Computers in Chemical Education Newsletter

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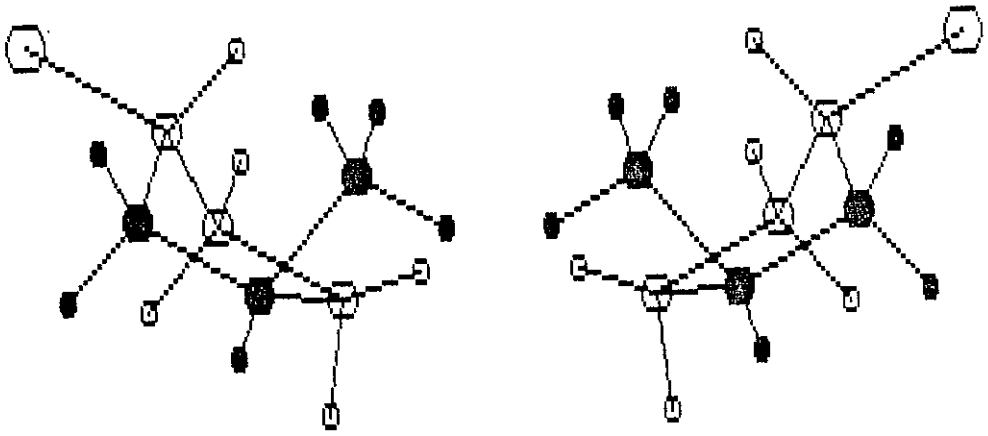
CHEMICAL STEREOGRAPHICS



OBJECT MIRROR IMAGE

trans-3-chloro-methylcyclopentane

COMMENTS FROM THE EDITOR

This Newsletter should have appeared in September 1986. I have edited the Newsletter since March 1981 and quite frankly I felt the need for an end to Newsletter deadlines. So I took a year off. I apologize to the editors, contributors and readers. All of the material from editors and contributors was received in time for a September 1986 issue. I appreciated the letters from those readers who wrote me asking why they were no longer receiving the Newsletter. I'm pleased to know that someone out there is reading the issues, which consume so much time and effort on the part of all those involved. Rather than trying to catch-up by putting out the four missing issues, this issue is to be considered a combined September 1986 and September 1987 issue. Subscriptions will be extended by one year. Thus, those of you who have subscriptions due to expire on September 1986 receive this the September 1987 issue as the last issue. The next issue will appear in December.

The June 1986 issue appeared prior to the 9th Biennial Conference on Chemical Education held on July 27 to July 31, 1986 at Montana State University, Bozeman, Montana. The meeting included a number of symposia, general papers, poster sessions and workshops on computing in chemistry. There was a computer graphics contest and exhibit sponsored by the Committee on Computers in Chemical Education. Also, project SERAPHIM sponsored a software contest and exhibit. Several of the exhibitors featured computer software and hardware. The total number of computer activities was most impressive. There was much more to be seen and heard about computing in chemical education than at previous biennial meetings, national and regional ACS meetings. The 10th Biennial Conference is scheduled for Purdue University during the summer of 1988. I would urge you to attend and make a presentation. It will be difficult, but not impossible, to surpass Bozeman.

Paul Cauchon, who has been a member of the Committee on Computers in Chemical Education and Chairman since 1984, stepped down as Chairman in 1987. Paul has been a prime mover on the Committee. Paul was the founder of the one-day high school chemistry teachers workshops which were originally sponsored by the Committee and held all over the country. These workshops are currently being sponsored by Project Seraphim. Paul has conducted many of the C.C.C.E. National Computer Workshops. He has written books and developed software for use in the classroom. It was recently announced that he will be recipient of the 1987 American Chemical Society Northeast Regional Award in High School Chemistry Teaching. Presentation of the award will occur during the 17th Northeast Regional ACS Meeting to be held in Rochester, New York in November. M. Lynn James from the Department of Chemistry, University of Northern Colorado, Greeley, CO 80639 succeeds Paul as Chairman.

In the June 1986 issue of the Newsletter Paul Cauchon asked for specific examples of computer applications which have proven successful in your own courses. He suggested you write a few paragraphs describing what you consider effective software. (It may be your own or commercial software.) Explain how and why it works for you. Pick at least one program you use on a regular basis and tell how you integrate it into your course. What do you expect students to get out of the program that they couldn't accomplish with the textbook or worksheet? What preparation do you give them? Exactly where does it fit into your course? How much computer time is required? How do you solve the problem of computer availability? How do you know that students use the program? The response to Paul's request has not been overwhelming. IS ANYONE REALLY OUT THERE?

COMMERCIAL SOFTWARE PREVIEW PACKAGE

The Committee on Computers in Chemical Education maintains two collections of commercial software which may be borrowed for up to five days by any school, college, university, or agency wishing to provide chemistry teachers in their institution or region with an opportunity to preview and evaluate computer-based instructional materials. Over 100 programs from a dozen publishers are contained in each of these collections. Although all disks are for the Apple II series of computers, many of the programs are also available for other types of hardware as well. The cost for using one of the collections is $75 to cover round-trip shipping by air express. Further information concerning specific contents and scheduling procedures is available:

East of the Mississippi: James Nelson, 148 Schuyler Road, Springfield, PA 19064.

West of the Mississippi: Don Murphy, 1920 Vine, West Des Moines, IA 50265.

MICROCOMPUTER GRAPHICS IN CHEMICAL EDUCATION

by Victor I. Bendall*

Microcomputer graphics are being used currently in several ways in chemical education software. Of course, microcomputer graphics can mean something as trivial as the display of the letter A on the axis of a graph or as complex as the display of a smoothly rotating molecular model. In this survey, the examples are taken from readily available software for the Apple II or IBM-PC series of microcomputers.

The simplest way that graphics are incorporated into software is as a static image used to illustrate some point. The image is prepared using a drawing utility such as Koala Painter and then stored for later use. This is by far the most common use of computer graphics and, although simple to produce, many more programs could benefit from this kind of graphic usage. It is easy to recognize because the images are commonly stored on disk so that the drive goes on and there is a short delay just before the image appears. Typically, such a program could show a Periodic Table on demand or a title page with an attractive image on it.

The better examples of the use of static images show up in the instrument simulations. These are intended for a tutorial or practice in the operation of a particular instrument. They can be useful when a student must practice the operation of a particular instrument before actually being allowed to operate it or when an instrument is not available but the skill to use it must be acquired anyway. These simulations can be relatively simple like the IR simulator of Krause for the MacIntosh (SERAPHIM MC1301). The user can control sample concentration and cell thickness before the simulation plots the spectrum of one of the available unknowns. A section of the program permits the user to make his own solution cell. The available parts have to be assembled in the right order and with some degree of precision.

More complex are the simulations of Paul Schatz (University of Wisconsin). The IR simulation mimics the Perkin-Elmer Model 1310 and the NMR models the Varian EH-360 instrument. The user must examine a mock-up of the main instrument panel and adjust the appropriate parameters just as in the actual machine. Then the spectrum is plotted.

HPLC by Rittenhouse and SPEC20 by Gable are under development through SERAPHIM. The former makes extensive use of very detailed, largely static images to simulate a High Pressure Liquid Chromatograph. The latter simulates the Spectronic - 20 visible-U.V. spectrophotometer. XENON by Whisnant (SERAPHIM AP606) simulates a vacuum line in which xenon and fluorine can react to form either or both of the xenon fluorides depending upon the temperature and concentration of the reactants initially chosen by the student user.

The most complex simulations use interactive animated graphics when the image on the screen responds to user input either directly, or indirectly, in that the image depends upon variables entered. The earliest examples were the Chem. Lab. simulations of Gelder. The one which illustrates the gas laws allows the student to vary P, V, N and T and to watch the simulated gas respond. Other modules available include acid-base titration, calorimetry and experiments involving equilibrium reactions. The simulations of Rittenhouse tend to favor re-enactments of famous historial experiments such as those of Rutherford. The user of this software can design and implement experiments on alpha particle scattering. The Rittenhouse simulations are excellent in that the graphics are very good and the user has to do the kind of thinking that the original experimenters did in order to reproduce the original results. The opportunity exists to accumulate extensive data from which the significant results must be culled.

