Empowering Student Learning with Molecular Visualization Tools in Discovery-based General Chemistry

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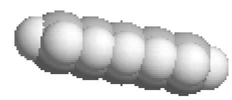
Do you fear that your students have this mental model of a hydrocarbon? The two dimensions of print materials and blackboard lectures could leave this image. Computer-based molecular visualization tools provide means to a more molecular approach in general chemistry, smoothing the transition into organic chemistry. How can chemistry educators take advantage of these technology tools and showcase the relevance of chemistry and its connections to other fields that are part of the molecular frontier (American Chemical Society, 2003; National Academies, 2003)? We present an inquiry-based approach developed in a community college that spans our general chemistry courses. Our approach involves adopting and supporting a common set of technology tools across courses and instructors in our two-year sequence of general and organic chemistry. Our students are predominately pre-professional students aspiring to enter the fields of medicine, pharmacy, dentistry, physical therapy, engineering, or biological research where understanding of chemistry is important. Students gain software competency in stages on a need-to-know basis. Our goal is to give students the ability to deal with multiple representations of molecules and forge connections between microscopic structure and macroscopic behavior. The different representations have various advantages depending on the molecule (simple, complex, or crystalline structure) and what is to be investigated.



Molecular Visualization Tools

The software applications that we use address 2D chemical structure drawing, molecular rendering, computation, and molecular dynamics and are summarized in Table 1 (opens in new window). The use of Chime has allowed us to build an extensive collection of web-based activities available online. Since this paper will use many links that utilize Chime we recommend that you install it now (if you do not have it) to benefit from the link displays (click here to get Chime). As often as possible, we use freeware applications to allow student accessibility from home at no cost. We selected Spartan, which has a significant cost, because it is a powerful research tool that students may see in upper-level courses at four-year institutions upon transfer. All applications are available to students on campus in

Table 1 - Molecular Visualization Tools

Software	Source	Features	Usage
ChemSketch	Freeware from ACD Laboratories	2D chemical structure drawing program with a large template collection of pre-built molecules Can export mol files for Chime/RasMol	Faculty and students Can copy/paste structures (or save as gif) into Word, PowerPoint, or html documents
Chime/RasMol	Both freeware – Chime from MDL RasMol from Bernstein Plus Sons	3D molecular rendering software with interactive multiple display modes and measurement capabilities (Chime operates as a browser software plug-in, RasMol is a stand alone application, 470 kB)	Faculty and students Can produce interactive web pages using Chime displays Animations of molecular motion and reaction mechanisms displayed with Chime
Spartan	Wavefunction Inc. (expensive) Faculty - full version Students - Student Edition available in computer labs	Molecular builder and research-level computational software Can export files for Chime/RasMol	Faculty and students Build and minimize energy of molecules Generate data for analysis Can produce avi file movies of animations
Odyssey	Wavefunction Inc. (reasonable?) Instructor's version	Molecular dynamics software – a systems approach to molecular motion and interactions	Faculty as demonstrations in class

open computer laboratories. Our holistic approach using technology has been described in Sinex and Gage (2003). Here we expand upon our use of molecular visualization tools. The capabilities of molecular visualization applications have been illustrated by Bradley (2002), Canning and Cox (2001), and Halpine (2001). Dori and Barak (2000) have demonstrated the molecular visualization enhances meaningful learning in organic chemistry.

In both second-semester general chemistry and again in second-semester organic chemistry, we require students to complete a written research paper and/or a PowerPoint presentation as a laboratory activity. The use of ChemSketch and Chime illustrations is required or highly encouraged as part of these projects. Individual faculty may require other uses, such as ChemSketch for laboratory reports in organic chemistry, as well as in projects.

To facilitate the use of all software applications for students, as well as faculty, we have produced online documentation which is available on our department webpage. The available documents, with numerous screen capture illustrations, are listed and linked in Table 2 below. To encourage faculty and student project use, we produced a guide to developing web pages in FrontPage using Chime, which includes how to install buttons, a feature that minimizes menu steps for beginners. We added support for RasMol because it is a small application, better for use on older computers, especially those without Internet access.

