Computers in Chemical Education Newsletter

Published by the ACS Division of Chemical Education
Committee on Computers in Chemical Education
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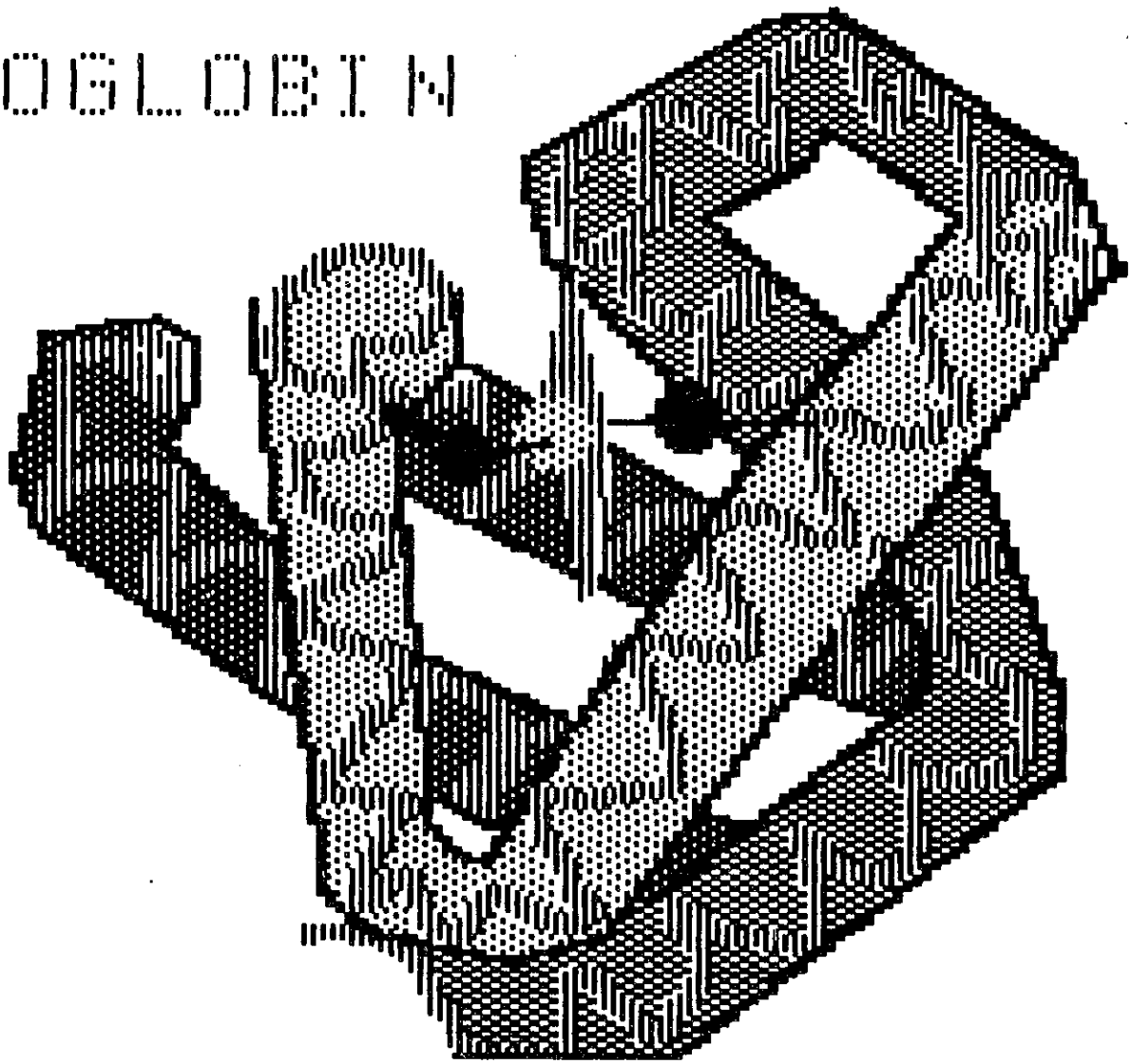
Volume VIII Number 1 **March 1985**



ON THE COVER

Dr. Charles E. Ophardt (Chemistry Department, Elmhurst College, 190 Prospect, Elmhurst, IL 60126) won second prize in the Computer Graphics Contest held at the Eighth Biennial Conference on Chemical Education for his entry entitled "Myoglobin". The figure was developed on an Apple II+ having 48 K bytes of core using the Micro Illustrator software package, an Apple Imagewriter and a Koala Pad. Professor Ophardt has indicated that the picture on page 47 of "The Structure and Action of Proteins" by R.E. Dickerson and I. Geis (W.A. Benjamin, Inc. 1969) served as the model for this figure.

MESSAGE FROM THE CHAIRMAN

Recently I came across a collection of "computer courseware evaluations" published by a regional educational agency. This group reviews software in a comprehensive, carefully structured process. The agency's efforts cover major curriculum areas and its findings are published periodically in a hefty 200 page catalog. In this particular issue, about 60 pages were devoted to science – with over 70 titles in chemistry alone, including the vast majority of what is currently available from commercial sources. About 50 programs or program sets had been evaluated, the others listed as "discontinued", "unavailable", or "outside the curriculum". Out of all those which had been screened, this group found only THREE it could recommend, and three more described as "still under review"; the other 46 were listed under the heading "unable to recommend due to unfavorable evaluation results". This I found alarming!