The animated simulations of Bendall are not so difficult for the user. The objective is made obvious and the program is much more linear, reducing the possibility of being side-tracked. A typical example is Backtiter (SERAPHIM AP604) in which the object is to determine the concentration of carbonates in a mixture by adding it to standard acid and back-titrating the excess. The simulation requires the user to weigh samples on a top-loading balance and to titrate using a simulated buret. Along the way, the carbonate is shown bubbling as the acid is added, the buret flame flickers and the gas is shown escaping when the carbonate is heated.

Molecular modellers illustrate another use of microcomputer graphics. Typical of these are MOLEC by Owen and Curry and Molecular Graphics by Henkel and Clark. MOLEC was reviewed in J. Chem. Ed. in September 1984. Molecular Graphics can display and manipulate structures with more than a thousand atoms and bonds. The image can be translated along any coordinate, rotated about any axis or bond, enlarged or reduced. Standard molecules such as chymotrypsin are available, or one may enter a molecule by supplying atomic coordinates and bond connection tables. The image can be space filling in which case each atom is represented by a large sphere or made up of lines or lines with a small sphere at each intersection. The structural manipulations are slow. This is a common

limitation of these packages. The calculation and drawing of a new view depends upon the number of atoms but can take up to eight seconds and is too slow for effective animation. Space filling representations take longer to draw than line drawings.

Plotting routines use graphics to plot graphs. The most general kind allows the user to enter data, process it, and present the plotted results. Data can be entered at the keyboard or directly from an instrument. ASYST is an elaborate example. It turns an IBM-PC into a data station where data can be collected, reduced and plotted. It has modules for graphical and statistical analyses. It uses the 8087 co-processor for computational speed. An interface board is required and about $1700 can purchase the complete system.

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If you are reasonably certain of how you wish to process data and proficient in programming, then you are best off writing your own software. You are more likely to get fast code because you can optimize it for your particular application. If you want elegant displays including bar and pie charts, you should consider using one of the packages used by business in conjunction with a utility like Lotus 1-2-3.

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Software which helps the programmer animate his graphics appears to have great potential. The latest software of this kind is Fantavision. If two different images are drawn using the Koala Pad, the software can transform one image into the other. Fantavision is easy to create a moving picture with up to eight colored objects moving smoothly around the screen. It is very impressive but the code is copy protected and the DOS is customized so that the disk you create must be specially formatted for that alone. To incorporate such a movie into CAI software would require the user to change disks for the animation and then return to the program disk when the animation concludes. The clumsy procedure effectively makes it impractical for incorporation into other packages.

CHANGE is a utility now available from SERAPHIM which is like Fantavision but is less sophisticated. It can animate only one unfilled object. If a triangle and a square are drawn, then CHANGE can smoothly change one into the other. The software automatically compensates for the different number of apexes in the two images. Since the points which define triangle and square are transformed on a one to one basis, then if the triangle is defined clockwise and the square defined anti-clockwise, the triangle will appear to turn over as it is transformed into the square.

I am pessimistic about the future of chemical educational software that uses animated graphics. There are two major problems. Graphically oriented software is very machine specific. Software that can only be used in locations which have identical hardware is not of great utility to the educational community at large. We need to standardize graphic software so that it will run on all common microcomputers or settle on the use of one or two microcomputers for CAI. Standardization of software means that the code will not be optimal for any one computer. There will be loss of animation speed. Standardization of hardware means that the introduction of new machines will be resisted. At the moment there is an unofficial unification in that the Apple II and IBM-PC are the two major microcomputers in education today. Unfortunately neither is particularly well suited for animation.

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The other major problem is the effort required to produce good animated software. There is little incentive for academic programmers to produce it. Creative work is done for money, glory or personal satisfaction. There is little profit in educational software. Good and bad are similarly priced and copying good software is rampant. The number of chemists who write educational software for use by students is not large and the number that use animation is smaller.

Most of the software referred to in this article is available from Project SERAPHIM with the following exceptions: Koala Pad, Koala Painter (Koala Technologies Corp.), Fantavision (Broderbund), MOLEC
(Cambridge Development Labs), Molecular Graphics (Academic Press), Asyst (McMillan), Chem. Lab Simulations (High Technology Software), GRAFIT (Golden Software), and Lotus 1-2-3 (Lotus Development Corp).

-Adapted in part from a paper presented at the 191st ACS Meeting in New York City on 17 April 1986.

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SOLVING QUADRATIC EQUATIONS

by Donald Rosenthal*

In the June 1986 issue of this Newsletter I described a program which has been used by students in lecture and laboratory courses to solve the equation f(x) = 0. Complicated equations of this form are easily developed even in a general chemistry course.

Paul Cauchon wrote to say that his secondary school students at Canterbury School write such a program. Alfred J. Lata at the University of Kansas has demonstrated Ken Ratzlaff's program which graphically helps to locate roots.

One of the commercial software exhibitors at the Biennial Meeting in Bozeman last summer saw my article and wrote to say that it makes much more sense to use sophisticated commercial software rather than trying to develop programs of your own. Many programmers have spent long hours developing programs where satisfactory or better commercial programs already exist. However, since all students at Clarkson have their own computers, a program is needed which can be distributed to all students. Students have to buy books for courses. Is it reasonable to ask them to spend $10 or more for a single program which they will only use a few times in a course? Usually, site licenses are very expensive. If students in computer programming courses are asked to write programs which will be used in other courses, this can have a very positive influence on student attitudes.

If any readers have additional thoughts on this or related subjects, please write.

In this issue, I'd like to consider the development and use of a program which will solve quadratic equations. Such a program is of possible use when the hydrogen ion concentration of a weak acid, HA, needs to be calculated or equilibrium involving a complex, MX, needs to be considered. Such problems are considered even in general chemistry courses. If the quadratic equation is written as:

$$AX^2 + BX + C = 0$$

everyone knows from high school algebra that

$$X = \frac{-B + (\text{or } -)SQR(B^2 - 4AC)}{2A}$$

This is a correct formula, but computers perform arithmetic with finite accuracy. In some cases large round off errors can occur. One situation where this can be true is when B*B is very much larger than 4AC. Under these circumstances, the value of the square root term in the above equation will be close to B. If the -B term and the square root term have opposite signs the computer can give an erroneous result. However, the root having the larger absolute value (-B and square root terms have the same sign) can be calculated quite accurately. The trick is to calculate the larger absolute value root, R1, and the other root, R2 is C/(A*R1).

To illustrate a situation in which the two formulas give different results, consider a complex MX whose dissociation constant is 1 (A = B = 1). If the initial concentration of complex is 1E-7 (C = - 1E-7), the quadratic formula gives 5.96E-8 on my microcomputer and C/(A*R1) is 1E-7. If the initial concentration of complex is 1E-8 (C = -1E-8), the quadratic formula gives 0 on my microcomputer and C/(A*R1) is 1E-8. (R1 = -1 in both cases.) These results indicate the complex is virtually completely dissociated. The concentration of undissociated complex is 1E-14 in the first case and 1E-16 in the second case.

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TEACHING STEREOCHEMISTRY WITH COMPUTER GRAPHICS

by Richard E. Partch*

Teaching molecular stereochemistry at Clarkson has taken a quantum leap forward as a result of the University's commitment to computer-based education. Commencing in the Fall of 1983, all entering freshmen received a Zenith computer. Thus, each student now has in his/her room the necessary hardware for using or creating software.

