

Advanced Chemistry Collection, 4th Edition

Abstract of Special Issue 28, a CD-ROM for Students

Would you like to help your students develop the ability to visualize molecules in three dimensions—even to imagine the vibrational motions of molecules? If so, 3DNormalModes is the program for you. And it's only one of more than 40 excellent, peer-reviewed instructional programs in the latest Advanced Chemistry Collection.

3DNormalModes

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3DNormalModes (for Windows-compatible computers) enables you or your students to choose one of 28 different molecules, orient it appropriately on the screen, choose any of its normal vibrational modes, and animate molecular vibrations in 3D. 3DNormalModes includes a database of experimental fundamental frequencies (1) and the corresponding normal modes of a representative sampling of inorganic and organic molecules. The normal modes have been obtained from ab initio HF/3-21G calculations (2, 3).

The main screen in 3DNormalModes is shown in Figure 1. Whatever molecule has been selected occupies the major portion of the screen, and all of the functions of the program are readily available via mouse clicks.

A molecule is selected from a list of 28 compounds (Figure 2), which may be sorted by name, chemical formula, or symmetry by clicking the appropriate word. Formaldehyde has already been selected, so 3DNormalModes displays a list of its normal-mode frequencies (Figure 3) along with simplified IR and Raman spectra (Figure 4).

A normal mode is selected by clicking on a frequency in the list, or on one of the lines in either the IR or Raman spectrum. In Figure 1, the third normal mode (1500 cm^{-1} ; CH_2 scissoring) has been selected for formaldehyde.

Figure 5 shows snapshots of the animation of this normal mode. Optional displacement vectors show the extent



Figure 1. The main screen from 3DNormalModes. Formaldehyde's 1500 cm^{-1} CH_2 scissoring normal mode has been selected.

and direction of motion for each atom in the molecule. With sliding controls, you can stop and restart the animation, change its speed, and change how far the atoms are displaced. You can also rotate (Figure 6), translate, and zoom (Figure 7) a molecule to reach the best vantage point from which to view its motion.

In summary, with 3DNormalModes you can:

- Animate each normal mode in a 3-D environment.
- Rotate, translate, and zoom to any viewpoint.
- Adjust the speed of the animation.
- Display atom displacement vectors.
- Adjust the length of the displacements of the atoms.
- Display simplified IR and Raman spectra and from them select a fundamental frequency.
- View information about the selected molecule and normal mode.

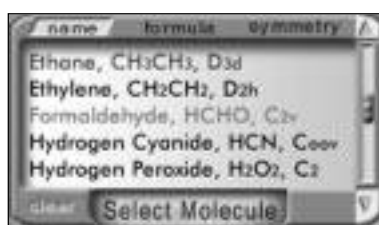


Figure 2. A molecule is selected from a scrolling list, by name, chemical formula, or symmetry.

Figure 3. You can select the mode you want to animate from a scrolling list of frequencies or types of motion.

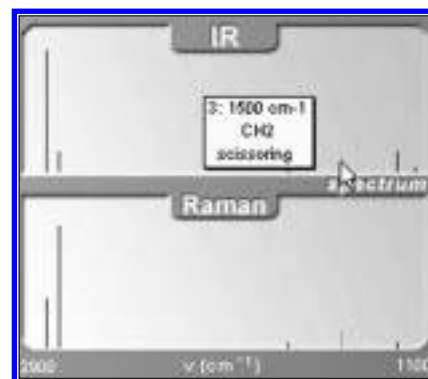


Figure 4. You can also select a mode to animate by clicking on one of the lines in the molecule's IR or Raman spectrum.

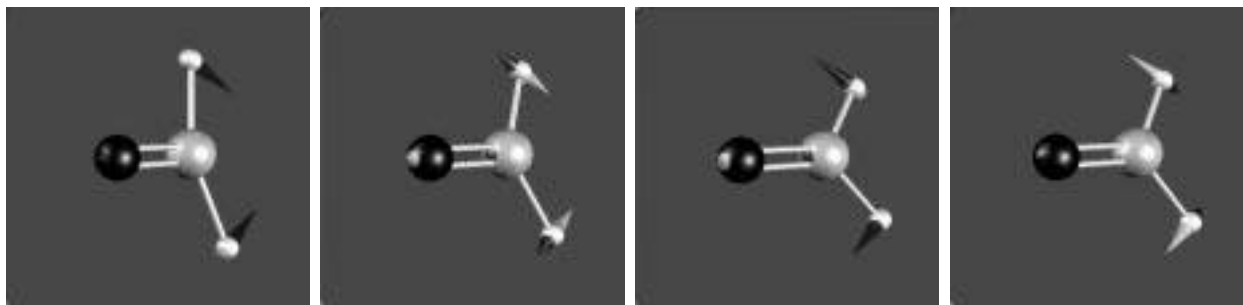


Figure 5. This series of images from 3DNormalModes illustrates the animation of the CH₂ scissoring normal mode (1500 cm⁻¹) of formaldehyde. The molecule has been rotated from its starting position (shown in Fig. 1) for a better view of the in-plane scissoring motion. Optional displacement vectors have been added to show the extent and direction of motion of each atom.

