Computational Chemistry as a Teaching Aid

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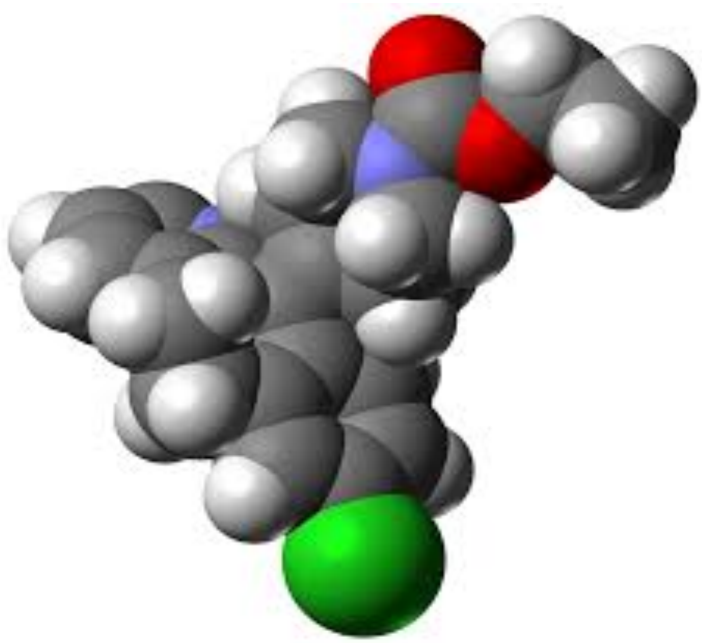

Approved by:

Professor N. Aaron Deskins

Abstract

Molecular modeling software has transformed the capabilities of researchers. Molecular modeling software has the potential to be a helpful teaching tool, though as of yet its efficacy as a teaching technique has yet to be proven. This project focused on determining the effectiveness of a particular molecular modeling software in high school classrooms. Our team researched what topics students struggled with, surveyed current high school chemistry teachers, chose a modeling software, and then developed a lesson plan around these topics. Lastly, we implemented the lesson in two separate high school classrooms. We concluded that these programs show promise for the future, but with the current limitations of high school technology, these tools may not be as impactful.

Acknowledgements

This project would not have been possible without the help of many great educators. Our advisor Professor N. Aaron Deskins provided driving force to ensure the research ran smoothly and efficiently. Mrs. Laurie Hanlan and Professor Drew Brodeur provided insight and guidance early in the development of our topic. Mr. Mark Taylor set-up our WebMO server and all our other technology needs. Lastly, Mrs. Pamela Graves and Mr. Eric Van Inwegen were instrumental by allowing us time in their classrooms to implement our lesson plans. Without the support of this diverse group of people this project would never have been possible.

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1. Introduction

Computational chemistry is a new technology that is critical in understanding the properties of molecules using computer simulations. Chemists quickly took advantage of computers, using them to solve problems since the 1950s. Early calculations were used to estimate the properties of single atoms and research eventually expanded to include more complex molecules. Today computational chemistry is used in a variety of ways. Chemists can use this technology to explore synthesis pathways, perform energy calculation on molecules, and to understand reaction mechanisms more clearly. This technology has helped innovate many fields in ways that would be impossible without it. Computational chemistry has been featured in many Nobel Prizes and has helped advance research on HIV such as Baker, Cooper, DiMaio, Gilski, Jaskolski, Kazmierczyk, and Zabranska (2011) found[1].

Chemical modeling is not just for chemists, however. Advanced chemical modeling software has been adapted to the skills of ordinary people. With the complex calculations hidden and the graphical interface simplified, anyone can take part in this new technology. Foldit[2] is an online puzzle game where people manipulate the structure of three dimensional proteins to find the lowest energy structures in an easy way. The best structures are analyzed by real biochemists and help innovate the biochemistry field.

Reaction mechanisms are often very difficult to determine. In the lab, tests such as temperature dependence and pressure dependence can be run. These and other experiments can give researchers clues as to how a reaction might proceed. Even with data from many lab tests it can be difficult or impossible to determine rate constants. Computational chemistry techniques, however, can give us the answers. Based off of lab data and a proposed mechanism, computational chemistry experiments can be used to confirm a proposed reaction pathway.

Chemical modeling software programs can also be used for education. Most professionals using computation chemistry software programs will perform massive, time consuming

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[1] Baker, D., Cooper, S., DiMaio, F., Gilski, M., Jaskolski, M., Kazmierczyk, M., ...Zabranska, H. (2011). Crystal structure of a monomeric retroviral protease solved by protein folding game players. *Nature Structural and Molecular Biology*, 18(10), 1175+. Retrieved from http://go.galegroup.com.ezproxy.wpi.edu/ps/i.do?id=GALE%7CA270363211&v=2.1&u=mlin_c_worpoly&it=r&p=HRCA&sw=w&asid=5db8be601ee5c2ab1cc0c38ca3a513a5

[2] What is protein folding? (n.d.). Retrieved January 27, 2015, from https://fold.it/portal/info/about

calculations to help answer questions. A chemistry student, however, can use the same principles the program uses to learn more about basic molecules. For example a biochemist might need a computation chemistry software program that can optimize the geometry of a protein containing many amino acids, but the student who wants to know what methane looks like in 3D space can use the same feature.

Our team hopes to take chemical modeling technology into high school classrooms to improve student's learning with these programs. Chemical modeling software programs were reviewed to find the program that would best fit the needs and skills of high school students. Aspects of the programs we considered included: installation, usability, and applicability to high school topics. Two software programs remained as finalists. Further research highlighted the areas of chemistry that high school students struggle with the most. Online sources were examined and many local teachers were surveyed to help determine the best topic to teach with a molecular modeling software. A lesson plan was developed around molecular geometry and then brought into the classroom. Students used computational chemistry software to visualize the complex geometry of molecules that they would otherwise only see on paper. By comparing the results from students using the software and those having an ordinary lesson, the effectiveness of molecular modeling software programs as a teaching tool could be evaluated. This report covers the fine points of software review, less plan creation, and implementation in the classroom.

2. Background

The following goals were decided upon at the commencement of this project in order to guide the project as it progressed:

- Evaluate existing free computational chemistry software
- Develop appropriate virtual chemistry experiments
- Implement the work in a local high school
- Ascertain effectiveness of computational chemistry software as a teaching aid

2.1 Computational Chemistry

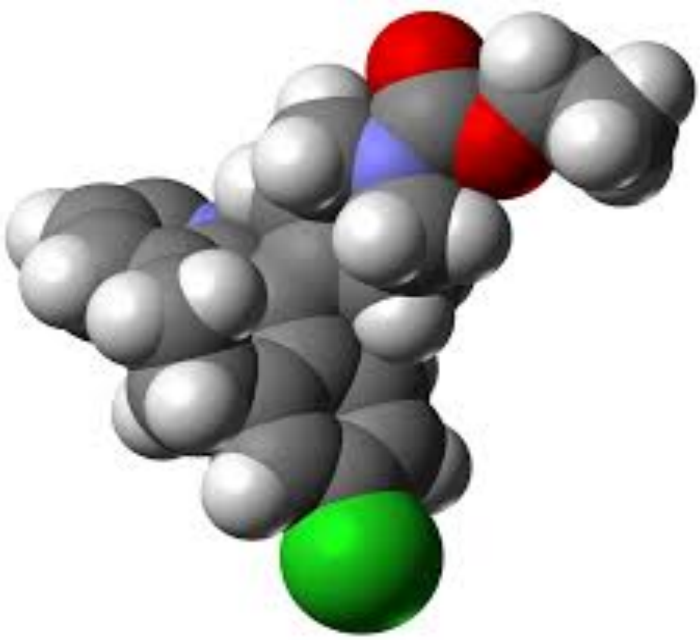

Figure 1: Computational chemistry in action

Figure 1 is a space filling model of the molecule Claritin, an allergy drug. The molecular formula for Claritin is $C_{22}H_{23}ClN_2O_2$. The model can be used to predict reaction pathways as well as functionality, in this case as an anti-histamine allergy drug. Computational Chemistry programs are mainly based off of the Schrodinger equation. The Schrodinger equation, also known as the Schrodinger Wave equation, is a partial differential equation that describes the change in the wave function of a physical system over time[3]. A wave function describes the quantum state of an isolated system, the wave function describes the entire system rather than there being individual wave functions for each particle within the system. The basic form of the Schrödinger equation is:

$$H\Psi = E\Psi \tag{1}$$

where H is the operator that describes the physics of the system, E is the energy of the system, and Ψ is the wave function that describes the location and velocity of the particle. Using this equation, the following properties can be calculated for modeled molecules:

- Electronic structure, which is the description of the location of an atom's electrons using orbitals.
- Geometry optimizations, which are the optimal geometric orientation of the atoms of a molecule.
- Frequency calculations, which are calculations that obtain the frequency with which the atoms of a molecule vibrate.
- Transition structures, which are the structures that exist at the highest energy on a one dimensional reaction coordinate graph.
- Protein calculations (such as docking), which are calculations that predict the folding of proteins, and how ligands will attach or "dock" onto the protein.
- Electron and charge distributions, are calculations that describe the way that positive and negative charges are distributed within a molecule.
- Potential energy surfaces (PES), which are a description of a molecules energy as a function of its geometry.
- Rate constants for chemical reactions (kinetics), which are a description of the rate and direction that a chemical reaction will take place.
- Thermodynamic calculations (heat of reactions, energy of activation), which describe the heat and energy that is either absorbed or released during a chemical reaction.

These properties can then be analyzed by chemists to better understand molecules, or to predict how certain chemical reactions may proceed. The three most common ways for

[3] Weisstein, E. W. (n.d.). Schrödinger Equation -- from Eric Weisstein's World of Physics [Text]. Retrieved April 25, 2015, from http://scienceworld.wolfram.com/physics/SchroedingerEquation.html

computational chemistry programs to run calculations are *ab initio,* semi-empirical numerical techniques, and molecular mechanics. *Ab initio* means "from scratch" in Latin and is a method of calculation that uses the Schrödinger equation, the atomic numbers of the atoms present, and fundamental constants. This method yields results that are very close to experimental results, but requires a good deal of time and processing power. Semi-empirical numerical techniques input experimentally obtained data into mathematical models. This method yields results that are slightly less accurate than those found using the *ab initio* method, but the calculations take less time and processing power to complete. Molecular mechanics utilizes "classical physics to explain and interpret the behavior of atoms and molecules". This method does not require much processing power and can be used for large molecules, but it does require experimental results to be inputted.[4]

Computational chemistry is a way to obtain chemical information when it is impractical to physically/experimentally obtain the data due to financial, safety, or time constraints. Computational chemistry programs can generate models of molecules to study quickly and efficiently. Some organic compounds would take weeks to synthesis in a lab setting where a scientist could "create" the same molecule in less than an hour using a computer. Computer models could give information that may assist in spotting potential issues in a proposed synthesis or reaction or other research areas. Researchers use computational chemistry to either to assist in understanding experimental data, or to predict the possibility of theorized molecules and reactions.

In an educational setting computational chemistry can be used to help students understand what molecules actually look like in three-dimensional space, as well as allowing them to better understand intermolecular forces and bonding. Computational chemistry also allows students to check the results of hand done calculations against calculations done by the software; this allows students to double check their work. In the scope of this project computational chemistry helped students learn molecular geometry by allowing them to build and visualize molecular structures.

2.2 ASSISTments

[4] Overview of Computational Chemistry. (n.d.). In *ChemViz Curriculum Support Resources*. Retrieved from http://www.shodor.org/chemviz/overview/ccbasics.html

In order to be able to better make practice problems, tests, and analyze test results this project utilized the ASSISTments program. ASSISTments is an online learning software developed at Worcester Polytechnic Institute in conjunction with Carnegie Mellon University. The software allows teachers to build online learning modules using text, images, videos, and media from other websites.

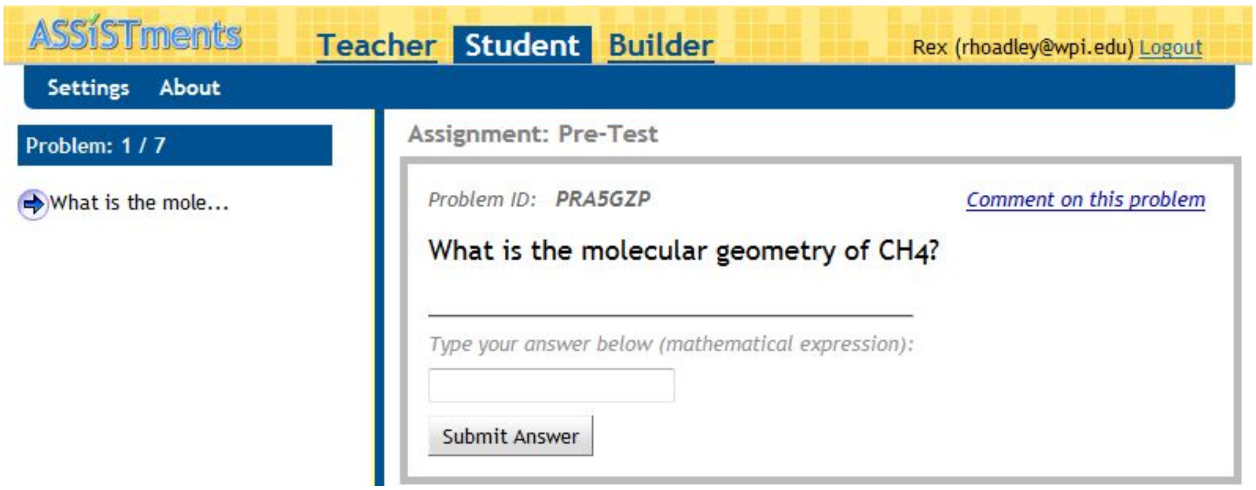

Figure 2 – A typical ASSISTments testing screen.

ASSISTments also includes many prebuilt problems sets for various topics including sciences, mathematics, and languages. ASSISTments problems could be: fill in the blank, check all that apply, multiple choice, open response, algebra, or externally processed questions. Fill in the blank problems require the student to type out the exact answer in an answer box. Check all that apply problems give students a list of answers that could be wrong or right with. The amount of choices is decided by the instructor and the students check the answers they think are right. Multiple choice problems, like check all that apply problems, give students a list of choice answer choices determined by the instructor. The students then choose the one answer they believe is correct. Open response allows students to type out their response to be graded later. These problems allow students to give a long answer but cannot provide immediate feedback. Similar to fill in the blank algebra questions have students type out their short answer in an answer box. These questions however can detect if there are missing variables in algebra expression and can provide feedback for that. Externally processed questions are for questions that involve outside web applications such as java and flash. The answers are built into these modules and graded outside of ASSISTments.

One of the most useful features of ASSISTments is the ability to include optional immediate feedback in problems. A custom feedback response could be set for different kinds of answers. Hints vary from simple suggestions to a detailed walkthrough. Different feedback could be set for different predicted wrong answers. This allows hints to guide students through the steps of solving a particular question, teaching the mechanism of solving rather than just providing the answer. Additionally, assignments can be given in a test mode that does not provide any feedback while students are taking the test. Students receive their score at the end of the test for all non-open response questions. Open response questions must be reviewed by a teacher and the grade entered manually.

Once a problem is built it is put into a problem set that teachers can then assign to their students. ASSISTments problems can be used in class to supplement a lesson, given as homework, or used to test students. When students log into the ASSISTments website they find their lesson with no additional software installed locally. After the results are in, the teacher can view the results and generate a report. Reports can be generated for an individual student, or the entire class.

The major advantage of ASSISTments was that it was already widely used in middle and high schools across Massachusetts. Because students have already used this software there is no learning curve. Additionally, because of the instant reports that can be generated, it is much easier to analyze students test results than with paper tests.

Furthermore, because ASSISTments was completely online, once an assignment had been made it can be given to any class that has access to the Internet. This allows for teachers to collaborate and to share assignments among their classes, no matter their location in the country. In cases like this project, teachers could give the assignments and tests to their own classes, no matter their location, and then report their data by simply sending the automatically generated report in ASSISTments. Without the limitation of needing to travel to each classroom, there is an opportunity for a much larger sample size in the future.

2.3 Challenging Topics in Chemistry

While every student faces different challenges in learning chemistry, there are some topics that many people struggle with. These hardest to learn topics are what were focused on for this project. To ascertain exactly what these topics were, AP test results as well as Massachusetts Education Standards were examined.