Prior to the release of the model 200 computer in mid-1986, very little educational software was commercially available for use on the Zenith. As a result, it was necessary for Clarkson faculty and students to write programs for use in study and research. One example, titled "Molecular Stereographics", was developed by three undergraduate computer science majors and myself. This software provides the user much more structural information about molecules than most other commercial programs written for use with the Apple and IBM PC's. Data has now been accumulated on the successful use of such software to enhance student understanding of molecular stereochemistry. In order to make this software more universally attractive, an IBM-PC compatible version was developed. (Professor O. B. Ramsay, Head, Department of Chemistry, Eastern Michigan University used the software to teach stereochemistry in China the Fall of 1986.) Brief descriptions of the stereochemical operations which can be performed and the type of study questions that have been assigned for students to solve are described below.

Table 1 lists the commands a user has at his/her disposal. Several commands are the same as those in software previously written by others, but, this stereographics program also allows one to

1) obtain interatomic distances (ethanol, Fig. 1)
2) view single, double and triple bonds as one, two and three lines, respectively (3,5-dimethylbenzoritrile, Fig. 2)
3) view in Newman or sawhorse projection conformational rotation about any bond (C_2-C_3 of propene, Fig. 3-4)
4) observe dihedral angle values for any pair of atoms while bond rotation is taking place
5) view a molecule and its mirror image at the same time and carry out any of the commands on either (trans-3-chloro-methylcyclopentane, see cover)
6) observe and carry out commands on two different molecules at the same time (butane, chloroethene, Fig. 5), and
7) delete one peripheral atom from each of two molecules in view and combine the remaining fragments to create a new, single molecule (1-hydroxyethyl + cyanomethyl —— 2-hydroxypropionitrile, Fig. 6).

A series of instructional pages are included in the software which describe, among other things, the 25 different elements that may be used to construct molecules (e.g., C, Li, B, Mg, Si, Fe, Pt, Eu), the 18 molecules already entered into the directory (Table 2), and the method of entering new molecules for stereographic study.

The software has been used over a two year period by 230 students in four different classes studying first semester organic chemistry. In every class, the average on quiz and exam questions dealing with stereochemical concepts, (e.g. chirality, conformation, unimolecular and biomolecular reaction mechanisms) was at least 12 points higher than the average on similar questions obtained in 12 years of teaching without graphics software. At the beginning level, the computer graphics program is apparently far better to learn from than student molecular models, possibly because molecules viewed and manipulated on video are more closely related to the format on written exams.

All students are asked to view aspects of the stereochemistry of several molecules already in the directory. Homework may include assignments like: 1) What is the dihedral angle relationship between the chlorine and nitrogen atoms in 2-chloroacetaldehyde imine? 2) Print out the highest and lowest energy Newman projections of ethyl-hydrogenperoxide about the C-O bond. 3) What is the interatomic distance between the C_4 ring carbon and a hydrogen on the methyl group attached to boat cyclohexane? 4) Construct a chiral molecule from any pair of non-chiral molecules and then print out the side-by-side view of the enantiomers of the molecules before and after they are overlapped to show non-superimposability.

After the student becomes familiar with the software by using the seven stereographic manipulations listed in the instructions and doing the homework described above, each student is assigned three unique molecules to enter into the directory of his/her disk. Examples of these assignments are: 2-chloropropane (least stable eclipsed) trans-2-bromo-methylcyclopentane, p-toluic acid; cyanogen, 1,3-dimethylcyclohexane (most stable), triphenylphosphine; diethylpropylboron, cis-ethylenediaminedichloroplatinum, europium acetylacetonate. Successful completion of this part of the homework requires each student to understand the relationship

TABLE 1

Press any key to view molecule again.

Movement Commands

(X)	X Axis Rotation
(Y)	Y Axis Rotation
(Z)	Z Axis Rotation
(-X)	-X Axis Rotation
(-Y)	-Y Axis Rotation
(-Z)	-Z Axis Rotation
(B)	Bond Rotation
(U)	Up
(D)	Down
(L)	Left
(R)	Right

Display Commands

(I)	In
(O)	Out
(S)	Stick
(G)	Globes
(F)	Full

Transpose Commands

(T)	Transpose
(M)	Mirror Image
(Q)	Quit Transposing or Mirror Image

Miscellaneous Commands

(J)	Interatomic distance
(B)	Dihedral Angle
(C)	Atom Deletion
(K)	Molecular Bonding
(E)	Exit
(H)	Halt
(HELP)	Help
(0-9)	Speed

Use capital commands for large movements, lower case for short movements.

FIGURE 1

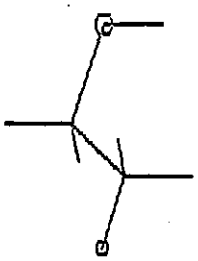
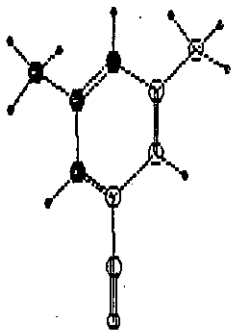


FIGURE 2



Distance equals 3.36

TABLE 2

3. THE DIRECTORY. The directory lists the file names for eighteen varied molecules already entered onto the disk. They are:

ETHANECL.REP	ethane (eclipsed)
ETOH.REP	ethanol
ETHPEROX.REP	ethylhydrogen peroxide
CLETHENE.REP	chloroethylene
CLACETIM.REP	2-chloroacetaldehyde imine
ACETCN.REP	acetonitrile
BRACET.REP	bromoacetone
PROPEN.REP	propene (eclipsed)
CLPROCN.REP	2-chloropropionitrile (most stable eclipsed)
BUTANE.REP	butane (staggered)
CLMECYPE.REP	trans-3-chloro-methylcyclopentane
BRCYHEX.REP	cis-1,2-dibromocyclohexane (most stable chair)
CYHEXB.REP	methylcyclohexane (boat)
BICYCLO.REP	bicyclo(2.2.1)heptane
CLMEBEN.REP	1-chloro-3-methylbenzene (m-chlorotoluene)
HOSTY.REP	o-hydroxystyrene
DIMEBECN.REP	3,5-dimethylbenzonitrile
TYLENOL.REP	tylenol

FIGURES 3-4

Dihedral angle =

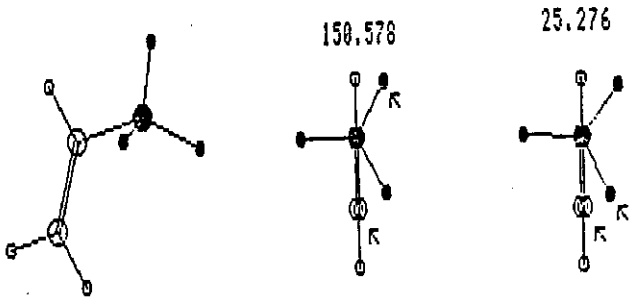


FIGURE 5
(ALSO SEE COVER)

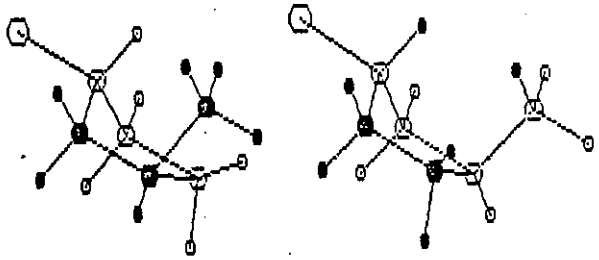


FIGURE 7

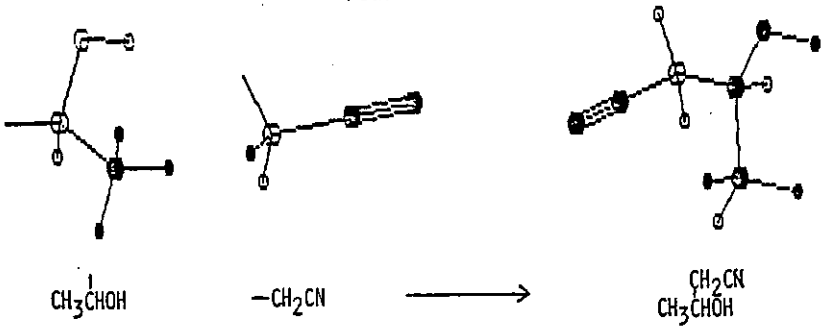
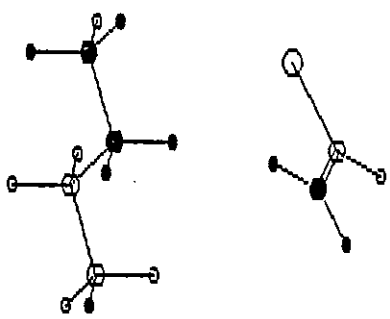


FIGURE 6



between bond lengths, bond angles and dihedral angles when representing a molecule in three dimensions. Disks are collected and evaluated to determine if the student has entered the molecules correctly.