In spite of the oft-heard lament that "most of the commercial software is junk", I feel that any reviewing agency which rejects almost 90% of the chemistry software currently being marketed should take a close look at the criteria and procedures it has established. Granted that much of the material for sale does not come close to making full use of a computer's potential value as an instructional tool, yet many programs offer excellent applications in many different ways, some much less "exiciting" than others, but still pedagogically quite sound. To me, such an overwhelming rejection of state-of-the-art software indicates incomplete understanding of the many roles computers can play and evaluation criteria that are too narrowly focused. In addition, some questions can be raised about the validity of at least one of the reviews which faulted a formula-writing lesson for being inaccurate because of "gold being shown with a +1 charge on the oxidation table"!

I am concerned about the newest level of educational bureaucracy that is appearing on the scene, establishing standards and checklists for evaluating software which sometimes seem to be more concerned with form than substance. It is far easier to rate a program on its appearance than to analyze its pedagogy. In fact, it is very difficult to appreciate just how bad or good a program will be until one has tried it with the student population for whom it was designed, in the context for which it was designed to be used. The nebulous, overworked criterion "is it user-friendly?" frequently has quite different answers, depending on who the user is and in what environment the software is being used.

Software evaluation is one of the most difficult tasks teachers are asked to perform these days, more difficult than textbook selection, I would say. All of us have used textbooks as students and as teachers. Hence, we know pretty much what works and what doesn't, based on experience from both ends of the process. Not so with software – the number of chemistry teachers who have used computers in teaching long enough to be able to look at a program and decide if and how a class will profit from it is still very small; the number of teachers who actually learned chemistry with computers is several orders of magnitude less! Each of us continues to discover new applications as some of the constraints (hardware costs, memory size) of just a few years ago are lifted.

So what do we do about it? How DO we decide what to buy, until that day arrives when most of what is being sold is really good? Well, for starters, I'd say read and save the software reviews in J. Chem. Ed. (They are also available through SERAPHIM). The approach taken in J. Chem. Ed. is to present in narrative form at least two viewpoints on a software package. Each reviewer is identified. You may draw your own conclusions, depending upon how closely your teaching situation parallels the reviewer's. Second, attend one of the SERAPHIM/CCCE Workshops or CHEM ED '85 where you'll have an opportunity to look at a sizeable sample of what's on the market, including some very good material from new, small publishers of whom you have never heard. Finally, share your experiences by writing a short article for this publication describing a program which you find useful, explaining what it does, how you use it, and why it is effective. (See Brian Pankuch's description of High Tech's Gas Laws in this issue, for example.) What works for you in your teaching situation may be just the thing someone else has been looking for, whereas the same piece of software may be relatively useless to someone with a different approach or learning environment. What we need is more specific information from a variety of sources, not broad generalized ratings based on arbitrary check lists. We each have our own "checklist" of what to look for, and I'm not sure one exists that suits all of us equally well. There is no denying the need for more good software – I think one way to get it is by vocally promoting the good material that is already available, thereby encouraging authors and publishers to move forward and invest time and money in an activity whose future financial success if far from assured.

COMMENTS FROM THE EDITOR

This is the next to the last issue of the Newsletter you will receive unless you renew your subscription by sending in the subscription renewal form before mid-July. Those who have already renewed their subscription will have the subscription expiration date appear on the first line of the mailing label (8609 is September 1986).

We are attempting to help organize a rather full program of contributed papers on computer uses in chemical education for the National Meeting to be held in New York City from April 6 to April 11,1986. We are interested in activities at the high school, first two years of college and advanced course level. Those of you who are willing to contribute papers or have suggestions for the high school program should contact Paul Cauchon, Canterbury School, New Milford, CT 06776, (203) 355-3103. Professor Patricia Flath, Paul Smith's College, Paul Smith, NY 12970, (518) 327-6264 will handle the first two years of college. I will help organize papers concerning the use of computers in advanced courses. (Professor Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam, NY 13676, (315) 268-2389). A symposium involving "Applications Software for Lecture and Laboratory Courses" is being considered. The symposium would involve the use of substantial program packages in education, i.e. the use of word processing, electronic spread sheets, data bases, statistical, numerical methods and graphics packages in courses. I would like to hear from anyone interested in participating in such a symposium. Anyone having suggestions for programs at future National Meetings (fall 1986 - Anaheim, CA and beyond) should contact Paul Cauchon.

Ken Ratzlaff has ably served as editor of the hardware QUERIES and WHO DONE IT sections of this Newsletter from the time this section was first established in 1981. Ken has contributed many articles to the Newsletter including articles on networks and the series on uses of the game port. Ken is presently Chairman of the Division of Computers in Chemistry and is writing a book. This, plus his activities at the University of Kansas where he heads the Instrument Design Laboratory makes for a very busy schedule. Ken has asked to be relieved of his duties as hardware editor and we have reluctantly accepted his resignation. Jim Beatty (Chemistry Department, Ripon College, Ripon,WI 54971, (414) 748-8123) has agreed to serve as new hardware editor. Please send QUERIES and WHO DONE IT materials to him.