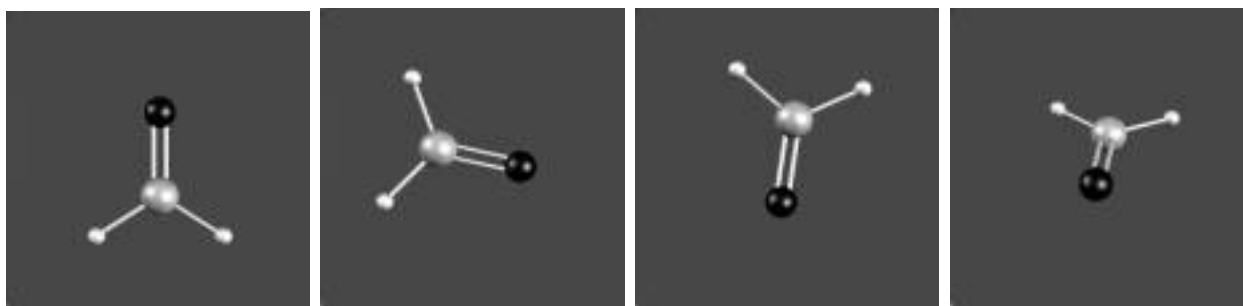


Figure 6. You can rotate a molecule in 3-D space, by any angle around any axis.

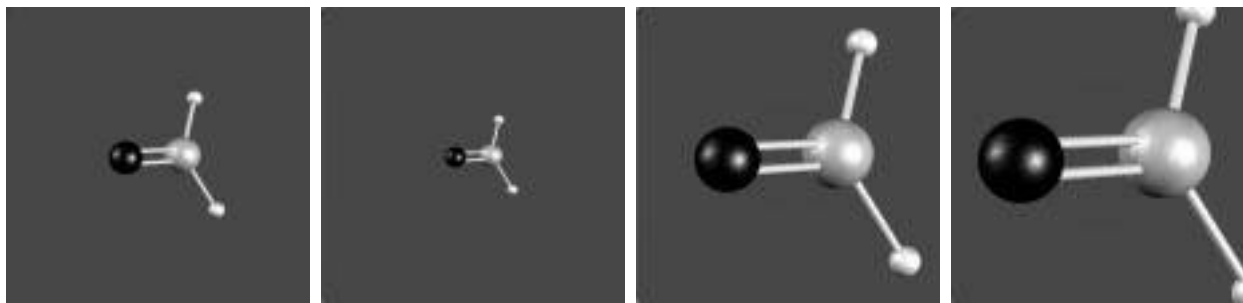


Figure 7. Zoom out or zoom in from the standard view of a molecule.

3DNormalModes can be used as a self-paced learning tool, as well as a classroom presentation. Students will be able to learn how to use the program from the built-in help screens, and the extensive selection of molecules allows for a broad range of student assignments to be made.

3DNormalModes can be used in conjunction with Alkanes in Motion (also on ACC) to compare individual normal modes with the overall vibrational motion of atoms in alkane molecules, thereby providing students with excellent visualizations of molecular motion.

MolVib is a similar program for Mac OS previously published by *JCE Software* (4) and also included in this edition of ACC. MolVib has limited capabilities of manipulation of the molecule in a real 3-D environment and includes a much smaller number of molecules. However, MolVib does allow users to add new molecules, a feature that is not available in 3DNormalModes.

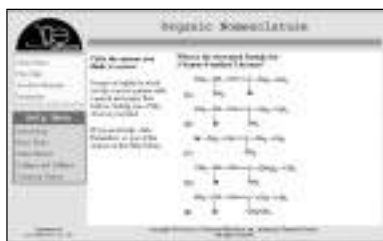
3DNormalModes requires Windows XP, 2000, ME, or

98. A 3-D accelerator such as DirectX 7.0 (recommended) or OpenGL is suggested, but not required.

Organic Nomenclature

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Organic Nomenclature is a drill-and-practice exercise in naming organic compounds (using both common and IUPAC names) and identifying structural formulas. Organic Nomenclature was originally published as a HyperCard stack for Mac OS computers (5). It is now available in HTML format for use by students with both Windows and Mac OS compatible computers. It consists of multiple-choice questions where a name or formula is given and the correct formula or name is chosen from a list of five pos-



A screen from Organic Nomenclature.