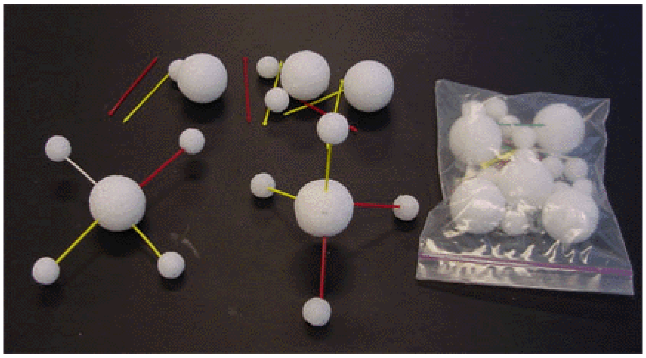
Table 2 – Online Software Documentation

Student Guide to the Use of Chime (requires Chime to be loaded)	Creating Web Pages in FrontPage using Chime
ChemSketch: A Guide to Drawing Chemical Structures	A Student's Guide to Spartan '04
A Quick Guide to RasMol	Odyssey (forthcoming)

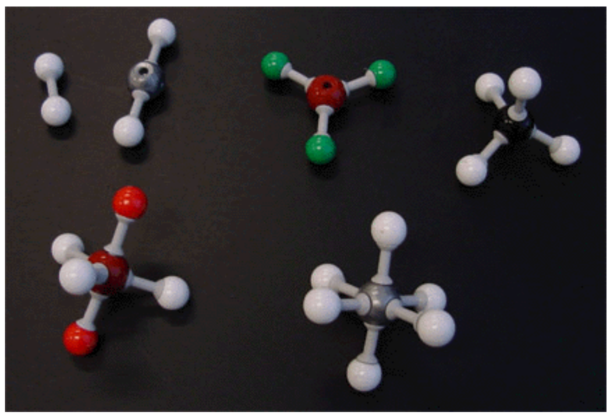
The tools we selected are compatible with each other and our Windows XP operating system on campus. They allow us to use 2D and 3D display modes of molecular structures to enhance our students' learning experience. We have incorporated these tools across multiple courses and instructors to ease students into their use and build on their utilization as students take our sequence of courses. Faculty training on these applications has come from external sources, such as conference or vendor workshops, and internal work sessions especially pertinent for our adjunct staff. All of the software usage compliments the increasing use of ball-and-stick models in our classes. We have invested in wooden and plastic ball-and-stick model kits to provide tactile experiences. We compare the advantages and disadvantages of both the tactile and virtual models in Table 3. The benefits of both tactile and virtual models are exploited in our courses.

Discovering the World of Molecular Geometry

Students get their first significant immersion into the world of molecular structure with VSEPR theory, which is introduced following chemical bonding and Lewis dot structures in the first semester of general chemistry. We start our student's experience with the discovery of the ideal geometries using Styrofoam balls and toothpicks in a laboratory activity called It's All in the Shape. The concept of maximizing distance between electron pairs to minimize repulsion is reinforced in this activity. Most students, with a little guidance, leave flatland (2D) and enter the 3D world.



After initial discovery, we use plastic ball-and-stick (Molymod) models from Indigo to be sure students understand the ideal geometries for 1 to 6 electron pairs around a central atom. They can also check the angles inherent in each geometry. The two colors shown in the trigonal bipyramidal geometry designate the two possible positions - axial (red) and equatorial (white).



We start the introduction of lone pair electrons with the ideal geometries, and then consider lone pair effects on the geometries. Students examine and manipulate the ideal geometries using web pages with Chime structures - Molecular Geometry and VSEPR: Ideal Structures. An instructor can introduce the use of Chime to the class. We provide an html interactive Guide to Chime for use by students and faculty. Many of our activities include instructions for the computer application. This allows the tactile and virtual models to reinforce each other and, more importantly, ensures that students correctly interpret what is viewed on the computer screen. Dori and