In this issue of the Newsletter Brian Pankuch has written an article describing the use of two computer programs in one of his courses. This was done in response to a suggestion by Paul Cauchon. I would be interested in receiving similar short articles describing novel uses of computer programs in courses or student responses to particular programs. Programs which are transportable either because they are commercial or in the public domain and which are likely to be of general interest should be described. Please send a typewritten copy of the article to me preferably double spaced.

I would be interested in receiving brief articles containing short routines that are likely to be of use to others. The article by Victor Bendall on page 5 of the December issue entitled "Embellish Your CAI Programs With Sound" is the sort of thing I mean. It contained a fifteen line listing of the program and twelve lines of text. In general, programs should be less than forty lines with one program statement per line. If possible, the listing should be letter quality so that it does not have to be retyped. Routines in BASIC, FORTRAN, PASCAL or assembly language are to be preferred.

USING COMPUTERS IN CHEMISTRY

by Brian Pankuch*

After being asked to comment on computer programs which I use, it was easy to choose my favorite two programs; not so easy to analyze why they are my favorites. Both do have several attributes in common. They:

1) Simulate moving particles that we can't see,
2) Give a more accurate model by showing movement and interaction at the same time,
3) Are interactive and give a wide choice of how information appears on the screen,
4) Allow the user to follow virtually any path desired through the program.

The first program demonstrates gas laws. It is available from High Technology Software Products, Inc., P. O. Box 14665, 8001 N. Classen Blvd., Oklahoma City, OK 73313 (405) 840-9900 for $100. You need an Apple with game paddles. The program draws a cylinder with a movable piston. You input the number of moles of gas using numbers 1-9. Other parameters such as temperature and pressure of the gas can be constantly changed using the game paddles. The gas molecules are shown bouncing around in the cylinder. If you increase the temperature or number of moles the volume is shown to increase by piston movement. At the same time, on the lower part of the screen, the current pressure, volume, number of moles, and absolute temperature are shown. The gas molecules move faster at higher temperature and slower at lower temperatures.

Before using the simulation in class, I discuss pressure, temperature, and volume measurements and units. The next period I wheel the computer and color monitor into lecture early enough to set it up and have a few students start using the program. Students choose the color of the cylinder, piston, and background on the screen, and the amount of noise molecules make when they collide with each other or the container. Enough time is provided to play with the game paddles to see what happens. In some classes students cluster around making suggestions, and agitating for their turn. In other classes you are lucky to convince one or two students to try the program.

Once class starts I begin to lecture on Boyle's law deriving the formula and emphasizing what's happening physically. I use the simulation to show an example of increasing the pressure emphasizing physically what is happening. We set up the problem on the board, not just solving the equation but using the computer simulation. For instance "What happens when we increase the pressure - see the volume gets smaller." The students can see the volume get smaller. We check the numbers on the screen. Pressure is bigger since we increased it and the volume is smaller.

How do you set the problem up mathematically? If you know the pressure is increasing in the problem and you understand physically that this has to decrease the volume, then you already know the final volume has to be smaller. We multiply the original volume by a pressure correction factor. Since we already know the final volume has to be smaller, we put the smaller pressure on top and the larger pressure on the bottom. We get the answer from the monitor, then solve Boyle's law mathematically and get the same answer. We check to be sure that the final volume is amller than the initial volume.

We go over a similar sequence with Charles' law. Combining these relationships, the ideal gas law is obtained. This is particularly useful since then we take the pressure and volume directly from the screen, multiply them (I usually set up numbers that are easily done in your head), then the number of moles and the absolute temperature from the screen and multiply these together with the ideal gas constant and show that the ideal gas law works for all examples we try. The simulation is part of the lecture.

I keep the equipment available for the next week or so during my conference hours to allow interested students to use it. Written evaluations and exams from students over seven semesters indicates that the program is very useful.

The second program is a molecular bonding simulation. I wrote this myself to bridge the gap between my concretely-thinking students and a rather abstract area. I was especially interested in showing the geometry of the molecules, that moving electrons are restricted to a probability space, and that two elements may form more than one compound.

This programs shows an abbreviated periodic table of about 70 elements. These are the elements included in the program. The program will only handle compounds containing two elements. The student is asked to choose the two elements, and is shown the three most likely oxidation states for each element. The student can then choose to see as many as three different molecules (appropriate messages are displayed if molecules are not formed). For lin-

ear, triangular planar, and tetrahedral molecules, bonding electrons are shown and the electrons may be animated in four different modes. With the trigonal bipyramid and the octahedron, stick models are presented on the screen.

My methodology is different with this program. I have previously covered VSEPR bonding thoroughly and have had students struggle with homework problems. As in the gas law case, I bring the computer in early before the lecture and get the students involved. In this case the students usually try a few simple molecules. Then someone gets the idea that the program may be used to solve problem 23h in the homework.

After a few students practice, I take over and use the animation in the HF to HI series to emphasize several points. The Lewis diagrams are useful but incomplete in visualizing what the electrons are doing. The electronegativity affects where the electrons spend most of their time. One of the animation modes allows you to leave a mark where the electron has been so that you get an approximate probability space or rough orbital pattern.

