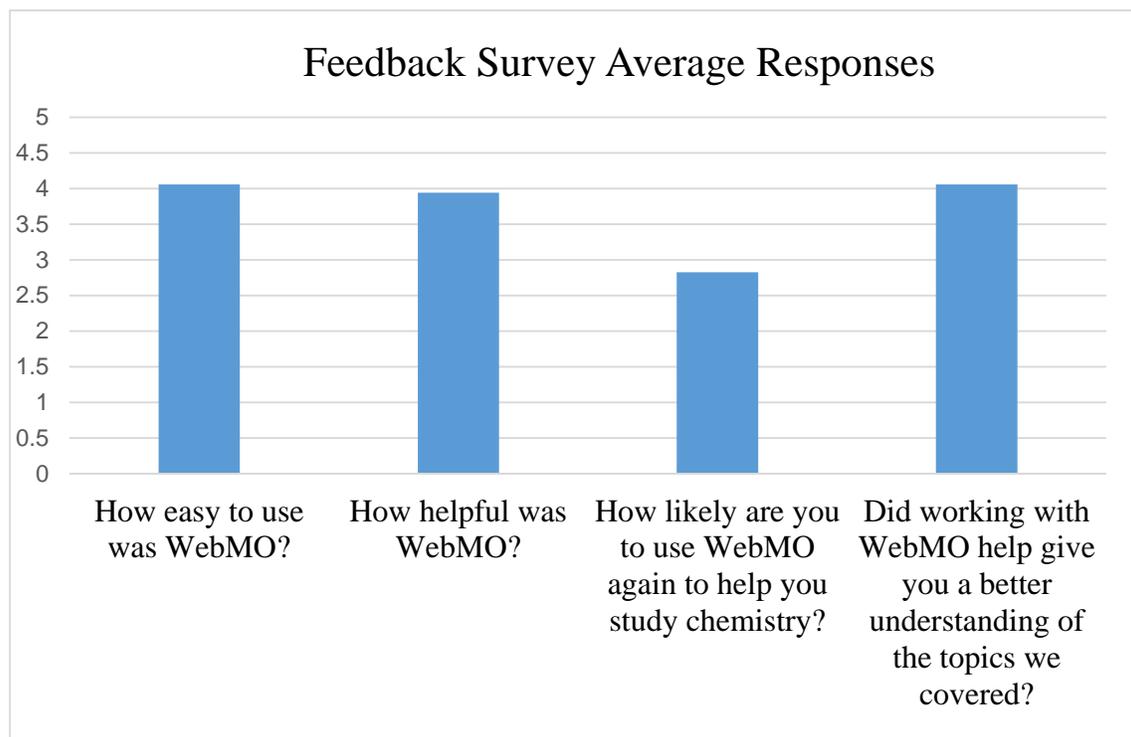
Overall, the average post-test scores for the entire class were higher than the average pre-test scores, indicated that WebMO was indeed an effective tool in helping the students understand the chemistry topics addressed. A more detailed analysis of the test results is given in Appendix P.

4.5.2.5. Student Feedback on WebMO

At the conclusion of our final visit to Millbury High School, we asked the students to fill out a brief feedback survey in order to get quantitative input from them about WebMO and its effectiveness in their class. This form asked a series of four questions based on a Likert-type rating scale, which is a rating scale used in surveys to assign numerical values to the degree to which people agree with or disagree with a statement. These questions asked the students' opinion of how easy to use WebMO was, how helpful WebMO was, how likely they were to use WebMO again to study chemistry, and whether working with WebMO helped them to better understand the topics we covered with them. Students were asked to rate their answers to each question on a scale of 1 to 5, where 1 indicated the program was not at all helpful, easy to use, or likely to be used again, and 5 indicated that the program was extremely helpful, easy to use, or likely to be used again. Based on class average results obtained, students generally felt that WebMO was fairly easy to use and helpful in understanding the topics covered in classes with us, both questions having an average response of approximately 4.05.

Students felt it was generally helpful overall (average score of approximately 3.94), but were on average unlikely to use the program again (average rating of 2.82). These averages are shown in Figure 8.

Figure 8 - Graph of average results obtained from student feedback from Millbury High School. The responses were on a scale of 1 to 5 where 1 corresponded to an answer of not at all or never again, etc., and 5 was a response of very easy to use, help-



A table of all of the individual responses can be found in Appendix P. There are a few possible reasons that may explain these trends. It may have been that the server failures encountered during the second session had discouraged the use of WebMO since calculations were very slow and in many cases the browser itself crashed, preventing visualization of the dipole moment vector. However, the large volume of computers trying to access the guest server at once may have been in conjunction with the age of the computers provided by the school, as these machines were several years old. Another possible explanation is simply the nature of the college prep class. As mentioned before, this class consisted of students that had less motivation to study than others, so while the program may have been useful and easy to use for them, they may not have wanted to go through the trouble of using this tool. Finally, the students were only familiar with the application of WebMO to the small group of topics that were introduced to them during the group's time at the school, so perhaps these students did not understand that the program could be used for a whole range of subjects and were thus not inclined to use the program again.

These ratings indicated that WebMO did in fact seem to meet the main goals of the project in providing a user-friendly tool to help high school students in their under-

standing of chemistry. However, a tool is only useful if students are willing to use it. Perhaps if WebMO was included as part of the coursework they would be open to using the program and taking advantage of the ability to visualize difficult chemistry concepts on the molecular level. But available simply as a tool to help them with homework or studying at home, students did not seem to be eager to use the program independently. One possible way to combat this would be to use a more simplified version of a molecular modeling program to avoid overloading students with all of the calculation options. Another option that may help would be providing students with more background information on each function of the program, so that they could understand how to best utilize the program for their needs. Based on problems seen within our testing at Millbury High School, another contributing factor may be inefficiency of the guest server which made it difficult for all of the students to try to log on and perform calculations at the same time. With solutions to stability problems resolved and more education specifically about WebMO and its capabilities, the students would have a better appreciation of working with the program and would be more likely to work with it independently.

5. Recommendations and conclusions

Here we discuss some of the ways in which, based on the data we have compiled through our initial testing with WPI students, the implementation at Millbury High School, and some of the feedback we have collected from these two student bodies, our molecular modeling-based curriculum can be improved. We also suggest some future work to fix the problems we encountered over the course of the project and how to expand the horizon of our curriculum goals.

5.1. Effectiveness of molecular modeling

While a glaring limiting factor of the implementation of WebMO at the high school was the low number of sessions with the students, some conclusions can be drawn about how effective this program was at helping students learn some of the basic chemistry concepts introduced at the college prep level. However, this proved to be helpful because the team could start the students off with basic topics. Considering that these fundamental concepts provide the groundwork for more advanced topics, it is perhaps better for a student to build knowledge upon a sturdy foundation rather than a shoddy one.

Given that the students the group worked with were only just beginning to grasp concepts such as the number of valence electrons each atom has and thus how many bonds an atom can make, or even simply the concept that more than one bond is possible between two atoms, the ability to build molecules from scratch was an essential lesson. As can be seen from the first week's pre-test in Appendix K, one can observe that before the students were exposed to WebMO building molecules was a matter of drawing rings around an atom and defining the presence of valence electrons. However, once introduced to the program and having had worked through building several sample molecules, the post-test results showed that the students better understood what it meant to build a molecule from a formula. This skill is one of the tenants of the Massachusetts standards described in section 2.4.1., but is more importantly crucial for understanding the vast majority of chemistry concepts, including how molecules react together, how some molecular properties arise, and so forth.

Generally, based on the data presented in Figure 4, it appears that the students improved from each pre-test to post-test on average by 16% and consistently so. What is interesting to note is that the largest improvement between the three sessions is the very first session, in which the average rise in test score was 33%. Additionally, test scores in the second and third session tended to remain high, so this may explain why increases from pre- to post-test in these latter sessions was smaller in magnitude. Considering that the first lesson focused solely on being able to draw molecules from scratch and visualizing them, a conclusion may be drawn that this lesson was most instrumental in helping students see molecules in a three-dimensional fashion, which was one of the major goals of the project. Being able to visualize molecules in this manner may have helped students answer questions in the pre-tests for sessions two and three, which asked questions pertaining to dipole moments and geometry, respectively. Thus, perhaps the most effective aspect of the molecular modeling program was bringing the two dimensional molecules of the white board to the three dimensions of the computer.

These observations beg the question, however, of why not simply use molecule model kits to demonstrate this same feature? The advantage of the computer program is the ability to perform more complex calculations, and to create and adjust the molecules much faster. While the only type of calculation ultimately used was dipole moment, geometric optimizations were also performed in order to correct the input geometry and accurately ascertain geometry type. In further classes with this group or with more advanced groups such as honors or advanced placement, more intricate calculations such as saddle point or vibrational frequencies could be used.

5.2. Future project work

Due to time constraints and other factors out of our control, we were unable to move on to the more advanced topics that we had designed many of our initial exercises for as well as address many of the common misconceptions, described in section 2.4.3., that we had planned to work on. Our research gave a good basis for future work, though, in showing that it is feasible to use WebMO with a classroom, and it is possible to design problems around the software in order to supplement student learning. WebMO was not overly complex for students to use and its visualization capabilities did help to improve student understanding of chemistry topics.

Future project groups can further design WebMO-based lesson plans to address the common chemistry misconceptions mentioned in the Background section of this report. Future groups may also choose to create a WebMO-based curriculum plan to meet other aspects of the Massachusetts Education Standards, such as the production or absorption of energy during reactions, balancing equations, and demonstrating the dynamic nature of molecules. In both of these scenarios, future project groups may benefit if they are able to allocate more of their time to be spent in class working with students. The following section further describes possible avenues for future projects to continue our efforts in bringing computational chemistry to the high school education system.

5.2.1. Program improvement

Considering the positive results obtained from the surveys from both the WPI and Millbury High School student body as well as the general improvement from pre- to post-tests, it appears as though the modeling program curriculum was effective as both an instructional tool and was easy to use as a software package. However, a large problem with the classroom use of the web-based program was that a large number of machines trying to access the web server at once slowed down the calculation process and often resulted in web browser crashes. While this problem was avoided in the third session, a more long-term fix is needed. This would most likely involve a local installation on the school computers, should the teacher wish to incorporate WebMO for extended use throughout their curriculum.

