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In the Classroom

Using Molecular Modeling to Enhance Visualization in the Organic Chemistry Classroom

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Computer-generated images present another visualization alternative for the classroom.

Organic reaction animations that include color and motion can supplement the use of traditional model kits to visualize molecules. Stereochemistry, Newman projections, steric interactions, and many other three-dimensional features can be easily seen with these animations. Computer-generated images and animations can go beyond simply *reproducing* “chalkboard” drawings or hand-held models. More abstract concepts, including electron density, molecular orbitals, and the mapping of properties such as electrostatic potentials onto an electron-density surface are easily visualized and interpreted using molecular modeling.

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QuickTime[1] animations of molecules and reactions are easy to generate from the graphical output of molecular modeling packages. This paper describes the use and preparation of these classroom visual aids, and provides nine QuickTime movies as examples.

Introduction

Simple visualization of molecules is an essential skill in chemistry, but one that is often challenging for beginning students. Conventional methods of visualization include chalkboard representations and hand-held models. Chalkboard representations can work well once students are familiar with the dense graphical language used to convey structures, but often do not clearly show the three-dimensional structure relationships to the untrained eye. Students (and all humans, for that matter) have grown up in a visual environment which prepares them to see and interpret spatial relationships quickly. In contrast, a printed black-and-white Fischer projection is far more challenging to interpret. The student must learn a whole new set of rules, including the nonintuitive idea that things in a horizontal line are coming towards you and things in a vertical line are going away from you. Chemists will, and should, continue to use the traditional line drawings and Fischer projections (they are very efficient ways of transmitting structural information), but we may be able to make the learning curve less steep for our students by first tying into the tremendous power of the visual system. Although physical models are extremely valuable for representing chemical structures, in a classroom setting their use is limited: the standard student versions are often too small to be easily seen, and the larger instructors' versions are often awkward to use. Computer-generated images present another visualization alternative for the classroom. Numerous others have presented detailed and critical reviews concerning the use of visualization techniques in the organic classroom. Casanova and Casanova's analysis is worthy of special note because of its range and cautions [1]. Their main thesis is that though animations clearly liven up the classroom environment, the information that students carry away can actually decrease unless they are given opportunities to rethink and reformulate the information in their own terms. (Note-taking has value as a learning process, not just as a transmission process.)

[1] QuickTime is a registered trademark of Apple Computer Corp.

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In a previous paper we explored ways to fill the gap between presentations based on simple formulas drawn on the board and more complex visual animations such as those presented in this paper [2]. Incorporation of multimedia as an aid to increase student interest and better illustrate concepts in traditional chemistry lectures is becoming more prevalent [3–5]. A number of excellent resources, both commercial and public, are available on CD-ROM or the Internet [3, 6, 7][2, 3].

A synergistic rise in desktop computing power and software development in the field of computational chemistry has delivered impressive visualization capabilities to the organic classroom. Many schools are now incorporating molecular modeling laboratories into the curriculum [4, 5, 8]. Beside introducing students to the methodology of modeling through computational laboratory experiments, an advantage of the computational packages is the generation of graphical output for simple molecular visualization. After examination of several molecular modeling packages, Spartan[4] was used at Middlebury College in the molecular modeling laboratory as it was user-friendly and had strong graphics capabilities [9]. MacSpartan[2] was also used to generate frames for these animations. However, other packages (e.g., CAChe[5], HyperChem[6], Sybyl[7], Cerius2[8], Chem 3-D[9]) could have been used as well [10]. The fierce competition between modeling programs has lead to rapid increases in power coupled with dramatic price decreases, a very favorable situation for those purchasing the programs.

Images of molecules are easily produced with molecular modeling software. Line or stick drawings conform most closely to what students see in their textbooks. Ball-and-stick models best illustrate atomic connectivity and spatial relationships but give a less-than-accurate picture of atomic and molecular sizes. Space-filling models emphasize the volume and shape of whole molecules while sometimes creating a false sense of “hardness” that must be dispelled. More subtle concepts can be illustrated by

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[2] Chem TV: Chem TV ® 1996, B Luceigh, Luceigh@chem.ucla.edu.
[3] SpartanLive! 1995, Wavefunction, Inc. URL: http://www.wavefun.com/.
[4] Spartan and McSpartan are trademarks of Wavefunction, Inc.
[5] CAChe is a trademark of CAChe Scientific, Inc.
[6] HyperChem is a trademark of Hypercube, Inc.
[7] Sybyl is a trademark of Tripos, Inc.
[8] Cerius2 is a trademark of Molecular Simulations, Inc.
[9] Chem3D is a trademark of CambridgeSoft Corp.