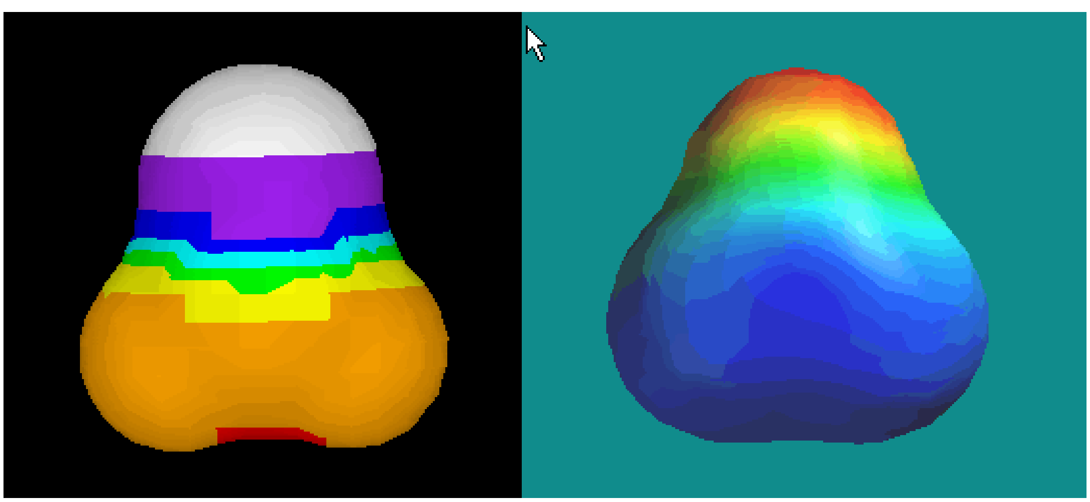
Table 3 – Interactive Molecular Visualization

	Tactile Models	Virtual Models
Advantages	✓ shows connectivity ✓ displays the real 3D in ideal state ✓ possibility of illustrating some intramolecular interactions (internal rotation) ✓ can test superposition of isomers ✓ can generate possible conformer structures by internal rotation	✓ shows true arrangement plus distortions – based on real experimental measurements or computations such as Spartan ✓ can change orientation and mode of display ("true" size with space fill) ✓ can make measurements -bond length -bond angle -torsion angle -molecular dimensions ✓ can visualize complicated molecules (DNA, proteins) with simplifying modes of display ✓ provides flexibility – animated vibrations (stretch, bend, internal rotation of bonds) ✓ can generate animated reaction mechanisms ✓ can display electrostatic potential maps -molecular polarity -attack points in reactions
Disadvantages	✓ is rigid (set bond lengths and angles) ✓ true molecule size and shape not possible ✓ can fall apart! (at least some)	✓ may encounter incorrect structure files ✓ may not grasp the 3D nature on flat computer screen

Barak (2001) recommend this to enhance learning. We constantly make this virtual-tactile connection by building the ball-and-stick models.

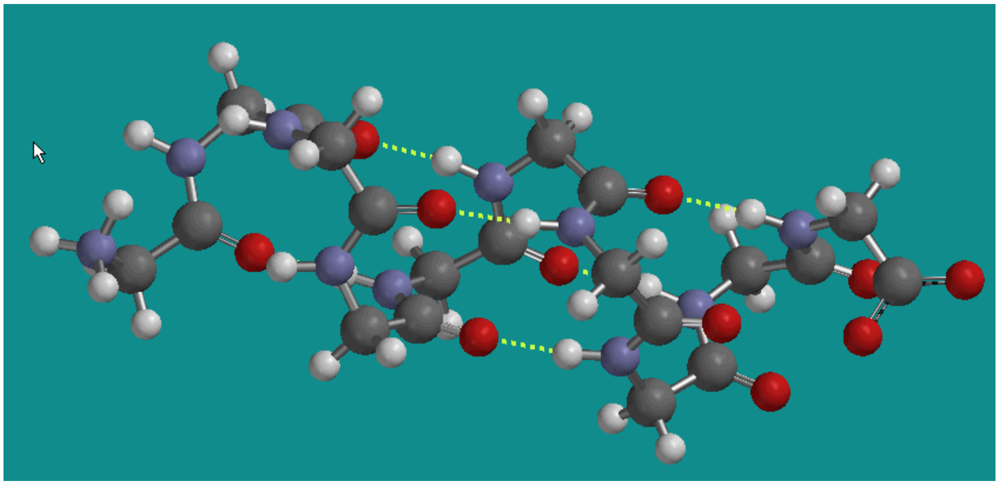
To discover the effects of lone pair electrons, one needs structures that show the distortion. This is accomplished using web pages with Chime structures – Molecular Geometry: When Lone Pair Electrons Rule. Now students must make measurements of bond angles in structures to discover the distortion caused by lone pair electrons. To make this as easy as possible for beginning students, we use buttons for features rather than multiple right click menu steps. This requires Chime structures with the correct bond angles based on x-ray measurements. The rules for positioning lone pairs on trigonal bipyramidal and octahedral structures can also be discovered. Many of the structures we use were built in Spartan, where angles can be set to values in the literature or generated as near-literature values by computational methods.

