## JOURNAL OF

# Chemical Education: Software

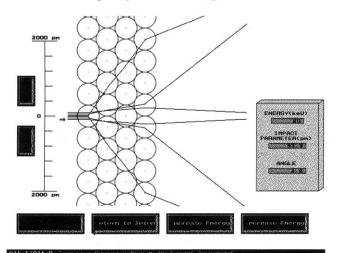
## Abstracts for Volume VB, Number 2

## Rutherford: Exploring the Scattering of Alpha Particles

Robert C. Rittenhouse Walla Walla College College Place, WA 99324

Ernest Rutherford's famous alpha particle scattering experiments led to the development of the nuclear model of the atom and therefore represent one of the major milestones in our understanding of the fundamental nature of matter. This simulation permits students to design and implement scattering experiments of the sort performed by Rutherford, Geiger, and Marsden. Radioactive sources and target metals may be selected from available supplies and a detector positioned around the target to record alpha particles scattered at various angles. A version of the Notebook program (I) has been incorporated into the simulation to facilitate exploration and analysis of scattering data.

In addition to the macroscopic scattering simulation, there are two atomic-level simulations designed to let students perform experiments that Rutherford could only have dreamed about. The first of these is called Trajectory Analyzer because students may use it to explore the scattering interaction between an incident alpha particle and a single atom. Particle energy, impact parameter, and magnification can all be adjusted by the student as part of the experimental design. Students can watch the trajectories develop and measure scattering angle and distance of closest approach to the nucleus. The second atomic-level simulation allows students to explore trajectories influenced by multiple atomic nuclei and investigate the effects of particle energy and target thickness (number of atom layers) on the scattering distribution. It is even possible to demonstrate single crystal channeling.



Screen from Rutherford showing scattering of alpha particles.

#### **Animated Demonstrations**

Philip I. Pavlik Northern Michigan University Marquette MI 49855-5343

Animated Demonstrations is a collection of five programs. The first three, PB1, PB2, and HCC, help students gain better understanding of quantum mechanical behavior by allowing them to observe it graphically. The last two, SALT and CLEAVE, illustrate on an atomic scale salt dissolution and crystal cleavage.

PB1 (1-D Particle in a Box) and PB2 (2-D Particle in a Box) are companion programs that depict accurate, animated, graphical representations of the wave functions (real parts), the probability density functions, and probability dot plots for the lowest four eigenstates of the system. PB1 displays three windows on the screen, one for each of the above-mentioned functions. PB2 makes use of two windows; the first one shows animated wave functions and the other alternately displays probability functions and dot plots.

HCC (Hydrogen-Atom Charge Clouds) displays accurate, three-dimensional pictures of all the electronic charge clouds for the 1s through 3d orbitals for the hydrogen atom. Each charge cloud is represented, to scale, by one thousand points in space, randomly distributed in accordance with the probability density function corresponding to its wave function. HCC also shows the charge clouds that result from the construction of 2sp, 2sp<sup>2</sup> and 2sp<sup>3</sup> hybrid orbitals from hydrogen atomic wave functions.

The HCC screen display consists of two windows. The first one shows an orbital graphic while the other presents a menu of all program options. The user may optionally choose to view single frames, or "slides", of the orbital charge cloud as it would appear from virtually any spatial direction or to see an animation that shows the charge cloud rotating around the desired coordinate axes.

SALT (Dissolution of Sodium Chloride) begins with a display of a sodium chloride crystal lattice under an animated assembly of water molecules. Water molecules are then shown hydrating and removing ions from the lattice and carrying them off into the solution. After several ions have dissolved the program simply recycles the animation sequence.

CLEAVE (Sodium Chloride Crystal Cleavage) depicts a section of a sodium chloride crystal lattice and a solid rectangular object above the crystal. The object pushes down on the lattice causing slippage of a lattice plane. This action subsequently brings like-charged ions into close proximity. The lattice is then seen to fly apart along the lattice plane due to the repulsive forces between these ions. This sequence repeats at user-controlled animation speeds.

Operation of all five programs in this collection is straightforward. PB1, PB2, and HCC include user instructions and are menu driven from the keyboard.

