Journal of Chemical Education Software

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Two Programs for Mac OS–Compatible Computers: Abstract of Volume 9C, Number 1

1. Alkanes in Motion

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The motion of gas molecules is very complicated owing to the combination of translation, rotation, and vibration. Such motion is difficult to depict using static media, such as the printed page. Also, simple animations tend to focus on only one aspect of molecular motion (*1*). So, to improve students' understanding of molecular motion, Alkanes in Motion, a collection of clip animations generated from molecular dynamics calculations, was produced. It depicts the molecular motion of hydrocarbons in the gas phase. Four animations from the collection are presented here. These four animations consist of two animations each of hexane and octadecane, one animation calculated to show translational motion, and one to show vibrational motion.

The molecular motion of alkane molecules was calculated using the molecular dynamics simulation (*2*, *3*) in HyperChem (*4*). The simulations were used to obtain the position of each atom of each molecule at each time step. Each simulated molecular system includes 18 carbons, (i.e., three hexanes) (Fig. 1) and one octadecane (Fig. 2) at a temperature of 600 K and is done using the MM+ method, based on the MM2 functional form, authored by Allinger (*5*).

The time increment of each molecular dynamics calculation was one femtosecond. The graphical display of the results of these calculations was then captured at periodic intervals. To accurately depict vibrational motion, animations were done capturing a frame each femtosecond. To show translational motion, a second animation captured at 25-femtosecond intervals was done. The individual frames were then compiled into a QuickTime animation.

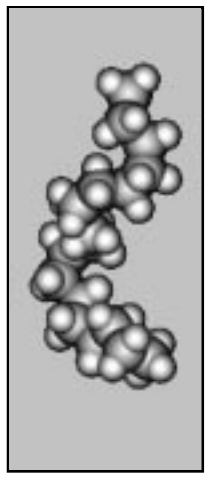

Figure 2. A frame from the *Octadecane in Motion* animation.

Each animation contains 900 frames. The molecules are rendered using a CPK-model; the color of carbon is cyan and the color of hydrogen, white. A time stamp was added to show the relative time of molecular motion. The total real time of the one-femtosecond interval animation is 0.9 picoseconds; at the 25-femtosecond capture rate the animation is 22.5 picoseconds in duration.

These animations of hydrocarbon systems clearly and accurately show the motion of molecules in the gas phase. In the one-femtosecond interval animations, the vibration and rotation of C–H and alkyl groups can be clearly seen. The 25-femtosecond interval animations show translation in addition to vibration and rotation. In some cases they show the detailed motion of atoms in molecules after a collision between two molecules. Previously, only rough and approximate movement of atoms vibrating, rotating, and translating could be shown. These animations depict the movement of molecules more realistically.

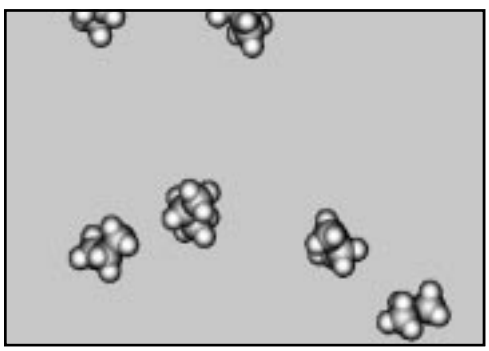

Figure 1. A frame from the *Propane in Motion* animation.

Acknowledgment

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Literature Cited

1. Huber, D.; Wagner, P. MolVib, *J. Chem. Educ. Software* **1995**, *7C(1)*.
2. van Gunsteren, W. F.; Berendsen, H. J. C. *Angew. Chem. Int. Ed. Eng.* **1990,** *29*, 992–1023.
3. Karplus, M.; Petsko, G. A. *Nature* **1990,** *347*, 631–639.
4. HyperChem; Hypercube, Inc., 419 Phillip Street, Waterloo, ON, Canada N2L 3X2, 1-800-960-1871.
5. Allinger, N. L. *J. Am. Chem. Soc.* **1977,** *99*, 8127–8134.

This issue contains two collections of software previously published for Windows computers. For information about obtaining these Windows versions, check the Order Form, or get in touch with *JCE Software* (see Ordering and Information on page 1016).