Students always want to do homework problems finding the molecule that is most likely formed between two elements. A number seem surprised that you can get many molecules from the same two elements.

The program works not by having structures stored in memory, but by storing basic facts such as the number of valence electrons, oxidation numbers, electronegativity, etc. It then "calculates" the number of ligand positions, lone pairs, etc. It is a primitive "expert system" in which I programmed my expertise as a step by step procedure to find the most probable molecular structure. In this case, I did not use anything which isn't present in popular freshman texts.

I wrote this algorithm in English, or perhaps "chemicalese" is more appropriate, and hand it out to the students. We then take a homework problem and step our way through as indicated in the algorithm. Then we have the computer work the problem. I keep emphasizing the movement of the electrons – both the actual change in position and the higher electron density near the more electronegative element. We discuss and show how we can get more than one molecule from two elements.

Students are encouraged to come in, use the programs, and make suggestions or improvements, which they do. Feedback and testing show that interest is increased and ability improved as a result of using this program.

As the author of this program, I found that creating a realistic moving model brought up many questions which required considerable thought and research. In building this "expert knowledge-based system" I gained considerable insight into the subject matter and why and where students frequently go wrong.

Many areas may benefit from teaching with an "expert system". Areas that appear particularly appropriate are those in which you can combine the computer's vast memory and speed with your intelligence and experience. To enumerate the 6000 or so possibilities in this program from my memory would be difficult, but by connecting my expertise via an algorithm to the computer's stored facts, a more useful tool is created.

Areas of application would be (a) helping students solve problems by setting them up specifically for the problem the student inputs, (b) helping analyze lab data. The step-by-step procedure to interpret results such as an IR spectra could be improved. Instead of using a general approach the program could consider the specific spectrum a student is solving and go through each step using that spectrum as an example. This type of program is difficult to write since the path is variable and determined by the user.

We have experimented letting students customize an existing program. As more students have programming skills we should get them involved in programming worthwhile chemistry problems – NOT problems done more easily with a calculator. Programs are particularly useful which simulate (a) something you can't see otherwise (electrons, atoms, molecules), or (b) something which is dangerous or very time consuming, or (c) instruments which are expensive or dangerous.

The programming itself is an excellent learning experience and may make the effort of including it in an already crowded course and curriculum worthwhile.

For further information on "expert systems" you will find Expert Systems - Myth or Reality? by Bruce D'Ambrosio, pp. 275-282 Byte, Jan. 1985, and The Fifth Generation - Artificial Intelligence and Japan's Computer Challenge to the World by Feigenbaum and McCorduck, interesting.

This last program will only run in Pascal on a Terak computer. It will not run on an Apple or IBM. See J. Chem. Ed. Sept. '84 for availability.

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A GAME APPROACH TO TEACHING FACTS
by R.W. Ramette*

A program named TRIVGAME, written in Microsoft BASIC for the TI Professional Computer, the IBM Personal Computer and capatibles, allows 1-8 contestants to choose 1-6 categories of questions to answer in the manner made so popular by the game Trivial Pursuit.

As play proceeds, an on-screen scoreboard displays the progress of each contestant. The first one to correctly answer a chosen number of questions in each category is the winner, and a song is played to honor the victory.

TRIVGAME uses random numbers to choose questions from text files residing on the disk. In contrast to the truly trivial questions that are included in the commercial board games, the object in an educational setting is to create files of questions that have a measure of significance. For example, it is not educational to ask for the birthplace of Linus Pauling, but a good question would be to ask the name of the American who won Nobel Prizes for both Chemistry and Peace.

The goal is to encourage students to learn a large number of "good things" about various subjects, to be exposed in a casual setting to numerous facts that almost never find their way into formal courses in spite of their inherent significance. For example, it is good for chemistry majors to know that helium gets its name from the Greek word for sun, because it was first "discovered" there by virtue of its spectral lines. They should somehow learn that our system of element symbols and formulas started in Sweden with the brilliance of Berzelius, that light bulbs are filled with argon to minimize evaporation of tungsten from the hot filament, that aluminum doesn't dissolve in the rain because of a tight thin layer of oxide.

Because TRIVGAME reads whatever question files are provided, it is possible for teachers and students to make up their own sets of questions in whatever categories they desire. There could be a file of questions for individual courses in the curriculum. Or perhaps an analytical professor would like to make a file dealing with modern instrumental analysis, or with environmental chemistry. An all-history collection could have separate files for organic chemistry, physical chemistry, nuclear chemistry, inorganic chemistry, chemical technology, and so on.

An important characteristic of such files is that they may easily grow larger, as participants suggest additional questions. Also, any one question might well be placed in more than one file. For example, a question on iodine clock reaction could be placed in the inorganic and the kinetics, and the miscellaneous file. A utility program, TRIVSORT, takes care of proper addition of new questions to existing files.

For those who are interested in obtaining the programs, please send $10.00. A disk containing the programs will be forwarded which will run on the TI or IBM PC.