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mapping a property onto a surface. An example of this is the color-coding of electrostatic potential data onto an electron-density surface in order to illustrate sites of excess charge (positive or negative). Each of these models can be interactively rotated and translated within the modeling program to illustrate important spacial and electronic concepts. Presentations can be turned into QuickTime movies, which allows for review of the material outside the classroom setting and for dissemination to others via local servers or Websites.

Using the Animations in the Classroom

The animations are easy to use in the classroom. The QuickTime movies are small files and need only a program such as SimplePlayer[10] to present them. Projection by an overhead panel (a practical tip: use the brightest possible overhead projector for best viewing) video projector or by a projection TV is sufficient. (If computer facilities permit, it is useful to actually display the molecules interactively directly from the modeling software. The QuickTime animations are, however, a satisfactory alternative.) Very smooth lectures or even kiosk presentations can be prepared by embedding the movies into multimedia authoring programs such as Microsoft PowerPoint[11] or Macromedia Director[12]. Although the images in the QuickTime frames cannot be actively rotated, careful planning can yield animation sequences that can be directly controlled and viewed in a “frame-by-frame” mode. This allows for repeated viewing of key steps in the sequence. Students in advanced courses can gain a much better appreciation for the spatial aspects of reactivity by building their own animations.

Having students build actual hand-held models corresponding to those being viewed is useful for simple three-dimensional visualization of structure. A written response or matching exercise (perhaps on a class handout) that gets the students beyond passively watching the animation are powerful ways to reinforce the concepts. Do not forget to explain the color schemes used in a presentation. We may know that the gray spheres represent carbon atoms; students may not.

[10] SimplePlayer is a copyrighted product of Apple Computer, Inc.
[11] Microsoft PowerPoint is a registered trademark of Microsoft.
[12] Macromedia Director is a registered trademark of Macromedia, Inc.

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Descriptions of Included Movies

The following animations are included as examples of the types of movies that we have found useful in the classroom situation. The different level of effort in making a movie from a simple reaction to adding text and backgrounds is also shown. The particulars of how to make the movies are included because, even though we recognize that the animation resources available are growing rapidly, most of us clearly experience times when we would like to have a custom display of one or more particular concepts. One of our main goals is to help other faculty discover the relative ease of producing their own animations.

Conformations of Butane

Newman projections of alkane conformers are classically used in the text book. This simple animation (Butane_1.mov 399 Kbytes)[13] shows the internal rotation of butane through 360° about the C_2–C_3 bond, with pauses every 60° to show steric interactions. A side view of the rotating molecule is also included (Butane_2.mov 438 Kbytes). It is useful to play both animations side-by-side on the screen. As for many of these animations, selecting the “Loop Back and Forth” option allows repeated viewing of the motion. A potential-energy reaction-coordinate diagram, created using any spreadsheet program, could be used to display the quantitative energetic differences of the conformers.

S_N2 Reaction

The back-side attack by the nucleophile and inversion in the S_N2 reaction is illustrated well in this ball-and-stick animation (SN2_1.mov 180 Kbytes) of the reaction of cyanide anion and chloromethane. The trigonal bipyramidal transition state of the reaction is clearly seen in this animation. The second S_N2 animation shows an electron-density surface. Now the concerted nature of the bond-making and bond-breaking processes are evident (SN2_2.mov 98 Kbytes). The third S_N2 animation shows the electrostatic potential mapped onto the electron-density surface (SN2_3.mov 205 Kbytes). Here the negative charge (deep red color) is seen passing from the nucleophile to the leaving group during the reaction. The formation of the new covalent bond (green) is also seen. The “Loop Back and Forth” option in

[13] All movies are available from the abstract page in either QuickTime or animated gif format.

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MoviePlayer[14] presents an unambiguous visualization of the reversible nature of the reaction. Again, all three movies can be displayed simultaneously.

Vibrations and Infrared Spectroscopy

It is difficult to use only a chalkboard to do justice to the concept of vibrational motion (although one alternative is generally enjoyed by most organic instructors as an amusing opportunity to practice some chemistry aerobics). The three normal-mode vibrations for water are shown, the symmetric (H2O_1.mov 67 Kbytes), asymmetric stretch (H2O_2.mov 438 Kbytes) and the bend (H2O_3.mov 120 Kbytes). The molecular vibrations are exaggerated in this animation for visual clarity in a lecture setting. For discussions of normal modes of vibration, it is helpful to display all three animations with the "Loop Back and Forth" option selected.