In terms of the larger picture, the high school student survey revealed that the students were not very likely to use WebMO again for their chemistry studies. While this may have been a result of the second session's server access failure, perhaps there ought to be a way for WebMO to appeal more to students of that particular demographic. Although the program was user-friendly, something is lacking that can attract students. These improvements may include faster loading times, fewer intermediate screens in order to perform calculations, and transforming the laundry-list nature of the job list page to something that will allow easier access of job information, such as an option to briefly see job results in the job list window. It would be useful to test WebMO on other chemistry students with different skill and knowledge sets to assess whether they would be willing to further use the program.

5.2.2. Long-term classroom incorporation

Based on the research completed for this project, it appears as though the incorporation of WebMO long-term into high school chemistry classroom use would be both feasible and beneficial to students. Because WebMO has a wide variety of applications from basic molecule building and geometry correction to more complex electron density and vibrational frequency calculations, the program could be useful to both basic chemistry students and advanced placement (AP) or perhaps even early college level students. For example, the vibrational frequencies calculation capability can be used to inform students about the different peaks present in infrared spectroscopy readings and the transition state calculation can be used to graph the energetics of a reaction as it progresses from reactants to products. The program proved useful in the test scores obtained from pre- and post-tests administered to the high school students in that scores were consistently higher on the post-test than on the pre-test taken before having a chance to work with WebMO. Even students' feedback indicated that they felt the program helped them to better understand the concepts presented by the tests, and that the program itself was generally easy and straightforward to use.

5.3. Final Conclusions

At the start of this project, three main project goals were outlined. The first was to achieve a satisfactory understanding of the theory behind computational chemistry programs in order to understand the modeling system to be incorporated into the high school classroom. This goal was successfully met by devoting the first seven-week term to research. The results are presented in the background section of this report as well as results section on software choice. The second goal was to build and develop a simple yet effective teaching module to present chemistry concepts in an educational manner which could help students better understand chemistry concepts. The entirety of the second seven-week term and approximately half of the third seven-week term were devoted to this goal, which was also successfully met. The results of this work are contained in the three-week teaching module which was implemented in the chemistry class at Millbury High School. The final goal established by the group was to measure the extent to which the teaching module was successful and propose improvements that could be made in the future. This goal was addressed during the second half of the third seven-week term, while teaching

the class of 16 juniors at Millbury High School. Throughout the three sessions, data was collected in the form of pre-tests and post-tests. By administering these tests immediately before and after the WebMO instruction, it was clear that any improvement was the direct result of using the software. Recommendations for further improvements are outlined in the following sections.

Minor setbacks that were encountered in this project can easily be minimized or even eliminated when planning for long-term classroom incorporation. This project has shown that for basic molecule building with no calculations, the WebMO sever is a suitable option, allowing students to take full advantage of the 3D workspace without having to worry about any system requirements outside of an internet connection and a browser with fully updated Java capabilities. For smaller classes working with some basic calculations, the guest server can still be used, but is perhaps better used with the class split into groups so as to not overload the server. If the software will be used long-term, a more efficient option would be for the school to request licenses and install WebMO locally on their computers, allowing students to use a school-owned server which would allow less restricted server operations and individual accounts in order to save calculations and be able to find them again later.

Overall, it would appear that the educational value offered by WebMO outweighs the work required of educators or IT staff to be done ahead of time. This valuable tool realistically can and should be incorporated into average high school chemistry classrooms to provide students with the visualization and calculations abilities otherwise unavailable to them.

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Appendices

Appendix A. Massachusetts chemistry educational standards

(Massachusetts Department of Education, 2006)

I. CONTENT STANDARDS

1. Properties of Matter

Central Concept: Physical and chemical properties reflect the nature of the interactions between molecules or atoms, and can be used to classify and describe matter.

- 1.1 Identify and explain physical properties (e.g., density, melting point, boiling point, conductivity, malleability) and chemical properties (e.g., the ability to form new substances). Distinguish between chemical and physical changes.
- 1.2 Explain the difference between pure substances (elements and compounds) and mixtures. Differentiate between heterogeneous and homogeneous mixtures.
- 1.3 Describe the three normal states of matter (solid, liquid, gas) in terms of energy, particle motion, and phase transitions.

2. Atomic Structure and Nuclear Chemistry

Central Concepts: Atomic models are used to explain atoms and help us understand the interaction of elements and compounds observed on a macroscopic scale. Nuclear chemistry deals with radioactivity, nuclear processes, and nuclear properties. Nuclear reactions produce tremendous amounts of energy and lead to the formation of elements.

- 2.1 Recognize discoveries from Dalton (atomic theory), Thomson (the electron), Rutherford (the nucleus), and Bohr (planetary model of atom), and understand how each discovery leads to modern theory.
- 2.2 Describe Rutherford's "gold foil" experiment that led to the discovery of the nuclear atom. Identify the major components (protons, neutrons, and electrons) of the nuclear atom and explain how they interact.
- 2.3 Interpret and apply the laws of conservation of mass, constant composition (definite proportions), and multiple proportions.

- 2.4 Write the electron configurations for the first twenty elements of the periodic table.
- 2.5 Identify the three main types of radioactive decay (alpha, beta, and gamma) and compare their properties (composition, mass, charge, and penetrating power).
- 2.6 Describe the process of radioactive decay by using nuclear equations, and explain the concept of half-life for an isotope (for example, C-14 is a powerful tool in determining the age of objects).
- 2.7 Compare and contrast nuclear fission and nuclear fusion.

3. Periodicity

Central Concepts: Repeating (periodic) patterns of physical and chemical properties occur among elements that define families with similar properties. The periodic table displays the repeating patterns, which are related to the atoms' outermost electrons.

- 3.1 Explain the relationship of an element's position on the periodic table to its atomic number. Identify families (groups) and periods on the periodic table.
- 3.2 Use the periodic table to identify the three classes of elements: metals, non-metals, and metalloids.
- 3.3 Relate the position of an element on the periodic table to its electron configuration and compare its reactivity to the reactivity of other elements in the table.
- 3.4 Identify trends on the periodic table (ionization energy, electronegativity, and relative sizes of atoms and ions).

4. Chemical Bonding

Central Concept: Atoms bond with each other by transferring or sharing valence electrons to form compounds.

- 4.1 Explain how atoms combine to form compounds through both ionic and covalent bonding. Predict chemical formulas based on the number of valence electrons.
- 4.2 Draw Lewis dot structures for simple molecules and ionic compounds.
- 4.3 Use electronegativity to explain the difference between polar and nonpolar covalent bonds.

- 4.4 Use valence-shell electron-pair repulsion theory (VSEPR) to predict the molecular geometry (linear, trigonal planar, and tetrahedral) of simple molecules.
- 4.5 Identify how hydrogen bonding in water affects a variety of physical, chemical, and biological phenomena (e.g., surface tension, capillary action, density, boiling point).
- 4.6 Name and write the chemical formulas for simple ionic and molecular compounds, including those that contain the polyatomic ions: ammonium, carbonate, hydroxide, nitrate, phosphate, and sulfate.

5. Chemical Reactions and Stoichiometry

Central Concepts: In a chemical reaction, one or more reactants are transformed into one or more new products. Chemical equations represent the reaction and must be balanced. The conservation of atoms in a chemical reaction leads to the ability to calculate the amount of products formed and reactants used (stoichiometry).

- 5.1 Balance chemical equations by applying the laws of conservation of mass and constant composition (definite proportions).
- 5.2 Classify chemical reactions as synthesis (combination), decomposition, single displacement (replacement), double displacement, and combustion.
- 5.3 Use the mole concept to determine number of particles and molar mass for elements and compounds.
- 5.4 Determine percent compositions, empirical formulas, and molecular formulas.
- 5.5 Calculate the mass-to-mass stoichiometry for a chemical reaction.
- 5.6 Calculate percent yield in a chemical reaction.

6. States of Matter, Kinetic Molecular Theory, and Thermochemistry

Central Concepts: Gas particles move independently of each other and are far apart. The behavior of gas particles can be modeled by the kinetic molecular theory. In liquids and solids, unlike gases, particles are close to each other. The driving forces of chemical reactions are energy and entropy. The reorganization of atoms in chemical reactions results in the release or absorption of heat energy.

- 6.1 Using the kinetic molecular theory, explain the behavior of gases and the relationship between pressure and volume (Boyle's law), volume and temperature (Charles's law), pressure and temperature (Gay-Lussac's law), and the num-

ber of particles in a gas sample (Avogadro's hypothesis). Use the combined gas law to determine changes in pressure, volume, and temperature.

- 6.2 Perform calculations using the ideal gas law. Understand the molar volume at 273 K and 1 atmosphere (STP).
- 6.3 Using the kinetic molecular theory, describe and contrast the properties of gases, liquids, and solids. Explain, at the molecular level, the behavior of matter as it undergoes phase transitions.
- 6.4 Describe the law of conservation of energy. Explain the difference between an endothermic process and an exothermic process.
- 6.5 Recognize that there is a natural tendency for systems to move in a direction of disorder or randomness (entropy).

7. Solutions, Rates of Reaction, and Equilibrium

Central Concepts: Solids, liquids, and gases dissolve to form solutions. Rates of reaction and chemical equilibrium are dynamic processes that are significant in many systems (e.g., biological, ecological, geological).

- 7.1 Describe the process by which solutes dissolve in solvents.
- 7.2 Calculate concentration in terms of molarity. Use molarity to perform solution dilution and solution stoichiometry.
- 7.3 Identify and explain the factors that affect the rate of dissolving (e.g., temperature, concentration, surface area, pressure, mixing).
- 7.4 Compare and contrast qualitatively the properties of solutions and pure solvents (colligative properties such as boiling point and freezing point).
- 7.5 Identify the factors that affect the rate of a chemical reaction (temperature, mixing, concentration, particle size, surface area, catalyst).
- 7.6 Predict the shift in equilibrium when a system is subjected to a stress (LeChatelier's principle) and identify the factors that can cause a shift in equilibrium (concentration, pressure, volume, temperature).

8. Acids and Bases and Oxidation-Reduction Reactions

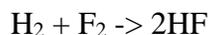
Central Concepts: Acids and bases are important in numerous chemical processes that occur around us, from industrial procedures to biological ones, from the laboratory to the

environment. Oxidation-reduction reactions occur when one substance transfers electrons to another substance, and constitute a major class of chemical reactions.

- 8.1 Define the Arrhenius theory of acids and bases in terms of the presence of hydronium and hydroxide ions in water and the Bronsted-Lowry theory of acids and bases in terms of proton donors and acceptors.
- 8.2 Relate hydrogen ion concentrations to the pH scale and to acidic, basic, and neutral solutions. Compare and contrast the strengths of various common acids and bases (e.g., vinegar, baking soda, soap, citrus juice).
- 8.3 Explain how a buffer works.
- 8.4 Describe oxidation and reduction reactions and give some everyday examples, such as fuel burning and corrosion. Assign oxidation numbers in a reaction.