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MULTITASKING OPERATING SYSTEMS FOR THE IBM PC
by G. Scott Owen*

With the decline in cost of memory and the increased processing power of 16 bit microcomputers, it is now feasible to use multitasking operating systems with these machines. By multitasking, I do not mean use by many users, but simply that the machine can execute several programs at the same time. This is a software development that I have eagerly awaited because it has seemed very inefficient to tie up my machine for extended periods performing some routine task, e.g. downloading files from a mainframe or performing some long calculation. I would like to report on my experience with one multitasking operating system Concurrent PC-DOS from Digital Research, the developers of the CP/M operating system.

This operating system started out as Concurrent CP/M-86 about two years ago. I bought the product at that time but soon realized that the CP/M-86 operating system was a loser in the new IBM world and all applications were being written for PC-DOS, or the generic MS-DOS. So, I put Concurrent on the shelf and hoped it might eventually be useful. I kept buying the upgrades and when DRI announced Concurrent PC-DOS (CC PC-DOS) and said that it would run all PC-DOS software, I quickly purchased the upgrade.

CC PC-DOS is an impressive piece of software which will allow you to execute up to four tasks at once and will even allow you to connect two dumb terminals to your PC for multiuser capability. It requires large machine resources and runs best on a 640K machine with a hard disk. The commands are very similar to those of PC-DOS and if you don't want to use commands there are programs included which allow you to perform the various DOS functions, e.g. formatting, copying, etc., entirely from menus. You can generate your own menus for custom work.

CC PC-DOS comes with a data communications program (very similar to PC-Talk), a full screen text editor, and a Card file program to store notes, addresses, etc. One problem is that all tasks must fit into memory at the same time and some programs require large amounts of memory. It is a windowing system and you can define windows of any size anywhere on the screen. If you have two monitors, (I have a graphics board and a monochrome adapter) then you can have one task displayed on each monitor). Switching from task to task is simple and you can have the task either continue to execute or be suspended when you switch to another one. This is useful as some programs write directly to the screen, e.g. Lotus 123, and so would show up even when you are looking at another task.

Being able to observe two tasks concurrently, by using two monitors, was very helpful. I could watch a file being sent or received using a data communications program while I was creating a program using a text editor. Another use was executing a program on one minitor while looking at the source code on the other. CC PC-DOS is very efficient and takes little overhead in switching from task to task, i.e. performing four calculations at the same time took very close to a factor of four of the time required to do only one task.

The documentation is reasonably good except that it doesn't really tell you what you shouldn't do. I was really enjoying using CC PC-DOS but there were some problems. Occasionally the machine would totally lock up and I would have to turn it off and then back on (a cold boot). It wasn't clear what was causing this problem but I thought I could live with it. But then DISASTER.

The machine locked up and when I turned it back on my hard disk would not boot up the system. I booted up the system on a floppy and then checked the hard disk with the PC-DOS utility CHKDSK. I got a very strange message for about twenty of my files as follows: "filename" CROSSLINKED ON CLUSTER 67 (or some such number). This esoteric message is not in the DOS manual. The two hidden system files on the hard disk (IBMDOS and IBMBIOS) were also crosslinked and this was why it wouldn't boot. I was able to erase and then replace the other files but I couldn't replace the two system files. Finally, my only recourse was to reformat the hard disk and start all over.

I removed the CC PC-DOS from the hard disk and put it in a box well away from my machine, where it remains. I refuse to use an operating system which destroys my files and makes me reformat and reconstrct my hard disk. Since it is impossible to get any support from DRI, unless you are a mega dealer, I don't know what I did wrong, but I'm not taking the chance that it might happen again. Oh well, maybe TOPVIEW will work.

BOOK REVIEWS

Regular readers of this column can look forward to a special treat if they plan to attend the Seventh C.C.C.E. Computer Workshop - East this summer in Potsdam. In addition to an extensive set of interesting workshops, there will be an exhibit of computer books and software which will be specially selected for their potential interest to chemists. Some of the books will be provided by the publishers, and some will be personal copies belonging to members of the conference organizing committee. The basis for selection in all cases will be the applicability of the book to the activities of chemists.

For those who have considered reviewing for this column but have hesitated to volunteer, the book exhibit may be an excellent opportunity. On the last day of the workshop sessions, those who wish to review one of the books provided by the publishers may take a book home with the understanding that they will submit a review of it within six weeks of the end of the conference. Of course, there is no reason to wait until summer to begin reviewing. Readers who would like to submit a book review for this column may write to Dr. Harry E. Pence (Department of Chemistry, SUNY-Oneonta, Oneonta, NY 13820) for further information and assistance. Even if you don't wish to write reviews at this time, please send suggestions for this column. There is room to discuss only a small fraction of the total number of computer books published, and your letters will help to identify the types of books that should be emphasized.

THE COLLEGE STUDENT'S PERSONAL COMPUTER HANDBOOK

by Bryan Pfaffenberger

SYBEX, 1984, 210 pgs., (paperback) $14.95

Reviewed by Harry E. Pence*

A recent television advertisement consisted of two contrasting scenes. In the first, an enthusiastic young man is boarding a train to leave for college. Though burdened with enough equipment to start a small boarding school, he isn't really prepared, or so the television voice assures us. The next scene shows the same young man returning home in dejection, a failure because he didn't have a personal computer. Pfaffenberger clearly agrees that a personal computer is a vital piece of equipment for the college student, but he completes the story only hinted at in the commercial, by showing that a college student can do much more with a personal computer than play computer games.