At this point, the concept of molecular polarity is introduced to students by using electrostatic potential maps that can be produced in Spartan and displayed with Chime (beware - the color scheme is nearly opposite in these two applications). Molecular polarity is crucial for understanding the physical properties of substances, such as boiling point and solubility, and in the interpreting reactive centers in chemical mechanisms. Polarity effects introduced in general chemistry are applied and reinforced in organic chemistry. Displayed here is formaldehyde (CH_2O), with the more electronegative oxygen at the top, shown as white in Chime (left) and red in Spartan (right). Note the red area between the hydrogens on the Chime map.

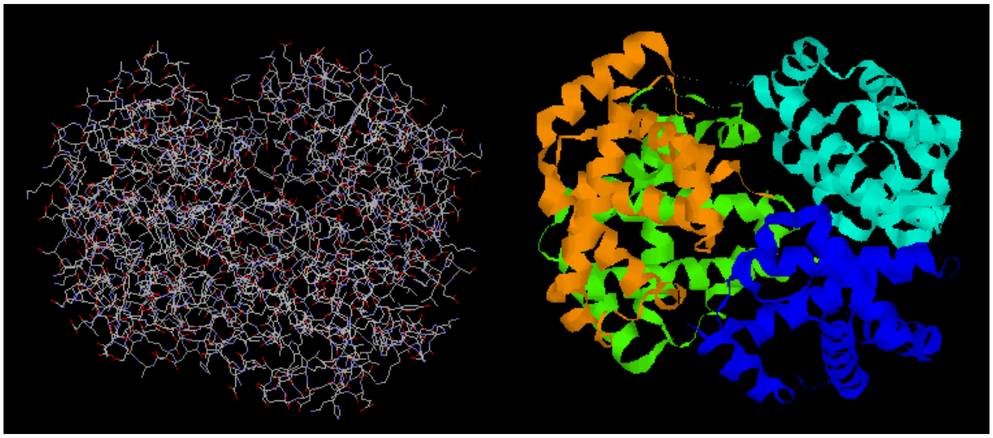


In our online activity, Looking at Molecular Polarity, we examine structures and ask students to predict the polarity (or lack thereof) of the molecules by first using their knowledge of molecular geometry and electronegativity differences in bonds. Then they can press a button to examine the electrostatic potential map for the molecule.

The real world of molecular structures is far from ideal and molecules are adaptive. Building on molecular structure, we introduce molecular distortion caused by other factors besides lone pair electrons. This is accomplished in Molecular Geometry: Getting Bent Out of Shape Again. Here large atoms, such as iodine, or bulky groups, such as t-butyl or phenyl, are examined. Polarity and steric concepts are used as we examine the behavior of liquids and solids, solutions, and acids and bases. See The Solid State for treatment of crystalline solids. The importance of intra/intermolecular forces (based on polarity) to biology can be illustrated with hydrogen bonding in DNA base pairs across the helical strands and in proteins. The illustration below, produced in Spartan 04, shows the hydrogen bonds (yellow dashed lines) in a helix of 10 glycine molecules.



Many comparable structures can be generated and concepts discovered using the builder in Spartan. Utilizing the ribbon mode of display is a great way to illustrate the helical and sheet nature of proteins or the double helical backbone of DNA. Below are the static images of hemoglobin as the wireframe model (left) and the four colored chains as ribbons (right). The helical secondary structure is seen immediately as is the quaternary structure.



A variety of concepts can be discovered by examining molecular structures and making interactive measurements such as bond lengths, bond angles, and torsion angles. Table 4 gives some examples from a larger collection of activities.

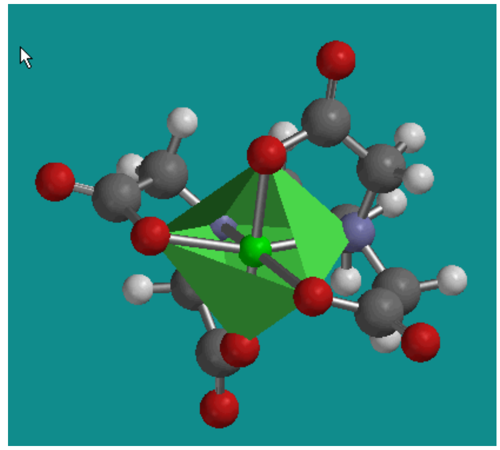
Table 4 – Web-based Chime Activities

Online Activity	Concepts discovered
The Carbon-Carbon Bond	Bond order-bond length-bond energy relationships; 1.5 bond order in benzene
Discovering Resonance	Resonance in carbonate ion
The Arrangement of Bonds	Isomers and differences in physical properties
The Flexibility of Bonds	Stretching, bending, and internal rotation of bonds using animated Chime files

The series Structure and Bonding includes use of interactive Excel simulations, Stella models, and animations to explore a variety of topics using many organic chemistry examples. Many comparisons of structure and reactivity can be made in acid-base equilibria (carboxylic acids, amines, and amino acids).