Appendix B. Questions used in Alpha & Beta Testing

1. The following reaction shows the synthesis of hydrogen fluoride from hydrogen and fluorine gas:



- Predict whether the total energy for the right-hand side of the equation is greater than, less than, or equal to the total energy of the unreacted H_2 and F_2 on the left-hand side of the equation. In other words, will the energy of the system increase, decrease, or stay the same when the forward reaction occurs?
- Run one Molecular Energy calculations for each of the molecules in the above reaction in WebMO using Firefly and the default calculation options. Taking the stoichiometry of the above equation into consideration, compare the total molecular energy of the right side to the right side. The program will calculate the energy of these molecules based on electrostatic, geometrical, and interactional states.
- In terms of the results obtained from this experiment, is the forward or reverse reaction energetically favored? Why?

2.

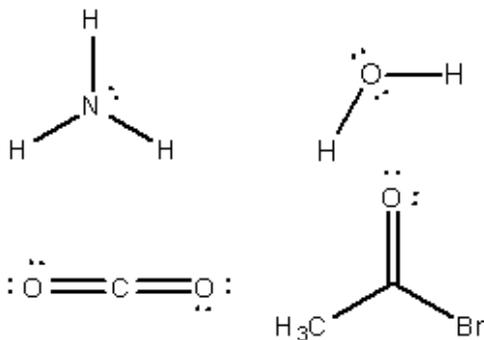
- Balance following chemical reaction:



- Construct only one of each of the reactant molecules in the WebMO workspace. Now construct the products using only the atoms you have just created with the following conditions:
 - Only reactant molecules can be used
 - Atoms cannot be deleted
 - Multiple copies of a reactant molecule are allowed, but keep track of how many you needed
 - Bonds can be broken and made between atoms

3.

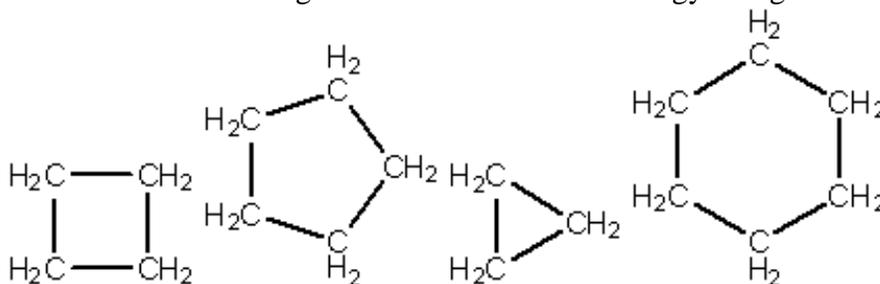
- Predict the dipole moments of the following molecules. Draw an arrow on the



molecule pointing from the most positive area to the most negative area. If the dipole moment points into or out of the page, please state it under the molecule. If no dipole moment exists, also mention that.

- b. Using WebMO, construct each of these structures and optimize the geometry using the Geometry option under the Clean-Up dropdown menu in order to see if you got the molecular structure correct. Then, please run a Molecular Energy job with Firefly in order to determine the right dipole moments for each molecule.

4. Please order the following molecules from lowest energy to highest energy:



- a. Using WebMO, run a Molecular Energy job after having built each of the above molecules in order to calculate the energies. Where do you think this strain energy comes from?
 - b. Explain why each of the molecular energy trends are what they are. What is contributing to the relative energies of the molecules? How does electronegativity of the atoms in parts ii and iii affect these energies?
5.
 - a. Build a dichloromethane molecule and perform a Vibrational Frequency job. Once the job is done, click on one of the clips at the bottom of the window in order to view the atoms in motion. Understand that molecules are not static and that each bond oscillates, much like a spring.
 - b. How do different size atoms affect the vibration of these bonds? Note that different types of bonds oscillate differently. Try to construct a double or triple bond with the same two atoms and see how that affects the frequency and bond length of the vibration.
 - c. What do you think causes this vibration in molecules?

Appendix C. Exercises Used at Millbury High School

Week 1:

Please draw the following molecules in WebMO:

1. H_2O
2. BF_3
3. CO_2

Week 2:

Please draw the following molecules in WebMO, and then run a molecular energy job to calculate the dipole moment:

1. H_2O
2. HF
3. H_2S
4. SCl_2
5. COH_2

Week 3:

Group 1: Please draw the following molecules and determine the geometry:

1. H_2O
2. CO_2
3. BF_3
4. CCl_4

Group 2: Please draw the following molecules and calculate the dipole moment:

1. CCl_4
2. HCCl_3
3. H_2CCl_2
4. H_3CCl

Appendix D. Table of Reviewed Software

Program	Site	Description	Reason for Dismissal
Abalone	http://www.biomolecular-modeling.com/Abalone/	Not really useful. The software focuses on biochemistry.	Biological
ACD/3D Viewer	http://www.acdlabs.com/resources/freeware/chemsketch/	ACD/ChemSketch Freeware is a software that able to offer a 2D and 3D structure for chemical structures. It also able to calculate some molecular properties, like molecular weight and density. To get the free version, you need register online. After download and install the software, there several PDF documents will help to get start. For the 3D viewer, there are 26 pages to read through. For the free version, the dictionary part is not work, so we cannot quick search our chemical structures by name. It may take a long time to draw a very complex structure. We are able to rotate our drawing in 3 Dimensional space, so it will much easier to draw a structure than some 2D drawing software. Also a table of Radicals offers plenty of common chemical groups. However, the 3D views requires you to draw a 3D structure. Thus, the software is useless when you just know the formula of a compound.	too Advanced

<p>ALOGPS 2.1</p>	<p>http://www.vcclab.org/lab/alogps/</p>	<p>ALOGPS 2.1 is an online software that help to predicted the partition coefficient, water solubility and pKa(s) of compounds. The software need to update. It just offer some shorted names for all the data. The links that led to some wiki pages could help us to understand what those data means, but many of those pages are no longer exist, like ALOGP and XLOGP2. Then those abbreviations mean nothing at all. Also even those links are working, it will take a long time and open tons of website to understand all the data. It will be very helpful if the software give some brief definition for those data. The molecule editor is very useful, which will help to determine properties for some unknown molecules.</p>	<p>Program stability problems</p>
<p>Ascalaph Designer</p>	<p>http://www.biomolecular-modeling.com/Ascalaph/Ascalaph_Designer.html</p>	<p>Created by the same company as Abalone, more about some complicated molecular and biochemistry.</p>	<p>Biological</p>
<p>Avogadro</p>	<p>http://avogadro.openmolecules.net/wiki/Main_Page</p>	<p>The data base is very limited, most time we need to draw the structure by ourselves. May useful. Detailed tutorials offered online. http://avogadro.openmolecules.net/wiki/Category:Tutorials</p>	<p>Limited database</p>

Chemitorium	http://sourceforge.net/projects/chemitorium/?source=dlp	A simple 3-D viewer, could not fix incorrect or unstable molecule structures. Complicated to draw a chemical structure. No fundamental groups that can choose, also no data bases to search any specific structure that we want. Just have a fancy wave effect that looks very cool. All in all it is not very useful.	Simple viewer
Cosmos	http://csciwww.etsu.edu/cosmos/	The software is too old, because the newest version is for Windows 95/NT. Everything work very slow. Not useful.	Program problems
Desmond	http://www.deshawresearch.com/resources_desmond.html	Seems to be specifically for biological systems, so probably not useful to us. The program is downloaded and free for “non-commercial use by universities and other not-for-profit research institutions”.	Biological
Fold It	http://fold.it/portal/	This program is a game that has something to do with protein folding...not useful at all for our purposes.	Biological
GoVASP		This program is not free, so probably not an option for us.	Not free
Jmol	http://jmol.sourceforge.net/	Jmol is a purely visualization tool. It allows users to construct molecules in a 3-D space and analyze features of the molecule such as bond length and bond angles, but does not allow calculations to be performed. Therefore, it is not useful for our purposes.	Viewer
MOIL	http://cbsu.tc.cornell.edu/software/moil/moil.html	MOIL is for protein structures, and it appears that you need to know a significant amount about coding to work the software. Probably not a good option.	Biological

MoleCools		Seems to be a molecular visualization tool, not useful for our purposes. Plus, I can't even find it anywhere on internet...	Simple viewer, and difficult to locate online
p4vasp	http://www.vasp.at/ ; http://www.castep.org/	This program seems to be a very specialized version of VASP. A brief look at VASP was promising, and it should be further looked into. Also ran into CASTEP while looking at VASP, which also looks promising.	Specialized
Qmol		Only calculates a molecular weight, given a molecular formula. Also returns percent weight of each element in the molecule. Probably not useful for our needs.	Viewer
RasMol		Much like JMol, this program is a molecular visualization program that can import any file type and allows the user to manipulate the molecule in a 3D workspace as well as set the type of view (ribbon, wire, etc.). The program also allows the user to output the molecule to any file type. Other than these few things, RasMol is not very useful.	Viewer
Raster3D		Purely command-line based and requires some command prompt knowledge. Most likely not useful for our needs.	too Advanced

UCSF Chi- mera		<p>This program has many different functions but is aimed primarily at analyzing proteins. While it cannot calculate MD or MC simulations, the user can import the trajectories from other programs and analyze them. Additionally, it can display various types of surfaces and intramolecular interactions. This program is worth looking into due to its wealth of tools for molecule analysis. As a note, Chimera is enormously more useful if the command line is used, so it may require the student to enter commands based on the manual.</p>	Biological
VegaZZ	http://www.vegazz.net/	<p>Similar to RasMol, VegaZZ does not actually provide a molecule builder, but allows import of molecules from other programs. Operations appear to be complex and require a lot of input about various methods, which seems inappropriate to ask of high school students. Not sure beyond that because I do not have molecule files to upload to test out, but in general the less things that need to be downloaded by our “subjects” (students), the better. VegaZZ also requires a registration, which is free, but is required for each individual student on each individual computer. It also requires e-mail access in order to receive the license file in order to complete installation, which also may be very inconvenient requirements for a student in class.</p>	too Advanced