Advanced Chemistry Collection, 4th edition (ACC) CD-ROM for Mac OS and Windows contains software that will enhance student learning in analytical, inorganic, organic, and physical chemistry courses, biochemistry courses, and many others. ACC includes both previously published and new peer-reviewed software on a single CD-ROM for convenient access by students. We expect students will find the programs included in ACC useful tools for learning chemistry outside the classroom as they progress through the chemistry curriculum.

The names of the programs included on the CD and the broad range of topics they address are listed on page 1224A. Descriptions of all programs on ACC may be found on the *JCE Software* Web site at <http://jchemed.chem.wisc.edu/JCESoft/Programs/ACC/contents.html>. Programs that are new or updated in this 4th edition are described in this abstract.

Licensing, Volume Discounts for Adoptions

ACC is intended for use by individual students. Institutions and faculty members may adopt Advanced Chemistry Collection as they would a textbook. We can arrange for CDs to be custom packaged with laboratory manuals or other course materials or to be sold to students through the campus bookstore. The cost per CD can be quite low when large numbers are ordered (as little as \$3 each), making this a cost-effective method of providing students access to the software they need whenever and wherever they desire. Network licenses to distribute the software to your students via your local campus network can also be arranged. Contact us for details on purchasing multiple-user licenses.

Price and Ordering

The price for this CD-ROM for a single user on a single machine is \$35 U.S./\$50 non-U.S. Adoption discounts are available for the purchase of 20 or more CDs. Call or email *JCE Software* for information about these bulk order prices.

sible answers. Selecting an incorrect answer generates a message explaining why the choice is incorrect. Students can then choose another answer or choose a different example. Once the correct answer has been chosen, a congratulatory message is displayed.

Organic Nomenclature requires the following software, which is available for free download from the Internet: Netscape Navigator, version 6.2 or higher, or Microsoft Internet Explorer, version 5.0 or higher.

An order form is inserted in this issue that also provides prices and other ordering information. Information about all of our publications (including abstracts, descriptions, updates, etc.) is available from our World Wide Web site at

<http://jchemed.chem.wisc.edu/JCESoft/>

Acknowledgments

ACC contains the work of many authors. The time and effort of these dedicated chemistry educators in producing these programs is gratefully acknowledged by the editors, along with the authors' generosity in contributing their work to the chemistry education community by submission to *JCE Software*. Thanks are also due the many peer reviewers who volunteered their time to test these programs, and the thousands of chemistry instructors all over the world who have made these programs available to their students. Their input has been invaluable in program development, revisions, and updates.

Hardware and Software Requirements

System requirements are in Table 1. Some programs have additional special requirements. For more specific information, see the individual program abstracts at *JCE Online* or the documentation included on the CD-ROM

Literature Cited

1. NIST Chemistry WebBook. <http://webbook.nist.gov/chemistry/> (accessed Aug 2003).
2. Computational Chemistry Comparison and Benchmark DataBase. <http://srdata.nist.gov/cccbdb/> (accessed Aug 2003).
3. Hehre, W. J.; Radom, L.; Schleyer, P. V.; Pople, J. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.
4. Huber, D.; Wagner, P. MolVib 2.0; *J. Chem. Educ. Software*, **1995**, 7C1.
5. Shaw, D. B. Organic Nomenclature; *J. Chem. Educ. Software* **1994**, 6C1.

Table 1. Hardware and Software Required

Computer	CPU	RAM	Drives	Graphics	Operating System	Other Software (required by one or more programs)
Mac OS Compatible	Power Mac	≥ 64 MB	CD-ROM; Hard Drive	≥ 800 × 600; thousands or millions of colors	System 8.6 or higher	Acrobat Reader; Mathcad; Mathematica; QuickTime; WWW browser; Chime plug-in; Flash Player; HyperCard Player
Windows Compatible	Pentium	≥ 64 MB	CD-ROM; Hard Drive	≥ 800 × 600; 16-bit or 24-bit color	Windows XP, 2000, ME, 98	Acrobat Reader; Mathcad; Mathematica; QuickTime; WWW browser; Chime plug-in; Flash Player; RasMol; HyperChem; Excel