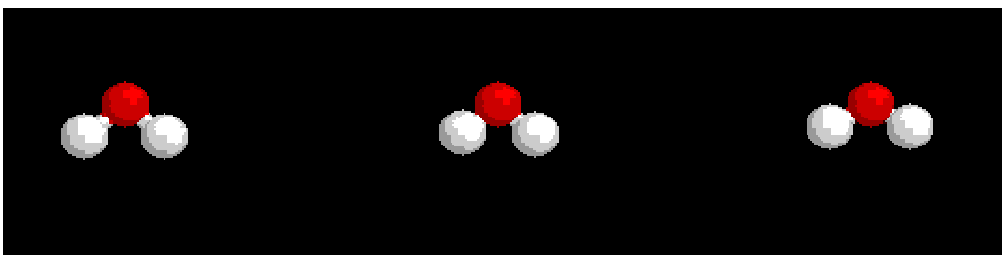
As an activity to reinforce the effects of both molar mass and intermolecular forces on boiling points, we examine the chlorination of benzene and the isomers produced for molecules with one to six chlorines. Students build ball-and-stick models to discover the possible isomers, draw the structures and predict boiling points of isomers, and then look up boiling points in the *CRC Handbook of Chemistry and Physics*. Students summarize resulting structures using ChemSketch. Predicting the rank of the polarity of a variety of bromochlorobenzene isomers is a valuable assessment question.

Use of Spartan allows students to build molecules and then minimize their energy with the push of a button. More sophisticated computations can be done and are often addressed in organic chemistry. A nice feature of Spartan for molecular geometry is the display of planes to produce faces in molecules. As an example, the octahedral coordination of the iron (III) ion in its EDTA complex ion is shown to the right. We have produced a number of movies using screen capture software to illustrate this in [Mathematical Shape and Molecular Geometry](#).

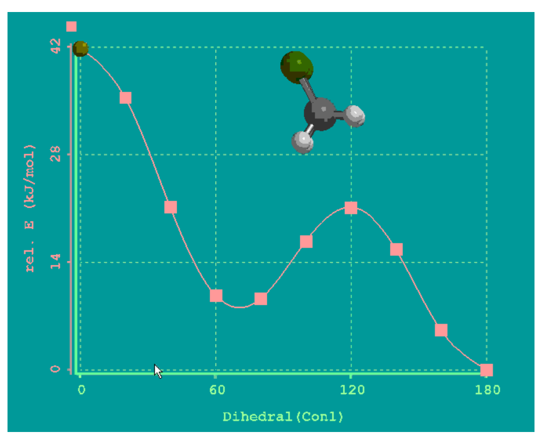


Examining Molecules in Motion

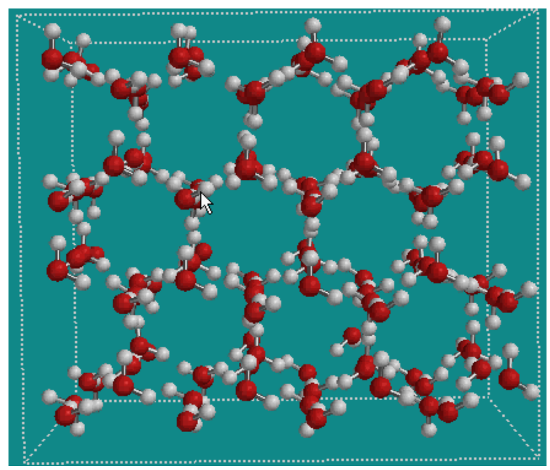
In first semester general chemistry, typically shortly after gases, we introduce students to vibrational motion, which is any motion that changes the shape of a molecule. This involves changing bond lengths (stretching vibrations) and bond angles (bending vibrations), as illustrated for water in the figure below.