#### **BCTC for Windows**

#### David M. Whisnant

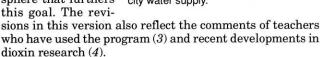
Wofford College Spartanburg, SC 29303

#### James McCormick

University of Wisconsin–Madison Madison, WI 53706

BCTC is an environmental simulation that is modeled after the dioxin controversy (2). In the simulation, students are involved in the investigation of a suspected carcinogen called BCTC, which has been found in a river below a chemical plant and above the water supply of a nearby city. The students have the options of taking water samples, analyzing the water (for BCTC, oxygen, metals, and pesticides), determining LD $_{50}$ 's in an animal lab, visiting a library, making economic analyses, and conferring with colleagues, all using the computer.

This version of BCTC has been rewritten to run under Windows 3.x using Microsoft Visual Basic, so that, along with being easier to use, the simulation is much improved visually. One of the intentions of BCTC is to involve students in an exercise (2) that closely approximates what scientists do. The realistic pictures in the new version, many of them captured with a video camera, create an atmosphere that furthers



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### **About This Issue**

#### John W. Moore Jon L. Holmes

University of Wisconsin–Madison Madison, WI 53706

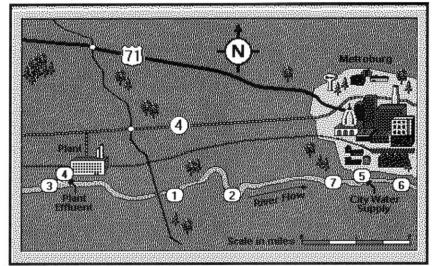
One of the best uses of the microcomputer as a tool in the teaching of chemistry is visualization of molecular- and atomic-scale concepts (such as atomic structure, quantum chemistry, and crystal lattices) that are difficult for students to grasp. Rutherford and Animated Demonstrations are excellent examples. Using the microcomputer to display graphical images and animations of these theories and concepts enhances students' understanding as no other medium can.

Rutherford is appropriate for introductory chemistry courses. It is designed primarily for interactive student use and includes brief tutorials that provide historical background and some theoretical explanation. It can also be used in the lecture to demonstrate the essential features of Rutherford's experiment. It is intentionally open ended to give students the freedom to design their own experiments—something not easily done in the conventional laboratory.

PB1 and PB2 are very useful as lecture tools to illustrate the relationship between the wave function, the probability density function, and the corresponding dot-plot representations of electronic orbitals commonly used in chemistry. HCC can be used either as a lecture supplement or a student tutorial. These five programs are appropriate for any chemistry (or physics) class where the quantum theory of atomic electronic structure is being studied. SALT and CLEAVE are designed primarily as lecture aids for introductory chemistry; they can be juxtaposed with demonstrations that illustrate conductivity by ions in solution and crystal cleavage.

BCTC for Windows explores the use of the microcom-

puter as a simulation tool. It allows the student to explore the scientific aspects of a typical environmental controversy. In their exploration many of the procedures used in the analysis of such a controversy introduced, are thereby demonstrating one of the roles of the scientist in today's society. Such linkage of science to everyday life shows the student how important scientific knowledge is to the human endeavor.



Screen from BCTC showing location of the entry of the effluent in the river, the city, and the city water supply.

BCTC can serve as the basis for a scientific report, class discussion, or a role-playing exercise (5). Because it requires no previous laboratory experience, this simulation can be used by students in middle and high school science classes, or in college courses for nonscience majors, as well as in introductory chemistry courses for science majors.

#### **Hardware Requirements**

The programs in this issue require a MS-DOS/IBM compatible computer. Rutherford requires 640K RAM and VGA graphics. An 80286 or better microprocessor, a hard drive, and Microsoft compatible mouse are recommended. Animated Demonstrations requires 512K of RAM and CGA or better graphics. BCTC for Windows requires more than 1M RAM, a hard disk drive, and any Windows 3.x compatible graphics. A mouse is highly recommended to take full advantage of the graphical interface. Windows 3.0 or greater is also required.

#### **Literature Cited**

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