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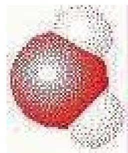
Paper 3

The Role of Molecular Structure and Modeling in General Chemistry

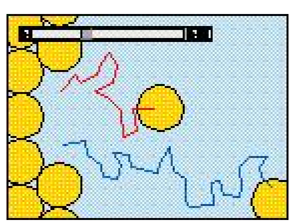


Loretta L. Jones
Department of Chemistry and Biochemistry, University of Northern Colorado
Greeley, CO 80639
lljones@bentley.univnorthco.edu

Abstract

Do introductory chemistry students believe in atoms and molecules or are they just humoring us? The three dimensional structure and dynamic interactions of molecules are difficult for many students to understand. Hand-held models help, but do not allow students to explore electronic structures or molecular energetics or to compare molecular skeletons with other representations. Can introductory chemistry students learn to use sophisticated molecular modeling tools? What guidance and training would be required? Can we develop a computer-supported learning environment for introductory chemistry students using molecular visualization software? Will students accept a technology- supported curriculum centered on molecular structure?

This paper will present preliminary findings of an exploration of the feasibility of using molecular modeling software in general chemistry and discuss the implications of an emphasis on molecular visualization for the general chemistry curriculum.



The Importance of Understanding the Particulate State of Matter

One of the most difficult problems in teaching introductory chemistry is conveying to students the three dimensional structure and dynamic interactions of molecules. Because of differences in ability to visualize unseen structures in three dimensions, many general chemistry students never adequately comprehend the molecular basis for chemical phenomena. Is it worth the effort? Most of us believe so and would agree with the following statement:

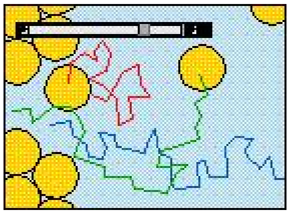
> *An understanding of the concepts of atom and molecule is fundamental to the learning of chemistry. Any misconceptions and alternative conceptions that students harbor about these concepts will impede further learning.*
> Griffiths and Preston (1992)

This implies that we need to ensure that students have a firm grasp of the particulate state of matter before pursuing advanced studies in chemistry. However, most of us will also recognize the following findings:

> *Recent studies of students' conceptual knowledge of chemistry indicate that students do not understand some of the fundamental ideas that form the basis of the discipline....*
>
> *although misconceptions diminish with schooling, they still persist in university students...*
>
> *students do not understand the meaning of the symbols chemists use to represent the macroscopic and microscopic levels...*
>
> *Students are able to use formulas in equations and even balance equations correctly without understanding the meaning of the formula in terms of particles that the symbols represent.*
>
> Gabel and Samuel (1987)

The problem is made more immediate by the growing emphasis in chemistry on research areas that require visual representations for understanding. Self-assembling monolayers of molecules, heterogeneous catalysis, conducting polymers, and liquid crystals are just a few of the research fields in which communication of ideas involves visual images. Some chemical phenomena are not obvious without visualization tools; they are difficult for chemists to study or describe without visualization aids such as molecular modeling programs. Since much future work in chemistry will require the use of visualization software and high performance computing, familiarity with these tools is fast becoming a literacy requirement for chemistry, the life sciences, and many engineering fields. Today's students will need to develop the ability to identify and make use of complex visualizations of molecular structures.

Our traditional text-based teaching practices were developed before the particulate state of matter was well characterized and may not be sufficient on their own to prepare students for the microscopic worlds of modern chemistry. Students need to become familiar with molecular level concepts and they must also learn to use the new tools of chemistry. The familiarization process can begin at the introductory level, when students are forming their embryonic mental models of the molecular world.