VMD+NAMD	http://www.ks.uiuc.edu/Research/vmd/	Requires download, registration, and agreement to a license, but all is free. However, VMD is yet another molecular visualization tool, not an actual molecular modeling program. It allows importing molecules (presumably built in other programs) but does not appear to have many options for calculations beyond that point. Both VMD and NAMD (both produced by University of Illinois at Urbana-Champaign) are described on the University of Illinois Theoretical and Computational Biophysics Group site as being for Biomolecular Simulation, which is outside of the realm of usefulness in our project. After several attempts to run NAMD, none have been successful. The file included in the download to help with troubleshooting is clearly written for someone who is far more experienced with computers than myself	Viewer
WebMO	http://www.WebMO.net	Straightforward interface, click to draw, can perform many calculations based on installed calculation package, WPI has a professional version that we can access, also has a free version that can be downloaded and installed locally, and a guest server that can be accessed for basic use without any installation or registration.	Chosen program

Xeo	http://sourceforge.net/projects/xeo/	Requires download, but no registration. Molecules are drawn in 2-D, and the commands/tools are difficult to navigate. Most things that can be manipulated require some other file or require input of x, y, z coordinates. Some of tools and utilities bring up a command prompt-like window, requires learning codes in order to use. Help file accessible in the program is very dense and long, difficult to navigate. Generally complex system, more intended for experts in molecular modeling computer programs.	too Advanced
Zodiac	http://www.zeden.org/index.php?option=com_content&view=article&id=46&Itemid=53	Requires a download but no registration. Can draw molecules in 2-D or build in 3-D, but in my testing the application crashed before I could try anything else. Could be useful for our purpose but need to figure out how to run in a more stable way before we can determine that.	Program problems

Appendix E. Instructions for Installation of WebMO on a computer running Windows 7 OS

- 1) Required programs
 - a) Java
 - i) For compatibility with current and future versions of WebMO, it is recommended that Sun Microsystem's Java Runtime Environment (JRE) version 1.5 or greater is recommended. Download and install the latest version version from www.java.com
 - ii) Note: Although WebMO 8 and earlier is compatible with Microsoft Java, this product has not been maintained since 2003 is not installed with Windows XP SP2 or Vista. Consequently, it is anticipated that WebMO 9 will discontinue support of Microsoft Java in order to take advantage the features associated with Sun Microsystem's Java.
 - b) Perl
 - i) Download and install ActiveState Perl ("ActivePerl") for Windows
 - ii) By default, perl will be installed to C:\Perl
 - iii) Verify installation by opening a command window and typing
 - (1) perl c:\Perl\eg\example.pl
 - iv) which should display
 - v) Hello from ActivePerl!
 - c) Apache
 - i) Download and install Apache for Windows
 - ii) By default, apache will be installed to C:\Program Files\Apache Software Foundation\Apache2.2
 - iii) You may need to unblock network access to this program after installation
 - iv) Verify operation of the webserver by browsing to
- 2) <http://localhost/>
- 3) which should display
- 4) It works!
- 5) Obtain a [WebMO license](#)
- 6) [Download](#) "WebMO for Windows" to your Windows PC

- 7) Extract the WebMO distribution
- 8) Right-click on the downloaded file and select "Extract all..."
- 9) Run the setup script
- 10) Navigate into to the extracted distribution and then into the WebMO.install directory
- 11) Double-click setup.pl
- 12) Follow the directions that are given in the setup script
- 13) Enter WebMO license number when prompted
- 14) Accept the default installation directories. **MAKE SURE THESE ARE THE RIGHT DIRECTORIES!**
- 15) Path to perl: C:/Perl/bin/perl.exe
 - i) HTML directory: C:/Program Files/Apache Software Foundation/Apache2.2/htdocs/WebMO
 - ii) HTML URL: /WebMO/
 - iii) CGI script directory: C:/Program Files/Apache Software Foundation/Apache2.2/cgi-bin/WebMO
 - iv) CGI script URL: /cgi-bin/WebMO
 - v) User files directory: c:/Program Files/WebMO
- 16) After the distribution files are copied, the command line portion of WebMO setup is complete
- 17) Follow the URL given at the end of setup process and continue with the online WebMO configuration. For a standard Windows installation, the login URL should be <http://localhost/cgi-bin/WebMO/login.cgi>
- 18) Login as user 'admin' with an empty password
- 19) Reset the admin password when prompted
- 20) Register your copy of WebMO when prompted
- 21) If the registration process fails (e.g., due to no internet connectivity), login again from the URL at the end of the setup process as user 'admin' with the new password
- 22) Click 'Interface Manager'
 - i) Click the 'Enable interface' icons to enable any computational chemistry packages that you have installed on your system

- ii) Click the 'Edit interface' icon and make any necessary changes in the interface configuration
 - iii) Click 'Submit' to commit the changes
 - iv) Click 'Return' and 'Return to Admin' to return to the WebMO administration page
- 23) Click on the 'User Manager'
- (i) vi. Click the 'New User' button
 - (ii) vii. Specify a Username and Password
 - (iii)viii. Click 'Submit' to create the user
 - (iv)ix. Click 'Return to User Manager' and 'Return to Admin' to return to the WebMO administration page
- 24) t. Setup is complete. Click the 'Logout' button to logout of the WebMO administration page
- 25) Login as the WebMO user that you created. In the job manager, click 'Create New' to run a test job

Appendix F. Instructions for Installing WebMO on a computer running Mac OS X

- i. Obtain a WebMO license at www.WebMO.net
- ii. Download "WebMO for Linux/Mac"(The WebMO.*.tar.gz distribution will automatically be expanded into a WebMO.*.tar file.)
- iii. Turn on the Apache web server

(For OS X 10.7 and below)

Under Apple: System Preferences, open the 'Sharing' control panel. Click the 'Start' button under the Web Sharing section (10.4) or check the Web Sharing item (10.5)

(For OS X 10.8+)

Start a terminal session (Applications/Utilities), and type:

```
$ sudo apachectl start
```

- iv. Configure Apache with Terminal
 - a) Start a Terminal program, which is located in the Applications/Utilities folder
 - b) Determine your home directory

```
$ echo $HOME
```

(/Users/USERNAME will show out)

- c) Create CGI directory

```
$ mkdir /Users/USERNAME/Sites/cgi-bin
```

- d) Move into apache configuration directory

```
$ cd /etc/httpd/users (OS X 10.4 and below)
```

```
or $ cd /etc/apache2/users (OS X 10.5+)
```

- e) Define CGI directory

```
nano /etc/apache2/users/USERNAME.conf
```

(enter administrative password)

- f) If the following lines do not already exist, add them:

```
<Directory "/Users/smit h/Sites/">
```

```
Options Indexes MultiViews
```

```
AllowOverride None
```

```
Order allow,deny
```

```
Allow from all
```

</Directory>

Then, add the following line to the end of the file

```
ScriptAlias /~smith/cgi-bin/ /Users/smith/Sites/cgi-bin/
```

g) After type in everything correctly

"Y" to save modified buffer (Which is this file).

"Control + X" exit the file

(During the process, if anything was typed wrong, please redo the whole process.

Also, if anything is not really work, just restart your computer, and then try again)

v. Run the setup script

a) Start a newTerminal program, which is located in the Applications/Utilities folder

b) Start the installtion

```
$ cd WebMO.install
```

```
$ perl setup.pl
```

(If WebMO. install is not found, try to find the folder of WebMO.install and use

```
$ cd /{the pathway to the place for WebMO.install} )
```

c) Follow the directions that are given in the setup script

- "Enter" to continue, then type in "y" and "Enter" again
- Enter WebMO license number when prompted
- Path to Perl binary: 1 (/usr/bin/perl)
- Webserver's name: localhost (or output of 'hostname' in Terminal)
 - (Do not use the example which the computer give you , like
 - USERNAME-macbook-pro.local, this will be too long. "localhost" works well.)
- HTML Directory: /Users/USERNAME/Sites/WebMO
 - (If that dictionary does not exist, then type in "y", this also apply for CGI Directory and User Directory after)
- HTML URL: /~ USERNAME /WebMO
- CGI Directory: /Users/ USERNAME /Sites/cgi-bin/WebMO
- User Directory: /Users/ USERNAME /WebMO
- Continue with installation to type in "y"

- (After the distribution files are copied, the command line portion of WebMO setup is complete)
- vi. Follow the URL given at the end of setup process (<http://localhost/~smith/cgi-bin/WebMO/login.cgi>) and continue with the on-line WebMO configuration
- a) Login as user 'admin' with an empty password
 - b) Reset the admin password when prompted
 - c) Register your copy of WebMO when prompted
 - d) If the registration process fails (e.g., due to no internet connectivity), login again from the URL at the end of the setup process as user 'admin' with the new password
 - e) Click 'Interface Manager'
 - Click the 'Enable interface' icons to enable any computational chemistry packages that you have installed on your system
 - Click the 'Edit interface' icon and make any necessary changes in the interface configuration
 - Click 'Submit' to commit the changes
 - Click 'Return' and 'Return to Admin' to return to the WebMO administration page
 - f) Click on the 'User Manager'
 - Click the 'New User' button
 - Specify a Username and Password
 - Click 'Submit' to create the user
 - Click 'Return to User Manager' and 'Return to Admin' to return to the WebMO administration page
 - g) Setup is complete. Click the 'Logout' button to logout of the WebMO administration page
- vii. Login as the WebMO user that you created. In the job manager, click 'Create New' to run a test job.

Appendix G. Installing calculation packages

Appendix G.1. Installing Firefly

- a. [Download](#) the PC-Gamess binary executable appropriate for your hardware
- b. Double-click firefly?.zip
- c. Read and follow the instructions in readme.txt to register and obtain a license key / decryption password.
- d. After receiving the password, double-click the ff?.rar file and use the password to extract all the files into c:\gamess

Appendix G.2. Installing MOPAC

- a. Request password (free for academic use) from MOPAC 2007 website
<http://www.openmopac.net/download-c.html>
- b. A password of the form 12345678a12345678 will be sent to you in an email message
- c. Download the "MOPAC2009 for DOS under any Windows" version ([Mopac2009 for all WINDOWS.zip](#)) from
- d. [http://www.openmopac.net/Download MOPAC Executable Step2.html](http://www.openmopac.net/Download_MOPAC_Executable_Step2.html)
- e. If using Vista (or Windows 7?), open Control Panel: User Accounts, and turn User Account Control off
- f. Create the mopac directory, which must be C:\Program Files\MOPAC
- g. Copy all the files ("Example data set.mop", "Installation instructions.txt", and "MOPAC2009.exe") from the downloaded distribution into this directory
- h. Install the password file
- i. Make a copy of "Example data set.mop" and rename it "12345678a12345678.mop" where 12345678a12345678 is your password.
- j. Open a Command Prompt window
> cd "C:\Programs Files\MOPAC"
> MOPAC2009.exe 12345678a12345678.mop
which will create the file "password for MOPAC2009"
- k. If using Vista (or Windows 7?), open Control Panel: User Accounts, and restore User Account Control to previous setting

Appendix H. Feedback Form from Alpha and Beta Testing

Computational Chemistry IQP Feedback Form

Thank you for participating in our computational chemistry testing! We would greatly appreciate any feedback you can provide regarding the exercise you just completed, the instructions provided, and your overall experience here today. Thanks again!