This is not another book on how to use a computer, but rather is a demonstration of how a personal computer can be especially valuable to a college student. This distinction is the key to understanding the author's selection of topics and the method of presentation. There is almost no discussion of programming or computer languages, because Pfaffenberger feels that user-friendly commercial programs are already available that serve the needs of the typical college student and represent the quickest way to make the computer productive.

Much of the book deals with the three types of commercial software that experienced users would expect; spreadsheets, word processors, and data base managers. In general, the author uses programs that are well-known, but the emphasis is not on learning how to use a specific program but on learning the capabilities of a general type of program. He discusses several typical problems in detail, showing the reader where a computer could be valuable. For example, he demonstrates a spreadsheet by statistically manipulating quiz grades from the grade book of a hypothetical student teacher and a word processor by writing and revising a section of a term paper. These and other examples are extensive and realistic.

The section dealing with on-line information services is especially helpful. Pfaffenberger recommends that students use the relatively inexpensive nighttime services, such as BRS/After Dark or Knowledge Index, and he also identifies which academic fields are poorly covered by these services. He describes a good example of a simple search and demonstrates how logical operators can be used to make a search more efficient. The treatment is brief but offers a good indication of the support these services provide.

For this reviewer, the most interesting section was the use of a database management system called Notebook (Pro/Tem Software) to record, retrieve, and reorganize a set of course notes. This discussion not only contained some valuable information about using the computer but also some useful tips on taking and organizing notes. Even though the method described probably requires more effort than most students are willing to invest, many instructors will find the technique interesting. On the other hand, the use of a database management system to do more traditional jobs, such as organizing references, addresses, etc. is discussed only briefly.

The introductory chapter on basic computer concepts is rather concise but contains a reasonable overview of what a beginner needs to know about computers. In addition, there is an appendix containing a brief glossary of commonly encountered terms. Other appendices provide a software and hardware buyer's guide and a guide to inexpensive on-line data base services. The number of recommendations in each category is limited, so that readers may find some personal favorites ommitted. Nevertheless, suggestions provide helpful guidance for a new user.

The author does a good job of showing how the computer can do a broad range of tasks, but probably in no case does the reader learn enough to actually use the software described. This is not a serious criticism, since the book is obviously intended to be an overview, rather than a tutorial. Once the reader understands what can be done, he or she will seek other sources of information to provide the necessary expertise. A more serious shortcoming of the book is the failure to provide a bibliography or reading list of books and journals telling the reader where to go for more information.

Readers of the CCE Newsletter will probably find that they are already familiary with much of the material in this book, but it can be a good resource for those who are inexperienced and wonder what can be done with a computer. That audience isn't limited to college students, and considering the background many students are obtaining in high school today, it is quite possible that the book may be equally useful to their parents and other adults. Pfaffenberger doesn't necessarily agree with the advertising claim that a student without a computer is doomed to fail at college, but he does suggest a number of areas where the computer may make a significant difference.

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KAREL THE ROBOT
by Richard Pattis
John Wiley Sons, 1981, 106 pgs., (paperback) $9.50
Reviewed by Harry E. Pence*

The fundamental concept of this book will be immediately obvious to anyone who has previously had the pleasure of using LOGO. Like the familiar LOGO turtle, Karel the Robot is simply another name for the cursor on the computer screen. His movements can be controlled by a relatively simple programming language. The subtitle of the book, "A Gentle Introduction to the Art of Programming with Pascal" indicates that Pattis has written his book not merely to provide pleasure for the reader, which it does, but also to provide an introduction to the fundamental concepts of Pascal.

The ground rules of Karel's universe are simple. The screen is divided into a ten by ten grid, described as streets and avenues. Movement across this grid is restricted by the presence of walls which are placed at different positions in each problem. Karel can move forward one grid space at a time, turn to his left, pick up or deposit markers ("beepers") in positions next to the cursor, and finally he can be turned off when the task is completed. If he is given an order which is impossible to execute, he turns himself off.

In each problem, the purpose is to move Karel across the screen, either picking up or depositing beepers in a predetermined fashion. Although the initial situations are relatively straight-forward, the problems become increasingly complex and are positively challenging by the end of the book. Students will find the approach to be non-threatening and conducive to learning. Numerical data, input-output methods, and data structures are de-emphasized, so that the student can develop a good foundation in the essentials of programming and problem solving.

Starting from the the primitive control structures described above, the instruction set becomes increasingly sophisticated, allowing for the development of block structures which are essentially equivalent to procedures in Pascal, conditional statements, such as IF/THEN/ELSE, and finally pretest loops, using the WHILE-DO command. Each of these new commands is integrated into a modular structure which closely resembles that used in Pascal.

The author has not only written a very readable introduction to structured programming, but he has also combined this with an excellent discussion of problem solving strategies. The method of stepwise refinement is introduced early and is employed consistently throughout the book. Pattis uses box of block diagrams to help the student to visualize the program structures, and he emphasizes that programs must be clear and understandable. The book doesn't teach Pascal, but a student who has completed this book will certainly find Pascal to be familiar and easy to learn.

