Journal of Chemical Education: Software

edited by
Jon L. Holmes
Nancy S. Gettys
University of Wisconsin–Madison
Madison, WI 53706

Four Programs for Windows: Abstract of Volume 4D, Number 2

1. PSL Photometer

Steven D. Gammon
Department of Chemistry, University of Idaho, Moscow, ID 83844

The majority of freshman chemistry laboratory programs include experiments that employ visible spectroscopy to teach Beer's law and derive related concentration information. These experiments are often done with a Baush & Lomb Spectronic 20 or Spectronic 21. While these experiments and equipment are "status quo" at most institutions, they do have a number of limitations. We have developed an alternative instrument and software that offers significant advantages over the above spectrometers.

The instrument is constructed from PVC "Tee" pipe, an LED, and employs the Team Labs Personal Science Lab interface (*1*) and a Radiometric Light Probe. Construction of the photometer from the PVC pipe is simple and inexpensive. The instrument has demonstrated both adequate sensitivity and selectivity to be an effective replacement for the above spectrometers in an undergraduate teaching laboratory (*2*).

In order to drive the instrument, PSL Photometer was developed to run under the Microsoft Windows™ operating system. In order to allow students to collect valid information without significant intervention by an instructor, a simple, user-friendly interface is employed. PSL Photometer allows students to create a standard calibration curve, take measurements on solutions of unknown concentration, and perform a linear least squares analysis on the calibration data. All the collected data are printable and can be saved as an ASCII file for spreadsheet use or inclusion in a computer-generated report. A sample screen from PSL Photometer is shown in Figure 2.

PSL Photometer has many unique features that make it ideally suited to undergraduate teaching laboratories and taking analytical sample measurements in the field. First of all, once launched, the program can detect whether the instrument is present and correctly configured. When printing, the Windows Print Manager handles printing problems. In all instances, if a problem is detected, feedback and suggestions to correct the problem are provided. There is also extensive on-line help that is fully searchable, has all the features common to most commercial Windows applications, and is available at any time. Help also contains content information on how calibration works and the configuration of the measurement hardware. All of these feedback mechanisms create an environment that ensures that students will be able to collect valid data.

Figure 1. The opening screen from PSL Photometer.

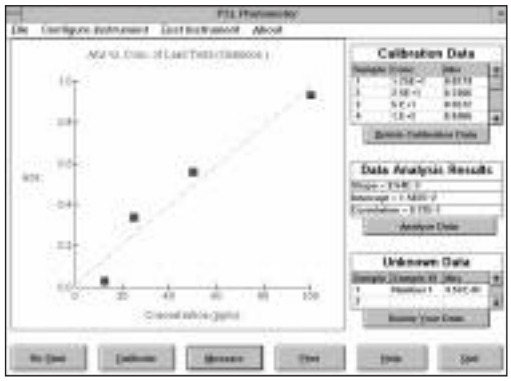

Figure 2. Sample data screen from PSL Photometer.

Another important feature of PSL Photometer is that the instructor has the flexibility to configure the "instrument" software for his or her teaching situation. Through the "Configure Instrument" option, the instructor may enable or disable printing, linear regression analysis of the calibration data, displaying the graph of the calibration data, and/or calculation of the unknown concentration(s). If all the configurable features are turned "off", one has the minimal instrument that behaves like the Spectronic 20. This may be desirable if the instructor feels the students need experience in graphing and linear regression. With the features turned "on" one has an instrument that provides all the possible information that can be obtained from a colorimeter. Finally, a custom configuration can be chosen with just the features that meet instructional goals. To prevent the students from changing the configuration of the instrument, this option is only accessible through a password.

Literature Cited

1. The product formerly called the IBM Personal Science Lab (PSL) is now the Team Labs PSL (Team Labs, 6390B Gunpark Dr. Boulder, CO 80301).
2. Pharr, C. M.; Malmberg, B. J.; Jegla, J. D.; Gammon, S. D. *J. Chem. Educ.* **1996**, *73*, 238–243.

