Journal of Chemical Education: Software

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Two Programs for Macintosh: Abstract of Volume 8C, Number 2

Schroedinger.m: A Mathematica Package for Solving the Time-Independent Schrödinger Equation

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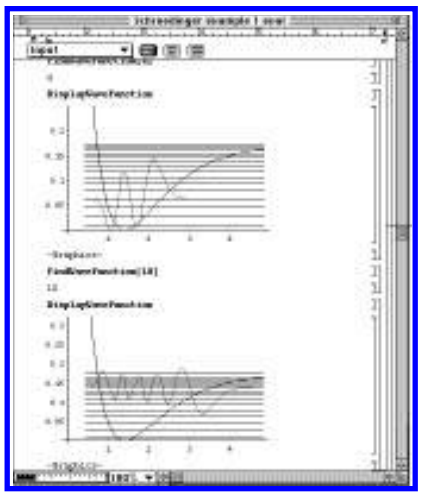
Schroedinger.m enables the user of Mathematica (*1*), to define a potential and determine bound-state energy eigenvalues for a one-dimensional Hamiltonian. A Windows version of this program (*2*) has recently been published. Schroedinger.m defines commands in Mathematica to set the potential, solve the Schrödinger equation to obtain both energies and wave functions, display the solutions graphically, and calculate certain integrals involving the wave functions. It is limited to one-dimensional bound-state problems with fixed boundary conditions; it cannot be applied to other one-dimensional problems with periodic boundary conditions. It is well suited to solving the one-dimensional R-dependent Schrödinger equation that describes most diatomic molecular potentials.

Students new to both quantum mechanics and Mathematica find Schroedinger.m easy to use. It can be used in a junior-level physical chemistry course to provide examples or to provide the means for students in such a course to carry out numerical experiments. The commands defined in the package require only elementary knowledge of Mathematica. However, the more Mathematica one knows, the further one can go with the applications. Knowing even a very few basic Mathematica functions enables a student to use solutions from this package to do some fairly sophisticated computations with one-dimensional wave functions.

A student does not need to know the details of Schroedinger.m in order to use it. However, it helps to be able to understand how the computer represents the solutions in order to move beyond the simplest applications or to understand the limitations of the package. The numerical method used is described in detail in the program documentation.



This screen from the first example notebook shows the n = 4 and n = 10 wavefunctions calculated by Schroedinger.m.

The user has direct control over parameters that define the extent of the grid, its spacing, and the range of solutions. In many cases, however, it is not necessary to worry about these numerical parameters. Simply using built-in defaults gives an adequate answer. However, to apply the method to an unusual or complex problem, it may be necessary to carefully consider how to set these parameters. Fortunately, the methods for doing so are fairly straightforward.

Literature Cited

1. Mathematica, Wolfram Research, Inc., P.O. Box 6059, Champaign, IL 61820-6059.
2. Hansen, J. C., Schroedinger.m: A Mathematica Package for Solving the Time-Independent Schrödinger Equation, *J. Chem. Educ.: Software*, **1996**, *4D Number 1.*

Symmetry Elements and Operations

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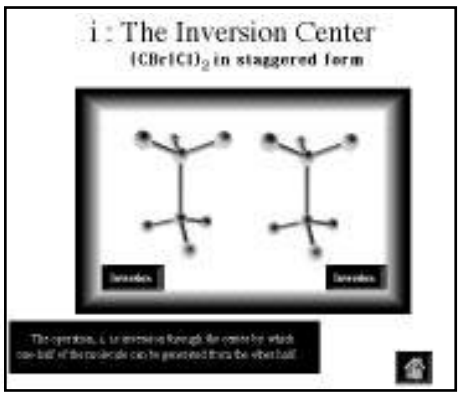
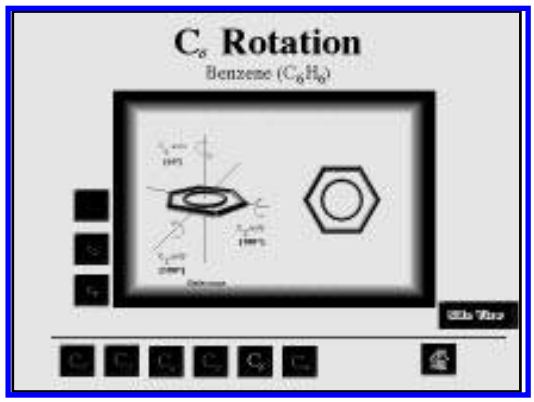
Symmetry Elements and Operations is a multimedia presentation that illustrates the basics of symmetry with three dimensional molecular models and simple text explanations. Three-dimensional graphics and animations are used to define and characterize the symmetry elements commonly encountered in chemical structures. They include identity (E), inversion center (i), proper rotation axis (C_n), plane of symmetry (σ), and improper (rotation-reflection) axis (S_n).