The AP, advanced placement, chemistry test is administered by The CollegeBoard, a not-for-profit organization which also administers the SAT. In addition to standardized testing, The CollegeBoard also provides resources for students to learn more about colleges and financial aid. The AP chemistry test is part of The CollegeBoard's Advanced Placement Program. This program allows students to take college-level classes while still in high school, and gives students the opportunity to obtain college-credit or other advanced placement. The AP Chemistry test has two sections, the first consists of sixty multiple-choice questions, and the second consists of seven free-response questions. Each section of the test accounts for fifty percent of the exam score. Looking at past year's AP Chemistry test results, it is clear that there are some areas in which the majority of students struggle. Some common mistakes on the AP test were not understanding acid/base chemistry, equilibrium constants, and knowing what reasonable values are.[5]

States set their own educational standards that they require all schools within the state to adhere to. For the Massachusetts Education Standards, there are certain learning standards that must be met for each topic. These learning standards are detailed in curriculum frameworks, the chemistry standards are detailed in the Massachusetts Science and Technology/Engineering Curriculum Framework[6]. The chemistry learning standards are arranged by grade, and for lower grades potential activities that complement each subtopic are given. However, as the grade level increases, the amount of activities provided decreases, and by the high school level no set activities are listed for any chemistry subtopic. For some subtopics an activity may be taught through a corresponding lab procedure, however for other subtopics there is no lab possible.

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[5] Student Performance Q&A: 2009 AP® Chemistry Free-Response Questions. (n.d.). The College Board. Retrieved from http://apcentral.collegeboard.com/apc/public/repository/ap09_chemistry_qa.pdf

[6] Massachusetts Science and Technology/Engineering Curriculum Framework. (n.d.). Massachusetts Department of Elementary & Secondary Education. Retrieved from http://www.doe.mass.edu/frameworks/scitech/1006.pdfhttp://doi.org/10.1119/1.1707018

According to the Massachusetts Education Standards, High School students are taught the following eight subtopics in chemistry: "*Properties of Matter; Atomic Structure and Nuclear Chemistry; Periodicity; Chemical Bonding; Chemical Reactions and Stoichiometry; States of Matter, Kinetic Molecular Theory, and Thermochemistry; Solutions, Rates of Reaction, and Equilibrium;* and *Acids and Bases and Oxidation-Reduction Reactions.*"[7] It is seen that Atomic Structure and Nuclear Chemistry, Periodicity, and Chemical Bonding do not have a possible lab component, this leaves a gap between these topics and the others that have a hands on component.

By looking at AP test results it was seen what subtopics students struggle with the most, and by looking at Massachusetts Education Standards it was seen what subtopics are lacking a corresponding activity. By combining the two the potential topics to be covered in this project were able to be narrowed down. A survey was sent to chemistry teachers to further narrow down this list of topics.

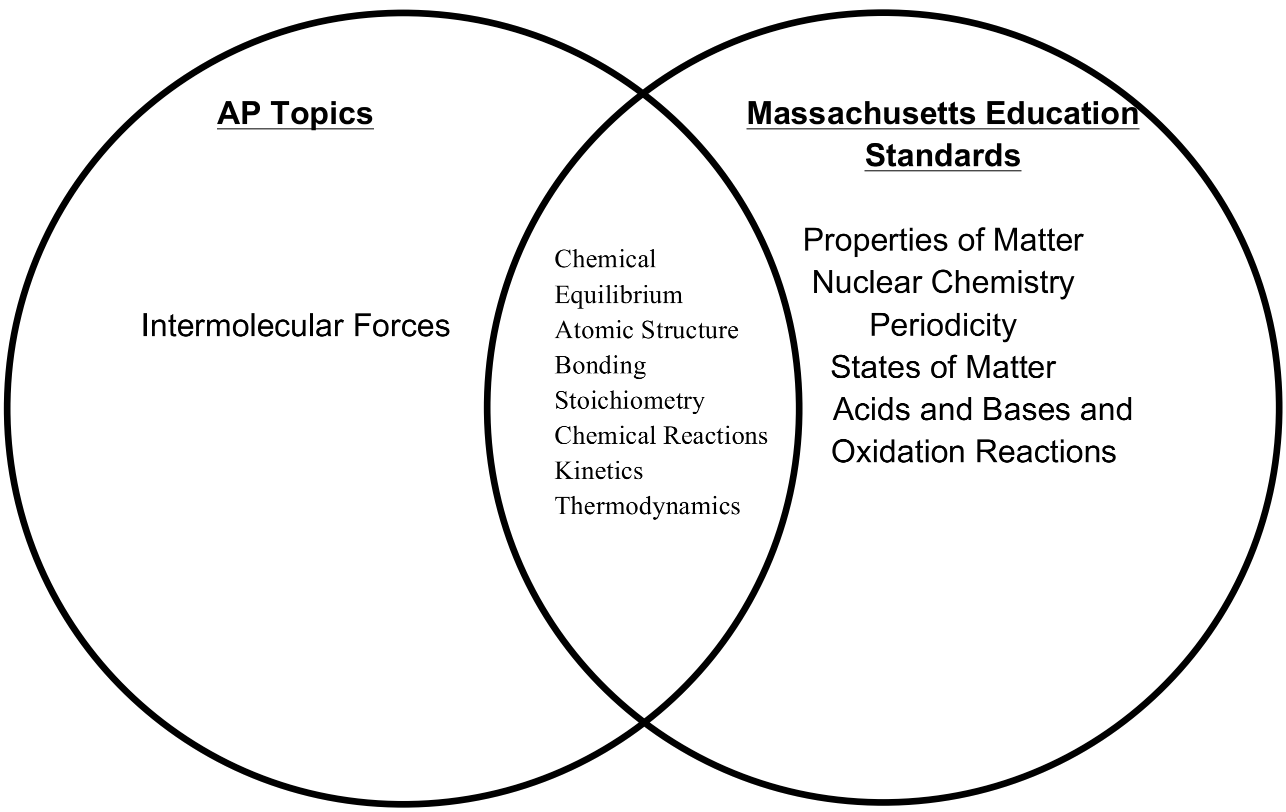

Figure 3 - Venn diagram of AP topics and Massachusetts Education Standards

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[7] Ibid

3. Methodology

The goal of this year's project was to determine if molecular modeling software could be an effective teaching tool. By improving upon previous work[8], the goal of this project was to reach a definitive conclusion on the usefulness of modeling software in the classroom. Once proof of principle was established, the construction of a lesson specific, user friendly software can be recommended. To start the project, potential programs were reviewed. Next, a survey was made and distributed to teachers to ascertain topics that their students struggle with, as well as the technology available to them. A lesson plan was then created around the results of the survey and program review. Once the lesson plan was completed it was then taken into classrooms. In the following section the specific details of this process are discussed.

3.1 Program Review

A quick search leads to numerous potential tools that could fit into the realm of molecular modeling software. There are many possibilities from the simple to the most complex. For this project the software should be easy to use but powerful enough to encompass the level of complexity encountered in a high school chemistry setting. A user-friendly interface would prevent students from becoming frustrated with the software and hindering learning. On the other hand, the software must be on a certain level where it allows enough freedom to make many types of models. An ideal software also needs to either be web based or easy to install with minimal requirements. This will prevent the program from being excluded due to high IT demands or difficult installations. High schools are very strict about what programs are installed and who has access to administrative controls, therefore the easier the program is to access the more favorable it will be for this application.

The first place to start was reviewing the list from previous IQP work[9] of possible software programs along with some searching to see if any other software had been developed in the past year. The choices were reviewed systematically and the list was soon narrowed down to just a few possibilities. The criteria used were ease of download, usability, level of the software, and capabilities. Some programs were extremely difficult to download and install, eliminating

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[8] Devaney, K., Hango, C., Lu, J., & Sigalovsky, D. (2014, March 10). Computational Chemistry in the High School Classroom. Worcester Polytechnic Institute. Retrieved from http://www.wpi.edu/Pubs/E-project/Available/E-project-031014-153531/

[9] Ibid

them quickly. After the programs were installed the next consideration was an easy to use user interface with the ability to perform molecular calculations. Some software programs included great graphical representations of molecules, but offered no calculations. Because the project goal is to teach chemistry concepts with calculations as one of the tools, these programs had to be eliminated as well.

3.2 Survey of Teachers

A survey was distributed to teachers to gain an understanding of what students have the most trouble with in chemistry, as well as, to gain insight into teacher's personal opinions on using computer models in the classroom. Information was pulled from the AACT and the Journal for Chemical Education. The AACT is the American Association of Chemistry Teachers. Unfortunately, most of the resources such as professional development and classroom resources were accessible only by members. General information such as the major topics of high school chemistry classes and some news articles about recent research were able to give us information for our survey. The major topics covered in classes were: acid & bases, atomic structure, chemistry basics, electrochemistry, energy & thermodynamics, equilibrium, gases, kinetics, molecules & bonding, nuclear chemistry, organic chemistry, quantitative chemistry, reactions & stoichiometry, solutions, and states of matter. These sources gave an understanding of the type of lecture topics and how teachers present the material.[10] The survey was developed using Qualtrics which is a survey generation and analysis tool. Qualtrics allows the user to create a survey and generate unique sharable links. This allows teachers to access the survey without the user generating personalized links to the survey for each teacher. Once the responses are recorded the results can be analyzed using Qualtrics report generator. The results of the survey are located in appendix B and are discussed later. Once a rough draft of the ten to fifteen minute survey was created Professor Brodeur, of the WPI chemistry department, reviewed the survey. He gave tips on clarifying individual questions and gave suggestions on other questions to ask. Once the initial review was complete, Ms. Katie Elmes of the WPI STEM Education Center review the survey one last time before she sent it out in the December monthly newsletter. The STEM Education Center is an organization at WPI that is focused on expanding science and engineering

[10] High School Topics. (n.d.). Retrieved from https://www.teachchemistry.org/content/aact/en/classroom-resources/high-school.html

educations in primary schools. Due to this goal they have a network of teachers across the country also working to improve early education. The monthly newsletter is an electronic publication sent out to teachers who signed up to receive information about upcoming events on campus, future research plans, or new research findings. The STEM Education Center was a great place to include the link to our survey because our project's main goal is the improvement of high school chemistry instruction. The recipients seemed eager to answer our questions and most of the responses came from teachers receiving the newsletter. Chemistry teachers that no longer received the newsletter were also sent personal emails requesting they take the survey. This helped open up the demographic as well as increase the number of responses.

The purpose of the survey was to gain an understanding of teachers' views toward technology in the classroom. If teachers were not open to changing current lesson plans to include chemistry software then further development of our project may be hindered. Teacher insight into which topics to focus on was also an expected result from the survey. Another constraint to computer software is teacher's access to computers for their class. Knowledge regarding the ratio of students to computers was vital. Lastly the survey was designed to allow the teachers using the lesson plan to give insight and ideas in the development phase. A copy of the survey distributed in the newsletters and by personal email is in appendix A.

3.3 Lesson Plan

Once a software program was chosen and the teaching material was in hand, lesson planning began. The lesson plan to be developed would cover three days of instruction. Day one of the lesson comprised a brief overview of geometry followed by a pretest on shapes up to four electron domains and time for the students to familiarize themselves with WebMO. The second day of the lesson plan had the students split into two groups. One group was taught using WebMO to assist them and the other group was taught conventionally with a whiteboard and lecture. The WebMO group also used ASSISTments during the lesson to get feedback. The ASSISTments page gave students instructions on what to do and gave the students questions to answer based off of what was seen in WebMO. At the end of the lesson the WebMO group used ASSISTments to test them. When the two groups finished a separate ASSISTments test was opened that neither group could use WebMO for, testing their ability. The classroom group did the same test on paper. Both groups focused on molecular geometry up to five bonding pairs while touching on six bonding pairs on the second day. At the end of the second day both groups took the same test. On the third day the two groups switched lesson styles. The WebMO group had a traditional lecture with whiteboard, and the other group moved into the computer lab. Similar to the second day both groups took a test at the end of the third day. Mrs. Grave's sophomore honors chemistry class was visited three separate times and the days went according to the lesson plan. Mr. Van Inwegen's junior AP chemistry class did the entire three day lesson plan during one extended period day. This way the results from the two different lesson styles could be compared to evaluate the effectiveness of WebMO as a teaching tool.

The two groups in the honors chemistry class were divided up after the pretest. Using the scores from the pretest, the groups were divided up so each group would have an equal amount of high scoring students and an equal amount of lower scoring students.

The AP chemistry class was split down the middle of the classroom. One side of the class was group one and the other was group two.

3.4 ASSISTments Lessons and Tests

The problems in ASSISTments reflected three major categories of problems: bond angles, molecular shape, and counting sigma and pi bonds. Bond angle problems provided students with a specific molecular geometry or a specific molecule. Using the structure given to them or determined by them; the students would then determine the bond angle between two atoms. Molecular shape problems provided students with a specific molecule or one described as having a certain number of lone pairs and bonding pairs. If students were provided with a specific molecule they would then have to determine the number of lone pairs and bonding pairs in the molecule. Using this information, students would give the corresponding molecule shape. Sigma and pi bond counting questions showed an organic molecule with varying types of bonds. Students would then have to determine how many sigma and pi bonds were in the molecule.

During lessons students could also use WebMO, the molecular modeling tool, to help them if they were in the WebMO group. Bond angles could be determined by building the molecule and measuring the bond angle by inspection or with the program. Molecules with certain numbers of lone pairs and bonding pairs could also be modeled to show the ideal molecular geometry. During the tests, after the lessons, both groups of students would not be able to use the WebMO tool and would have to draw upon their own knowledge.

3.5 WebMO Server

There are a variety of calculation methods that computers can use to perform chemical calculations. WebMO uses GAMESS, Gaussian, TINKER, NWChem, MOPAC, and Firefly, and allows the user to select which one to use. These programs run the calculations in the background and WebMO shows us their results. For our project Gaussian was used due to the fact that WPI already had the required license. A personal server is not required to use WebMO because a demo server exists for users to try it out. The WebMO demo server had a limited amount of processing ability and could become very slow if too many users are trying to run calculations at once. To prevent some of the issues last year's group faced, such as the server crashing, a local server of WebMO was set up. The system used for our server was an IBM x3755 with 4 Quad Core 2.6 Ghz Opteron 8435 Processors. It has 128GB of DDR2 RAM. The hard disks are 450GB Seagate Cheetah 15000 rpm drives in a software Raid 1. The new server was tested to gauge its capacity to handle a classroom of students. Twelve computers ran the WebMO program on the same account, mimicking what would happen in the classroom setting. The server provided very stable and reliable modeling results even with twelve computers running at the same time. After this stress test the server was deemed adequate for the needs of the lessons. In Mrs. Graves's classroom, the larger of the two, only 10 students would be on the WebMO server at any one time.

4. Results and Discussion

4.1 Program Review

Initially, many programs were reviewed to see how they met the following criteria: web based application, mac compatibility, if it was mobile friendly, ease of installation (if applicable), and ease of use. The evaluated programs are outlined in Table 1. Two programs fit the needs of the project, WebMO and Avogadro. WebMO is a web-based modeling program that can run extensive calculations and Avogadro is a downloadable program that can run simple calculations, further details on these programs are given in sections 4.1.2 and 4.1.4 respectively. WebMO can be run in any browser that has java and can be installed locally. Avogadro cannot be run in a browser and must be installed locally. Avogadro's installation, however, is very simple. Avogadro would be a better choice than WebMO if class wide usage were a problem. Avogadro could also be used anytime a WebMO server might be down. To help finalize our decision, a survey was sent out to local high school chemistry teachers.

Program	Web Based	Mac Compatible	Mobile App	Easy to Install	Ease of Use 1=very difficult 5=very easy	Finalist
ACD	No	No	No	Yes	2	No
WebMO	Yes	Yes	Yes	No	4	Yes
Avogadro	No	Yes	No	Yes	5	Yes
Chemitorium	No	Yes	No	Yes	1	No
Virtual Lab	No	Yes	No	Yes	5	No

Table 1. Comparison of Potential Programs

4.1.1 Eliminated Programs

Some programs were eliminated immediately due to major flaws in installation, or user friendliness that made them incompatible with our project. Despite being very user friendly, Virtual Lab was discarded because it did not suit our needs. Virtual lab did not offer any calculation capacity and tended to be aimed at running basic lab experiments such as acid/base titration virtually instead of constructing molecules. Chemitorium was very easy to download and had many useful features, but was extremely difficult to operate and was therefore eliminated as well. ACD/ChemSketch was eliminated due to the fact that it is only a viewer and cannot perform calculations.