2. HIPPO-CNMRS: Highly Improved Prediction Program of Carbon Nuclear Magnetic Resonance Shifts

Helmut Hönig
Technical University Graz, Graz, Austria

HIPPO-CNMRS is a "highly improved" version of a ^{13}C-NMR program previously available from the author. It can predict the ^{13}C NMR spectrum for most substituted alicyclic saturated and aromatic ring systems (cyclopropane to cyclooctane; benzene, naphthalene, anthracene; *cis*- and *trans*-decaline; some heterocyclic systems like furan, tetrahydrofuran, pyridine, piperidine and quinoline; most substituted acyclic compounds with up to six carbons in the parent structure; and simple olefins and alkynes. Also included is a database of 1700 molecules that permit you to add to, edit, display, and print data or spectra from user experiments and/or from the literature.

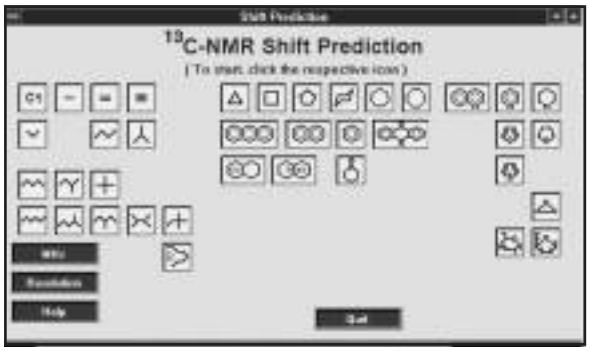

Figure 1. Shift prediction mode.

To do a shift prediction you start by selecting the basic structure. You can then select substituents for the base structure from a scrolling list and drag them to the desired position. Both the frequency and the resolution can be adjusted. With the click of a button you calculate the ppm values for each carbon atom and then display the spectrum.

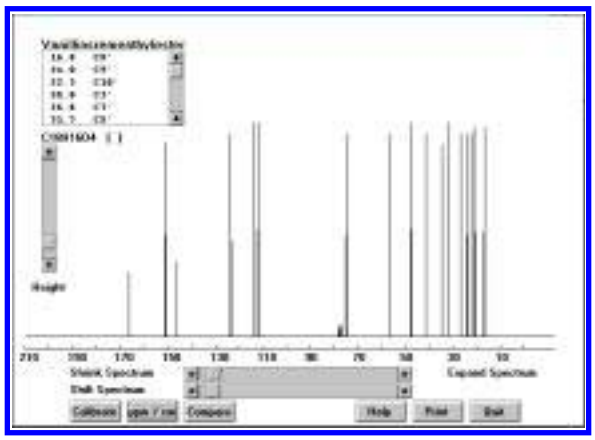

Figure 2. A ^{13}C NMR spectrum displayed in HIPPO-CNMRS.

The HIPPO-CNMRS database is searchable or you can scroll through a list of included molecules. Data for each molecule are saved as a separate data file. You can view the spectrum, print it, and even compare two spectra on the same screen. Spectra can be scaled or shifted on the screen.

HIPPO-CNMRS has several advantages over other ^{13}C-NMR programs. The program is small, requiring only about 1 MB of space on the hard disk. Data files for a ^{13}C spectrum require only about 200 bytes. It does not require any other software, except Windows. It combines prediction of unknown spectra with retrieval of stored spectra and has a very fast retrieval time. The prediction mode gives rise to very good representations of carbon shifts for cyclohexane systems, including axial and equatorial substituents, and for polysubstituted aromatics.

3. SPECPNMR: A Proton NMR Slide Show

Adrian J. Blackman
University of Tasmania, Hobart, Tasmania, Australia 7001

SPECPNMR is one of a set of programs developed as an aid for teaching introductory spectroscopy to organic chemistry students (*1*). It includes a brief introduction to nuclear magnetic resonance spectroscopy followed by a detailed look at proton magnetic resonance spectroscopy. The program generates electronic slides for display in a lecture theatre on a large screen using a video projector or LCD panel and overhead projector. The slides are designed to help a lecturer teach spectroscopy. They are visual aids for a lecturer who can provide accompanying verbal explanations. Although the slides are not intended for direct use by students they are sufficiently self explanatory to allow them to be used as a hands-on teaching module.