Helping Students to Visualize the Particulate State of Matter

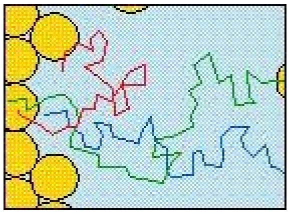
New approaches are emerging that help to close the gap between chemistry as a molecular science and student understanding. Because molecular level concepts are not visible to the eye, they appear complex and abstract to beginners. Hence, these new approaches have focused on helping students visualize what they cannot see. For example, illustrations of the molecular level of matter in have become richer and more numerous than they were just a few years ago (See Figure 1).

Figure 1: A molecular-level textbook illustration of the reaction of a methane molecule with excess oxygen (Atkins and Jones)

Hand-held models help students learn about molecular structure through touch as well as sight, but do not allow students to explore electronic structures, molecular skeletons, and molecular energetics and motions in real time and from many viewpoints. Thus, interest has risen in the use of computers to represent atoms and molecules. Selected images of still or moving molecules can be displayed on demand or students can use molecular modeling programs to specify and manipulate molecular level systems and collect information about them.

Literature reports of the impact of computer representations of molecular structures, simulations and animations on student understanding and motivation find promise in these approaches. For example, Bergandine, Koker, and Veltman (1993) found that high school students who constructed electron density maps of molecules became motivated to do their own research and asked for more time on the computer. Hakerem, Dobrynina, and Shore (1993) found that high school students who studied computer-generated simulations of water molecules overcame significant misconceptions about the structure, composition, size, shape, bonding, and energy of water molecules. Williamson and Abraham (1995) found that students who viewed molecular animations achieved higher test scores than students who had viewed still images of the same molecular-level situations.

Recent research on the use of pictures in assessing understanding (Smith and Metz) shows that even experienced chemists can have difficulty interpreting pictorial representations of the molecular level of matter. This raises the possibility that the mechanisms used for understanding images may be different from the mechanisms used to understand text. Because abilities to learn from the two mechanisms vary, it may be that our text-based approaches to teaching are leaving behind students who learn more easily from visual imagery (Nakhleh).



Instructional Computer Programs

The availability of reasonably-priced molecular modeling programs makes the incorporation of visualizations of molecular structure and dynamics into the curriculum practical. However, these programs were designed for expert bench chemists, not first-year chemistry students, and the impact of these programs on novice users is not well understood. A chemist knows which substances will result in fruitful study, but a student needs guidance to make good use of sophisticated research software (diSessa). In addition, people see different things when viewing complex structures: what one sees depends on one's background in chemistry and preparation (Millar and Driver).

One solution is to create structured environments for students that provide training in the use of the software and assignments that they must complete with its help. Another solution is to create desired images, label them, and use them within an instructional program. By this means, sophisticated routines beyond the abilities of most introductory chemistry students can be used to generate instructional materials. For example, the following three images (Figures 2-4) are part of a program that introduces students to molecular polarity by displaying images generated in a powerful modeling program (*Inorganic Molecules: A Visual Database*, Ophardt). Visual representations of complex phenomena such as electron density gradients can make the concepts of electron distribution and polarity more meaningful for the novice.

Figure 2: Electron distribution in the ammonia molecule is presented in various forms that are not possible to display with molecular models.

Figure 3: Electron density contours and isosurface of the ammonia molecule

Figure 4: Electrostatic potential of the ammonia molecule visualized as color differences

A third approach that is less common, but can be very powerful, is to provide students with a molecular design and construction program imbedded in a comprehensive instructional setting. For example, in the *ChemQuest* computer programs (Agapova, Jones, and Ushakov) students construct the world from the bottom up, beginning with subatomic particles and moving up to atomic orbitals (Figure 5):

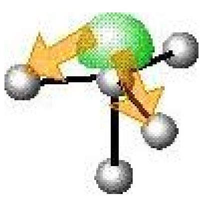
Figure 5: Construction of atomic orbitals. The atom may be rotated and viewed from any angle.