4.1.2 WebMO

WebMO has an online demo server for users to test out without installing any local software. As long as the user has a web browser that can run java plugins, the demo server can be used. WebMO can also be installed on a custom server. Many schools have WebMO installed on their own servers for students and faculty to use in a web browser just like the demo server. The process to download and install the program locally is very complex relative to the other visualization software programs. WebMO requires the installation of a few other programs to run properly. Ordinary users might find it difficult to fully install WebMO on their computer. Once WebMO is installed, however, it has a variety of features. The interface for building molecules is very easy to learn. The program supports ninety two elements, calculations for bond angles, molecular geometry optimization, and more. WebMO also supports a wide variety of computation engines including Gaussian, GAMESS, PC-GAMESS, MolPro, Mopac, NWChem, PQS, PSI 4, PWSCF, VASP, QChem, and Tinker. This program includes a mobile app version for iPads and iPhones. Surprisingly, more and more classrooms have do not have access to computers and instead use only tablets such as iPads to run programs making WebMO more widely available. It should be noted without a locally installed program or separate server the demo server alone will not be able to support a full classroom of students. Even with the simplest calculations the server will be slow if many users run calculations at the same time.

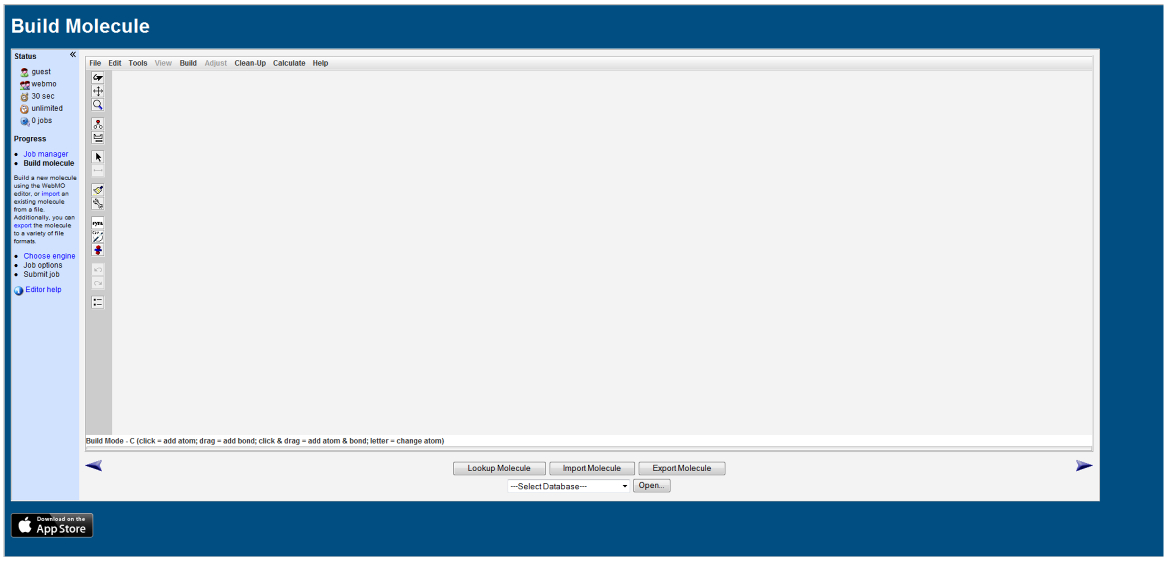

Figure 4 – WebMO user interface

4.1.3 ACD/ChemSketch

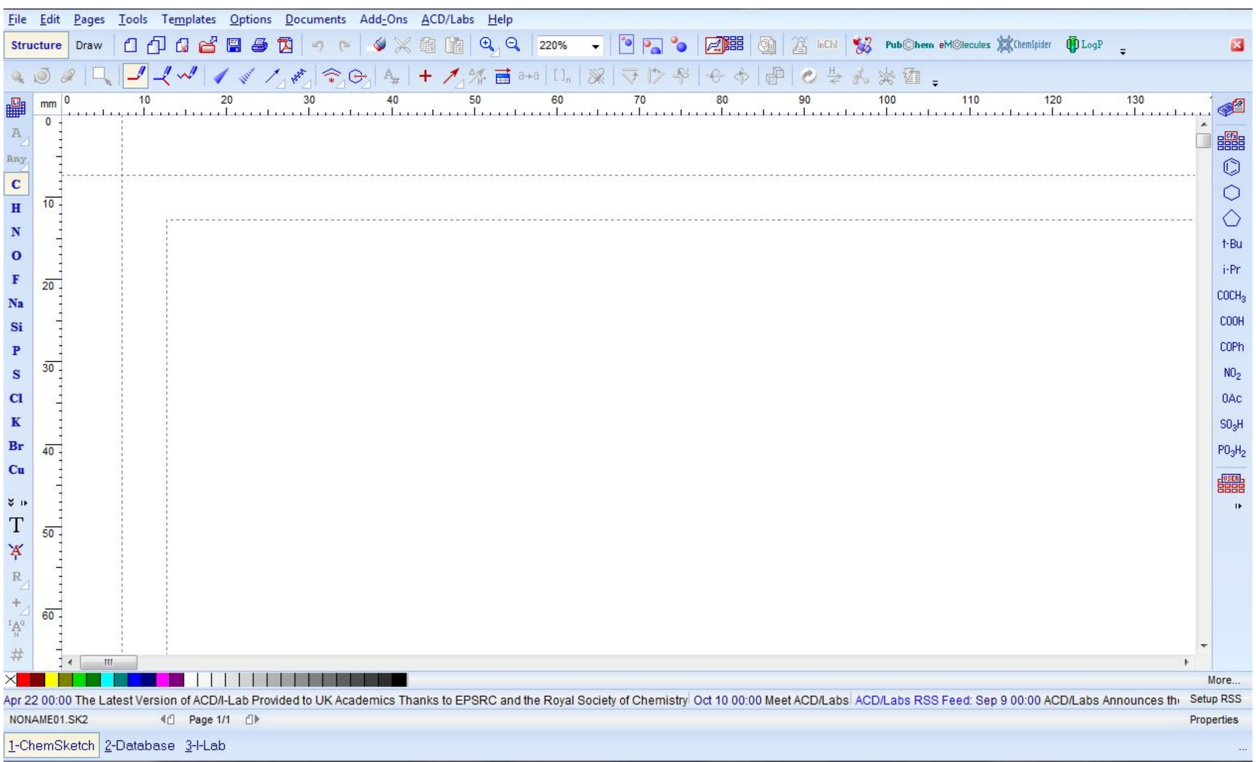

Figure 5 – ACD/ChemSketch user interface

ACD/ChemSketch is an easy-to-install program available for Windows. This program has a free version that includes most of the periodic table like WebMO. This program allows users to build molecules and visualize them in 3D space. First molecules are built in 2D space using atoms and lines to connect them and can be transferred to 3D space. ACD/ChemSketch includes many features including, links to PubMed for a structure, showing aromaticity, and structure optimization. The interface, however, might be a little overwhelming for high school level students. There are many more functional buttons than the other programs and might lend itself to confusion. There are many functions that ordinary high school students may not have a use for. For this reason and the fact that ACD/ChemSketch must be installed locally it was not made the software choice for this project.

4.1.4 Avogadro

Avogadro, like ACD/ChemSketch is a very easy to install program. This program, like WebMO, has a very easy to use interface. Unlike WebMO, this program does not include a web based version. Similar to the other programs, Avogadro includes a wide variety of elements to build molecules with. These molecules are built in 3D space and their geometry can be optimized. Avogadro does include some features that may not be suitable for high school students but not many. The molecular model can viewed in many different ways including ball and stick, wireframe, and Van der Waals spheres. The interface is not overwhelming and this program was chosen as a finalist to consider for our modeling software.

Most of the free programs available online were quickly eliminated. The two programs left after the evaluation were WebMO and Avogadro. The final program was decided by surveying chemistry teachers and using their feedback to decide. Some chemistry teachers had access only to iPads, not computers. Because WebMO is also compatible on mobile Apple devices, the case for WebMO became stronger. Another consideration was program setup. WebMO requires only that a web browser can run java, although it can also be installed locally. Avogadro can only be run locally. Some but not all schools might have trouble installing a new program on computers in a computer lab. These considerations along with other results from the teacher survey lead to the choice of the WebMO software for classroom use.

4.2 Survey Results

Besides the teachers receiving the STEM newsletter most of the teachers receiving personal emails were happy to help us by answering our questions. From the results of thirty of teachers we concluded that the lesson plan should encompass molecular geometry. The survey results can be found in appendix B. Almost all teachers felt computer technologies had a place in high school classrooms. 94% answered yes to the question “Are you open to incorporating software into your classroom”. More importantly, more than half the respondents said they could achieve a 2:1 or 1:1 ratio of students to computers if they went into a lab or library. This is promising for the future of technology in classrooms as almost every student has access to a computer. Of all the teachers with access twenty-four of twenty-nine claimed to already use computer labs. The five teachers that did not use their schools resources mostly attributed it to accessibility and reliability concerns. Scheduling lab time can be difficult when an entire school is using the computers. Furthermore some topics have a limited amount of useful material to draw from. This was voiced by one teacher specifically when they wrote, “The lack of high quality instructional material online” in response to why they did not use computers more. Still even this teacher was open to technology as long as it is an effective tool for learning. Teachers tended to want to engage their students with technology, but felt it was either unreliable or ineffective as a teaching aid. In the survey we attempted to gain a direction for our lesson plan. Teachers were asked to rank topics from easiest being to hardest relative to each other. In the Qualtrics analysis each position was given a number. 1 being easiest. The teacher’s rankings were then averaged to give an average placement for each topic. The average placement was about the same for every topic. A range from 4.2 to 5 was common. Only Gases and Organic Chemistry above 5. Because no one topic stood out as a clearly difficult topic it seemed the difficulty tended to depend upon the class. One teacher may think gasses were the hardest while another ranked organic chemistry the hardest. This in turn led to the variance in the data to be large. One explanation for the inconclusive results of the survey was the difference in the level of students. Where an AP teacher has a different curriculum than an honors or general chemistry teacher. Our survey simply asked all teachers to rank the topics based on their opinion. If the teachers were separated by level or asked specifically what each level of student has the most trouble with maybe the results would be more homogeneous. This could be a better way to gauge topic difficulty in the future and a better measure the needs of each level. Because the mean was clustered and no one topic was significantly harder than any other topic we decided to choose atomic structure. This did have the lowest mean value of 4.21 meaning it could be one of the more difficult topics. The variance in the data however makes this conclusion suspect. A better reason for choosing atomic structure for the lesson was modeling software lends itself well to teaching atomic structure. Teachers were also asked to rank the usefulness of computer aid from not useful to very useful. Teachers thought that the most benefit would be to the highest level of students. AP and dedicated organic chemistry classes could receive the most support. While teachers thought AP could benefit the most from modeling software even for general chemistry the scores were still positive. The scale used for this question was not useful to very useful. The lowest average was for general chemistry yet it was still in the "somewhat useful" category. Teacher thought that computer programs would still have a positive impact on the general classes but the higher levels would gain more form the lessons. This reinforces that all levels of high school chemistry students can gain something from having their lessons use technology.

4.3 Lesson Development

The lesson plan was developed based upon survey results, the level of the classes, and time constraints. Based upon survey results (see appendix B), and conversations with Mrs. Graves and Mr. Van Inwegen, the honors class and AP class instructors respectively, molecular geometry was decided as the topic to be covered by the lesson plan. The structure of the lesson is given in section 3.3. This structure was dictated by time constraints; because of scheduling conflicts we were only able to visit the honors class three times and the AP class once. After deciding on the topic and the structure of the lesson, a rough draft of the lesson plan was made. Mrs. Graves and Mr. Van Inwegen then reviewed this plan for clarity and time. The lesson plan was extended to include molecules with more bonding pairs, and to stay within the allotted time the amount of practice problems was cut down. Additionally, it was decided that if the class finished the lesson early for any reason that they would do additional practice problems.

4.4 Test Results - Honors Class

The honors class was divided into two groups. Group one had a lecture on the first lesson day and group two had a lesson using WebMO on the first lesson day. Both groups worked together on the very first day with a brief WebMO overview, so that the students would be familiar with the program before using it in lessons, and took the pretest.

After taking the pre-test at the end of the first day, the students took post-test one at the end of the second day, and then took post-test two at the end of the third day. On average group one scored 65% on the pre-test, 52% on post-test one, and 28% on post-test two. One average group two scored 75% on the pre-test, 68% on post-test one, and 72% on post-test two.

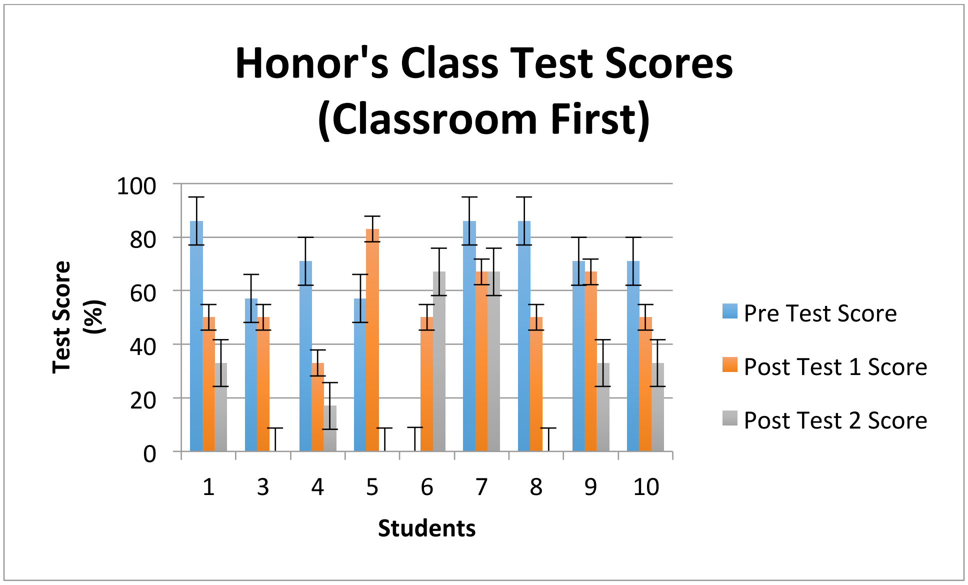

Figure 6 – Honor's class test results where students were given classroom instruction in the first session and WebMO instruction in the second session.

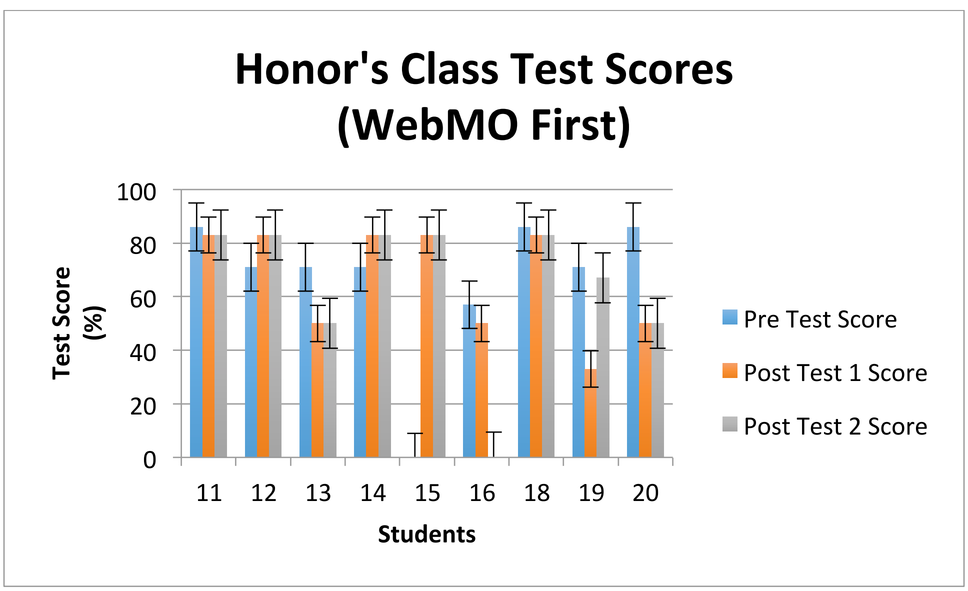

Figure 7 – Honor's class test results where students were given WebMO instruction in the first session and classroom instruction in the second session.