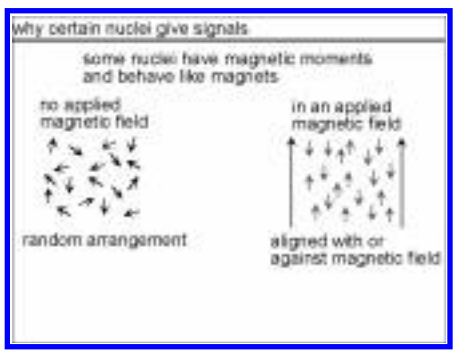

Figure 1. An early slide from SPECPNMR.

The slides have been carefully designed to be visible under projection conditions. They have a consistent appearance and style. Minimum use has been made of special effects and other "gimmicks" that can be distracting to students. Many of the slides use the "build" principle. New information appears to be added to the previous slide thereby allowing progressive development of a topic. This spectroscopy slide show has been in use at the University of Tasmania for several years.

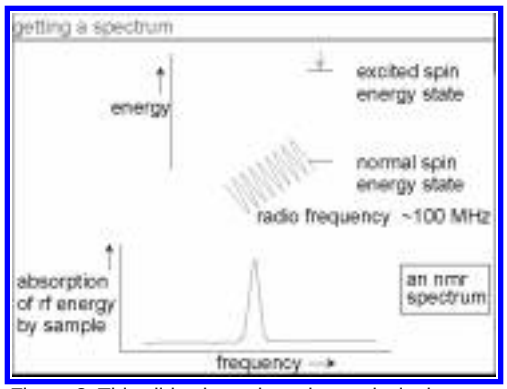

Figure 2. This slide shows how the peaks in the spectrum are generated.

SPECPNMR contains 90 slides. Navigation between slides is easy—simply click the left and right arrow keys. In addition, a pop-up menu of all slides is available so that you can move to any slide in the presentation. A click of the mouse produces a bright green marker that can be used to draw on the slides for emphasis. Marks are erased when you leave the slide by pressing the Delete key.

Literature Cited

1. The full set of spectroscopy slide show software is available for purchase from the author. Contact: A. J. Blackman, Department of Chemistry, University of Tasmania, GPO Box 252C, Hobart, Tasmania, 7001, Australia; email: Adrian.Blackman@chem.utas.edu.au.

4. Alkanes in Motion

Jae Hyun Kim

Kongju National University, Kogjusi, Chungnam, Republic of Korea 314-701

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.

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

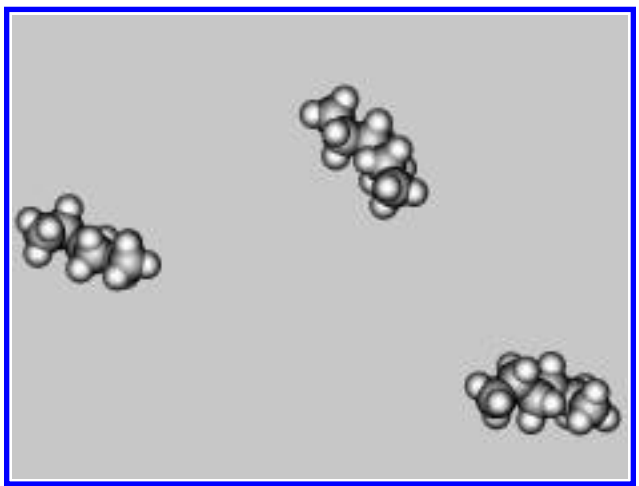

Figure 1. Frame from the animation of hexane.