In summary, there is strong evidence that students of organic chemistry substantially enhance their understanding of molecular structure when they are assigned computer graphics homework. Therefore, whenever possible, instructors should incorporate such software in their courses. In fact, the stereographics program we have developed has application even in freshman college and high school advanced placement courses.

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BOOK REVIEWS

Darnell Salyer, a Professor of Chemistry at Eastern Kentucky University, reviews a book on animation techniques for the Apple II in this issue. Based on his description, this book should be quite helpful to those readers who wish to spice up their programs with some eye-catching graphics. This is Darnell's first appearance in this column, but his article on the Apple random number generator appeared in the Newsletter two years ago. Also, he has worked with John Moore at Project SERAPHIM reviewing Apple software. In the second review, Dennis Seivers continues his fine series of book reviews on interfacing. This time the focus of attention is the IBM-PC. The final review looks at computer applications in the flavor and fragrance industries, an area that is probably somewhat unfamiliar to many readers.

Do you have some special area of computer expertise that you would like to share with your colleagues? If so, why not write to me and ask if there are books in your field of interest that you might review. Of course, it is always interesting to hear from the readers. Even if you don't wish to review a book, but want to share some comments or suggestions, write to Dr. Harry E. Pence, Book Review Editor, Department of Chemistry, SUNY-Oneonta, Oneonta, NY 13820.

ANIMATION MAGIC WITH YOUR APPLE IIE AND IIc

by Ron Person

Osborne McGraw-Hill, 2600 Tenth St., Berkeley, CA 94710

1985, 274 pages, paperbound, $15.95

Reviewed by Darnell Salyer*

Animation Magic is a veritable treasure chest of useful tools for creating animation sequences, graphics, and games. The book should be of considerable interest and value to intermediate or advanced programmers who are producing CAI and computer applications materials, and wish to add enhanced graphics and animation. A familiarity with Applesoft Basic is needed, but Person presents demonstrations and explanations of all programs and routines which will expand the user's programming skills. Non-chemical examples are used, but the techniques should be generally applicable. The programs will also execute on II, II+, and Apple look-a-like machines with at least 48 K of memory and DOS 3.3 or ProDOS.

The initial chapter,"An Animation Primer", is a general discussion with no programming, followed by Programming Your Game, which emphasizes structured programming with a master control and carefully arranged subroutines. Chapter Three gives an elementary introduction to creating, saving, loading, relocating, and using shape tables; table directories, and memory mapping. The relationship of color to shapes is considered.

Chapter Four extends the discussions and examples to shape animation. Easy to follow steps are given for using two large utility programs, Shape Maker and Advanced Shape Maker, to create cells for sequences and motions. Featuring a flashing cursor "pen" and enlarged grid, these are menu-driven and provide operation modes of pen-up, pen-down, draft, plot, edit, save, etc. The utilities eliminate much of the work of creating figures or shapes. They require relatively little direct use of machine language programming. A third utility, Table Maker, groups collections of shapes in a single shape table. Advanced programmers may be led to create their own utility programs.

Many useful small routines are found in Chapter Five on Backgrounds. Among the most notable are:

Color Pattern Fill (painting areas) Via XDRAW a closed boundary on the graphics screen is filled with single color or a pattern. This is useful for easily filling a buret, volumetric flask, etc.

Cut and Paste/Copying Screen Sections An original image can be duplicated at a different screen location, reproduced upside down or mirrored.

Rubber Band Box Via XDRAW, SCALE, AND ROT, the programmer-turned-artist can create rectangles and ovals of various sizes at a desired screen location.

Excellent paragraphs and small demo programs summarize the use of software switches to change graphics pages and page-flipping animation.

Collision detection and target identification are covered in Chapter Six, while Chapter Seven moves away from programming details to a brief discussion of form, objectives, strategies, and visual features of programs or games, which will lead to more effective interaction.

Chapter Eight concerns refining programs and includes lettering, titles, pull-down and pull-up menus, icons, and creation of function keys. Special Effects of Chapter Nine include motions of a bouncing ball, collisions, and rebound, calculated or manually entered motion paths, and motions under the influence of gravity.

TURTLE, ROUNDUP, and JERRI THE JUGGLER are demo programs which illustrate various forms of simple motions up to that of an animated runner.

The SCREEN ARTIST utility is introduced for creating backgrounds. It may be used independently of the animation programs to create bit-map files for title screens, enhanced graphics, or pictures. Programs may then add/remove other features by way of other utilities which write on the HIRES screens or by HPLOTing.

Approximately one-third of the pages of Animation Magic are listings of the programs, and these were found to be remarkably error free. A printer's error was found on page 2, where Apple III should be II. It is instructional to type the programs as they are studied, executed , and debugged, but the time saved may be worth $19.95 for the Animation Magic Toolkit, which may be ordered from an address in the book. The reviewer's order was filled in eight weeks.

Companion works by Person include Macintosh Game Animation, and the IBM PC and PCjr version of Animation Magic, both from Osborne McGraw-Hill. Corresponding toolkit diskettes are also available, the former from Person and the latter from Osborne McGraw-Hill.

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INTERFACING TO THE IBM PERSONAL COMPUTER
by Lewis C. Eggbrecht
Howard W. Sams Co., Inc., 1985, 246 pages, paperbound, $15.95
available from Group Technology, Ltd., Box 87, Check, VA 24072
Reviewed by Dennis Seivers*

Interfacing to the IBM Personal Computer is a valuable reference for those seriously interested in designing interface projects for the IBM PC computer. This fully indexed book is written in moderately technical language. Illustrations are well-placed and accent the text very well. Unlike many books in this field, a relatively small number of pages are devoted to specific project construction. Rather, the discussion is more generic in nature and explores bus and circuit design.

The discussion begins with a full exploration of the 8088 microprocessor. Each feature is fully described along with its use and means of access. This permits direct use of the microprocessor in circuit interfacing. This is one of the better descriptions of the 8088 done in a moderately technical, abbreviated manner.

The expansion bus configuration is explored in a similar manner. The author provides readers with some interesting ideas for application of the bus circuit but does not design the circuit.

The section on timing cycles is extremely well done and quite useful. The author develops the use of the internal clock as well as several other possible sources of timing signals. In this chapter information is given on the machine language needed to access these timing circuits. Most of the program considerations are found elsewhere. This material is further explored by consideration of both the hardware and software triggers of timing devices.

The chapter on interrupt usage is fairly typical of the use of computer interrupts for data collection and transmission. Machine language and BASIC techniques for programming the interrupts are supplied without any specific application in mind. I rather prefer this, as it allows for the construction of a library of useful routines to be created for future use.

The system and memory maps are comprehensive. This chapter is mostly a series of charts with a minimum of explanation. Dialogue is rarely needed, as this material is used chiefly for reference.

The section on data transmission and acquisition speed synchronization is one not generally found in most interfacing books. The treatment is clear and detailed. Many unique problems are associated with high speed data transfer, and several solutions are discussed.