Students can then construct the molecular shape corresponding to any simple molecular formula and examine its properties. The constructed shape must match the chosen number of electron pairs and bonds. It can then be rotated and viewed as either a molecule or an arrangement of bonds and electron pairs (Figure 6):

Figure 6: Construction of molecular shapes. The molecular structure may be rotated and viewed from any angle.

Metallic and ionic crystal lattices of various sizes can also be constructed in three dimensions and examined from various perspectives so that the relationships among the particles can be seen (Figure 7):

Figure 7: Construction of an ionic crystal. The student builds the crystal by placing ions in the appropriate locations. The crystal can then be rotated and enlarged, and lattice planes can be identified.



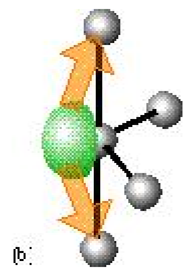
Molecular Modeling in a General Chemistry Course

The programs illustrated in the preceding section were not available three years ago, when molecular modeling was introduced into the general chemistry curriculum at the University of Northern Colorado (Jones et al.). Thus, *HyperChem* software was introduced into the laboratory program. *HyperChem* is a molecular modeling program that has a simple interface and can be used to construct simple systems after a short period of training. It also functions reasonably well with inorganic compounds. A user-friendly student interface is very important for molecular modeling programs to be effective in introductory courses. For example, Bergandine, Koker, and Veltman (1993) found that, although research visualization software could be used by introductory students, the addition of a simpler interface greatly reduced the time required for students to generate images.

Only one three-hour laboratory period is available for students to learn how to use the modeling program and complete the assignments. Thus, a set of paper handouts was generated that includes a brief tutorial introduction to the program functions students will use and assignment sheets. Students are asked to write the Lewis structures of a set of molecules as a pre-laboratory assignment. During the laboratory period, with a teaching assistant available for support, they complete the tutorial and then build the structures of the molecules for which they wrote Lewis structures. They optimize the geometry of each molecule, view it represented as spheres, sticks, and dots, measure its bond angles, and then explain deviations of the bond angles from predicted values. In this way, students discover the effect of lone pairs on bond angles, something that is not possible to teach with hand-held models---in most model kits, the bond angles in water, ammonia, and methane, are an identical 109.5 degrees. Once students have completed building the structures and printing them out for their reports (Electronic lab notebooks have not yet arrived on our campus!), they tackle independent investigations, in which they must use the modeling program to collect data on the properties of molecules in order to solve a problem. For example, students can investigate the effect of substituting various numbers of fluorine atoms on the polarity of methane. They build methane and each fluoromethane, view and print the electron density distributions, and calculate the electrostatic potential at each atom. In this way they learn that methane and tetrafluoromethane are both nonpolar molecules, despite the high polarity of the C-F bond. Another investigation they might choose is the effect of bond order on bond length and bond angles.

Hand-held models are also used in the same laboratory period, to provide students with an opportunity to feel the three- dimensional shapes. After each molecule is constructed on the computer, students build it with a model kit, to better see the limitations of each representation (See Figure 8).

Figure 8: Molecular modeling programs can be used to display electron density plots, which help students visualize molecular polarity. Here, *HyperChem* has been used to build a representation of methylamine, optimize its geometry, and superimpose a topographical plot of its electron density.



Assessing the Feasibility

Before molecular modeling could be introduced into the general chemistry course, certain questions needed to be answered:

- Can introductory chemistry students learn to use sophisticated molecular modeling tools?
- To what extent is guidance and training in the use of these tools required?
- Will students accept a technology-supported curriculum centered on molecular structure?
- Is it feasible, given costs and equipment availability, to incorporate instructional software into general chemistry lab and/or lecture?
- Will it be possible to revise the general chemistry curriculum to center it more on molecular structure and dynamics?