Symmetry is an important concept in chemistry. A firm understanding of the basic concept of symmetry is extremely useful in studying molecular structure, stereochemistry, spectroscopy, group theory, and reaction mechanisms. Often it is difficult and requires quite a bit of imagination to visualize the symmetry properties within a molecule presented on a two-dimensional printed page. Use of molecular models may help, but such models are typically difficult for students to see when demonstrated by an instructor in the classroom. Symmetry Elements and Operations was designed to help students identify the symmetry properties of a particular structure by performing on-screen symmetry operations and then comparing the structure of the molecule before and after the symmetry operation. The screens can be easily projected using a large monitor or a



Inversion Center Symmetry is illustrated using $(CBrICl)_2$ as an example. Two methods of inverting the atoms about the center of symmetry can be animated by clicking buttons on the screen.



The C_6 rotation of benzene is animated in two views.

LCD panel or projector for classroom use.

Symmetry is generally first introduced in organic chemistry when stereochemistry and optical isomerism are discussed. Only simple symmetry elements such as point of symmetry (i) and plane of symmetry (σ) are usually discussed at that level. A more thorough treatment is done in inorganic and/or physical chemistry courses when point group classification and group theory are introduced. Symmetry Elements and Operations can be used at either the introductory or more advanced level. Organic, inorganic, and organometallic molecules are used as examples.

In Symmetry Elements and Operations, definitions of each symmetry element with specific molecules are presented first as examples. Second, the symmetry operations with reference to the symmetry elements within a molecule can be carried out on-screen. For example, rotations around a C_n axis or reflection across a plane are animated using three-dimensional models.

Finally, several examples (cyclopropane, NH_3, SF_6, and H_2O_2) are used to give the student additional practice in identifying symmetry elements and their respective operations. In the sections on each individual symmetry element, the symmetry operations concerned are treated in detail with full illustration to build up the basic concepts. However, in the Example Section, some additional symmetry elements are present that are not dealt with in the program. These are labeled without full illustration. Students should be able to identify these additional symmetry elements by applying the basic concepts learned in previous sections.

Using This Software in the Classroom

How To Use These Programs

Schroedinger.m is intended for use in physical chemistry or introductory quantum chemistry courses. It comes with three example notebooks and a student lesson with a separate complete solution. It is a powerful package that is very useful in teaching topics in quantum chemistry. Originally developed on the Macintosh, Schroedinger.m will run with any Mathematica system. A Windows version was published by *JCE: Software* earlier this year (*2*).

Symmetry Elements and Operations can be used at any time symmetry is introduced in the chemistry curriculum. It is especially appropriate for introductory discussions of the topic in organic, inorganic, and physical chemistry classes. Symmetry Elements and Operations is suitable for either a lecture presentation or for use by individual students as a tutorial or review.

Hardware and Software Requirements

Software in Series C of *JCE: Software* requires an Apple Macintosh computer with 4 MB RAM, a hard drive, and a SuperDrive floppy disk drive. System software version 7 or later is required. The programs in this issue have additional requirements as noted below:

Schroedinger.m requires

- a version of the Mathematica program with notebook-type interface;
- at least 8 MB of RAM.

Symmetry Elements and Operations requires

- approximately 4 MB of free space on a hard drive;
- a color monitor capable of displaying at least 256 colors at 640 × 480 resolution (13-in. or larger monitor).

How to Order This Issue

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