A few projects are described in detail and include the use of the cassette port for TTL output and the use of the parallel printer card for data output. The methods described are not new, but many users are unaware of the techniques needed for these simple interface designs. The ever-popular game card is a standard interface port, and the author describes several uses. A variety of high voltage and high current control devices are described. These include a lamp driver, stepper motor driver (two types), and a classic relay driver. Schematic diagrams and software routines are provided, and these projects should find many applications.

BASIC programming techniques are described to utilize these interface projects. The use of BASIC and machine language drivers teaches many important concepts. The programming chapter is very well done but does assume some prior experience with machine language entry and BASIC.

If you are looking for predesigned projects and software, this book is not for you. Should you be interested in designing a special interface for your laboratory, this book could answer many technical questions related to the hardware and software components. The experienced user will find this a useful reference, while the intermediate user should learn a great deal from this book.

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COMPUTERS IN FLAVOR AND FRAGRANCE RESEARCH

Craig B. Warren and John P. Walradt, editors
American Chemical Society, Washington, D.C.
1984, 164 pages, hardbound, $29.95
Reviewed by Harry E. Pence*

Computer use has been expanding rapidly in all types of industrial chemical laboratories, so it should surprise few readers that this trend also extends to the flavor and fragrance industries. Since changes in these industries are not always widely followed, the specific directions of computer development may not be familiar to most of us. This book consists of a series of papers presented at a symposium sponsored by the Division of Agricultural and Food Chemistry at the 186th Meeting of the American Chemical Society, Washington, DC, August 28-September 2, 1983.

The first five articles deal with using computers for structure-activity correlations, information handling, and statistical analysis. Many of the processes in these articles, such as computer-assisted molecular design, information storage, and information retrieval, will be familiar to those who regularly follow computer developments in chemistry, but the specific applications are sufficiently different to be of interest. In addition, sensory scientists must collect and process data from evaluation panels, individuals who express their opinions about the flavor and/or odor of possible new products. These panels play a key part in product development, and the computer can contribute significantly to this work.

Most chemists are aware that the pharmaceutical industry has played a pioneering role in research on computer-assisted molecular synthesis but may not be familiar with similar work done in the flavor and fragrance industry. These papers discuss several methods that are being studied to find structure- activity correlations. Taken together, they present a useful perspective on some of the progress in this area. Even though the relation between sensory properties of flavor compounds and their molecular properties is not yet understood, progress is being made towards predicting the odor and/or taste of new products.

Computer processing of information from evaluation panels is especially important since it can both decrease the cost and increase the reliability of these procedures. The criteria here can be complicated. As an example, the public may associate effectiveness of medicines with unpleasant taste, and consumers can be just as likely to reject a product that tastes too good as one that tastes too bad. To quantitatively measure these trends, statistical analysis plays a role that is as important as analytical instrumentation and measures of organic reactivity.

Of course, the computer is not essential for this work. Acceptable products were produced long before the development of the microprocessor, but the computer offers savings of both time and expense when used for product modeling and optimization. It can streamline the process by recording evaluations, organizing data, and determining the most effective new product formulations.

Chapter Six discusses how to determine whether the purchase of a Laboratory Information Management System (LIMS) is economically justified. Papers on this topic often point out the technical advantages but fail to consider economic factors. This treatment is not detailed, but it does identify the major financial and workload considerations which should be surveyed. It may provide an interesting perspective for those who are thinking about purchasing a LIMS system as well as those who don't normally deal with factors like interest payments, analyst workload, and speed of analysis.

Those readers who feel that instrumentation is overemphasized at the expense of human capabilities should be encouraged by a statement in the next chapter (page 75) that, "Despite the inherent sensitivity and wide applicability of conventional GC and GC/MS techniques, they will never replace the well trained nose as a means of identifying odiferous components." Unfortunately the ego boost is of limited duration, since the author goes on to explain how a new instrument, the Atmospheric Pressure Chemical Ionization Tandem Triple Quadrupole Mass Spectrometer (APCI/MS/MS), is able to analyze air-borne fragrances directly from the atmosphere without intermediate trapping or concentration steps, just like the human nose. The applications used to test this instrument are quite interesting, including a determination of whether men emit different chemicals from their skin than women, and also an investigation of the advertising claims that a certain perfume creates a different aroma on every woman who wears it.

The next three chapters describe other computer-based analytical instruments that are used in the flavor and fragrance industry. An article on near infrared reflectance analysis (NIRA) states that this procedure is becoming very popular for food analysis because it is not only rapid and non-destructive but usually requires little, if any, sample preparation. These advantages should also make the method useful in other areas of chemistry. Gas chromatography has been used for many years to analyze the individual compounds responsible for product flavor, but the effectiveness of this instrument is increased by coupling it with multivariate methods of statistical analysis. The efficacy of this combination is demonstrated here by two studies, an aroma analysis of cigarette smoke from different tobaccos and the correlation of analytical and sensory data for quality control.

The last article on instrumentation describes the use of a commercially available laboratory automation system for chromatographic analysis, data processing, and data analysis of flavor extracts from food. The data treatment again includes statistical procedures known as multivariate analysis. The final chapter concerns the use of a laboratory robot system for routine analytical tasks. This study reports that sample preparation by the robot system offers significant time savings over manual methods. Accuracy and precision are almost identical by robot and manual methods.

The book is printed from camera-ready copy, but all of the chapters are quite clear and readable. Each article provides a short bibliography with references through 1983, and the book includes an adequate index.

Although the computer applications outlined in this book are derived from the fields of flavor and fragrance research, many of the techniques should be applicable to other areas of chemistry. These articles could provide an interesting perspective both for those who are currently involved in computer applications in the industrial laboratory, as well as for those who only wish to keep informed of recent developments.

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Hardware QUERIES

Send Hardware QUERIES and REPLIES to Jim Beatty, Chemistry Department, Ripon College, Ripon, WI 54971, (414) 748-8123.

Software QUERIES and REPLIES should be sent to Ken Loach, SUNY at Plattsburgh, Plattsburgh, NY 12901, (518) 564-2230.

WHO DONE IT?

WHO DONE IT? information should be sent to the appropriate section editor (Hardware or Software - see QUERIES above).

Jim Beatty (see address above) is interested in receiving WHO DONE IT? items or more extensive reviews from users of data acquisition systems such as the Keithley 500 Scientific workstation and the Keithley System 570 Data Acquisition workstation.

WHO-167 (Sept. '86)

Consumer Reports, March 1986, 51 (3), 166-169 reviews the following IBM-compatible computers: Epson Equity I, Kaypro PC, Leading Edge Model D, and the Zenith Z-148.
October 1985, 50 (10), 576-580 reviews of IBM-compatible computers included the Compaq Portable, Kaypro 16, Leading Edge Model D, Panasonic Sr. Partner, Sanyo MBS-775, Tandy 1000, and the IBM-PC. (J.B.)

WHO-168 (Sept. '86)

The Apple Macintosh is reviewed in Consumer Reports, January 1985, 50 (1), 28-31. (J.B.)

WHO-169 (Sept. '86)

Two Apple II compatibles, the Franklin Ace 2000 and the Laser 128, are compared to the IIc and IIe in Apple+, June 1986 4 (6), 26-44. (J.B.)

WHO-170 (Sept. '86)

Consumer Reports, August 1985, 50 (8), 467-471 gives a review of the Apple IIe Professional, TRS-80 Model 4P and Kaypro IIx. A comparison of these machines with the IBM-PC and the Apple Macintosh is given.

WHO-171 (Sept. '86)

Consumer Reports, June 1985, 50 (6), 338-343 reviews the following Dot-matrix printers: Panasonic KX-P1081, Smith Corona D200, Apple Imagewriter, C. Itoh 8510 BPI, Diablo P12CQI, Epson RX-80 F/T, IBM Graphics, Mannesman Tally Spirit 80, Okidata 92P, Radio Shack DMP-120, Star Delta-10, Star Gemini 10-X, Hewlett-Packard ThinkJet, Apple Scribe, and the Okidata 92S. Also, the following daisy-wheel printers are reviewed: Juki 6100, Brother HR 15, NEC 15LQ, Silver Reed EXP 400, and Smith Corona L1000.