The first term that molecular modeling was used in general chemistry, a study of the feasibility of its use was conducted in order to try to answer these questions (Jones et al, 1993). At this time only a few computers were available to the students. Thus, only half of the 100 students completed the *HyperChem* modeling assignments, the other half worked with hand-held models to complete the same assignments. Each group also completed additional inquiry-based investigations. The computer modeling group completed the independent investigations described above and the group working with physical models used clay and sticks to complete an inquiry assignment in which they discovered the bond angles that best reduce repulsion in molecules with different numbers of atoms around the central atom. At the end of the semester, students took a quiz on the topics taught in that laboratory session and completed an attitude survey. Comments and suggestions were also solicited from students, teaching assistants, and faculty members.

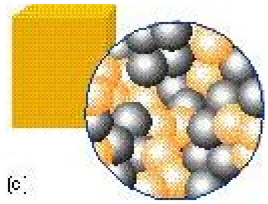
There was no difference in achievement between the two groups, nor was a difference in attitude reported. Most of the students were able to learn to use the modeling program and complete the assignments during the three-hour laboratory period, but a few still had difficulty, suggesting that an interface especially designed to facilitate student interaction would be beneficial. The majority of the students reported that they enjoyed using the molecular modeling program, felt they learned from it, and found it a valuable part of the course. Both groups of students expressed a strong preference for an increased emphasis on molecular structure in the curriculum. Each learning environment was found to have its advantages:

Comparison of the Two Environments

Molecular Modeling Software
Can read bond angles.

Allows for lone pairs.
Computes optimal structure.
Allows different renderings.
Shows electron density.
Shows molecular orbitals.
Shows molecular skeletons.
Gives information on energetics.
Students check their predictions themselves with the computer.
Students learn to use a valuable research tool.

Hand-held Models
Structures can be felt as well as seen.
Structures are truly three-dimensional.
Structures are portable, so students can compare structures across the room.
Using clay centers, students can explore effect of electron repulsion on molecular shape.
Student predictions are checked by the instructor.



Conclusions

Molecular modeling is now an integral part of the general chemistry curriculum at the University of Northern Colorado. The molecular modeling laboratory is only one part of a comprehensive molecular introduction to chemistry that has been incorporated into the general chemistry course. Near the beginning of the first semester and prior to the molecular modeling laboratory class, students complete a lecture hall activity in which they repeat the clay center inquiry laboratory activity, but this time with gum drops, toothpicks, and protractors. The curriculum has been revised to take advantage of the familiarity students gain with molecular structure (Jones et al., 1995). Nomenclature is delayed until after molecular structure has been taught, so that polyatomic ions can be introduced as three-dimensional structures, rather than just as formulas. Chemical reactions and stoichiometry are also taught after molecular structure, so that students can better understand chemical equations and how chemical processes differ from physical ones.

Students report that they enjoy learning from both computer programs and models and appreciate the opportunity to learn a useful research technique that can be applied in later courses and in their careers. It is likely that the use of molecular modeling in general chemistry courses will continue to grow around the world, as the tools become more readily available. For example, the program *Rasmol* is a powerful molecular modeling program available free on the World Wide Web. It is also possible to obtain from Cambridge Software a free copy of a program that allows the user to display many of the chemical structures available at Web sites. The *HyperChem* home page contains information on how to link to many of the molecular modeling web sites. These modeling programs can be used on a variety of workstations and computers.

There remain many unexplored possibilities and little is yet known about how giving students the opportunity to explore and build structures in the molecular world affects learning. An important feature of the use of modeling and construction programs is the active participation required of the student. The student must constantly make decisions while using the software. Research has shown (Friedler et al.) that successful learners employ different learning strategies from those used by immature learners and that those strategies can be taught. Successful learners have been found to implement a variety of active cognitive strategies; for example, they relate new knowledge to old, they monitor their understanding, they infer unstated information, and they review, reorganize and reconsider their knowledge. On the other hand, immature learners tend to employ passive strategies.