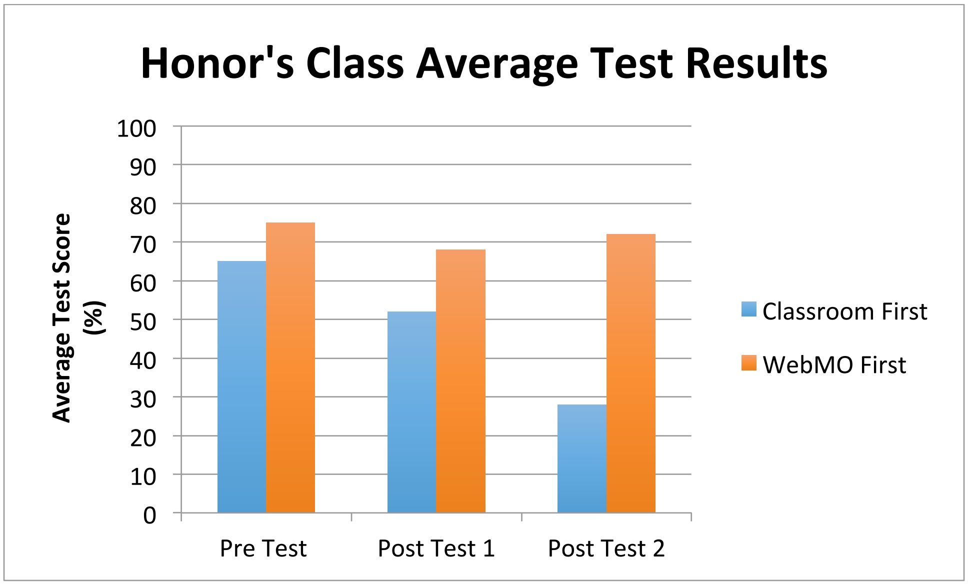

Figure 8 – Honor's test results

These results show that WebMO helped group two score a better average on the first post-test material. The data also shows that despite the use of WebMO group one did not show an increase in its test average from post-test one to post-test two. This could be due to post-test two being more difficult than post-test one, or because of the two week gap between day two and day three. Group two, in the classroom on day two, scored forty four percent higher on average. Comparing the two groups shows that WebMO was more effective for teaching the background knowledge necessary to learn the harder parts of a topic. In this case, group one was introduced to molecular geometry in the classroom first and then taught the geometry of molecules with more bonding pairs using WebMO and showed a 24% drop in post-test scores. Whereas, group two was introduced to molecular geometry using WebMO and taught the geometry of molecules with more bonding pairs in the classroom and showed a 44% increase in post-test scores.

Both days in the classroom two of the IQP team members were present to teach. This allowed for one member to prepare practice problems and solve technical problems while the other continued the lesson. One IQP member was in the labs on both days. Mrs. Graves was also present in the lab on both days. Her lack of familiarity with WebMO, may have caused her to be less of a help as another WebMO project team member could have been. The groups in the classroom also had more time to learn, in a more familiar way. Although the groups easily picked up WebMO and had used ASSISTments before, they still had to take time to load up computers and log in, which took up valuable lesson time. Group two took the post-tests on paper the day they learned the material because of a lack of computer availability. Group one experienced some technical difficulties in the lab, the school was installing testing software onto all of the school computers that day and therefore the school's servers were extremely slow. Because of state-wide computer testing their test was postponed by two weeks and was taken on paper at the beginning of day three.

Additionally the sample size was small. Although most classrooms would not be much larger than twenty students, more data would be better.

4.5 Test Results - AP Class

The AP class was divided into two groups similar to the honors class. Both of the groups were given a brief demo of the WebMO program, so that the students would be familiar with the program before using it in lessons, first and then took the pre-test. Group one was then given the first lesson using WebMO and group two was given the same lesson using a traditional lecture. After the first test the two groups switched for the second lesson. Group one had a lecture and group two learned using WebMO.

On average group one scored 67% on the pretest and group two score an average of 69% on the pretest. This showed that the two groups had similar abilities in molecular chemistry before teaching began. On the first post-test group one scored an average of 78% and group two scored an average of 69%. This showed that WebMO helped group one score an average of 9% higher on the first lesson. For the second lesson group two, the lecture group, scored an average of 64%. The lecture group, group one, scored an average of 67%. These averages are closer than the averages from day one, with a difference of 3%, but it does show that WebMO did not lead to higher scores on the second lesson. This could be because the material was review material for this class, so both groups came in with about the same prior knowledge of the material.

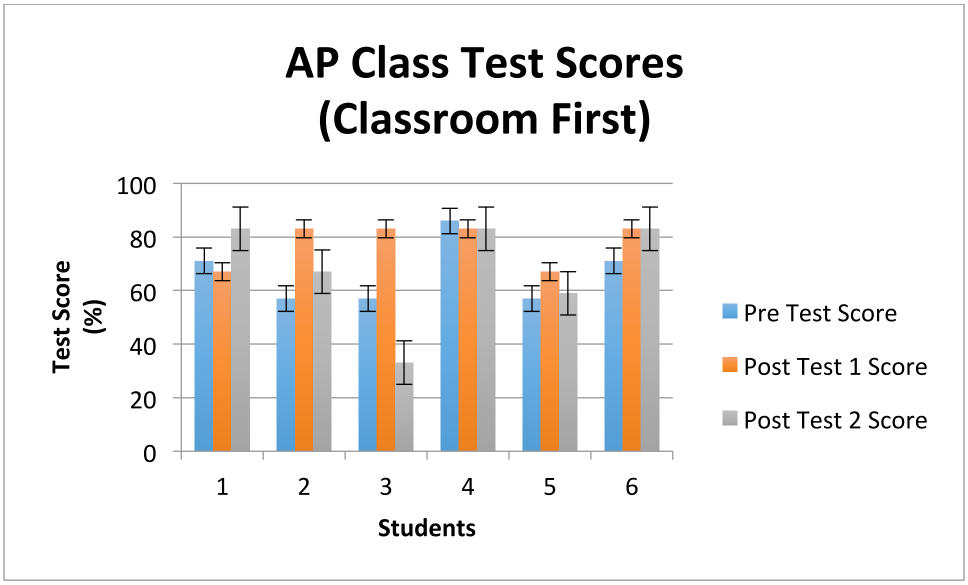

Figure 9 –Advanced placement test results

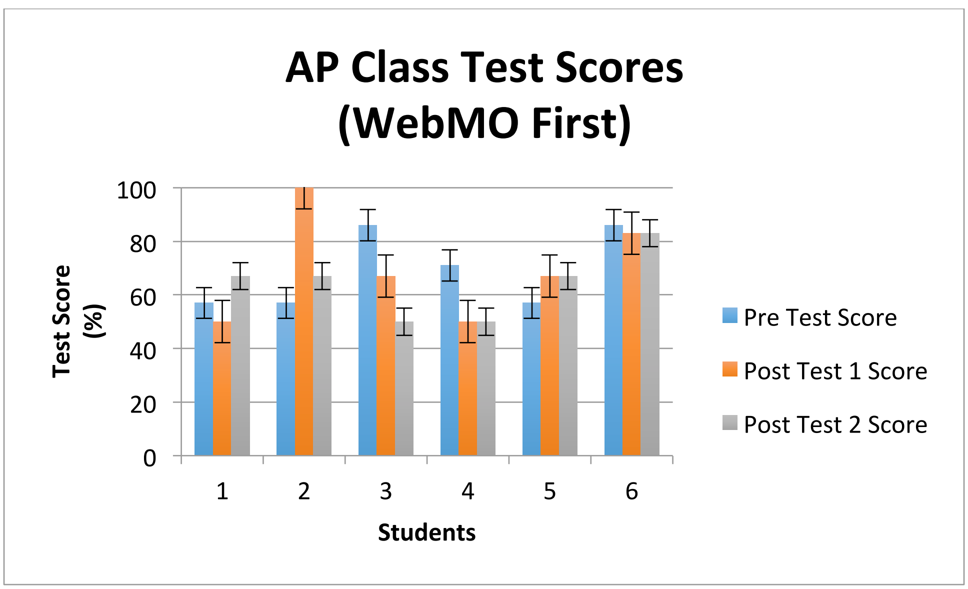

Figure 10 –Advanced placement test results

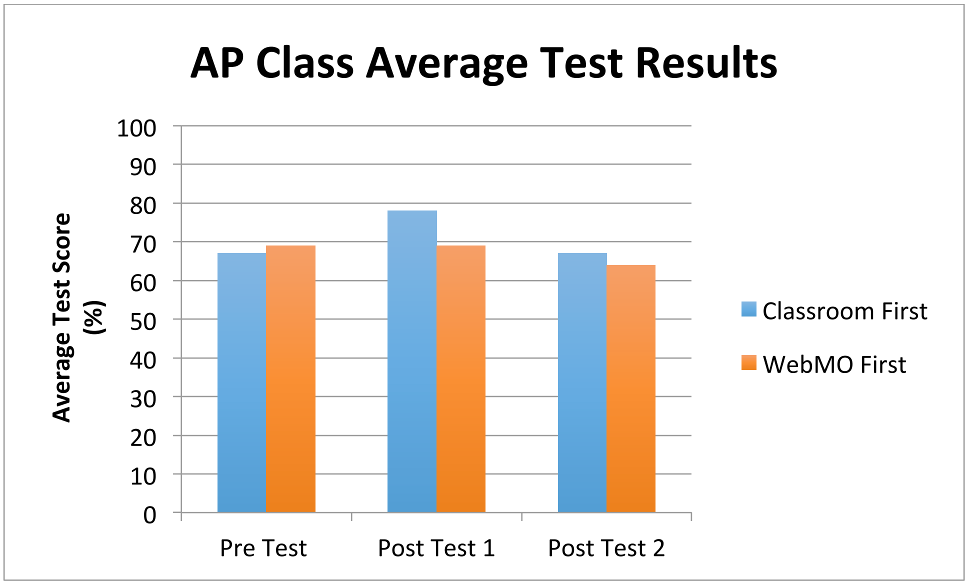

Figure 11 –Advanced placement test results

As with Mrs. Graves Honors class, the AP class showed that WebMO helped more in providing a solid foundation than in teaching advanced topics. It is seen that group one, who was taught the basics of molecular geometry in the classroom, experienced an 11% drop in post-test scores. Whereas group two, who was taught the basics of molecular geometry using WebMO, experienced a mere 5% drop in post-test scores. This reinforces what was found with the honors class, that WebMO helps best with building a foundation for learning harder subjects.

Similar to the way the honors class was instructed, two IQP members stayed in the classroom to lecture while one IQP member along with the instructor, Mr. Van Inwegen, assisted the students using WebMO. Although the instructor was not familiar with WebMO Mr. Van Inwegen, the instructor for the AP class, was very familiar with ASSISTments, providing some additional help in the computer lab.

One problem with these results is the size of the class. Similar to many AP classes, there were fewer students than a general or honors class. This very small group of students did not lead to very reliable results. With such a small sample any outliers or deviations cause large effects on the average of the data.

4.6 Classroom Dynamics

There were some noted differences between the attitudes of the Honor's class and the AP class that may have had an impact on the student's test results. The AP class was much more serious about the lessons and tests than the Honor's class. This is most likely due to the fact that the material being taught was relevant to the upcoming AP test but not relevant to any tests or class work for the Honor's class.

In the computer lab AP students tended to be self-starters and more focused on the lesson. Once told what to do they got quiet and worked diligently only pausing to ask questions. Normally they asked the instructors for help and not each other. The honors class, on the other hand, needed to be more closely monitored to keep them on task. They had many more questions, because of the new material. Instead of always asking the instructors they would first ask each other fostering a disruptive environment. Both classrooms were very receptive and interested in the lesson, but the AP students certainly gained more from exercises. They were much more thorough in their classwork, and learned during the periods. The AP students also had an advantage because the lessons were administered consecutively due to a block schedule where that day was two periods, roughly two hours.

The honors class was gaining a preview of what topics would be covered in the AP class the following year. Unfortunately, the material tended to be new and difficult to grasp with little introduction. The WebMO lessons tended to fall short on introducing new material to the honors class. The AP class, on the other hand, used the lesson as a review of prior material for the AP test. The lesson worked well at refreshing and reinforcing learned knowledge for these students. The conclusions that can be drawn from these observations are minimal because the group had very little lesson planning experience. While our lesson plans may not have taught new material well this is not to say someone cannot use a similar lesson plan to greater effect.

4. 7 Challenges Faced

4. 7.1 State Wide Testing

During the first major lesson in the honors chemistry class the students in the WebMO faced Internet problems while using ASSISTments. That day many classes in the school were downloading software for testing purposes. The wide use of bandwidth across the school slowed down the online program for our students. Our students were able to finish the lesson using WebMO and ASSISTments but they found difficulty making it through the test for the day. Because of this these students took the test the following week at the beginning of class after a brief review. The students in the classroom group did finish the first test because they took the same test on paper. This could lend itself to some discrepancies in the test results data because the classroom students had just taken the lesson. Although the other group did manage to finish the lesson, and had a brief review the next week, they did have a week in between the main lesson and the test.

4.7.2 Communication

WPI runs on an accelerated schedule compared other places, which can make communication with people who are not WPI students very difficult. Terms at WPI are seven weeks. Coordinating with teachers must be done concurrently with other lesson development. Sometimes people from outside WPI do not understand the time constraints of the college school year due to differences with the high school calendar. Because of this, a lot of time was lost while emailing back and forth with various people connected to the high schools visited. In many cases, meetings were impossible due to scheduling or other factors, and therefore email was the only viable method of communication. Because so much time was lost due to waiting for replies to emails, we were only able to go into two classrooms, which limited our sample size.

4.7.3 Current Curriculum Schedules

Lessons with Mrs. Graves' class and Mr. Van Inwegen's class were planned to be around early March. This was because by that point students would have a solid foundation in chemistry and the lesson plan would be finalized. Unfortunately Mr. Van Inwegen's class, being an AP class, had a very tight schedule closer to the end of the year as they prepare for the AP test. Thankfully the extended period he offered for use was about the same amount of time used in Mrs. Graves' class but the students had the entire three day lesson at once. By the time our lesson plan was completed Mrs. Graves' students were ready to tackle molecular geometry but were in the middle of doing work on other topics. Ideally the lessons would be administered during the time of year students learn molecular geometry.

4.7.4 Lack of teaching/lesson planning experience

As current college students with no knowledge of classroom planning or teaching techniques it was difficult to create a high school lesson. Professor Brodeur was kind enough to give tips for measuring how long students should take compared to how long it took the test maker to complete the task. Besides timing issues, classroom control was sometimes difficult. As guests in a classroom it was at times awkward to correct or refocus students when they got off task. Determining how to teach the portion of the class that received instruction in a traditional classroom setting was not difficult. Actually going into the classroom and using the techniques researched proved more demanding. In future projects observation of chemistry classes either at WPI or a local high school before attempting to teach a group of students may prove beneficial. Team members could also consider practicing on volunteer peers prior to entering a classroom. Finally closer collaboration with the class's teacher may improve the instruction from the IQP team.

4.7.5 Time constraints

Ideally WebMO would be used to supplement the entire molecular geometry portion of the high school chemistry curriculum. Mrs. Graves and Mr. Van Inwegen were kind enough to give us some of their time but it would be unreasonable to administer the tests every day for possibly weeks. Because we were only able to use three hours of each class' time, our results do not reflect what a fully WebMO integrated lesson might show.

4.7.6 Attendance

Ideally our team would have tracked the performance of all the students in the groups, showing where they did better than their classmates and where not. Unfortunately, there were some students that did not take all three tests. The AP class lesson was done all in one day, making the data set complete. The honors class, however, was instructed on three separate days. Some students failed to take the pretest, and some failed to take the post tests. Two to three students were absent each day of the project. For this study, however, only students with complete data were included in the results to make for more reliable data.

4.7.7 Small Sample Sizes

Ideally more classrooms would be tested to determine whether or not molecular modeling software is helpful in the classroom. In the AP classroom there were only six students in each group. This could lead to some misleading results. Although the two groups were split up using two different methods for each of the lessons, the sample size was too small to account for outlying scores. For example a student could do well on the pretest using his or her existing knowledge and then choose to pay little attention to the lesson knowing the scores would not affect their final grade. In the honors classroom each group had ten students. Although this sample is bigger, it is still not big enough considering the huge impact on low or high score can have on the groups' average. For example, one student scoring a zero on any of the test in the honors class would bring down the average by 10% and one student in the AP groups would bring the average down 17% with a zero score.

To determine whether or not WebMO and other molecular modeling software help in the classroom, many more classrooms will need to be tested using these methods.