Both mainframe and microprocessor versions of Karel are available, but personal experience suggests that this support is not essential. Running the programs on a computer does help to catch subtle errors, but the author is quite right when he suggests that if time is limited, it is equally effective to do the programs by hand. The preface indicates that this entire book is covered in four class days at Stanford. This seems a little rapid for those who have never programmed before, but it accurately suggests that the book is clearly written and easy to understand.

Pattis has written a book which is not only fun to read but also teaches many of the basic ideas of computer programming. It is a good introduction to structured programming for the beginner and can also serve as a transition to Pascal for someone who is already familiar with a non-structured language, such as BASIC. It is a pleasure to recommend this delightful little book.

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ANNOUNCEMENTS FROM PROJECT SERAPHIM

Project SERAPHIM, the NSF sponsored clearinghouse for microcomputer information and software for chemistry instruction, has just released some new items of interest. These include:

Apple Disks, new series. There are 26 (full) diskettes in the new series of reorganized, debugged, and corrected programs for Apple II/II+/IIe. These are available individually for $5 each or as a set of 26 disks for $125; available documentation is supplies with each program, on the disk itself. The reorganization has classified these programs into ten subject areas:

-Series 100: Methods of Chemistry
-Series 200: Atomic Structure/Periodicity
-Series 300: Bonding/Formulas/Stoichiometry
-Series 400: Solids/Liquids/Gases
-Series 500: Solutions Processes/Acid-Base
-Series 600: Chemical Reactions/Equilibrium-Kinetics-Redox
-Series 700: Organic Chemistry
-Series 800: Environmental/Industrial Chemistry
-Series 900: Analytical/Qual
-Series 1000: Nuclear Chemistry

To order copies of these disks or to obtain descriptions of the contents of each, contact Project SERAPHIM (address below) to obtain a Catalogue.

Project SERAPHIM Catalogue: The Project SERAPHIM Catalogue has been completely revised as of January 1985. It contains complete information about the new series of Apple disks, new Commodore disks, new TRS-80 disks, new written materials, etc. The Catalogue is free. Write for one at the address below.

Project SERAPHIM Software List: The Software List is a compilation of all chemistry-related instructional computer programs about which the Project has been able to gather information. This includes commercially and noncommercially-available programs as well as Project materials. The Software List has been revised and is now available in its Fifth Edition, February 1985. It contains 429 listings of individual programs and software packages. It is indexed by author, subject, publisher, and by availability of reviews. The cost remains at $5/copy.

Other new publications: These include a microcomputer version of the Project CHEMLAB database for the IBM PC -- a database of all laboratory experiments published in the Journal of Chemical Education from 1957 through 1982; written materials for teachers of biology, physics, or mathematics suggesting sources of and information about software in these disciplines; written materials about interfacing the TRS-80 Color Computer; and many other items.

To obtain any of the above items or to get on the Project SERAPHIM mailing list to receive regular announcements, write to: John W. Moore, Director, Project SERAPHIM, Department of Chemistry, Eastern Michigan University, Ypsilanti, MI 48197. (Phone (313) 487-0368 or 387-0106).

ESTABLISHING A UNIVERSAL CHEMISTRY NETWORK

by Kenneth Ratzlaff, Chairman of COMP Division*

It has become increasingly clear to many of us that the chemical community must have a communications network. This might not be obvious to those who do not use a network. However, one rapidly becomes convinced upon observing how much a network is used by those who have one available.

I hope that during this year, the COMP division and the CHED division, both of whom have shown interest, will set up a prototype network for division members. With this memo, I would like to solicit more information and some opinions. Then we might be able to move ahead toward a proposal by summer and possible implementation of a prototype system by fall.

In the following sections, I have tried to list

(a) some of the possible applications that I see for the network,
(b) the characteristics which I think the ideal network should have and,
(c) some of the available options and how they fit the ideal characteristics.

This list is incomplete and may contain errors but is meant to serve as an initial attempt to formulate what is needed. I would appreciate receiving your comments regarding applications, characteristics, and options which you believe are most important.

Some Suggested Network Applications

1. Transmission of messages. The entire chemical community would benefit from regular and convenient communication. In particular, committees could improve their operations. Persons who have networks available find that they prefer this method to phone calls in many cases because (a) they do not need to depend on the call going through, and (b) the message is left accurately.

2. Transmission of documents between collaborators. Manuscript drafts and data sets can be rapidly sent to research collaborators. Although the technology for handling technical symbols is not yet universally available, it is possible to pass drafts back and forth. This is already frequently done by workers having this capability.

3. Electronic transmission of messages to organizations. If a journal editor had an electronic mailbox, reviews could easily be sent even though we might have a hard time passing final copies of technical manuscripts. Society program chairpersons could transmit program information to the Society office.

4. Maintenance of shared information. Division directories with names, addresses, phones, and mail codes might be made public (with a warning against commercial use). The Society programs could be listed as soon as they are finalized, and the tentative programs could be made available to program chairpersons while in process.

5. Bulletin boards for announcements. A bulletin board could be maintained for public announcements with special areas for specific subjects.