WHO-172 (Sept. '86)

Twenty-five monochrome and color computer monitors are reviwed in Consumer Reports, July 1985, 50 (7), 420-422.

WHO-173 (Sept. '86)

Patricia Wirth and Lincoln Ford in Byte, July 1986, 11 (7), 303-310 review five laboratory interfacing packages to go with the interfacing boards, Techmar Lab Master and Data Translation DT2801, for the IBM PC. (J.B.)

WHO-174 (Sept. '86)

Byte, May 1986, 11 (5), 215-224 includes a Rich Mallory review of current optical disk drives for those wishing increased storage for the IBM-PC. (J.B.)

WHO-175 (Sept. '86)

There is a special issue on applications of expert systems (AI) to CAI in J. of Computer Based Instruction, Spring 1986, 13(2), 29-61: the eight articles cover principles and practice of the application of 'intelligent' teaching systems to Department of Defense training, but the techniques obviously could have wider applications. (K.L.)

WHO-176 (Sept. '86)

T. Mirecki, PC Tech J., June 1986, 4(6), 52-75: this is a review of the new wave of 'enhanced-BASIC' interpreters now coming onto the market: BASICA, BetterBasic, BusinessBasic, MegaBasic, ProBasic, TrueBasic, and Whatcom Basic. (K.L.)

WHO-177 (Sept. '86)

V. E. Wright, PC Tech J., June 1986, 4(6), 110-123: a review of Formula/One, an equation-solving system patterned after TKSolver! It can be used to solve complex systems of equations and for curve-fitting and regression analaysis. (K.L.)

WHO-178 (Sept. '86)

Byte, May 1986, 158-246: this is a group of seven articles on Mass Storage. All but one of them are on CD-ROM optical disk systems, which are beginning to come into educational and library use as data-base systems for full-text searching. (K.L.)

WHO-179 (Sept. '86)

Users of the IBM-PC should consult the Fall 1986 Special Issue of Byte for a collection of articles on technical features of the IBM-PC. The following two articles should be of special interest:

D. E. Crabb, "Annotated Bibliography of Recent Books: Technical Topics for the IBM-PC Family", idem, 11-35.

J. R. Edwards, "Public Domain Utilities", idem, 39-54: this has information on many free software utilities for the IBM-PC, with sources. (K.L.)

WHO-180 (Sept. '86)

R. E. Dessy has a continuing series of articles on instrument interfacing called "The PC Connection" in Analytical Chemistry. So far, three parts of this series have appeared: Part I, May 1986, 58 (6), 678A-690A; Part II, June 1986, idem, 793A-804A; Part III, July 1986, idem, 919A-925A. (K.L.)

WHO-181 (Sept. '86)

The following papers and poster-computer hands-on sessions were presented at the 9th Biennial Conference on Chemical Education at Montana State University, Bozeman, Montana on July 28-30, 1986.

Stanley G. Smith and Loretta L. Jones (School of Chemical Sciences, University of Illinois, 601 S. Mathews, Urbana, IL 61801): "Computer-Assisted Videodisc Lessons in Chemistry."

H. Saltsburg, R. H. Heist, and T. Olsen, (Dept. of Chemical Engineering, University of Rochester, Rochester, NY 14627): "A New Way to Teach High School Chemistry Laboratory."

Joseph J. Lagowski, (Dept. of Chemistry, The University of Texas at Austin, Austin, TX 78712): "The Simulation of Laboratory Experiences."

Leonard J. Soltzberg, (Dept. of Chemistry, Simmons College, 300 The Fenway, Boston, MA 02115): "The Computer-Assisted Blackboard", "Far-From-Equilibrium Model Systems" and "Improving Student Attentiveness with a Classroom Computer."

William Torop (Dept. of Chemistry, West Chester University, West Chester, PA 19383): "Chemistry Laboratory Reports Using a Spreadsheet Computer Program."

David B. Shaw (Madison Area Technical College, 3550 Anderson Street, Madison, WI 53704): "Teaching the Concepts of Accuracy and Precision as You Introduce Your Computers."

Douglas A. Coe (Dept. of Chemistry and Geochemistry, Montana College of Mineral Science & Technology, Butte, MT 59701): "Numerical Methods on a Spreadsheet."

Gilbert Pollnow (Dept. of Chemistry, University of Wisconsin, Oshkosh, WI 54901): "Enjoying Chemical Data Processing with 'Minitab'."

Merlyn D. Schuh (Dept. of Chemistry, Davidson College, Davidson, NC 28036): "Biophysical Chemistry Experiment: Micro-Computer Analysed Initial Rate Kinetics of Benzene-Enhanced Unfolding of Myoglobin."

Daniel Cabrol and Claude Cachet (Universite de Nice, 06034 Nice, France), Richard Cornelius (Lebanon Valley College, Annville, PA 17003): "The Computer as a Problem-Solving Partner -- A Program Written in Prolog."

Allan L. Smith (Chemistry Dept., Drexel University, Philadelphia, PA 19104): "Undergraduate Use of Equation Solvers for Chemical Computations", "Computer-Based Molecular Graphics for Learning Molecular Structure", and "Two Computer Simulations for Learning Equilibrium and Kinetics."

Donald B. Stierle and Donald J. McBride (Dept. of Chemistry and Geochemistry, Montana College of Mineral Science and Technology, West Park Street, Butte, MT 59701): "Using Three Computer Assisted Instructional Programs in Teaching Organic Chemistry."

Edward A. Mottel (Dept. of Chemistry, Rose-Hulman Institute of Technology, Terre Haute, IN 47803-3999): "Dynamic Computer Programming: Allowing Students to Design and Solve Their Own Problems."

Robert M. Dreyfuss (Mercy College, Dobbs Ferry, NY 10522): "Tutorial Software for General Chemistry."

Dr. Donna Bogner (Box 51, Wichita State University, Wichita, KS 67208): "So, You Only Have One Computer."

R. W. Ramette (Carleton College, Northfield, MA 55057): "Some Useful Computer Programs."

George C. Lisensky (Chemistry Dept., Beloit College, Beloit, WI 53511): "Tuning an NMR Spectrometer: A Computer Simulation" and "Using Record/Recall: Event-Driven Data Acquisition with ADALAB, Followed by Plotter or Screen Comparison of Stored Spectra."

James T. Streator (Dept. of Chemistry, Manchester College, North Manchester, IN 46962): "Computer Use in the Classroom."

J. A. Weyh and J. R. Crook (Dept. of Chemistry, Western Washington University, Bellingham, WA 98225); L. Hauge (Spokane, WA 99223): "Reactions in Aqueous Solution."

David A. Wing (Dept. of Natural Sciences and Mathematics, Grand Canyon College, Box 11097, Phoenix, AZ 85061): "Using a Spreadsheet in Advanced Chemistry Courses."

John S. Martin (Dept. of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2): "Demystifying Bronsted: A Computer Course in Acid-Base Equilibrium."

F. J. Rowe (Northport High School, Northport, NY): "Classroom Usage of Computer Graphing."

J. I. Gelder and R. E. Snelling (Dept. of Chemistry, Oklahoma State University, Stillwater, OK 74078): "A Quantitative Microcomputer Lecture Demonstration of an Equilibrium Reaction."

Nancy Whiteside Brickhouse and Derek A. Davenport (Dept. of Chemistry, Purdue University, West Lafayette, IN 47907): "The Blue-Bottle and Your Basic Phenolphthalein-phade Reaction Revisited."

Bruce W. Gutzmann and John P. Walters (Dept. of Chemistry, St. Olaf College, Northfield, MA 55057): "Chemically Driven Interfacing in the Analytical Laboratory."