5. Recommendations

The single most important step moving forward is lesson plan development. Future IQP teams should attempt to work more in conjunction with high school teachers while developing a lesson. Chemistry teachers' jobs revolve around using teaching techniques to help students learn the material. College students do not have the background needed to plan the most effective lessons. Instead of making a lesson then taking it into a classroom it is recommended to develop the lesson with a teacher. This will require more time and possibly off campus travel but should provide better results. This is where ASSISTments can be beneficial for collecting data. Once a lesson plan is created, teachers around the country could incorporate the lesson simply by knowing the assignment ID number. Future IQP students would not necessarily need to go into classrooms, but could instead contact teachers and have the teacher use the assignment. This would also solve the problem of teaching a lesson that the students are not currently focused on. If the assignment is available teachers could use it when they reach the topic in their curriculum. All the data from all the classrooms could then be collected for the student researchers without leaving the campus. Furthermore, allowing teachers to use the lessons in their classroom without the intrusion of new instructors could produce more accurate and reliable data. Teaches have a unique way of controlling and interacting with their students. Anytime this delicate balance and normalcy is interrupted students can act differently. As the school year progresses teachers determine the best way for each student to learn. As outsiders in any particular classroom an IQP team cannot curtail a certain lesson to individual students as effectively as their everyday teacher. Also an IQP team that has little teaching experience would not be able to defuse situations that arise in the classroom to the same extent as the teacher who works with his or her students daily. These factors ultimately point toward data collected from teachers using the lesson independent of the IQP team would be more accurate than any data collected first hand.

Another focus for future project work could be a software program strictly developed for this project. WebMO has numerous features that were not utilized by this project. It also requires numerical analysis tools to be installed locally to work. Numerical analysis tools are the way in which a program, in this case, WebMO approximates the location of electrons and thus the structure. Gaussian was used for this project. At the high school level the geometry was considered to be ideal. The numerical tools, therefore, were extremely powerful for the application, but there was not a program that met the defined criteria that did not use one form or another of numerical approximation. A school using a server for WebMO could avoid local installation of these numerical analysis tools on all computers. A software program specifically developed for this project could be easily downloadable and only as complex as needed for high school chemistry needs. This would save on calculation time, extraneous buttons or functions, and usability. The ideal program would have the lesson and teaching tool integrated allowing students to submit answers and get feedback within the teaching tool. The ideal program would likely include features for ideal geometry, charges, naming, and organic elements. Other features may be overly complex for use in high school classrooms.

As mentioned above, this project ran into a few problems. Future project work should be cognizant of the potential problems involved when using unreliable networks, and focus on proving without a doubt the merit of computer software in high school classrooms. The data collected indicates a possibility of benefits but does not prove satisfactorily that computational chemistry is useful. Future projects should continue to refine the lesson plan using WebMO to make a definitive case for this technology in high school level chemistry classes.

6. Conclusions

WebMO proved to be a robust software capable of facilitating learning in a high school classroom. ASSISTments worked well as a lesson building tool. Unfortunately, the success of new technology in the classroom was limited by the quality of the network. The bandwidth and Internet speed constrain the number of students able to use this technology at a time, especially due to the fact that molecular modeling software are highly demanding programs. WPI created a dedicated server on campus to ensure the problems faced while using the molecular modeling software were not due to a lack of processing power. This clearly points to the school's Internet not being able to handle the demands of the molecular modeling software. Computational chemistry programs can be developed and functioning, but until they can be reliably used in high schools teachers will not take the chance of losing a day of instruction to possible IT problems. Teachers tend to be completely open and willing to try technologies but are leery of finicky technology. Many teachers are apprehensive of using new technologies, because they expect to encounter many problems when using computer technologies. This expectation prevents further implementation of technology in classrooms. The most disappointing realization in this result is that regardless of what is done to make curriculums better and more appropriate the real blockage lies with variables outside of our control. School networks and Internet bandwidth limit what a teacher can have his or her students complete while in school. Therefore, teachers tend to refrain from trying new programs or forms of instruction, because they know the students may encounter technical difficulties. Until schools have much better systems across the board it is realistic to think that new technologies will be a novelty and not a mainstay in our primary education system. However, WebMO does show promise as an effective teaching technique. WebMO, or other molecular modeling programs, help best with establishing a foundation before moving on to more challenging subjects.

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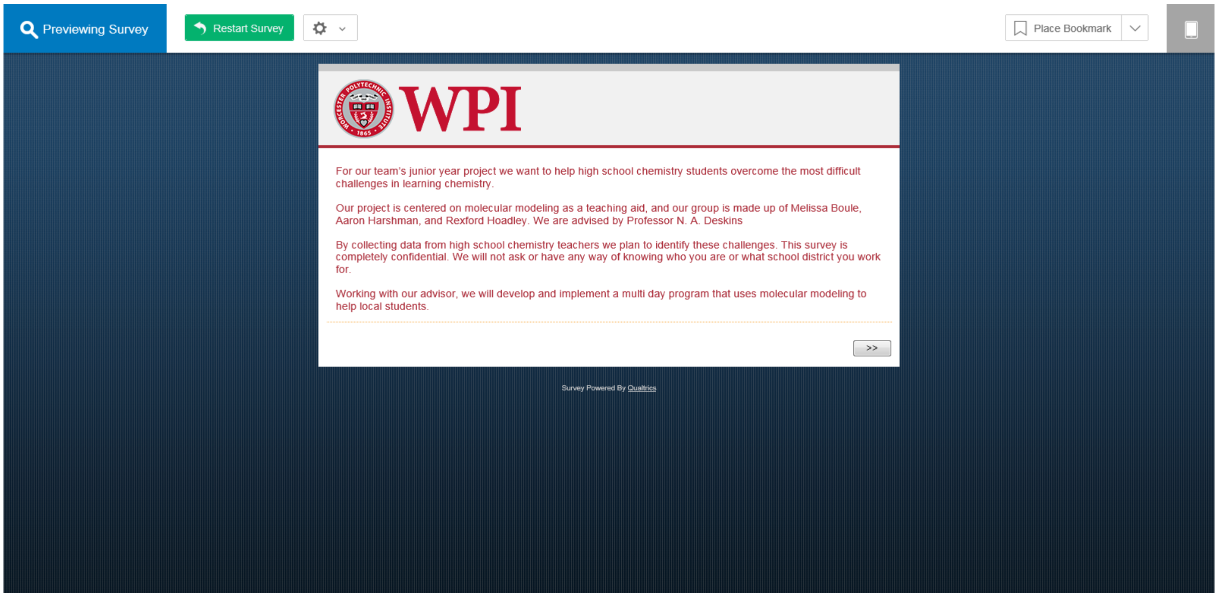
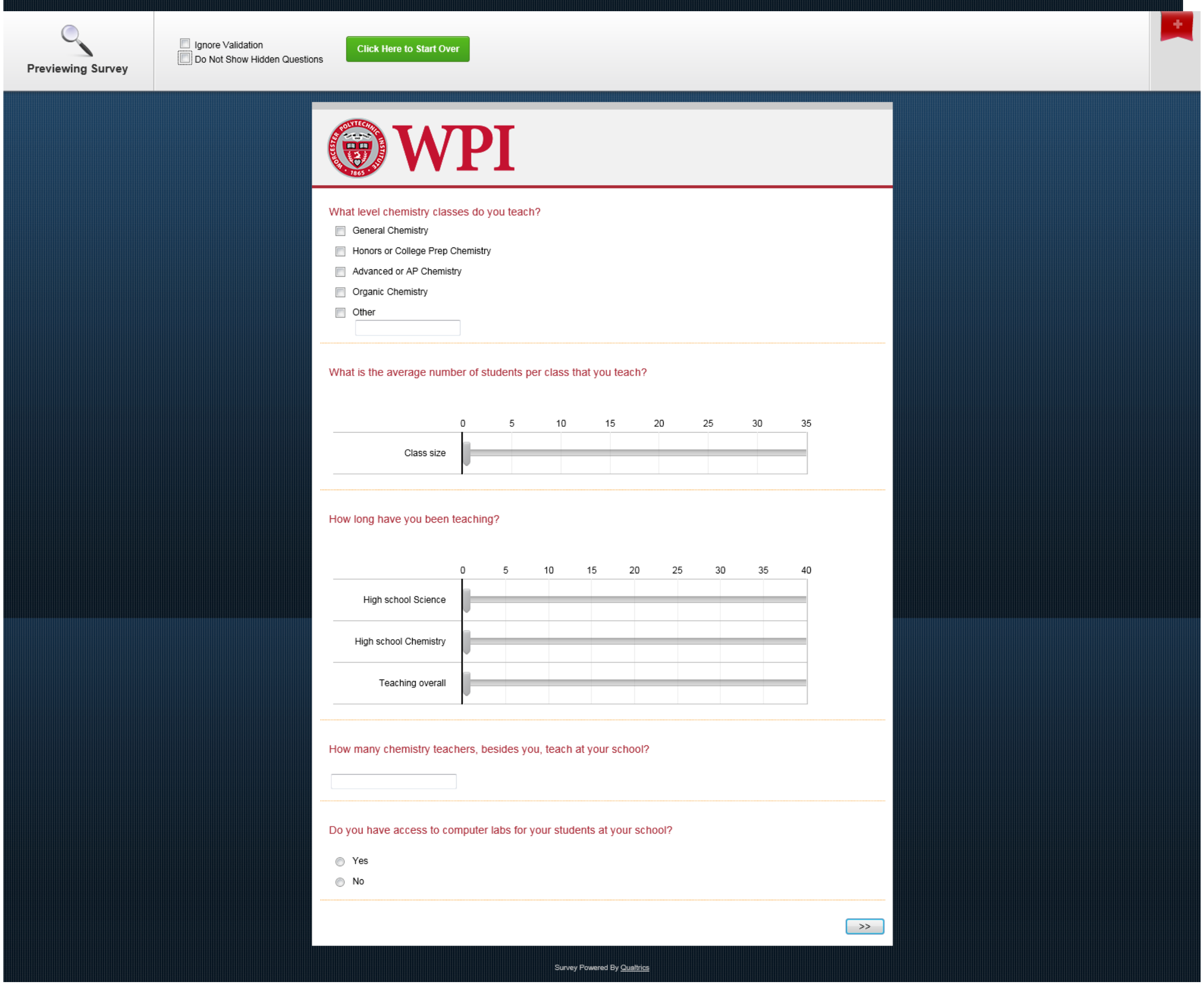
Appendixes

Appendix A. Survey for Teachers





Previewing Survey

Ignore Validation
Do Not Show Hidden Questions

Click Here to Start Over

WPI

Are you open to incorporating technology into your lesson plans and why?

- Yes
- No

What chemistry topics do you feel your students have the most trouble with. Please rank, by dragging the topics, from most difficult being 1 to least difficult being 9.

- Acid & Bases
- Atomic Structure
- Electrochemistry
- Equilibrium
- Gases
- Kinetics
- Molecules & Bonding
- Organic Chemistry
- Reactions & Stoichiometry

What topics typically require extended time to teach or frequent revisits? Why do students seem to have difficulty grasping these topics?

How easy or difficult are each general reaction class for students to understand?

	Very Difficult	Difficult	Somewhat Difficult	Neutral	Somewhat Easy	Easy	Very Easy
Oxidation and Reduction reactions							
Acid base reactions							
combustion reactions							
Decomposition							
Single Displacement							
Double Displacement							
Synthesis							
Other							

Do you think computer software, capable of modeling molecules and preforming basic calculations regarding bond lengths and energies, could increase students understanding of course material?

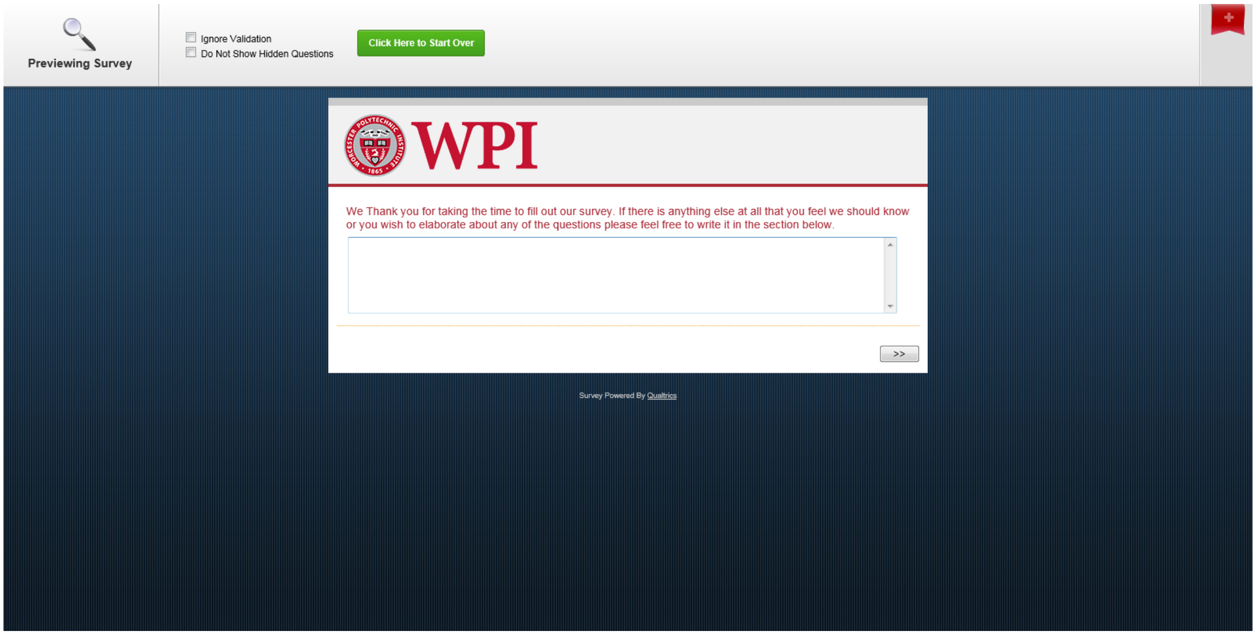
	Very Useless	Useless	Somewhat Useless	Neutral	Somewhat Useful	Useful	Very Useful
AP or Advanced Students							
Honors or College Prep Students							
General Chemistry Students							
Organic Students							

Do you think a molecular modeling software is beneficial to students understanding of chemistry topics, when used in the classroom?

- Yes
- No

Why?

>>


Previewing Survey
Ignore Validation
Do Not Show Hidden Questions
Click Here to Start Over
WPI
We Thank you for taking the time to fill out our survey. If there is anything else at all that you feel we should know or you wish to elaborate about any of the questions please feel free to write it in the section below.
>>
Survey Powered By Qualtrics

Appendix B. Survey Results

My Report

Last Modified: 05/05/2015

1. What level chemistry classes do you teach?

#	Answer		Response	%
1	General Chemistry		16	53%
2	Honors or College Prep Chemistry		25	83%
3	Advanced or AP Chemistry		16	53%
4	Organic Chemistry		2	7%
5	Other		4	13%

Other
IB Chemistry
Integrated science & math

Statistic	Value
Min Value	1
Max Value	5
Total Responses	30

2. What is the average number of students per class that you teach?

#	Answer	Min Value	Max Value	Average Value	Standard Deviation	Responses
1	Class size	10.00	30.00	20.84	5.22	31

3. How long have you been teaching?

#	Answer	Min Value	Max Value	Average Value	Standard Deviation	Responses
1	High school Science	1.00	40.00	17.83	11.25	29
2	High school Chemistry	2.00	40.00	18.36	11.17	28
3	Teaching overall	4.00	40.00	19.97	10.84	30

4. How many chemistry teachers, besides you, teach at your school?

Text Response
1
1
6
3
0
3
0
1
1
3
0
3
3 others
3
2
1.5
2
3
3
3
5
1
0
2
7
2
0
3
2
3
2

Statistic	Value
Total Responses	31

5. Do you have access to computer labs for your students at your school?

#	Answer		Response	%
1	Yes		29	94%
2	No		2	6%
	Total		31	100%

Statistic	Value
Min Value	1
Max Value	2
Mean	1.06
Variance	0.06
Standard Deviation	0.25
Total Responses	31

6. Do you currently utilize the computers at your school?

#	Answer		Response	%
1	Yes		24	83%
2	No		5	17%
	Total		29	100%

Statistic	Value
Min Value	1
Max Value	2
Mean	1.17
Variance	0.15
Standard Deviation	0.38
Total Responses	29

7. why do you not use the computers in your classroom?