* Required

*Which is the highest level of chemistry you have taken? **

- CH 1010
- CH 1020
- CH 1030
- CH 1040
- CH 2000 level
- CH 3000 level
- CH 4000 level
- Other:

* Required

Computational Chemistry IQP Feedback Form

*What comments can you provide about the instructional video provided? **

Was the video easy to understand and easy to follow? Did the video cover everything you needed to know to complete your problem? Was everything in the video explained thoroughly enough? Was the video excessively informative? Etc.



* Required

Computational Chemistry IQP Feedback Form

*Which question did you work on? **

*Was the question asking about material you have learned previously? **

- Yes, I already had a good understanding of this topic
- No, I have never learned this material
- I was somewhat familiar with the material covered
- Other:

*Do you feel that you have a better understanding of this topic after completing this exercise? **

*What feedback can you provide about the question itself? **

Was the wording clear and concise? Did you know exactly what the question was asking you to do? Was the question easy to understand? Did you feel you had sufficient time to complete the entire exercise? Etc.

Computational Chemistry IQP Feedback Form

*How effective do you think the modeling program was in completing the task? **

Was the program easy to navigate? Did the program provide all of the capabilities you needed to solve your program? Was the question easier thanks to the program? Etc.

Would you use WebMO yourself to study chemistry concepts?

- Yes I would use this myself to study chemistry
- No, I would never willingly touch this program again
- This program could be useful if I was forced to use it again
- Other:

Raffle Entry!!!

Don't forget to provide your information so we can enter you in the raffle for the GRAND PRIZE!!!!

What is your full name (first and last)?

What is your WPI (@wpi.edu) email address?

Please only use your WPI e-mail address

Which is the highest level of chemistry you have taken?	What comments can you provide about the instructional video provided?	Which question did you work on?	Was the question asking about material you have learned previously?	What feedback can you provide about the question itself?	How effective do you think the modeling program was in completing the task?	Would you use WebMO yourself to study chemistry concepts?
CH 4000 level	It was very thorough	Question 4	Yes, I already had a good understanding of this topic	The question was well worded and straight forward. I knew exactly what was being asked.	The modeling software worked smoothly and queuing up results made comparison easy. Overall it worked perfectly	Yes I would use this myself to study chemistry
CH 1010	Great	Question 2	Yes, I already had a good understanding of this topic	It was easy to understand and do.	A hotkey for adjust would have made things much easier and faster. Other than that hotkey, the program worked well. It was easy to place molecules and create bonds.	This program could be useful if I was forced to use it again
CH 3000 level	OK	Question 5	Yes, I already had a good understanding of this topic	OK	OK	This program could be useful if I was forced to use it again
CH 2000 level	None, easy to understand	Question 2	Yes, I already had a good understanding of this topic	I have no idea how or where to submit the question or if not that get the	Could not run it on my ipad	I am not taking any more of these classes so it would not be useful for me

				answer to understand if it right or wrong. I am also working on an iPad so that may be why		
CH 4000 level	Provided a good general overview of material	Question 3	Yes, I already had a good understanding of this topic	Understood well, clear	Intuitive design	Yes I would use this myself to study chemistry
CH 3000 level	Very instructional and straight forward. I believe it was easier to use than Hyperchem and other similar programs. The convenience of a web based molecular modeling program is fantastic. Very well done.	Question 5	Yes, I already had a good understanding of this topic	The question was about vibration frequency and how it is effect by different bonds and molecule sizes. The question was worded well and clearly outlined what one needed to do.	Again, it was more efficient and easier to navigate than Hyperchem, which is what I have been using most often. Question 5 was much easier to do in a modeling program than trying to calculate the vibration frequency by hand in dichloromethane.	Yes I would use this myself to study chemistry
CH 1040	I couldn't find the video..?	Question 5	I was somewhat familiar with the material covered	The question was worded well and straight forward. I had no trouble understanding it.	The program made the question easier to complete. Once I figured out how to use the program I could solve the problem quickly.	This program could be useful if I was forced to use it again

CH 4000 level	To be completely honest, I didn't have the patience to actually watch the whole video. I just skipped forward to what I needed to know (namely, how to proceed to the job) and that's it.	Question 4	Yes, I already had a good understanding of this topic	Yes, I thought the wording was clear. My problem was more of figuring out how to do what was necessary in the software.	I think more guidance would be helpful, as many college students (like me) will not have the patience to watch the video. It'd be best if buttons that created a new job and proceeded to the job from the molecule builder were more obvious, and if the program itself made it clear how you could analyze multiple molecules. After that though, the program threw a pop-up that ended up freezing Chrome (something I haven't had happen before), so I couldn't go any farther with the exercise.	This program could be useful if I was forced to use it again
CH 1020		Question 4	I was somewhat familiar with the material covered			This program could be useful if I was forced to use it again
CH 2000 level	The video was easy to follow up until the molecule was ready to be published. I could not find the firefly option, however other options were available, so I used another option instead. The video was fairly informative however and it made it	Question 1	Yes, I already had a good understanding of this topic	The wording was fine, I had no trouble understanding the material and what it was asking, I had enough time to complete the problem.	The program was extremely easy to navigate after the tutorial video. Before the video it was more difficult to navigate, but not impossible. The program makes it easy to understand the properties and geometry of the molecules in question, which in respect made it easier to do the problem.	This program could be useful if I was forced to use it again

	really easy to learn how to use the software.					
CH 4000 level	<p>Ya'll did a really nice job developing this and I really hope it ends up being implemented. I had some problems as well. My computer could not display the molecule in the energy modeling stage when I went to calculate the total molecular energy as directed in the prompt. I went to the "View Job 145773: HF, Molecular Energy - Gaussian" to do this and got all of the tool bars loaded but nothing in the working space. Also from an observers stand point; these high schoolers are probably not up to WPI chemistry standards so terms like "stoichiometry", while</p>	Question 1	Yes, I already had a good understanding of this topic	<p>It's a good question about the spontaneity of a given reaction given the total molecular energy. However the question may be advanced relative to your target audience. I found one typo, "compare the total molecular energy of the right side to the right side". Overall the question really is good, I just wonder how equipped students are to handle it.</p>	<p>Not at all effective. I could not get it to function. I am also running ancient software (>6 years old) so probably an issue on my side. The idea is very cool though and would probably be engaging to the audience you are looking at.</p>	<p>I was not able to evaluate fully</p>

	<p>accurate and precise, are probably beyond their grasp. Even energy is often left to the middle-end of year in some curriculums.</p> <p>Love the idea though and keep up the hard work!</p>					
CH 3000 level	<p>The video was not easy to follow, nor did it cover everything I needed to know. I could not access firefly nor could I figure out how to draw arrows on the molecule. The video was very monotone and the speaker was awful. It would have been helpful to show the buttons you needed to press, like circle them or something.</p> <p>Also an outline of what the video was going to go through at the beginning would have been helpful.</p>	Question 3	<p>Yes, I already had a good understanding of this topic</p>	<p>The question confused me because I was not sure what I needed to submit for it. Should I have submitted each molecule individually or put them all on the same drawing? There was also no way for me to draw arrows on the program so I was not sure if I was supposed to do that or if that question</p>	<p>I don't think the program was very effective. It is more convenient than a physical model but the program has some issues that need to be worked on.</p>	<p>This program could be useful if I was forced to use it again</p>

				<p>was more of a guess and then check your answer type thing. It also wasn't clear how to draw the molecules. I drew the molecules according to the video, which said to use the Clean-up drop down menu. The second part of the problem then said, check your answer using the clean-up drop down menu. The instructions were very unclear.</p>		
CH 1020	<p>Everything explained covered my problem quite well! Not sure if a beginner would be able to follow the explanations, though.</p>	Question 4	<p>Yes, I already had a good understanding of this topic</p>	<p>The wording was a bit confusing. Could have been more concise and lose the "tech terms". Those</p>	<p>It completed the task reasonably well. The program saved some calculations, or critical thinking, but no knowledge was necessarily acquired through use of the program.</p>	<p>This program could be useful if I was forced to use it again</p>

				are the most difficult. They are distracting. " now you simply run this pro- gram"....		
--	--	--	--	---	--	--

Appendix I. Javascript Code to Randomize Questions in Beta Testing

```

<!DOCTYPE html PUBLIC "-//W3C//DTD HTML 4.01 Transitional//EN">
<html>
<head>
<meta name="generator" content="HTML Tidy for Linux (vers 6 November 2007), see
www.w3.org">
<title>Dan's Website</title>
<link type="text/css" rel="stylesheet" href="new%201.css">
<style type="text/css">
body {
background-color: #FFFFFF;
}
span.c5 {font-family: Baskerville; font-size: 80% }
h2.c4 {font-family: Baskerville; font-size: 80% }
div.c3 {color:#FFFFFF}
img.c2 {position:absolute; TOP:300px; LEFT:260px; WIDTH:608.4px;
HEIGHT:434.2px}
div.c1 {text-align: center}
</style>
</head>
<body>
<script type="text/javascript">
function random_5(){
var myrandom=Math.round(Math.random()*4)
var link1="Problem_1.html"
var link2="Problem_2.html"
var link3="Problem_3.html"
var link4="Problem_4.html"
var link5="Problem_5.html"
if (myrandom==0)
window.location=link1
else if (myrandom==1)
window.location=link2
else if (myrandom==2)
window.location=link3
else if (myrandom==3)
window.location=link4

```

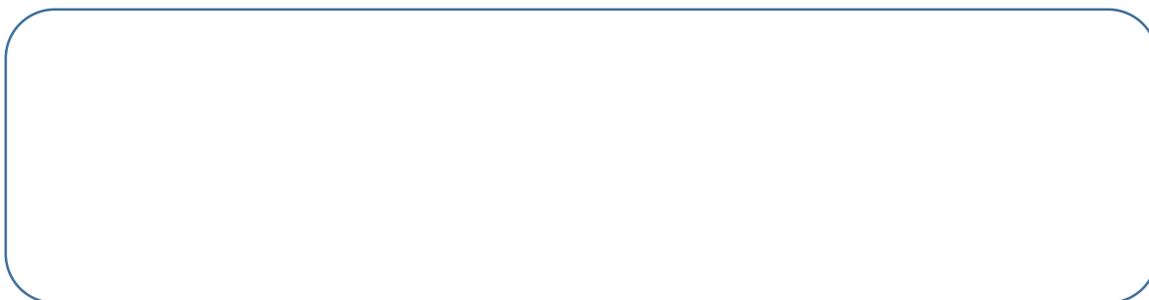
```
else if (myrandom==4)
window.location=link5
}
</script>
<form>
<input type="button" value="Random Problem!" onClick="random_5()">
</form>
</body>
</html>
```