2. Enriching Quantum Chemistry with Mathcad (for Macintosh)

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Mathcad is a comprehensive, inexpensive program for doing numeric and symbolic mathematics on a computer. Mathcad handles data, text, mathematics, and graphics in a single live document and has an appealing, user-friendly graphical interface. Mathcad has a wide variety of applications in the undergraduate chemistry curriculum, but is especially useful in the mathematically intensive courses traditionally found in the physical chemistry sequence (*1–4*). As the title suggests, Enriching Quantum Chemistry with Mathcad (for Macintosh) presents applications of Mathcad in the area of quantum chemistry selected from those previously published for Windows (*5*, *6*).

Students generally find quantum chemistry to be highly mathematical, quite difficult, and very abstract. They are right on all counts. However, the subject is also extremely important today, even at the undergraduate level. There is, therefore, a need for relatively simple computer exercises that bridge the gap between the formalism of quantum theory and its various computational methods (7). All of the Mathcad documents presented here attempt to do this in one way or another. Some exercises involve relatively elementary problem solving, while others, for example, illustrate the basics of molecular orbital theory and the variational method.

Enriching Quantum Chemistry with Mathcad (for Macintosh) includes Mathcad documents in the following areas:

- Routine problem solving and units management
- Linear, nonlinear, and polynomial regression analysis
- Numerical solutions for Schrödinger's equation
- The variational method
- Hückel molecular orbital theory
- Semi-empirical MO calculation on hydrogen fluoride
- A really simple SCF calculation
- Spectroscopic transitions for an electron in a 1-D box
- Finding roots

Literature Cited

1. Coleman, W. F. *J. Chem. Educ.* **1990,** *67*, A203.
2. Adravkoski, Z. *J. Chem. Educ.* **1991,** *68*, A95.
3. Rioux, F. *J. Chem. Educ.* **1992,** *69*, A240.
4. Turner, D. E. *J. Chem. Educ.* **1993,** *70*, A185.
5. Rioux, F. Enriching Quantum Chemistry with Mathcad; *J. Chem. Educ. Software* **1994,** *1D2*.
6. Rioux, F. Enriching Quantum Chemistry with Mathcad, Part II, J. *Chem. Educ. Software* **1995,** *3D1*.
7. Montgomery, H. E., Jr. *J. Chem. Educ.* **1977,** *54*, 748.

Using These *JCE Software* Programs in the Classroom

This issue contains two collections of software previously published for Windows computers. For information about obtaining these Windows versions, check the Order Form, or get in touch with *JCE Software* (see Ordering and Information).

Alkanes in Motion is a collection of animations generated using molecular dynamics. It is appropriate for use in almost any level of chemistry. In high school or general chemistry it can be used to illustrate the constant motion—translation, rotations, and vibrations—of molecules. In organic chemistry, it can illustrate the shapes, motions, and interactions of simple organic molecules. In physical chemistry, it can be used as an introduction to molecular dynamics calculations.

Enriching Quantum Chemistry with Mathcad for Macintosh is designed to be used in physical chemistry or in a separate course on quantum chemistry. It is an electronic textbook of quantum chemistry in which the equations and graphs are "live". Changing a parameter or equation causes all calculations to be redone. The new results are displayed either as a table of numbers or as a graph or both. The opportunities for exploration and enhanced understanding of the meaning of quantum chemical equations are nearly infinite. This is a preview of what the textbook of the future might look like.

Ordering and Information

Journal of Chemical Education Software (often called *JCE Software*) is a publication of the *Journal of Chemical Education*. There is an Order Form inserted in this issue that provides prices and other ordering information. If this card is not available or if you need additional information, contact: *JCE Software*, University of Wisconsin–Madison, 1101 University Avenue, Madison, WI 53706-1396; Phone; 608/262-5153 or 1-800-991-5534; FAX: 608/ 265-8094; email: *jcesoft@chem.wisc.edu*. Information about all of our publications (abstracts, descriptions, updates, etc.) is available from our World Wide Web site:

http://jchemed.chem.wisc.edu/

Hardware and Software Requirements

	Computer	CPU	RAM	Drives	Free Disk Space	Graphics	System	Other
Alkanes in Motion	Mac OS compatible	68020 or higher, or Power Macintosh	≥8 MB	Hard disk, High-density (1.44 MB) floppy	10 MB	≥256 colors, 640 × 480	System 7 or later	QuickTime, Movie Player
Enriching Quantum Chemistry with Mathcad	Mac OS compatible	68030 or higher with FPU, or Power Macintosh	≥8 MB	Hard disk, High-density (1.44 MB) floppy	1 MB	≥256 colors, 640 × 480	System 7.1 or later for 680X0; 7.5 or later for Power Macintosh	Mathcad 6 or Mathcad PLUS 6 for Macintosh