Text Response
The lack of high quality instructional materials online. Next year, students will all have iPads, so I will have constant access, but I still feel that quality assessments are lacking. I also feel that the quantitative aspects of Chemistry are better suited for writing where I can see the steps used in problem solving.
too difficult to schedule time - too many students in the school, not enough computers
low accessibility
Computers are in library and require signing up for the time period. They are first come first serve for all classes during that period.
Too difficult to schedule

Statistic	Value
Total Responses	5

8. What is the general ratio of students to computers?

Text Response
1:1
4:1
1:1
We have 3 computer labs that each have enough computers for a class; we are going 1:1 ipads next year.
1:1
1:1 in computer labs
1 to 1

2 students to 1 computer (lap top); 1 student to 1 pc (computer lab)
1:1 for iPads only, not computers
13:1
1/1
not sure
1 computer per classroom so 1:29
1:1
1:1
1:1
100:1
2:1 with a laptop cart
2:1
1:1 if the computer lab isn't being used by someone else
1:1
In computer lab 1:1, but only 2 computer labs available.
in the classroom there is one computer, in the computer lab there are 30 computers
1:1
10 to 1
10 to1
1:1   In mobile labs that we sign up for to use of the teaching block
4:1
1:1 but we have to sign up to use the mobile lab

Statistic	Value
Total Responses	29

9. Are you open to incorporating technology into your lesson plans and why?

#	Answer		Response	%
1	Yes		30	100%
2	No		0	0%
	Total		30	100%

Yes	No
I think it is useful for visualizing things you cannot see and you can try things that might be hazardous or unsafe in the lab.	
It is necessary to incoporate technology into lessons to further student understanding and engagement.	
Only if it is useful for a high school student, is relevant to the curriculum, and is not too time consuming.	
I can't imagine lessons without it....calculators, data loggers, computers, excel, wolfram, desmo	
Students will have 1:1 iPad access, so I would like to make use of them.	
Allows for student exploration of certain topics that we might not be able to do during lab time.	
The animated molecular programs assist student in visualizing the interactions of particles.	
Helps students visualize	
Staying current with emerging technologies is important as it gives the student	

more real world experience.	
Its the way of the world particularly with the youngsteers	
I already do and find it to be highly useful in student growth and understanding	
kids are more technology knowledgable so it does enhance the learning experience	
I currently use technology in my room and it is required for the IB curriculum	
Fact of life. Enables so much more visually for understanding......WHEN IT WORKS!..(and the tech people are available to solve problems)	
Students enjoy using technology.	
gives students access to projects, simulations	
Technology can be used to create models that help to explain abstract concepts.	
Lab probes11	
Kids love it	
I currently use technology when it seems to enhance the instruction but compatibility btw programs and machines is an ongoing problem.	
I use technology now and find that it is helpful to students.	
Students will need those skills	
My students complete online web-based homework and have access to an e book	
like any tool it can play a role	
I think it has the ability to help students see things on a molecular level	

Statistic	Value
Min Value	1
Max Value	1
Mean	1.00
Variance	0.00
Standard Deviation	0.00
Total Responses	30

10. What chemistry topics do you feel your students have the most trouble with. Please rank, by dragging the topics, from most difficult being 1 to least difficult being 9.

#	Answer	1	2	3	4	5	6	7	8	9	Total Responses
1	Acid & Bases	1	3	8	4	5	2	2	1	2	28
2	Atomic Structure	8	4	3	1	1	2	4	1	4	28
3	Electrochemistry	2	5	4	3	3	2	5	3	1	28
4	Equilibrium	5	3	1	4	4	3	2	3	3	28
5	Gases	0	3	2	1	6	4	3	4	5	28
6	Kinetics	3	1	3	2	3	7	4	5	0	28
7	Molecules & Bonding	1	6	3	4	1	5	5	2	1	28
8	Organic Chemistry	2	3	0	3	5	1	2	5	7	28
9	Reactions & Stoichiometry	6	0	4	6	0	2	1	4	5	28
	Total	28	28	28	28	28	28	28	28	28	-

Statistic	Acid &	Atomic	Electro-	Equilibr	Gases	Kinet	Molecules	Organic	Reactions

	Bases	Structure	chemistry	-ium		-ics	& Bonding	Chemist -ry	& Stoichiom -etry
Min Value	1	1	1	1	2	1	1	1	1
Max Value	9	9	9	9	9	8	9	9	9
Mean	4.43	4.21	4.68	4.75	6.00	5.25	4.75	6.00	4.93
Variance	4.48	9.29	5.86	7.38	5.19	5.08	5.31	7.41	8.88
Standard Deviation	2.12	3.05	2.42	2.72	2.28	2.25	2.30	2.72	2.98
Total Responses	28	28	28	28	28	28	28	28	28

11. What topics typically require extended time to teach or frequent revisits? Why do students seem to have difficulty grasping these topics?

Text Response
Students struggle with the abstract nature of chemical bonding and intermolecular attractions. The concept of equilibrium is very abstract and difficult to understand, while the problems are very math based, which makes the topic challenging for students. Students who find mathematical problems difficult find stoichiometry challenging.
Stoichiometry needs to be revisited throughout the year because it is used so frequently and many students fail to understand the first time. They have difficulty because their math skills are low and have difficulty with ratios.
- THERMOCHEMISTRY (not on your list), Electrochemistry, equilibrium, kinetics, bonding, molecular geometry, atomic structure - all deal with concepts that students cannot visualize well. Students have difficulty constructing knowledge about the molecular interactions of matter, especially 1st year chemistry students. 2nd year AP Chemistry students are better able to interpret graphs, stoichiometry calculations, and visualize movement of molecules at the particulate level.
Depends on the level; in general, stoichiometry, formula writing/names, equilibrium (for AP)
The ones I find myself cycling back to and spreading out throughout the year are stoichiometry and atomic structure. Using mathematics, particularly with units they don't regularly use outside the class seems to frighten some. Atomic structure is a big item because we need to unlearn their fixed definitions of atoms, ions, electrons..etc.
In general, for college-prep courses, any quantitive topic (e.g. stoichiometry, gases, etc.) require more time due to the complexity of the thought process and the mathematics required. For Honors and AP students, less extended time and revisits are required because students are generally more focused and have more advanced mathematical abilities.
Aqueous equilibrium and pH problems. They do not think the problems through. They try to remember a method that worked in one case, but not necessarily in all cases. In addition, students have problems with significant figures with pH (a log function).
(I don't teach organic - not a state framework and not an AP standard - don't have time.) (I do not get to kinetics and equilibrium in my CP and Honors chemistry classes because they arrive to me with practically NO chemistry background from middle school - simply the bohr model of the atom and a rudimentary understanding of chemical reactions. As a result, I must begin at the very beginning and I don't get to the advanced topics.) Stoichiometry requires the most time because their math background is very week. Any conceptual understanding (molecular bonding, the currently accepted model of the atom) are difficult.
Valence as an idea arises again and again requiring an evolution of thinking about it

Polyatomic ions, and ionic bonding. It requires memorization to a certain extent.
Equilibrium and Stoichiometry, concept is both mathematical and somewhat abstract
Stoichiometry is one of the worst depending on the class. They really struggle with just the idea of essentially a "made" up unit like the mole. For some reason it just takes them a while to get over the fact that it acts the same way that a dozen or other unit works. Don't think conversions are the problem, more just the unit itself.
if math based, students math skills are usually behind what chemistry requires
Stoichiometry is something that we have to come back to a lot due to its recurrence throughout the different sections. Nomenclature is also a difficult thing to retain.
Note to the above ranking- Topics below gases are not usually taught in a one semester course in HS. Look at the state standards to see why. Also I spend much time on simple basics like measuring, metrics, review of math skills, reading skills, unit conversions and writing effectively. Please also see PHET from U Colorado Boulder. They are currently in use here for simulations and some interactives. Now on to the question..Atomic theory experiments, quantum. bonding, VSEPR, measurement, electromagnetic spectrum calculations are some topics that require extra time. Kids that are not developmentally ready to visualize spatial concepts have difficulty with simple VSEPR diagrams. I (and the department) do not even try MO theory. It is in their text. Some students are simply not willing to commit time to reading, understanding and taking sufficient notes or doodling to get the concepts in their heads. Other students can do all the math, drawing, writing and reading in their sleep. The diversity of students is a major issue that needs to be addressed in the current classroom for chemistry. Placement is based on algebra I pace. If they got through algebra I with a B or better in the regular course (not the year long or enrichment) then they come into college bound Chemistry. Otherwise they go into Elements of Chemistry and we have to adjust to accommodate their abilities. Also learning support students are funneled into the Elements course. They have many academic and visual issues, not to mention lack of skill sets to reason and use computers.
Equilibrium and Acid/Base calculations involving weak acids and weak bases. The problems are complex. Students have trouble applying the concepts and thinking through the process of solving the problem.
Stoichiometry Math
equilibrium - stoichiometry - in CP chemistry often times dimensional analysis / problem solving skills are a weakness for students
In Honors chemistry, I would say that most students struggle with molecular shapes and relating class material to actual molecules and atoms.
Kinetics. 2nd order reactions.
Balancing chemical equations and concentration problems. They don't have a good base of math skills.
Thermo - all new concepts
Quantum mechanics and thermodynamics (though not on your list) are the most difficult for them to grasp. Equilibrium is next most difficult as they struggle to make the larger connections or recognized the limited connection between strength and concentration
Stoichiometry (Honors Chemistry students) - math and sorting values from the problem to an equation is challenging for students. ions and Ionic Compounds (College Prep students) - Determining the chemical formula for an ionic compound requires several steps (determining the charge on the cation and anion and then determining the ratio of the ions that are stable).
Periodic trends
Electrochemistry is the most difficult. Students have trouble with calorimeter questions and what to do with the calorimeter constant and why you don't always have to use it. There are also a tremendous number of equations involved in this chapter. My students also have trouble with buffer problems, especially problems needing the amount of acid or base to add to change the pH.

energy is the hardest topic for students. They learn a lot about KE in 9th grade physics. We then layer PE on top of that. They will often say 'it's endothermic, so it needed energy so it created energy". PE can't be felt; therefore it's abstract, so difficult. Also, teenagers are the center of the universe so if they feel a beaker and the beaker got warm then it's EZ for them to say the Rxn was endo since they are the reaction-they are the center of all. So, we do a lot of experiential activities (simple endo and exo Rxns in a test tube, evaporative cooling experiments) and reinforce that if KE goes up then PE goes down. Sometimes I break it into energy transfer between system and surroundings and sometimes whitewash this and just claim that if one goes up the other goes down. Also - I didn't order your list above b/c you didn't say at which level (college prep or AP). It matters.
Electrochemistry. There are a lot of formulas such as the Nernst equation that students have to be able to use. Students have trouble grasping the difference between electrochemical reaction and electrolytic.

Statistic	Value
Total Responses	28

12. How easy or difficult are each general reaction class for students to understand?

#	Question	Very Difficult	Difficult	Somewhat Difficult	Neutral	Somewhat Easy	Easy	Very Easy	Total responses	Mean
1	Oxidation and Reduction reactions	6	7	10	1	2	2	0	28	2.71
2	Acid base reactions	0	4	13	1	6	3	1	28	3.79
3	combustion reactions	0	0	7	5	10	4	2	28	4.61
4	Decomposition	0	0	4	7	5	10	2	28	4.96
5	Single Displacement	0	3	5	5	7	6	2	28	4.50
6	Double Displacement	0	3	5	5	6	8	1	28	4.50
7	Synthesis	1	2	3	7	6	7	3	29	4.66
8	Other	0	2	1	0	0	0	0	3	2.33

Other
Biochem reactions
balancing
Kinetics

Statistic	Oxidation and Reduction reactions	Acid base reactions	combustion reactions	Decomposition	Single Displacement	Double Displacement	Synthesis	Other

Min Value	1	2	3	3	2	2	1	2
Max Value	6	7	7	7	7	7	7	3
Mean	2.71	3.79	4.61	4.96	4.50	4.50	4.66	2.33
Variance	2.06	2.03	1.51	1.52	2.19	2.11	2.45	0.33
Standard Deviation	1.44	1.42	1.23	1.23	1.48	1.45	1.56	0.58
Total Responses	28	28	28	28	28	28	29	3

13. Do you think computer software, capable of modeling molecules and preforming basic calculations regarding bond lengths and energies, could increase students understanding of course material?

#	Question	Very Useless	Useless	Somewhat Useless	Neut -ral	Somewhat Useful	Use -ful	Very Useful	Total Respon- ses	Mean
1	AP or Advanced Students	1	0	0	1	5	11	11	29	5.97
2	Honors or College Prep Students	1	2	2	0	10	7	7	29	5.24
3	General Chemistry Students	2	3	4	1	9	7	3	29	4.55
4	Organic Students	0	0	0	3	5	5	10	23	5.96

Statistic	AP or Advanced Students	Honors or College Prep Students	General Chemistry Students	Organic Students
Min Value	1	1	1	4
Max Value	7	7	7	7
Mean	5.97	5.24	4.55	5.96
Variance	1.61	2.69	3.18	1.23
Standard Deviation	1.27	1.64	1.78	1.11
Total Responses	29	29	29	23

14. Do you think a molecular modeling software is beneficial to students understanding of chemistry topics, when used in the classroom?

#	Answer		Response	%
1	Yes		28	97%
2	No		1	3%
	Total		29	100%

Statistic	Value
Min Value	1
Max Value	2
Mean	1.03
Variance	0.03
Standard Deviation	0.19
Total Responses	29

15. Why?

Text Response
It would need to be carefully structured if students are exploring modelling software for the first time as part of a classroom lesson. Done well, it could be very illuminating.
Students have difficulty visualizing shapes and symmetry when it comes to polarity. Much of the software designed for modeling is very complex. It could be beneficial to have software targeted to high school curriculum in the same way some modeling kits are targeted to high school classes.
If students could manipulate molecules, they would have a richer understanding of particulate interactions.
I would have to look at the software; Thinking back to the molecular modeling program used in the pharmaceutical industry, it is far too complex and would be useless in the classroom.
I used a modeling software for a few years between 2005-2008?, MoluCad, which was developed for HS students, and then I stopped using it and stuck totally to the modeling kits. But my decision was based on computer availability and dodgy technology. I strongly believe there is a role for modeling software in chemistry class
To be able to see a molecule in 3-dimensions makes understanding many of the properties of the molecule easier.
The visualization of molecules would be most beneficial.
Limited usefulness... Probably only helpful for very complication biochem reactions that are hard to visualize. But I am open to the concept!
It aids in comprehension by visual representation, especially in students that are visual learners.
helps the visual learners
I've seen it before in workshops and it seems like it could be highly useful. Never really had the chance to test it on my students. The ability to see molecules and atoms interact when otherwise you couldn't see them could be a very useful tool.
Gives them a visual or manipulative to support the theory
Chemistry is an abstract science, students cannot see or manipulate atoms and therefore have trouble grasping their properties. Having software that can bridge this gap might be very helpful for all learners.

Molecular modeling allows visualization of concepts that they can't envision.
It may give them interactives to use when prediction geometries, shape, interactions, but it cannot get too complicated from use or running requirements since the time to commit to this topic and the computer network use would be both limited.
It is easy to manipulate the model and examine 3D aspects of molecules.
it can be difficult to see the three dimensional shapes / structures in a text. Not all students are kinesthetic learners where using molecular modeling kits in class is beneficial
I think anytime one can view abstract concepts such as breaking and creating bonds, transfer of electrons, concentration gradients, and atomic structure, through models that allow manipulation, their true understanding is greatly enhanced.
It's is difficult to model these molecular shapes in 2D the 3D on-line sources are very useful. We need good software with good questions.
Some students need to see the models to understand such microscopic substances.
If easy to use, it can make these abstract topics more clear and allow them to see beyond the ideal problem presented in the reading.
When used appropriately, software can help students visualize the chemistry happening at a microscopic scale.
Let's them visually see the theory being taught
If students can actually see what is happening on the molecular level they will better understand the concept
For VSEPR, hybridization, MO theory, yes. For Orgo students looking at different SN or E reactions, yes. Would see quite limited use in my classes overall however.
Students can see what is happening at the molecular level

Statistic	Value
Total Responses	26

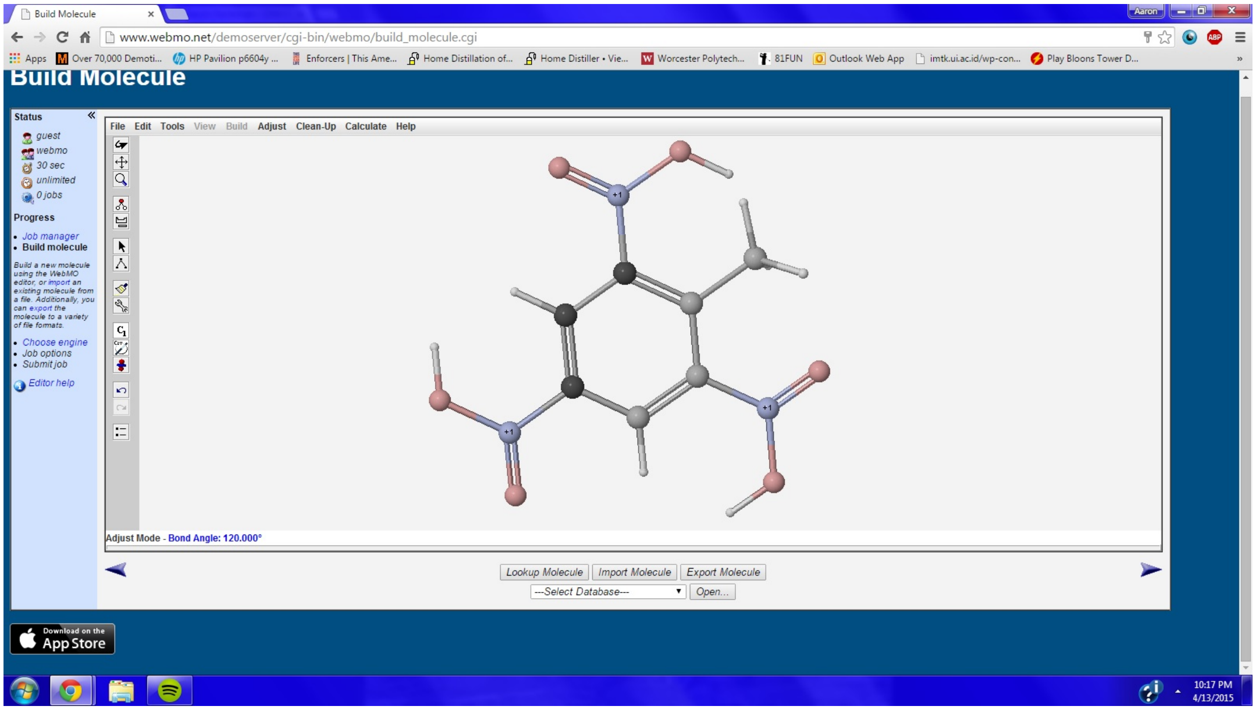
16. We Thank you for taking the time to fill out our survey. If there is anything else at all that you feel we should know or you wish to elaborate about any of the questions please feel free to write it in the section below.