Appendix J. Pre- and Post-tests Used at Millbury High School

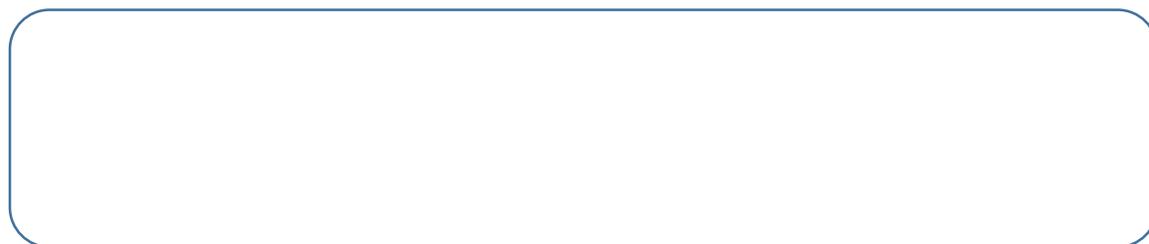
Pre-test Week 1:

Using your knowledge of valence electrons and bonds, draw the molecules for each of the formulas below.

1. O₂



2. C₂H₆

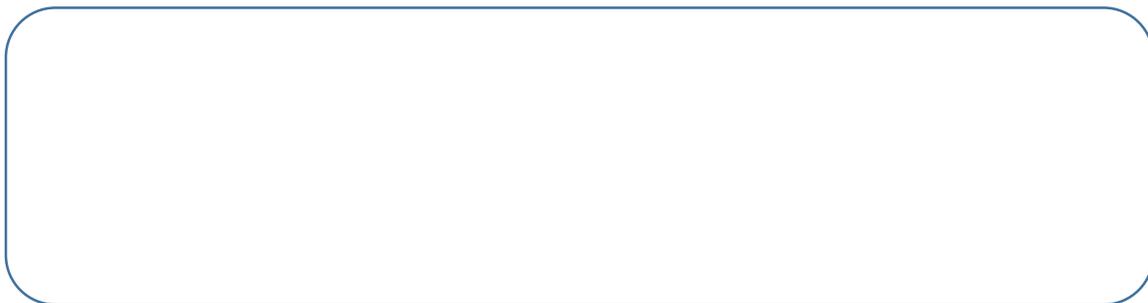
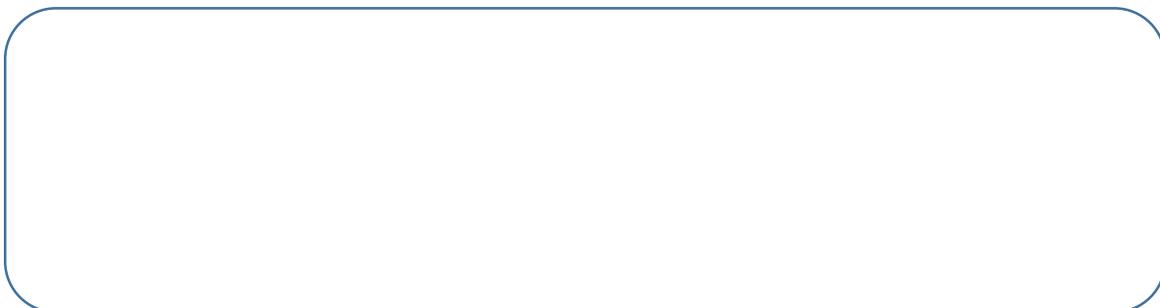


3. CO₂



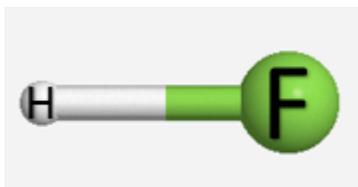
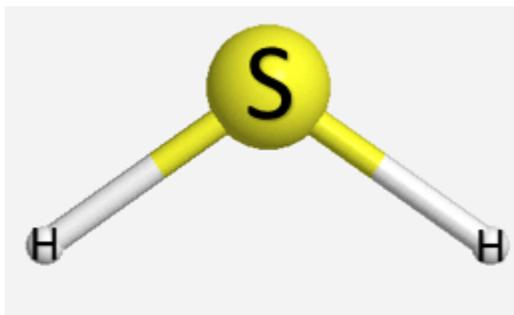
Post-test Week 1:

Using your knowledge of valence electrons and bonds in addition to what you've learned after working with WebMO, draw the molecules for each of the formulas below.

1. CO**2. N₂****3. C₃H₈**

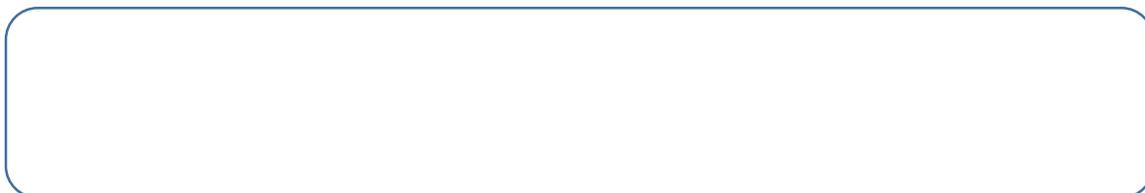
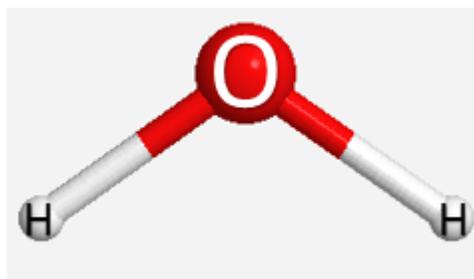
Pre-test Week 2:

Using your knowledge of valence electrons and bonds, draw the molecules for each of the formulas in problems 1 and 2. Based on periodic trends, draw an arrow pointing toward the most electronegative atom in problems 3 and 4.

1. H₂O**2. O₂****3. HF****4. H₂S**

Post-test Week 2:

Using your knowledge of valence electrons and bonds in addition to what you've learned after working with WebMO, draw the molecules for each of the formulas in problems 1 and 2. Based on periodic trends, draw an arrow on problems 3 and 4 pointing toward the most electronegative atom.

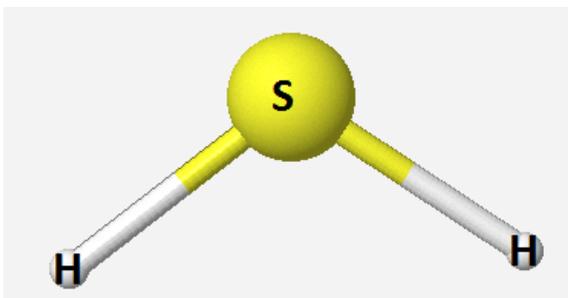
1. BF₃**2. SO₂****3. HBr****4. H₂O**

Pre-test Week 3:

Using your knowledge of valence electrons and bonds, please draw the molecule for the molecular formula below. Once you have a structure, please draw an arrow pointing from the most negative area to the most positive area, based on the relative electronegativities. Don't forget that molecules can have double bonds!

1. CH₂O

Given the 3D structure of this molecule, name the shape.

**2. H₂S**

Given the molecular formula below, draw the molecule and then name the shape.

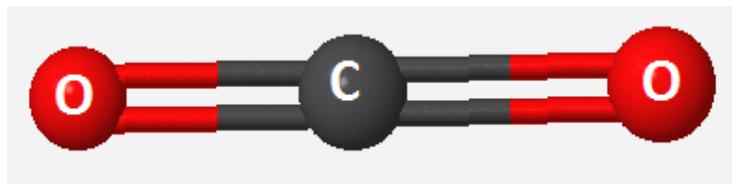
3. HF

Post-test Week 3:

Using your knowledge of valence electrons and bonds, please draw the molecule for the molecular formula below. Once you have a structure, please draw an arrow pointing from the most negative area to the most positive area, based on the relative electronegativities. Don't forget that molecules can have double or even triple bonds!

1. HCN

Given the 3D structure of this molecule, name the shape.

2. CO₂

Given the molecular formula below, draw the molecule and then name the shape.

3. BF₃

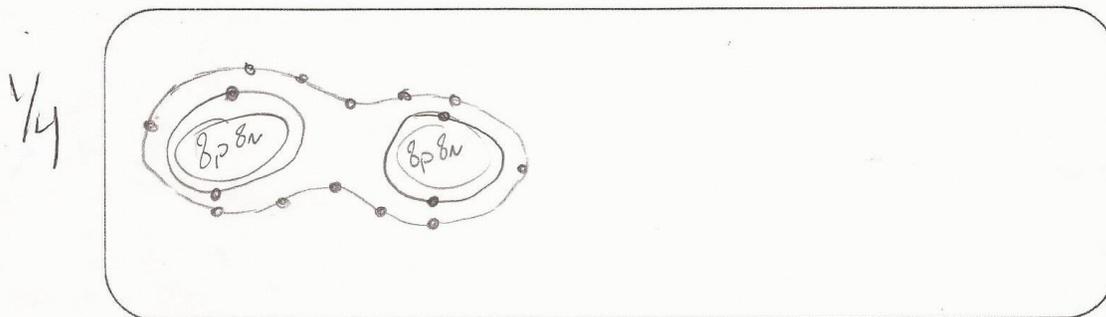
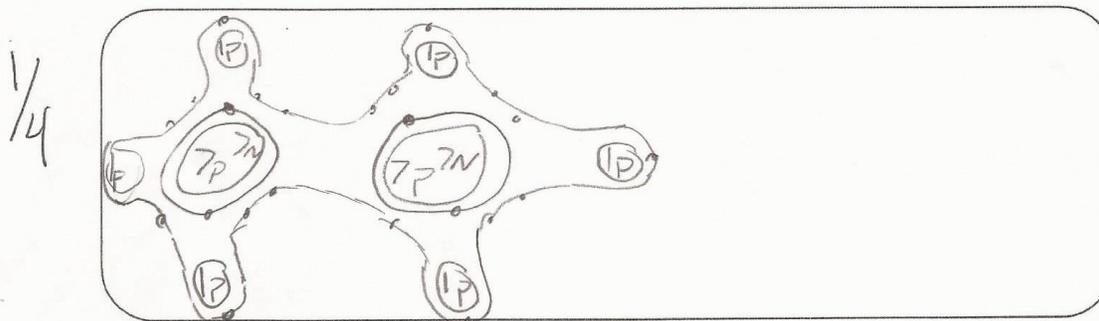
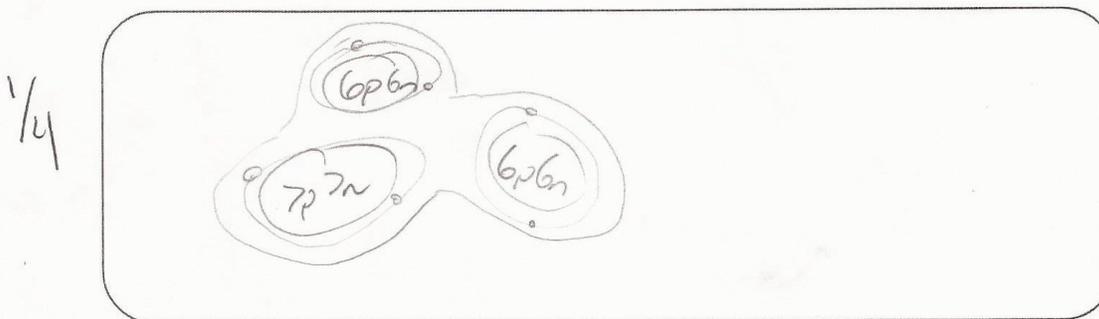
Appendix K. Examples of Student Performance on Pre- and Post-tests