Methyl Vinyl Ketone

This progressive representation of an α,β-unsaturated ketone (MVK.mov 477 Kbytes) shows a series of different model types. The animation finishes with a complex plot of the magnitude of the LUMO color-coded onto the electron-density surface. This graphic clearly illustrates the susceptibility of the enone to nucleophilic attack at both the β-carbon and the carbonyl carbon. The visual power of the graphical image is helpful in interpreting and predicting reaction chemistry.

Generation of Animations

Three basic steps are needed in the generation of all animations: a) generation of desired images; b) conversion of these images to PICT files; and c) compression of the PICT files to produce a QuickTime movie. There are *numerous* programs and methods to accomplish each of these steps; some methods for each step are suggested below.

Generation of Graphical Images

Color images for these particular animations were generated on an SGI workstation using Spartan 4.0 or on a Power Macintosh® using MacSpartan. Again, other molecular modeling programs can be used to generate the images for the animations.

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[14] MoviePlayer is a trademark of Silicon Graphics, Inc.

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An IBM-compatible PC also can be used as a platform to produce the images and animations. The molecules were structurally optimized and the graphical properties were calculated using semiempirical or ab initio methods. For animations, a number of sequential images will be needed. Obviously, the more images in the sequence, the smoother the animation will be. Generally, about 20 frames will produce an animation of very reasonable quality for classroom use.

Creation of PICT Files

Images for each sequential frame were saved as PICT files. On the SGI workstation, the molecular modeling graphics were saved as RGB files using the Snapshot desk accessory. Text can be added to the frames (before creating the animation) by inserting the images into Showcase and saving the files as RGB files. The movie can be made directly on the workstation (*vide infra*) or the RGB files can be converted to PICT files using the desktop accessory TOPICT and then exported to the Macintosh.

On the Power Macintosh, the images from MacSpartan were exported directly as PICT files. The images can also be captured with a program such as Snap[15] and pasted into a program such as ClarisWorks[16] or ChemDraw.[13] This allows the addition of text and line drawings before saving the sequence of PICT files.

It is important to number the frames sequentially (frame.01, frame.02 etc.) so the movie can be generated all at once. Personal need will determine the number of frames generated and how much additional text is added to the PICT files.

Making the Movie

For images generated on the SGI workstation, the PICT files were transferred to a Macintosh using Fetch[17] and the animation was made on the personal computer. (Alternatively, the movie can be actually generated on the workstation and transferred afterwards. MovieMaker[18] was used on the SGI Workstation[15] to create some

[15] SNAP ver. 1.1.4; John L. Hayes, 175B North Magnolia, Anaheim, CA 92801.
[16] ClarisWorks and ChemDraw Pro are trademarks of Claris Corp.
[17] Fetch, v. 3.0, Copyright 1995 Trustees of Dartmouth College.
[18] MovieMaker and Workstation, are trademarks of Silicon Graphics, Inc.

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animations. Then the complete movies were transferred with Fetch.[19]) Several programs are available on the Macintosh to make the movies; PICTS to Movie[20] was used to generate several of these animations. It is sometimes necessary to use some cleanup and compression routines if the QuickTime movies consume too much space. This is a simple process and can be done with a program such as ConvertToMovie.[21] This is also a useful program to change the frames-per-second setting and other parameters of the movie.

QuickTime movies generated on the Macintosh computer can be played on an IBM compatible computer by using the program flattenMooV on the finish movie. This small and easy-to-use program copies and duplicates the moov resource of QuickTime files into the movie's data fork allowing playback on Intel-based computers. Commercial products such as Adobe Premiere[22] or Avid Video Shop[23] can produce a cross-platform movie directly from either the sequence of graphics files or from an existing Quicktime movie.

Conclusions

Teaching methodology in the organic classroom is rapidly changing with modern technology. Visualization of graphical images can help explain complex topics in organic chemistry and be used to help predict chemical reactivity. The preparation of QuickTime animations can now be done quickly and efficiently by an organic professor on the desktop computer, as part of routine lecture preparation. While the animations are not refined to a professional level, they are accurate and useful in the classroom. With a little practice, the file compression and movie-making are neither time-intensive nor memory-consuming processes. Each movie took under an hour to complete; the most time-intensive step was the creation of the individual PICT files. The actual creation of the animation from the sequence of frames takes only seconds.

[19] You will need to select file type:binary, Type: MooV, Creator: TVOD. Note, these are *case sensitive*.
[20] PICTS to Movie, Copyright 1992, David Rees.
[21] ConvertToMovie, QuickTime Release, Apple Computer Co.
[22] Adobe Premiere is a registered trademark of Adobe Systems Inc.
[23] Avid VideoShop is a trademark of Avid Technology, Inc.

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Please feel free to use the animations included in this paper in your classrooms! Other animation examples are also available[11].

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