Text Response
Your survey would benefit from some editing--several questions were poorly worded or contained grammatical errors.
It was difficult to organize the topics in order of difficulty because many of the topics are not taught in an Honors or General Chemistry class, such as electrochemistry and others are only briefly touched upon, such as kinetics, equilibrium or organic chemistry. The level of depth on these topics is surface and therefore not difficult for the class to understand.
Too many students do not have a fundamental understanding of the classification of matter and atomic structure that I need to spend time on these concepts and do not get to the higher level concepts in chemistry. As a result, when students take AP chemistry, I need to spend too much time on the fundamentals and not enough time on the topics of equilibrium, kinetics, thermodynamics and electrochemistry.
Real reactions with real chemicals are most educational... Software could be helpful only after foundations are laid through hands on lab experience and discussion.
Good luck with your project
Good luck! Have any of you actually taught in a HS setting or looked at a typical semester HS course in chem?

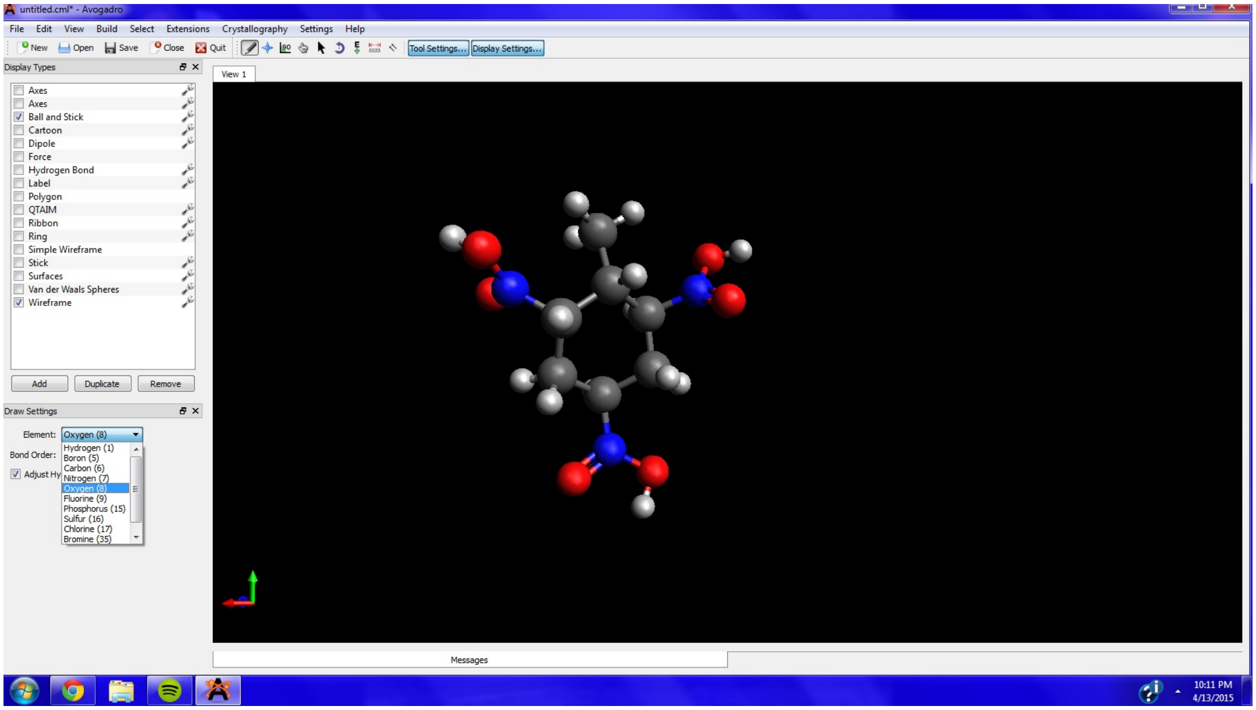
Just keep me informed of your progress and if you need anyone to pilot your software. Keep up the great work!
Lesson design need to include detailed answers to all questions to help the teacher who may be asked to teach a course they are not familiar with.
I would love it if you would contact me. I am both a HS Chemistry teacher and a PhD student at WPI. I work with Neil Heffernan and co. on ASSISTments; I have been developing ASSISTments content for Chemistry. eric.vaninwegen@gmail.com or egvaninwegen@wpi.edu If you google: Chemistry Eric ASSISTments, you should get my website
Bond length and bond energies are not helpful to most high school students because these topics are more advanced that what is covered in Honors or College Prep curriculum. These concepts are included in the AP Chemistry curriculum but on a somewhat limited basis.
I like modelling. Sometime the software is too complicated or too expensive to use.

Statistic	Value
Total Responses	11

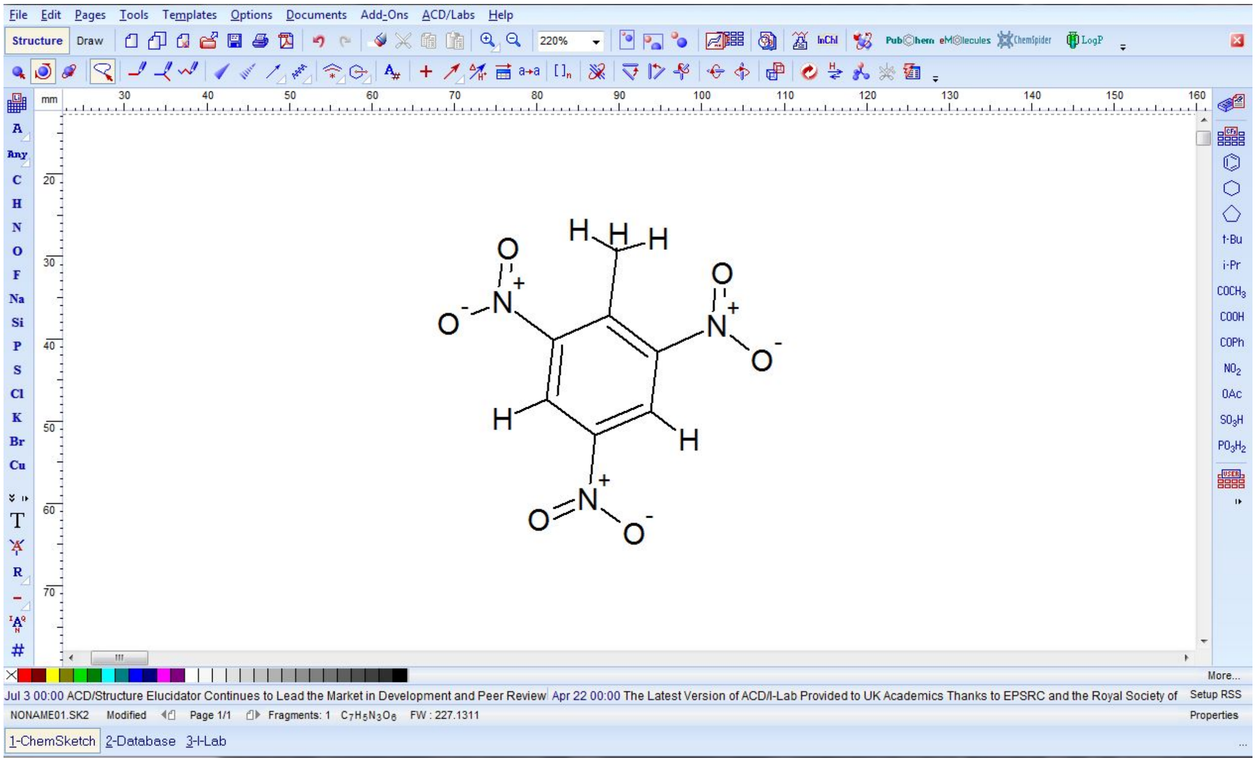
Appendix C. WebMO screenshot

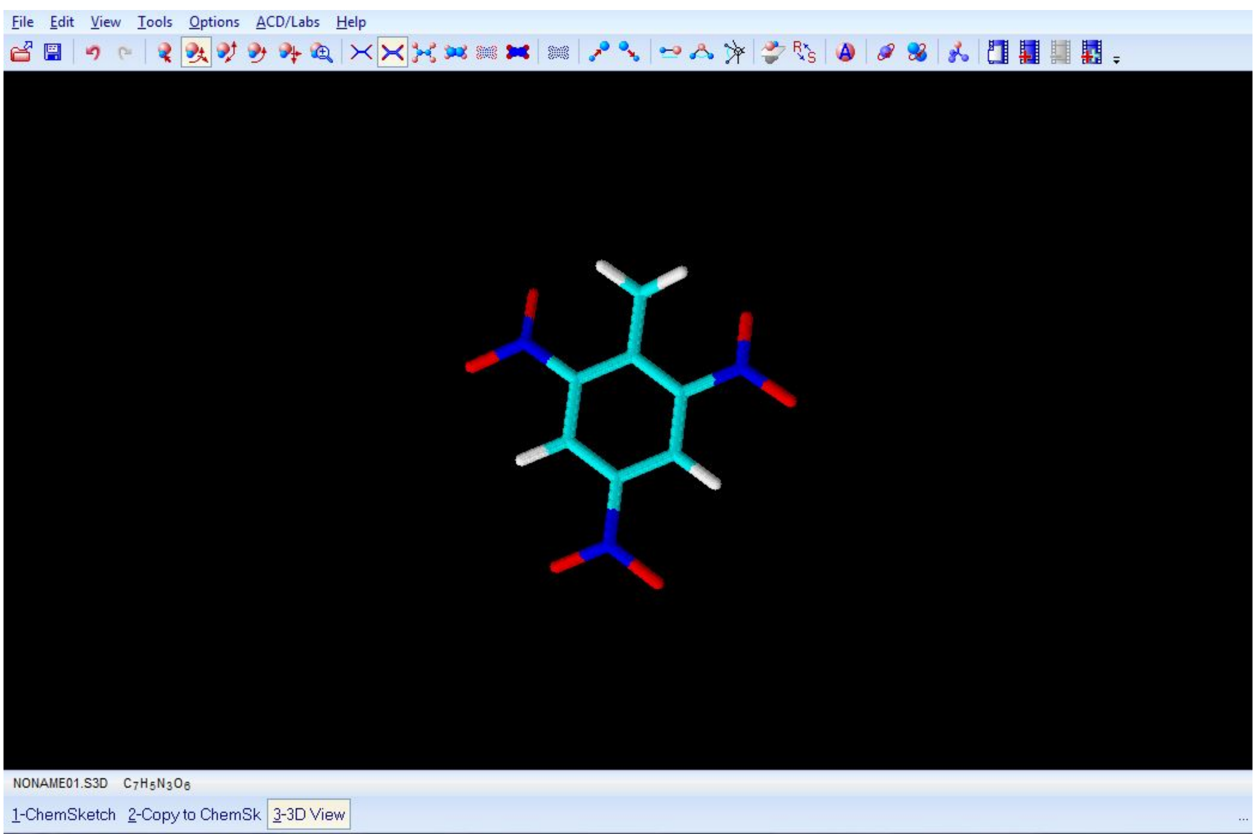


Appendix D. Avogadro Screenshot



Appendix E. ACD/ChemSketch Screenshots





Appendix F. WebMO Tutorial Video

https://www.youtube.com/watch?v=X_JbEtytasE

Appendix G. Approval Email from WebMO Employee

Harshman, Aaron J

Sent Items

Friday, January 30, 2015 4:31 PM

To whom it may concern,

My name is Aaron and I am working with a team to study computational chemistry as a teaching aid in high school classrooms. We are Juniors at Worcester Polytechnic Institute (WPI). We would like to use Webmo as a software to facilitated the learning of molecular geometry. Our goal is to go into multiple classrooms and test students learning with and without a software such as Webmo. We are not the best with computers and were wondering if there is a way for our school to set us up a webmo server. This way we will not cause excessive traffic on your servers as well as having a dedicated reliable server for us. We also wanted to make sure this is legal and acceptable to do so. We do not want to use your software for our study without your approval.

Thank you for providing a great software and we hope we can come to an agreement that allows us to use it.

-Aaron Harshman

JR Schmidt [schmidt@chem.wisc.edu]

Actions

To: Harshman, Aaron J

Cc: webmo@webmo.net; lulu@wpi.edu; Hoadley, Rexford; polik@hope.edu

Inbox

Saturday, January 31, 2015 2:50 PM

- You replied on 2/1/2015 12:16 PM.

Aaron,

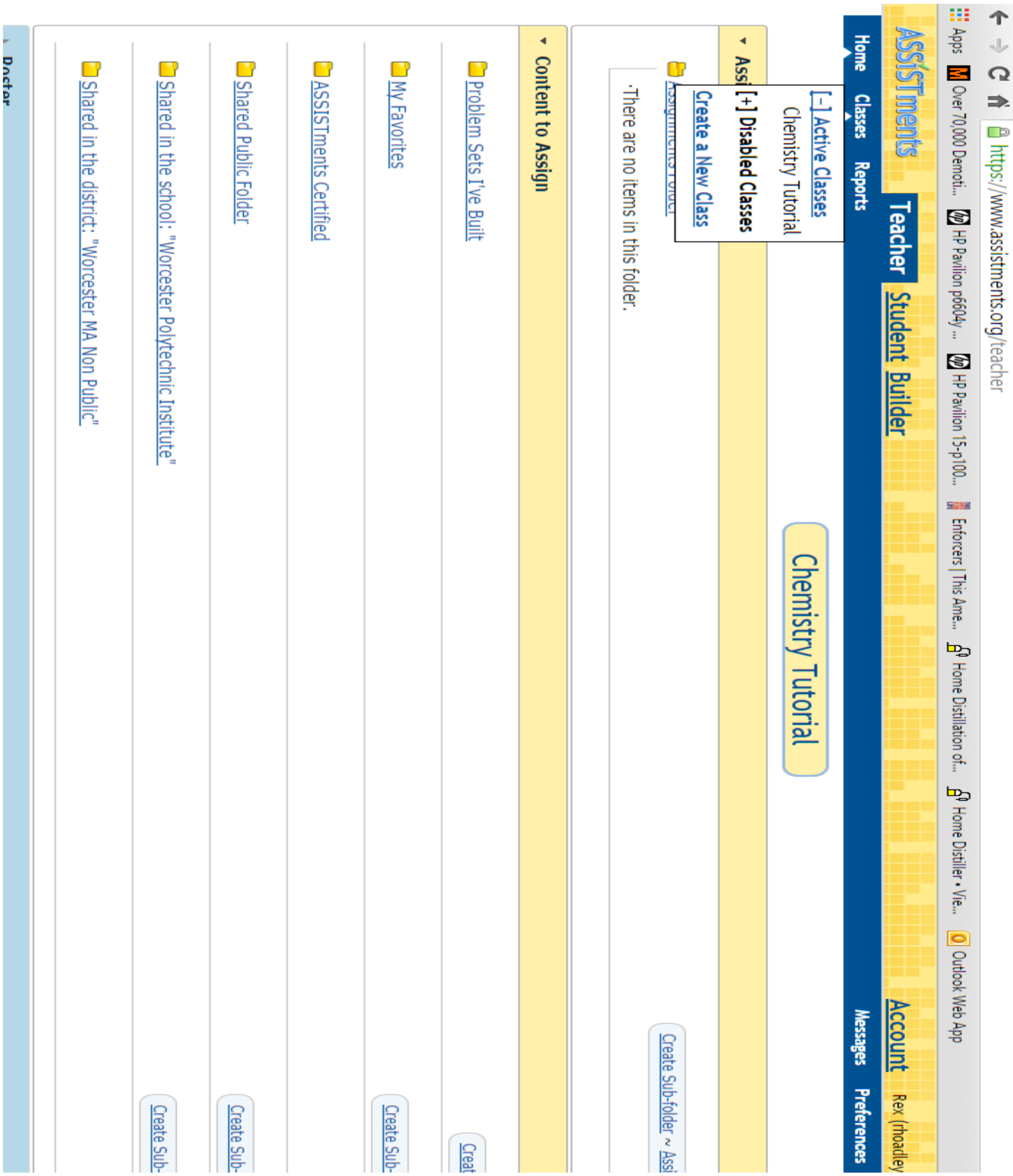
I have some good news for you: WPI actually is running at LEAST one local WebMO server already. You might talk with Robert E. Connors in Chemistry as (based on our registration data) he has got a server up and running. Since the basic version of the software is free (and should do everything you want), he could get you up and running with your own server. Installation, particularly on Windows server, is straightforward if you have a bit of local expertise.