Week 1 Pre-Test - Student #12

12%

WebMO Week 1

Using your knowledge of valence electrons and bonds, draw the molecules for each of the formulas below.

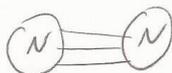
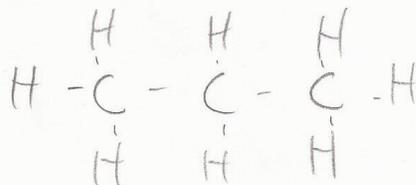
1. O_2 2. C_2H_6 3. CO_2 

Week 1 Post-Test - Student #12

100%

WebMO Week 1

Using your knowledge of valence electrons and bonds in addition to what you've learned after working with WebMO, draw the molecules for each of the formulas below.

~~1.~~ CO2. N₂3. C₃H₈

Week 2 Pre-Test - Student #3

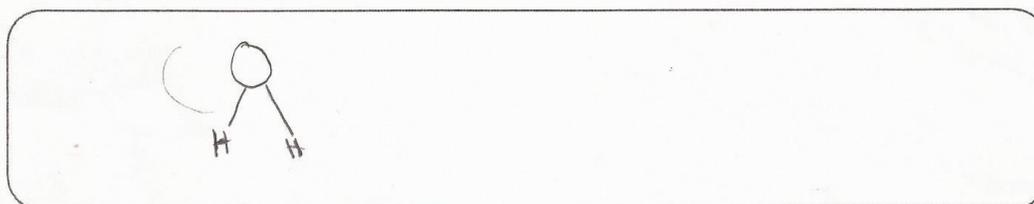
38%

WebMO Week 2

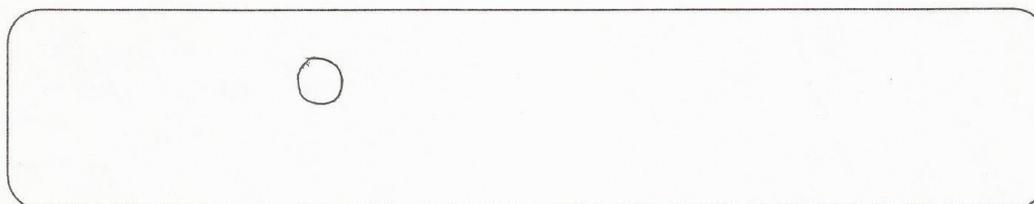
Using your knowledge of valence electrons and bonds, draw the molecules for each of the formulas in problems 1 and 2. Based on periodic trends, draw an arrow pointing toward the most electronegative atom in problems 3 and 4.

1. H₂O

4

2. O₂

1

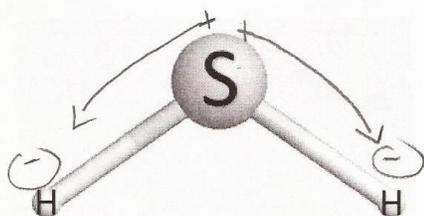


3. HF

0

4. H₂S

1

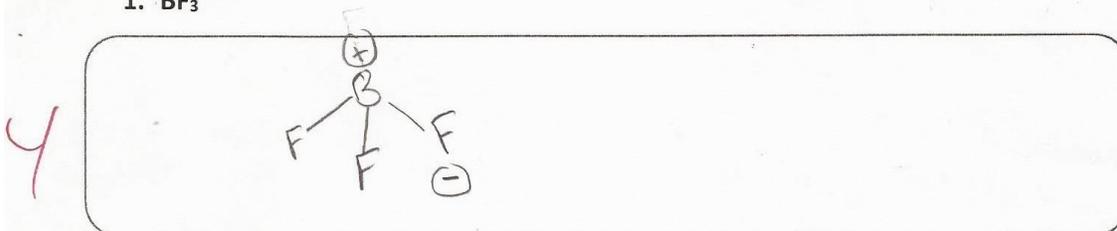
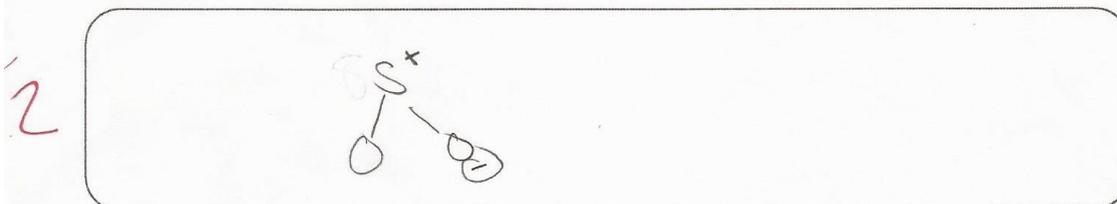
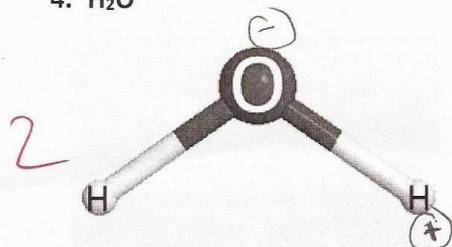


Week 2 Post-Test - Student #3

63%

WebMO Week 2

Using your knowledge of valence electrons and bonds in addition to what you've learned after working with WebMO, draw the molecules for each of the formulas in problems 1 and 2. Based on periodic trends, draw an arrow on problems 3 and 4 pointing toward the most electronegative atom.

1. BF_3 2. SO_2 3. HBr 4. H_2O 

Week 3 Pre-Test - Student #9

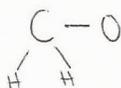
42%

WebMO Week 3 (Pre)

Using your knowledge of valence electrons and bonds, please draw the molecule for the molecular formula below. Once you have a structure, please draw an arrow pointing from the most negative area to the most positive area, based on the relative electronegativities. Don't forget that molecules can have double bonds!

1. CH₂O

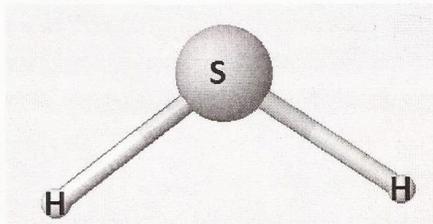
2/4



Given the 3D structure of this molecule, name the shape.

2. H₂S

1/4



Linear X

Given the molecular formula below, draw the molecule and then name the shape.

3. HF

2/4



shape: bent

Week 3 Post-Test - Student #9

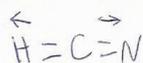
83%

WebMO Week 3 (Post)

Using your knowledge of valence electrons and bonds, please draw the molecule for the molecular formula below. Once you have a structure, please draw an arrow pointing from the most negative area to the most positive area, based on the relative electronegativities. Don't forget that molecules can have double or even triple bonds!

1. HCN

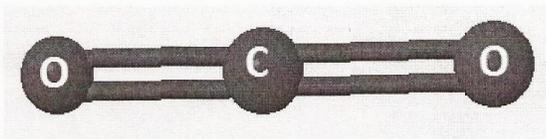
2



Given the 3D structure of this molecule, name the shape.

2. CO₂

4



Linear

Given the molecular formula below, draw the molecule and then name the shape.

3. BF₃

4



Trigonal planar

Appendix L. Feedback Form Used at Millbury High School

WebMO Feedback Form

1. How easy to use was WebMO?

Very difficult to use

Somewhat easy to use

Very easy and straightforward to use

2. How helpful was WebMO?

Not at all helpful

Somewhat helpful

Extremely helpful

3. How likely are you to use WebMO again to help you study chemistry?

I will NEVER use WebMO again

I might use WebMO again to study

I will DEFINITELY use WebMO again to study

4. Did working with WebMO help give you a better understanding of the topics we covered?

WebMO did not help me at all in understanding the topics covered

WebMO was somewhat helpful in learning these topics

WebMO was very helpful in understanding these topics

Appendix N. WebMO Cheat Sheet

File | **Edit** | **Tools**

File: New, Open..., Save As..., Save Image..., Print..., Preferences...
Edit: Undo, Redo, Cut, Copy, Paste, Find
Tools: View, Build, Adjust, PBC..., Edit Cartesian..., Edit ZMatrix...

Change Different Modes

Build: C, H, O, N, Other..., Fragment...