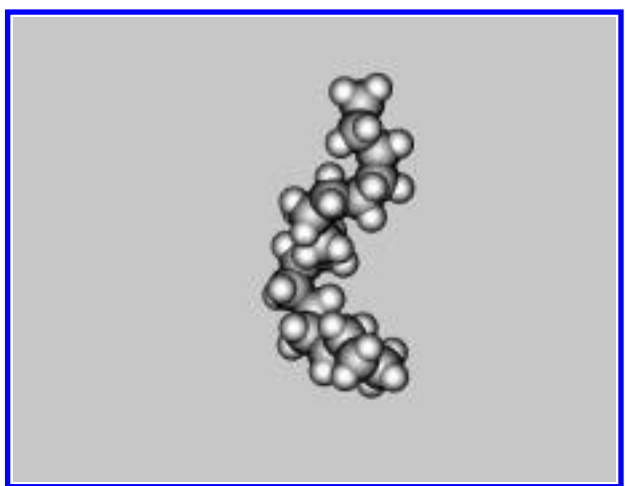

Figure 2. Frame from the animation of octadecane.

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.

Acknowledgment

These animations were produced with the support of the Yonam Foundation in the Republic of Korea.

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.

Using This *JCE: Software* Issue in the Classroom

This issue contains four programs on a variety of topics that use a variety of presentation styles from standard applications to clip animations and a slide show. Two pertain to nuclear magnetic resonance spectroscopy; another is for use in the general chemistry laboratory; and finally computer generated animations depict alkane molecules in motion. There should be something here of interest to almost any chemistry instructor.

Using These Programs

NMR is one of the most widely used instrumental analytical methods. The two NMR programs in this issue should be useful additions in instructional strategies for teaching this important area. HIPPO-CNMRS is used for prediction and comparison of ^{13}C NMR spectra. It could be used to help introduce the topic, to allow students to study and compare spectra from the extensive database, or to examine experimental data. SPECPNMR is a slide show intended as in introduction to proton NMR for sophomore level organic chemistry students. Both of these programs are useful as lecture aids or for direct student use.

PSL Photometer is software to control the Personal Science Lab interface (*1*). Users of *JCE: Software*'s KineticsLab (*2*) and Beer's Law (*3*) programs will appreciate the convenience and flexibility of this new program for Windows. Included are four laboratory exercises you can use in your student laboratories.

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.

Hardware and Software Requirements

Programs in Series D of *JCE: Software* require Microsoft Windows version 3.1 or later and a compatible computer. We recommend an IBM-PC or compatible with a 80386 or higher processor, a minimum of 4 MB of memory, a hard disk, one floppy disk drive to install the software, a mouse, and a Windows-compatible graphics card, such as an IBM VGA or Super VGA adapter with a compatible color monitor. DOS 5.0 or later is highly recommended. The issue is supplied on 3.5-in. disks. Additional requirements are noted below:

PSL Photometer requires Team Labs Personal Science Lab (*1*) equipment with radiometric light probe and a PVC photometer (*4*).

SPECPNMR requires a monitor capable of displaying at least 256 colors at 640 × 480 pixel resolution.

Alkanes in Motion requires QuickTime for Windows (5), supplied with the issue.

Literature Cited

1. The product formerly called the IBM Personal Science Lab (PSL) is now the Team Labs PSL (Team Labs, 6390B Gunpark Dr. Boulder, CO 80301).
2. Cannon, J. F.; Gammon, S. D.; Hunsberger, L. R. KineticsLab: The Crystal Violet Sodium Hydroxide Reaction, *J. Chem. Educ.: Software*, **1994**, *7B*(1).
3. Scott, J. L. Beer's Law: a Computerized Experiment, *J. Chem. Educ.: Software*, **1996**, *9B*(1).
4. Pharr, C. M.; Malmberg, B. J.; Jegla, J. D.; Gammon, S. D. *J. Chem. Educ.* **1996**, *73*, 238–243.
5. QuickTime, Apple Computer, Inc., 20525 Mariani Avenue, Cupertino, CA 95014-6299.

How to Order This Issue

Journal of Chemical Education: Software (often called *JCE: Softwar*e) 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.

For More Information Visit our WWW Site

Information about all of our publications (abstracts, descriptions, updates, etc.) is available from our World Wide Web site:

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