To build on the knowledge of molecular structure from our first semester of general chemistry, we have introduced two web-based laboratory activities to our second-semester course. These two activities include Chime images plus data and movies from Spartan to introduce students to Discovering Intramolecular Interactions by examining a series of molecules where internal rotation around a bond causes a variety of interactions. The starting point is 1,1-dichloroethane as illustrated on the graph to the right, where relative energy is a function of Cl-C-C-Cl torsion angle (dihedral angle as labeled by Spartan). We examine data generated by Spartan to see how the bond lengths and bond angles vary as the torsion angle changes. We



then examine dimethyl peroxide and di-t-butyl peroxide. Newman projections could be introduced at this point with their construction aided by ChemSketch. As an assessment, students complete Helical Structures as a take-home project, which compares a helical protein to a helical hydrocarbon and the coiling of helicenes. Molecular motion is also extensively covered in second-semester general chemistry as a prelude to entropy by examining Molecules in Motion, which ties the three states of matter, conformers, and reaction mechanisms together using a number of animated Chime files. By the end of the semester, students are Studying Vibrations in Molecules, which introduces them to IR spectroscopy. This primes them for its use in organic chemistry, where it is classically treated more as a tool with minimal theoretical background. Ultimately, students come away with the knowledge that molecules are flexible and ever changing due to vibrational motions. We have truly left flatland and molecules are now dynamic entities. Before computers, we could only preach this; now students can view and manipulate virtual molecules.



Odyssey, a molecular dynamic package (based on computational methods) with instructional modules, allows you to investigate a collection of molecules or a system while changing variables such as temperature. All three modes of molecular motion (translational, rotational, and vibrational) can be examined in single phases, during phase changes, and during reactions. Our initial use has been with the instructor's version, presenting systems in class with an LCD projector. The static image to the right shows the crystalline structure of ice (click here for a screen capture from Odyssey showing the vibrational motion and hydrogen bonds, yellow dashed lines that appear mid-way through – 6 MB avi file).

Designing Template-based Web Pages

As a means to engage students in the chemical literature and use molecular visualization tools, the eMolecules Project has been developed. This project, in its early stages, is designed to be an Internet collection of student-generated web pages from a variety of disciplines that use or discuss chemical substances. Included in the disciplines that might participate in such a project are chemistry, biology, nutrition, forensics, and the health-related programs such as nursing or respiratory therapy. As the database grows through student contributions, other courses may use the collection as a resource for further projects, such as comparing chemical structures of drugs or gathering molecular data. The eMolecules Project will be a truly interdisciplinary project produced by students with the assistance of faculty as content authorities and editors. The project reinforces the critical connection of chemistry to other disciplines while encouraging students to use and develop technological resources.

Students gather atomic and molecular information from a variety of sources, online and print materials, to create a webpage based on a template design. The template is used to provide uniformity in layout and basic information; however, it can be expanded or modified to allow student creativity. To adapt the eMolecules Project across disciplines, a variety of templates that provide a starting point for students will be produced. Each template requires different information depending on its purpose and some templates, of necessity, will be more complex. Proper citation methods for all information will be required and all writing must be original to the student. Since many disciplines and their textbooks show classical 2D structural formulas for chemicals, we will expect students to use a chemical structure drawing program (ChemSketch). All templates include an interactive Chime structure in the traditional ball-and-stick mode, as well as the space fill mode to illustrate a more molecular-realistic size and shape. Use of a template will allow a Chime image to be embedded with preset code so that students do not struggle with unknown program language code. Each template will allow comparison of the 2-dimensional drawing with the 3-dimensional Chime image.

Some Final Thoughts

The combination of tactile and virtual molecular models strengthens student understanding of the three-dimensional nature of the structures, especially as the structures become more complex. The dynamic aspects of molecular motion are also introduced. Having students work in multiple modalities, especially employing two-dimensional structure drawing software necessary for print media, starts building the capability in students to mentally convert between modalities, a skill that is very beneficial to scientists. The molecular visualization tools we have adopted provide students with a variety of opportunities to develop technology skills that will serve them well in their future coursework and professional employment. An engaging, interactive learning environment is also created, which is in line with national reform efforts (Siebert and McIntosh, 2001). The tools also allow us to strengthen our approach to developing conceptual understanding (Sinex and Gage, 2003) and provide a smooth transition into organic chemistry. A vast variety of other applications, mostly freeware, can be found at the World Index of

Molecular Visualization Resources. Our future efforts are geared to addressing assessment in an interactive computer environment to model the learner-centered environment.

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