J. W. Beatty (Dept. of Chemistry, Ripon College, Ripon, WI 54971): "Interfacing of Chemistry Experiments at a Small Liberal Arts College."

D. T. Magnuson (Dept. of Chemistry, Texas A&M University, College Station, TX 77843): "Interfacing for Real-Time Data Acquisition and Analysis in an Undergraduate Potentiometric Titration Experiment."

John K. Estell (Dept. of Computer Science, University of Illinois, 1304 West Springfield Ave., Urbana, IL 61801): "The Operation and Modification of the Apple Paddle Input."

J. R. Amend, R. A. Howald and E. S. Hood (Chemistry Dept., Montana State University, Bozeman, MT 59717): "How Can One Spend Equipment Dollars Effectively to Bring Interfacing Into Undergraduate Labs?"

R. Roe, Jr. and W. W. Schulz (Highland Park High School, Dallas, TX 75205): "Making Computer Slide Shows."

Frank Rioux (Dept. of Chemistry, Saint John's University, Collegeville, MN 56321): "Microcomputer Graphics and Quantum Mechanics."

Bhairav D. Joshi (Dept. of Chemistry, State University College, Geneseo, NY 14454): "Electronic Spreadsheets - New Tools for Scientific Problem Solving."

W. A. Whitla (Dept. of Chemistry, Mount Allison University, Sackville, New Brunswick, Canada, E0A 3C0): "An Inexpensive A/D Interface for the Commodore C-64 Computer: An Automated Titration Experiment."

M. Lynn James (Dept. of Chemistry, University of Northern Colorado, Greeley, CO 80639): Symposium on "Implementing the Computer as an Integral Aid to the Chemistry Teacher."

Sherry Berman-Robinson and Lee Marek (Sandburg High School, Orland Park, IL 60462): "Computer Interfacing as Useful Tools in the Science Classroom."

R. Roe, Jr. (Highland Park High School, Dallas, TX 75205): "Making Computers and Related Technology in Integral Part of Your Classroom."

James W. Beatty and Thomas J. Oyster (Chemistry Dept., Ripon College, Ripon, WI 54971): "The First Decade of PC Usage in a Liberal Arts College Chemistry Department."

K. A. Hartman (Ames Senior High School, 20th and Ridgewood, Ames, IA 50010): "Chemical Education and the Computer: Marriage, Live-In Companion, or Peaceful Coexistence."

Howard P. Williams and J. Emory Howell (Dept. of Chemistry, University of Southern Mississippi, Hattiesburg, MS 39406-5043), Joseph L. Russell (Dept. of Chemistry and Physics, Alcorn State University, Lorman, MS 39096): "Structured Chemical Problem Solving and Basic."

R. G. Kooser (Knox College, Galesburg, IL 61401) and R. Ditchfield (Dartmouth College, Hanover, NH 03755): "Kinetic Mechanism Modeling on the Macintosh."

Dr. Larry M. Julien (Dept. of Chemistry and Chemical Engineering, Michigan Technological University, Houghton, MI 49931): "Animated Interactive Simulations of Chemical Phenomena on Microcomputers."

F. J. Juergens (Dept. of Chemistry, University of Wisconsin-Madison), J. I. Gelder (Dept. of Chemistry, Oklahoma State University) and S. Sellin (Dept. of Manufacturing Systems Engineering, University of Wisconsin-Madison): "Displaying Titration Curves on an Apple IIE With the ADALAB(TM) Interface Board and Interfacing Utility Programs."

Fred D. Williams (Dept. of Chemistry and Chemical Engineering, Michigan Technological University, Houghton, MI 49931): "Participational Fiction in Education."

R. C. Rittenhouse (Dept. of Chemistry, Eastern Michigan University, Ypsilanti, MI 48197): "Computer Simulation of Advanced Instrumentation."

Geoff Rayner-Canham (Sir Wilfred Grenfell College, Corner Brook, NF, Canada A2H 6P9): "Two Uses of Microcomputers in a Small College Environment."

John V. Clevenger (Truckee Meadows Community College, Reno, NV 89512): "Bring in a Trojan Horse."

John L. Burmeister (Dept. of Chemistry, University of Deleware, Newark, DE 19716): "Dynamics of a Three-Cornered Duel: The Creation of a Complete Computer-Based General Chemistry Course."

R. W. Gable (Dept. of Chemistry, Davidson College, Davidson, NC 28036): "Keeping the User Happy: Examples and Suggestions for Better Programs."

D. Cabrol (Centre de Recherche Pedagogique et de Renovation Didactique de Chemie, Universite de Nice, Parc Valrose, 06034 Nice Cedex, France): "Prolog and Artificial Intelligence Techniques for Chemical Education."

Tom Aanerud (P. O. Box 1828, Riverton, WY 82501): "Spreadsheet Templates for Vocabulary Development."

James L. Fasching, Duane C. Costa, Richard B. Suarez (Dept. of Chemistry) and James G. Kowalski (Dept. of Philosophy, University of Rhode Island, Kingston, RI 02881): "Chem-Tutor: An ICAI System for Teaching Chemistry."

Roy W. Clark (Dept. of Chemistry and Physics, Middle Tennessee State University, Murfreesboro, TN 37132): "Microcomputers in the Chemistry Teacher's Office."

Raymond F. Beamish (Chemistry Dept., Wilson High School, Tacoma, WA 98406): "Computer Assisted Science Labs for Chemistry."

H. Donato, Jr. and C. Metz (College of Charleston, Charleston, SC 29424): Estimation of Error in the Physical Chemistry Laboratory Using Lotus."

C. R. Ward (Dept. of Chemistry, University of North Carolina at Wilmington, Wilmington, NC 28403): "Microcomputer Applications in Chemistry: A One Semester Course for Majors."

Lucy T. Pryde (Dept. of Chemistry, Southwestern College, 900 Otay Lakes Rd., Chula Vista, CA 92010): "Using SERAPHIM/ChemCom Interface Software in the Classroom."

COMPUTERS IN CHEMICAL EDUCATION NEWSLETTER

SUBSCRIPTION RENEWAL FORM

The mailing list will be updated for the next issue of the Newsletter. If you wish to renew or initiate your subscription please fill out this form completely and return it with your remittance to:

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Clarkson University
Potsdam, NY 13676

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Back issues from 1981 to the present may be obtained at $1.50 per issue. Issues appear in (1) March, (2)June, (3)September and (4)December.
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NAME _____

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CITY _____ STATE____ ZIP_____

PHONE NUMBERS Work (___) _____ Home (___) _____

Courses which you teach _____

Name of school or professional affiliation, if not indicated in the above address.

_____

Please provide all information requested on the other side of this sheet.

OVER PLEASE

1. Are you a member of the ACS? __ Yes __ No
   Division of Chemical Education __ Yes __ No
   Division of Computers in Chemistry __ Yes __ No

2. Brief description of hardware and software which you use.

3. Do you have telecommunications capabilities? __ Yes __ No
4. What communicates with what? Indicate any special software or hardware.

5. Do you have access to any networks? __ Yes __ No
   If so, please identify. _____

6. Areas of Computer Activity and Interest

Leave the space provided below blank if you have no present interest or activity. 1 means a little, 2 means moderate, 3 considerable, and 4 with a consuming passion.

Use the space on the right to identify the courses in which the software or hardware is used. Identify the programming language(s), computer and any specialized hardware or instruments used.

	Degree of Interest	Activity	Description of Use
CAI Drill and Practice			
CATC (Comp. Assisted Test Construction)			
CMI (Comp. Managed Instruction)			
Simulation			
Numerical Methods and Statistics			
Graphics			
Software development other than above			
Interfacing			
Laboratory Automation			
Other (specify)			

	Personal Use	Administrative Use	Use in Instruction
Word Processing			
Software Used			
Electronic Spreadsheets			
Software Used			
Data Bases			
Software Used			

WORKSHOPS, MEETINGS, CONFERENCES & COURSES

Please send information to Donald Rosenthal, Editor. Describe the program, include location sponsoring group, dates, costs and who to contact for further details (name, address, and phone number). Information should be sent as far in advance as possible.