Clean-Up: Generate bonds, Add hydrogens, Hybridization, Geometry, Mechanics, Comprehensive - Idealized, Comprehensive - Mechanics (Selection Only)

Fix the structure of the molecule

Periodic Table

Adjust the molecule

Rotate (drag = XY; alt-drag = Z)

Translate (drag = XY)

Zoom (drag up = bigger; drag down = smaller)

Built (click = add atom; drag = add bond)

Adjust the molecule

Comprehensive clean-up - Geometry

Comprehensive clean-up - Mechanics

Back to Job Manager

Undo

Redo

Left click

Right click

Continue to Select Calculations

Lookup Molecule | **Import Molecule** | **Export Molecule**

---Select Database--- | **Open...**

File | **Edit** | **Tools** | **View** | **Build** | **Adjust** | **Clean-Up** | **Symmetry** | **Huckel** | **Help**

1. = select

2. Shift + = multiple select

3. on one Atom

4. on a Bond

sp
 sp2
 sp3
 dsp3
 d2sp3

Charge...
 Delete

Single
 Double
 Triple
 Delete

Refresh Running Jobs to see if they are complete

Create New Job

Refresh | **Download** | **Move To** | **Delete** | **Utilities** | **Logout**

New Job | **Refresh** | **Download** | **Move To** | **Delete** | **Utilities** | **Logout**

Appendix O. WebMO Video Tutorial

A video tutorial on using WebMO (titled “Webmo_Tutorial”) developed for and submitted with this project can be found at the WPI project site:

<http://www.wpi.edu/academics/library/find/iqp-mqp.html>

Appendix P. The Results for the High School Students' Tests

Table P 1 - Pre- and Post-Test score results.

Student Number	Week 1 - Scores		Week 2 - Scores		Week 3 - Scores		Average - Scores	
	Pre- Test	Post- Test	Pre- Test	Post- Test	Pre- Test	Post- Test	Pre- Test	Post- Test
1	0.75	0.83	0.56	0.44	0.58	0.42	0.63	0.56
2	0.25	0.63	0.94	1.00	0.75	0.67	0.65	0.76
3	0.25	0.75	0.38	0.63	0.58	0.83	0.40	0.74
4	0.25	0.63	0.50	0.88	0.58	0.83	0.44	0.78
5	0.92	0.63	1.00	1.00	0.92	0.75	0.94	0.79
6	0.25	0.88	1.00	0.88	0.67	1.00	0.64	0.92
7	0.25	0.25	0.25	0.88	0.50	0.83	0.33	0.65
8	0.25	0.88	0.50	0.69	0.67	0.58	0.47	0.72
9	0.25	0.25	0.81	0.69	0.42	0.83	0.49	0.59
10	0.33	0.63	0.50	0.63	0.83	0.75	0.56	0.67
11	0.00	0.63	1.00	0.94	0.67	0.75	0.56	0.77
12	0.25	1.00	0.75	0.81	0.92	1.00	0.64	0.94
13	0.33	0.50	1.00	0.88	0.58	0.83	0.64	0.74
14	0.25	0.50	0.94	1.00	0.33	0.33	0.51	0.61
15	0.58	0.75	0.94	0.75	0.75	0.67	0.76	0.72
16	0.00	0.75	0.81	0.81	0.58	0.67	0.47	0.74
Average	0.32	0.65	0.74	0.80	0.65	0.73	0.57	0.73
Standard Deviation	0.24	0.21	0.26	0.16	0.16	0.18	0.22	0.18

Table P 2 - Test score statistics.

		Average	Standard Deviation
Week 1	Pre- Test	0.32	0.24
	Post- Test	0.65	0.21
Week 2	Pre- Test	0.74	0.26
	Post- Test	0.8	0.16
Week 3	Pre- Test	0.65	0.16
	Post- Test	0.73	0.18
Average	Pre- Test	0.57	0.22
	Post- Test	0.73	0.18

Table P 3 - Plots of test score vs. student number, depicting individual test scores for pre-test and post-test for each week.

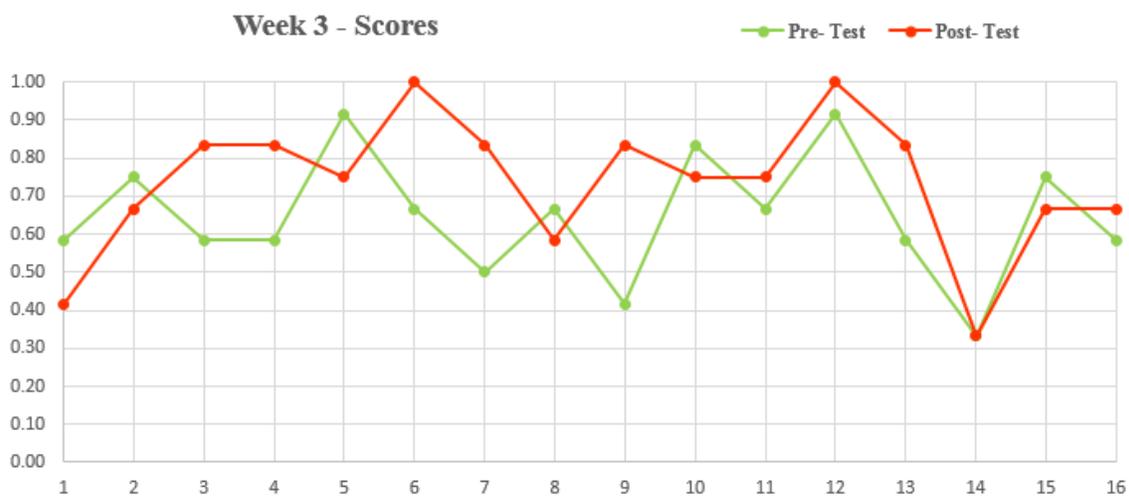
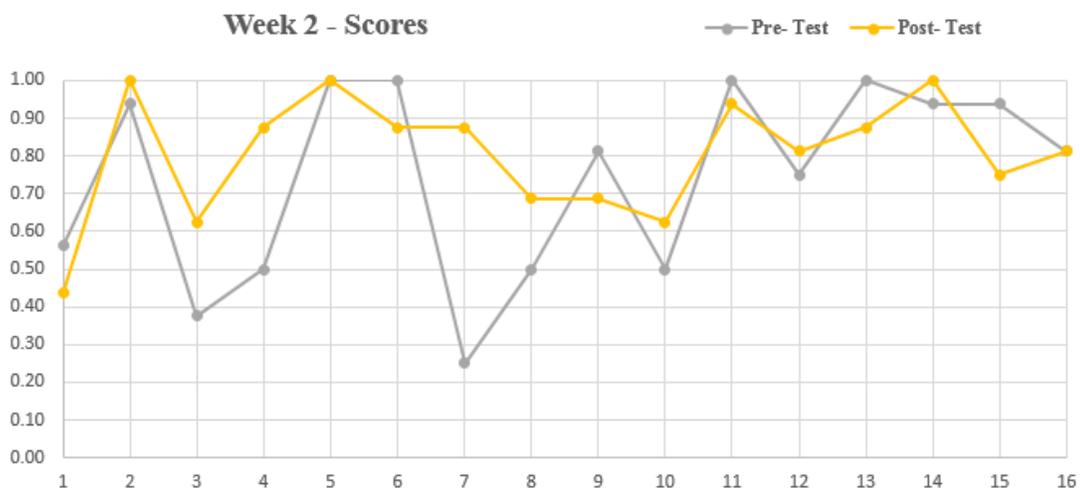
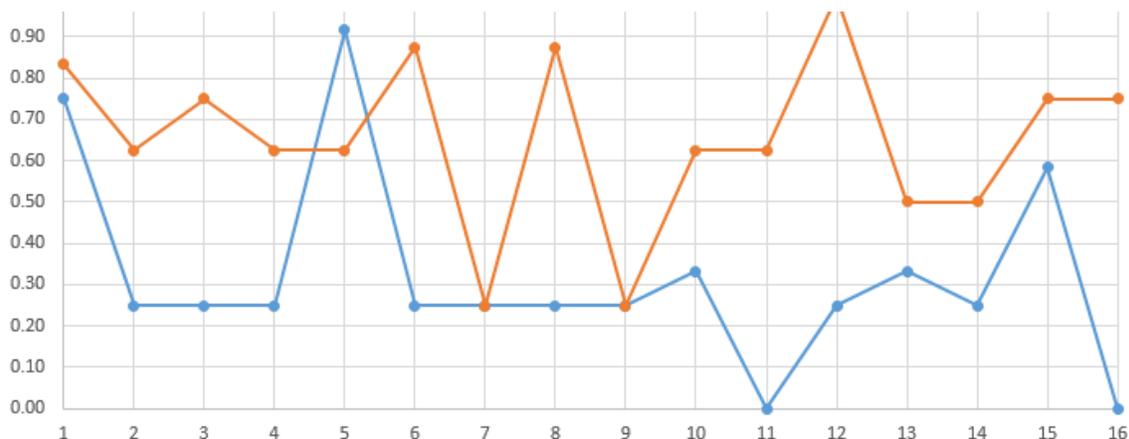


Table P 4 - Plot of pre- and post-test score vs. student number, depicting individual test scores averaged over the three weeks.

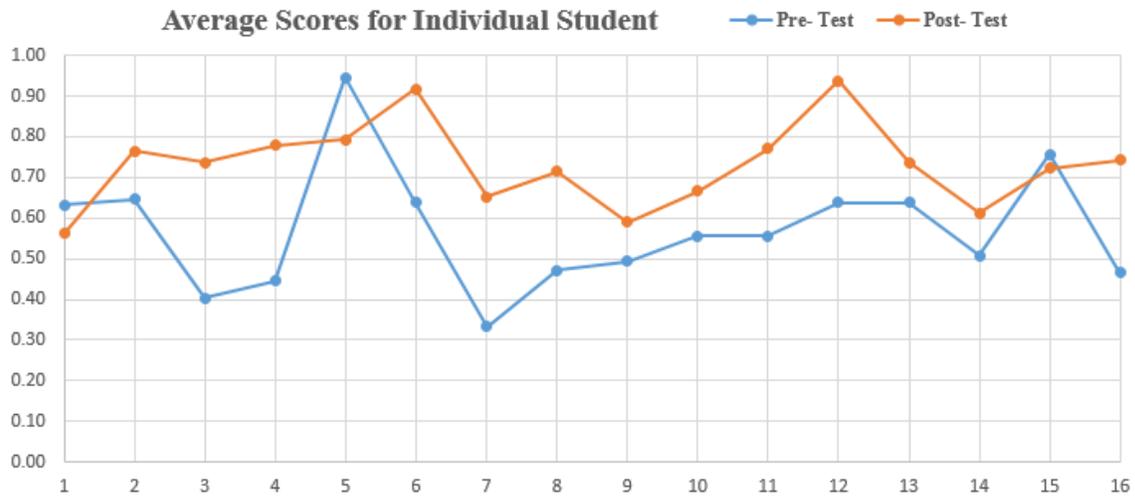


Table P 5 - Graph of weekly average test scores and overall teaching module average.