If you have access to iPads, you might also consider using the WebMO app for iOS. This should be able to do almost everything you want, without even require a server.

There is absolutely no issue with using WebMO for this purpose. We are curious to learn more about your results!

Sincerely,
JR Schmidt

Appendix H. ASSISTments Screenshot



Appendix I. Test Questions

Problem Set "Pre-Test" id:[PSATNFF]

☐ **Select All**

☐ **1) Problem #PRA5GY8 "PRA5GY8 - NH3 shape"**

What is the molecular geometry of NH_3?

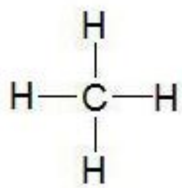
☐ **2) Problem #PRA5GZP "PRA5GZP - CH4 shape"**

What is the molecular geometry of CH_4?

☐ **3) Problem #PRA5CWU "PRA5CWU - Carbon Dioxide Doulbe Bonds"**

How many double bonds are there in carbon dioxide?
(Use a number character eg. 1, 2, 3, . . .)

4) Problem #PRA442Q "PRA442Q - Tetrahedral Angels"



In a tetrahedral structure such as methane the bond angels between the hydrogen atoms are exactly 90 degrees.
True or false?

- True
- False

5) Problem #PRA5CWV "PRA5CWV - Central Molecule LP BP"

A central molecule with no lone pairs and two electron bonding pairs takes what shape?

6) Problem #PRA5EYN "PRA5EYN - sp3 Angles"

In a tetrahedral structure the angles between the sp3 hybridized orbitals are how many degrees?

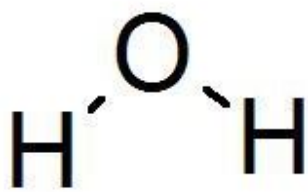
7) Problem #PRA5E86 "PRA5E86 - TeF4 Angles"

TeF_4 has seesaw geometry. What is the bond angle between either non-axial Florine atom and the lone pair in the molecule?

Problem Set "Test 1" id:[PSATNFC]

☐ **Select All**

☐ **1) Problem #PRA5C2T "PRA5C2T - Water Bent"**



A)
Water is not a linear molecule because

- ○ The hydrogen atoms are attracted to each other
- ○ The electronegative oxygen pushes the hydrogens away
- ○ oxygen has two electron lone pairs
- ○ Linear molecules require double bonds

B) What is the angle between the hydrogen atoms in the water molecule?

☐ **2) Problem #PRA5EZB "PRA5EZB - Tshape Angles"**

The bond angles in a T shaped molecule between the nearest groups, such as ClF_3 are:

☐ **3) Problem #PRA5EYQ "PRA5EYQ - Square Planar # LP #BE"**

A square planar molecule has 4 bonding electron pairs and how many lone pairs?

☐ **4) Problem #PRA5FHB "PRA5FHB - SO2 shape"**

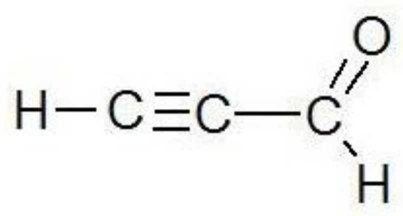
What is the geometry of SO_2?

- ○ Linear
- ○ Tetrahedral Bent
- ○ Trigonal Planar Bent
- ○ T-Shaped

Problem Set "Test 2" id:[PSATNFE]

☐ **Select All**

☐ **1) Problem #PRA5FRN "PRA5FRN - Count Bonds 4"**



The above molecule has how many Pi bonds?

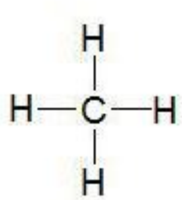
☐ **2) Problem #PRA5EZD "PRA5EZD - Square Pyramidal LP"**

A square pyramidal molecule has how many lone pairs?

☐ **3) Problem #PRA5EZC "PRA5EZC - Square Planar Bond Angles"**

The bond angles in a square planar molecule with 4 bonding electron pairs and 2 lone pairs are:

☐ **4) Problem #PRA5EYM "PRA5EYM - Hybrid Orbitals Methane"**



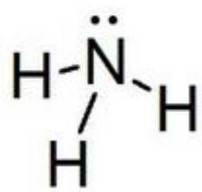
In a tetrahedral structure such as methane the central carbon has what type of hybrid orbitals?

- sp
- sp2
- sp3
- sp4

5) Problem #PRA5EYN "PRA5EYN - sp3 Angles"

In a tetrahedral structure the angles between the sp3 hybridized orbitals are how many degrees?

6) Problem #PRA5C2X "PRA5C2X - NH3"



What is the molecular geometry of this molecule?

Appendix J. Sample test answers

[redacted]

1. A. the electronegative oxygen pushes the hydrogen away

B. 109.5

2. 120°

3. 1 lone pair

4. trigonal planar Bent

5. 9 Sigma, 1 pi

[redacted]

1. a oxesen has two electron lone pairs
   b. 109.5

2. 60

3. 1

4. Linear

5. 9 sigma, 1 Pi

[redacted]

1. A. the electronegative oxygen pushes the hydrogen away

B. 109.5

2. 120°

3. 1 lone pair

4. trigonal planar Bent

5. 9 Sigma, 1 pi

Appendix K. WebMO lesson

Problem Set "WebMo lesson. 5/6 Groups" id:[PSATM4Y]

☐ **Select All**

☐ **1) Problem #PRA5EE9 "PRA5EE9 - Problem #778564"**

A) Open up the WebMo App by clicking on the link below.

cchem.wpi.edu

The username and password is.

ajharshman
ajharshman

When you are logged on type yes in the answer field to continue to the next exercise.

B) Today we are going to start with Trigonal Bipyrimidal geometry. This is anything with 6 groups around the central atom. A good example is PF_5.

1. Construct a model in WebMo of PF_5.
2. Use the comprehensive-idealized button under the clean-up drop down Menu.
3. This molecule has two different positions for atoms. Axial and non-axial. The non-axial atoms will be removed first.

What are the angles between the axial-axial atoms?

C) Still using the same model what are the bond angles between the non-axial atoms?

☐ **2) Problem #PRA5EGB "PRA5EGB - Problem #778597"**

A) Instead of having 5 atoms around a central atom. What happens if there is still 5 groups but one is a lone pair.

1. Build a molecule of PCl_4.
2. Optimize the geometry with the clean-up drop down.
3. Look at the change in geometry from the last structure.

This structure is called Trigonal Bypyrimidal See-Saw.

What is the angle between the 2 non-axial atoms and the lone pair?

B) On the last molecule click on a Cholorine atom and delete one.
Now optimize the geometry again.
Study how the geometry has changed with the deletion of another atom.
This is called T-Shaped.
Scientists aren't the most creative with naming.
Answer next when ready for the next part.

C) Finally if one more Chlorine is removed you will reach a linear geometry.
Remove a Chlorine and optimize the geometry.

Then answer done.

3) Problem #PRA5EGC "PRA5EGC - Problem #778598"

A) Now we will explore the geometry of a central atom with 6 groups around it.

Like before we will first consider a molecule with all 6 groups being atoms.

Make the octahedral molecule SF_6.

What are the bond angles between all of the atoms?

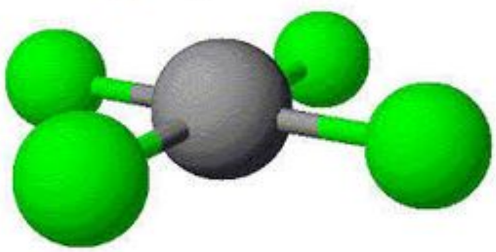
B) Again as before begin removing Florine atoms one by one and see how the geometry changes each time.

SF_5 - Square pyramidal

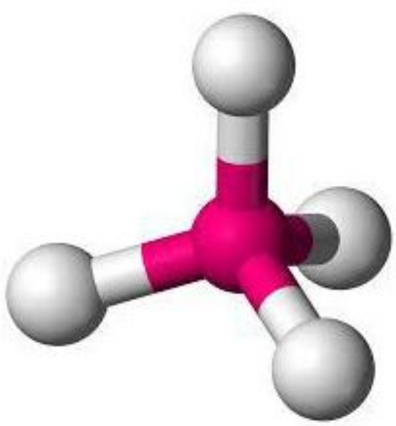
SF_4 - Square Planer

It is mechanically impossible to remove another group and stay within the octahedral geometry.

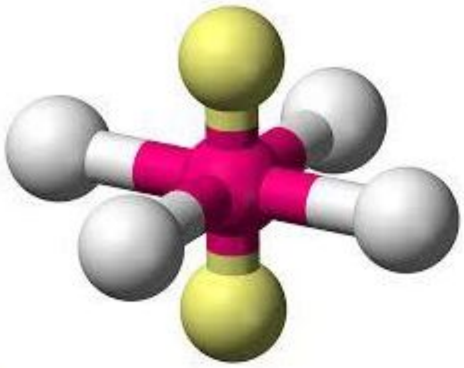
What does Square pyramidal look like?



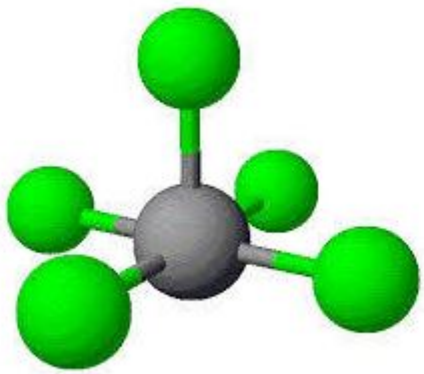
A)



B)



C)



D)

- A
- B
- C
- D

Appendix N. Practice Problems

Problem Set "Practice problems " id:[PSAS4GB]

☐ **Select All**

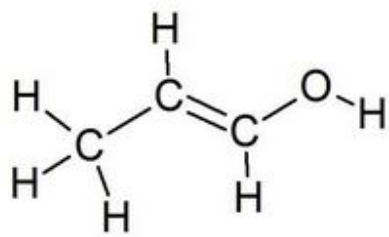
☐ **1) Problem #PRA5GZN "PRA5GZN - H2O shape"**

What is the molecular geometry of H_2O?

☐ **2) Problem #PRA5GY9 "PRA5GY9 - BF3 shape"**

What is the molecular geometry of BF_3?

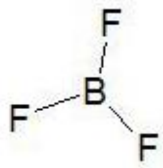
☐ **3) Problem #PRA5AQM "PRA5AQM - Count Bonds"**



Count the amount of pi bonds and sigma bonds in the above molecule.

- 7 Pi bonds, 2 Sigma Bonds
- 2 Pi Bonds, 7 Sigma Bonds
- 1 Pi Bond, 9 Sigma Bonds
- 1 Pi Bond, 8 Sigma Bonds

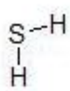
4) Problem #PRA5C2K "PRA5C2K - BF3 Bond Angles"



In a trigonal planar structure such as boron fluoride the bond angles between the fluorine atoms are exactly 120 degrees. True or false?

- True
- False

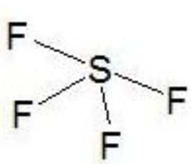
5) Problem #PRA442P "PRA442P - SH2 BP LP"



The above molecule has two pairs of bonding electrons and two lone pairs, what is the molecular geometry?

- Tetrahedral
- Bent
- Trigonal Planar
- Linear
- Trigonal Pyramidal

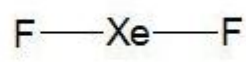
6) Problem #PRA5EY9 "PRA5EY9 - SF4"



Sulfur tetrafluoride has what molecular geometry?

- Bent
- Tetrahedral Bent
- Seesaw
- Pyramidal Bent

☐ **7) Problem #PRA5EZA "PRA5EZA - XeF2 Angle"**



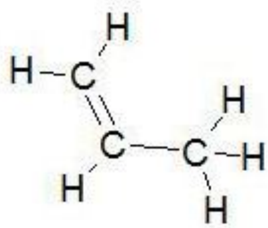
Xenon difluroide has the same bond angles as what molecule?

- SF6
- H2O
- CO2
- NH3

Problem Set "Practice problems day 2" id:[PSATNFH]

☐ **Select All**

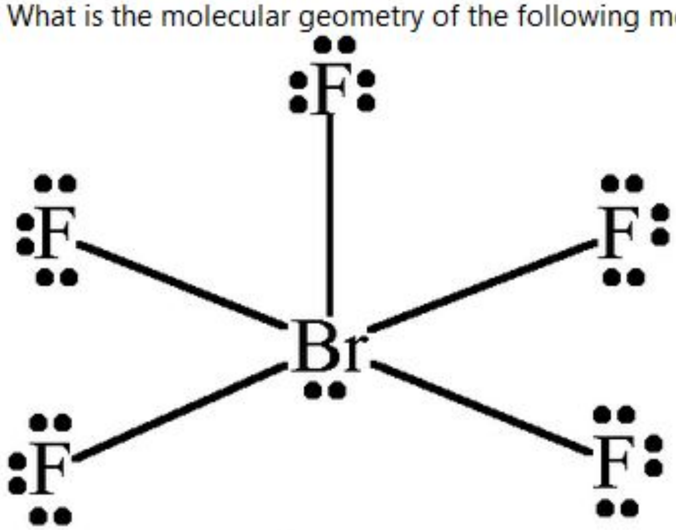
☐ **1) Problem #PRA5FRH "PRA5FRH - Count Bonds 3"**



The above molecule has how many sigma bonds?

☐ **2) Problem #PRA5FHK "PRA5FHK - BrF5 shape"**

What is the molecular geometry of the following molecule?



☐ **3) Problem #PRA5E86 "PRA5E86 - TeF4 Angles"**

TeF_4 has seesaw geometry. What is the bond angle between either non-axial Florine atom and the lone pair in the molecule?

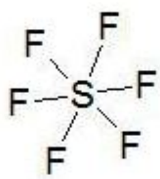
☐ **4) Problem #PRA5FHJ "PRA5FHJ - AlCl3 shape"**

What is the molecular geometry of $AlCl_3$?

5) Problem #PRA5GZF "PRA5GZF - ClF5 shape"

What is the molecular geometry of ClF_5?

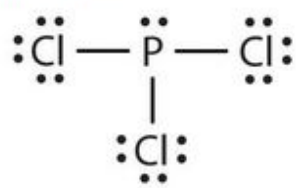
6) Problem #PRA5EYP "PRA5EYP - SF6 Geometry #LP #BE"



A molecule with 6 bonding electron pairs and no lone pairs takes what shape?

- Square Planar
- Hexahedral
- Square Pyramidal
- Octahedral

7) Problem #PRA5FHC "PRA5FHC - PCl3 shape"



What is the molecular geometry of the above molecule?

8) Problem #PRA5EYR "PRA5EYR - PCl5"

A central atom with 5 bonding electron pairs and no lone pairs such as PCl_5 takes the trigonal bypyramidal shape.
True or false?

- True
- False