April 20: SERAPHIM - C.C.C.E. High School Teacher Workshop at Marion College, Marion, IN.
This workshop has two basic objectives- To illustrate how microcomputers can be of use to a chemistry teacher and to provide an opportunity to preview representative samples of commercially available software. Joe Rich, Blackhawk Christian School, Fort Wayne, IN is the workshop leader. Contact Dr. Vickie Hess, 4201 South Washington Street, Marion, IN 46952 for additional information.

April 28 - May 3: ACS National Meeting at Miami Beach, FL
Symposia and general papers. High school and student affiliate programs. CHED meeting chair is Richard Steiner, Department of Chemistry, University of Utah, Salt Lake City, UT 84112; (801-581-6681). A symposium on Bachelor Degree Programs in Computational Chemistry is being organized in the Division of Computers in Chemistry by Dr. Peter Lykos, Illinois Institute of Technology, Chicago, IL 60616.

May 17: SERAPHIM - C.C.C.E. Teacher Workshop at Carl Sandberg H.S., 133rd and La Grange Road, Orlando Park, IL 60462.
See April 20 listing for details. Contact Sherry Berman at the above addresss for additional information.

May 30 - June 1: Personal Computer and STD Computer Interfacing for Scientific Instrument Automation at V.P.I. and State University, Blacksburg, VA.
A hands-on workshop with each participant wiring and testing interfaces. Directed by Mr. David E. Larsen and Dr. Paul E. Field. $450 for 3 days. For more information contact Dr. Linda Leffel, C.E.C., V.P.I. State University, Blacksburg, VA 24061. (703) 961-4848

June 1: SERAPHIM - C.C.C.E. Teacher Workshop at Columbia Greene Community College, Hudson, NY 12534.
See April 20 listing for details. Contact Dr. Jeanne Gizare at the above addresss for additional information.

June 10 - 14: VIIth International Conference on Computers in Chemical Research and Education at Garmisch-Partenkirchen in the Bavarian Alps, Federal Republic of Germany.
Plenary lectures, poster presentations and a computer exhibit. For further information write Conference Office, Gesellschaft Deutscher Chemiker, Abt. Tagungen, P.O. Box 900440, D-6000 Frankfurt am Main 90, Federal Republic of Germany.

June 24 - 26: Northeast Regional Meeting of the A.C.S., SUNY at New Paltz, New Paltz, NY 12561
Symposia on Computers in the Chemical Laboratory, Computing for Every College Student, and computer literature searching. General papers on computer applications. Contact J. Malmgreen, Eastern Alloys, Henry Henning Drive, Maybrook, NY 12543.

July 28 - August 1: Seventh C.C.C.E. National Computer Workshops - East at Clarkson University, Potsdam, NY 13676
Six intensive workshops are planned. See detailed information elsewhere in this Newsletter. Contact: Donald Rosenthal at the above address (315-268-6647).

July 29 - August 2: World Conference on Computers in Education in Norfolk, VA.
Contact Gerald Engel, WCCE/85, Department of Computer Science, Christopher Newport College, Newport News, VA 23606.

August 2 - 5: CHEM ED '85 at Montclair State College, Upper Montclair, NJ.
Workshops, demonstrations, presentations, poster sessions and computer sessions. Individual presentations demonstrating effective use of currently available software and hardware which can be used in the classroom. Approaches to problem solving as illustrated by TK! Solver (Alan Smith) and George (Dick Cornelius). Computer Assisted Testing (Darell Beach). Workshops on laboratory instrument interfacing; and spread sheets, word processors and other aids to the chemistry teacher. A C.C.C.E./SERAPHIM software evaluation center will operate throughout the conference. Contact CHEMED '85, C/O Dorothy Lehmkuhl,56 Normal Avenue, Upper Montclair, NJ 07043 for further details.

August 11 - 15: Seventh C.C.C.E. National Computer Workshops - West at Truckee Meadows Community College, 7000 Dandini Blvd., Reno, NV 89512
Five intensive workshops are planned. See detailed information elsewhere in this Newsletter. Contact John Clevenger at the above address for additional details (Phone 702-673-7221).

August 22 - 24: Personal Computer and STD Computer Interfacing for Scientific Instrument Automation, Washington, DC
Similar to workshop being held May 30 - June 1. Refer to this entry for further details.
Workshop repeated in Greensboro, NC September 19 - 21.

August 23 - 28: IUPAC-sponsored 8th International Conference on Chemical Education in Tokyo
Write J. T. Shimozawa, Chemical Society of Japan, 1-5 Kanda-Surugadia, Chiyoda-ku, Tokyo, 101 Japan.

September 8 - 13: 190th ACS National Meeting in Chicago, IL Symposia, general papers and exhibits. Those wishing to present papers must submit four copies of an abstract with the original on an ACS abstract form by May 1 to William F. Coleman, Department of Chemistry, Wellesley College, Wellesley, MA 02181 (617-235-0320, ext. 3129)

October 18 - 19: First Eastern Small College Computing Conference at the University of Scranton and the Hilton at Lackawana Station.
Designed to promote a free exchange of information among small college personnel concerned with the use of computers in the academic environment. Intended to span all academic disciplines. Topics include software, simulation, course management, curriculum development, computer literacy, the computing laboratory and micro/mini/mainframe. Extended abstracts are due on February 15th, notification of acceptance May 17th, completed papers are due by July 15th. Contact Professors Meinke and Beidler, ESCCC, University of Scranton, Scranton, PA 18510.

WEST COAST COMPUTER WORKSHOPS SET FOR AUGUST 11-14 AT RENO, NEVADA

Unanticipated circumstances have necessitated rescheduling the Seventh CCCE National Computer Workshops-WEST, previously announced for the Los Angeles area. Instead, the Workshops will be hosted in Reno, Nevada at Truckee Meadows Community College beginning Sunday, August 11 and running through Thursday, August 15. The meeting is co-chaired by Dr. John Clevenger, Department of Chemistry, Truckee Meadows Community College 700 Dandini Blvd., Reno, NV 89512 and Dr. M. Lynn James, Department of Chemistry, University of Northern Colorado, Greeley, CO 80639. Workshops to be presented include "Getting Started", Dr. Pat McIntyre, St. Martin's College; "Development and Design of CAI", Dr. Stanley Smith, University of Illinois; "Computer Graphics for Chemistry", Dr. Jess Schilling, Trinity University; "Interfacing Laboratory Instruments and Microcomputers", Dr. James Currie, Pacific University; and "Software Evaluation", Dr. M. Lynn James.

Located in a well-known resort area, Truckee Meadows is only an hour's drive from Lake Tahoe. Registrants will be housed in casino hotels at special conference rates. For registration details, costs and other information, contact John Clevenger at the above address (phone (702) 673-7221). Additional information on these workshops will be available in the June Newsletter.

SEVENTH C.C.C.E. NATIONAL COMPUTER WORKSHOPS-EAST

The registration form for the National Workshops to be held in Potsdam, NY, July 28th to August 1st, 1985 appears on the following page. Only the registration fee needs to accompany the Registration Form. Checks or money orders should be made out to Clarkson University. Housing will be provided in dormitory rooms with a shared bath between two rooms. The cost for single occupancy for four nights is $52. Double occupancy is $35 per person. This revised rate is less than is indicated in the registration form. Those interested in making Potsdam the home base for a vacation may be interested in weekly room rates which are $57 for single occupancy and $43 per person for double occupancy. In addition to local recreation Potsdam is within easy driving distance of the Adirondacks and Lake Placid, the Thousand Islands, Ottawa and Montreal. Persons planning to stay five or more days should request weekly rates.

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Potsdam, New York 13676

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