Computer software can provide the facilitating structure and tools to guide not only learning, but the development of student learning capability (Linn et al., 1990). In other words, students can be prompted by the computer to develop more successful, more active cognitive learning strategies. Attempts to address this challenge have been made in the *Exploring Chemistry* series (Jones and Smith, 1988) and in other highly interactive instructional software packages. Active learning strategies are also the foundation underlying the development of the new *ChemQuest* chemistry curriculum, which integrates text, software, and hands-on activities. The challenge we face when introducing students to molecular modeling software is how to provide the structured learning environment that best leads to understanding.

Acknowledgements

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The reader should be aware that every illustration in this paper was converted into a new format somewhat inexpertly by the author, which has resulted in some degeneration of the image. The original of each figure is of much higher quality than it appears here. The same is true of the small graphics at the head of each section, which were all excerpted from original illustrations by Peter Atkins (Atkins and Jones).

References

Agapova, O., Jones, L., and Ushakov, A. (in preparation) *ChemQuest: Chemistry for the Information Age* Software Component.

Atkins, P., and Jones, L. (in preparation) *Chemistry: Molecules, Matter and Change*. New York: W. H. Freeman.

Bergandine, D., Koker, T., and Veltman, T. (1993) Visualization in chemistry education. Presented at the Meeting of the American Chemical Society, Denver, CO, March 31.

diSessa, A. A. (1987) The third revolution in computers and education. *Journal of Research in Science Teaching*, **24**, 343-367.

Friedler, Y., Nachmias, R., and Songer, N. B. (1989). Teaching scientific reasoning skills: a case study of a microcomputer- based curriculum. *School Science and Mathematics*, **89**, 58-67.

Gabel, D. L., Samuel, K. V., and Hunn, D. (1987) Understanding the Particulate Nature of Matter, *Journal of Chemical Education*, **64**, 695-697.

Griffiths, A., and Preston, K. (1992) Grade 12 students' misconceptions relating to fundamental characteristics of atoms and molecules, *Journal of Research in Science Teaching*, **29**, 611-628.

Hakerem, G., Dobrynina, G., and Shore, L. (1993). The effect of interactive, three dimensional, high speed simulations on high school science students' conceptions of the molecular structure of water. Presented at the Meeting of the *National Association of Research in Science Teaching*, Atlanta, GA, April 17.

Jones, L., Thomas, P., Fields, C., Geiger, L., James, M., Cooper, N., Henderleiter, J. (1995). A conceptual approach to general chemistry, *Gordon Conference on Innovations in College Chemistry*, Ventura, CA, January 11.

Jones, L., Thomas, P., Fields, C., Geiger, L., James, M., Schwenz, R., Cooney, J. (1993). Molecules, multimedia, and general chemistry. Presented at the University of Northern Colorado Center for Research in Teaching and Learning, October 12.

Jones, L. L., and Smith, S. G. (1988). *Exploring Chemistry*. Wellesley, MA: Falcon Software.

Linn, M. C., Songer, N. B., Lewis, E. L., and Stern, J. (1990). Using technology to teach thermodynamics: achieving integrated understanding. in D. L. Ferguson (ed.) *Advanced Technologies in the Teaching of Mathematics and Science*. Berlin: Springer-Verlag.

Millar, R., and Driver, R. (1987) Beyond processes. *Studies in Science Education*, **14**, 33-62.

Nakhleh, M. B. (1993) Are our students conceptual thinkers or algorithmic problem solvers? *Journal of Chemical Education*, **70**, 52-55.

Ophardt, C. E. (in press). Inorganic molecules: a visual database, *JCE:Software*, **8C**, no. 1.

Smith, K. J., and Metz, P. A. (1996) Evaluating student understanding of solution chemistry through microscopic representations, *Journal of Chemical Education*, **64**, 695-697.

Williamson, V., and Abraham, M. (1995) The effects of computer animation on the particulate mental models of college chemistry students. *Journal of Research in Science Teaching*, **32**, 521-534.