6. Bulletin boards for individuals. In some areas, such as in electronics and microcomputer use, bulletin boards are used widely to help solve problems. One person might put up a message asking where one might get a chemical or to find out if someone else has solved a given problem, or even to find a good restaurant for a committee meeting. Other persons see this message when they log on and have an opportunity to respond.

Characteristics of an Ideal Network

1. It must be universally accessible by the chemical community, a community which includes chemists in large industries, chemists in small consultantships, chemists in major universities, and chemists in very small colleges. The accessibility requirement would seem to exclude networks which are available to only people doing certain types of research (e.g., ARPANET or CSNET), networks which are available only to certain types of organizations (e.g., BITNET), or networks used only by certain subsets of users (e.g., USENET).

2. It must have the capability of transmitting mail, each individual user having an electronic mailbox. That mailbox could be located either on a central computer which is the hub for an entire network, or the mailbox could be in a local computer system if the network primarily passes messages.

3. Enough file space should be available for the transmission of large manuscripts between collaborators or reviewers, etc. Both protected storage (with several levels of protection possible) and public storage should be available.

4. The network should provide for direct communication between any pair of users.

5. Conferencing should be possible where a larger number of users log on to one discussion simultaneously.

6. There should be bulletin board capability. The bulletin board should be segmented by discipline and sub-discipline and allow any user to leave a question, announcement, or problem to which any other person can respond.

7. The ideal methods of connection should be either by toll-free call or by direct connection to one's local computer.

8. The cost of using the network should be low to the end-user. There are several possibilities. A small connect-time charge could be billed to the employer, the cost of the network could be borne by the institutions which use it, or it could be supported by one or more funding agencies eager to improve the quality of science in the country (NSF, NIH, PRF, DOD, etc.).

9. Transmission speeds at least to 1200 baud and preferably from 300 to 19,200 baud should be supported. The speed would depend on the lines available to an individual user or site.

Networks Known to be Used by Chemists

1. CHYMNET. This is a prototype hub-based network which is now functioning. It was implemented through an NSF grant to the SERAPHIM program for which John Moore is PI. Software to achieve most of the goals (mail, conferencing, etc.) listed above runs on the Amdahl computer at the University of Michigan. I do not know what the potential is for expanding this particular implementation.

2. Commercial Information Utilities. CompuServe and The Source are the best known. These are available to anyone for a sign-up charge, a monthly minimum fee, and a connect-time charge. They allow mail and storage, have low-cost phone numbers, and include bulletin-board facility. They can be accessed only by phone at 300 and 1200 baud.

3. USENET. I believe this is a network of UNIX computers. The cost of supporting a leased line and the operating software is apparently borne by the individual computer facilities.

4. ARPANET. A network which is available to users who hold DOD contracts. Apparently at Berkeley there is a gateway into ARPANET.

5. CSNET. Like ARPANET, CSNET is a restricted network, restricted to persons or departments performing computer science research.

6. BITNET. This is a network of universities using software provided by IBM. My understanding is that the costs are borne by each university which must run the software on its local IBM computer and pay the cost of a leased line to the nearest other installation.

7. Microcomputer Bulletin Boards. Throughout the country there are literally thousands of public-access bulletin board systems. Most specialize in a specific group of users, either by geographic location or by subject interest. There is software available for setting it up. A proposal has been made that I set up such a system from one of our computers; we would need to add 2-3 telephone lines and the appropriate software. The disadvantage is small capacity. The advantage is that the user need only pay toll charges.

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WHO DONE IT?

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

WHO-107 (March '85)

At the ACS Great Lakes and Central Regional Meeting at Western Michigan University in May, 1984, the following papers were presented:

P. A. Wong (Chemistry Department, Andrews University, Berien Springs, MI 49104): use of a microcomputer to simulate differential pulse polarography.

R. E. Harmon, E. M. Harmon (Chemistry Department, Western Michigan University, Kalamazoo, MI 49008): computerized literature searching in undergraduate and graduate research. (K.L.)

WHO-108 (March '85)

At the ACS Midwest Regional Meeting at Southwest Missouri State University in October 1984, the following papers were presented in the area of chemical educational computing:

A. M. Watson, M. E. Sandler, P. A. Plume (Chemistry Department, Wichita State University, Wichita, KS 67208): maintenance of records of student store-room window transactions on low-cost dedicated microcomputers.

S. M. Condren, B. Durham (Chemistry Department, Christian Brother College, Memphis, TN 38104) and Chemistry Department, University of Arkansas, Fayetteville, AR 72701): interfacing Corning pH meters to PET microcomputers.

K. J. Lissant (Petrolite Corporation, 639 Marshall Ave., St. Louis, MO 63119): use of personal computers and X-Y plotters in displaying chemical data.

D. J. Clevette, J. E. Bauman (Chemistry Department, University of Missouri-Columbia, Columbia, MD 65211): interfacing a Tronac solution calorimeter with an Apple IIe microcomputer. (K.L.)

WHO-109 (March '85)

At the NERCOMP Conference on Computers in Biology and Life Science Education, March 2, 1985, Wellesley College, Wellesley, MA, the following papers were presented:

M. S. Coyne (Biology Department, Wellesley College, Wellesley, MA): programs and simulations for use in student laboratories, in the PILOT language.

R. F. Olivo (Biology Department, Smith College, Northampton, MA): acquiring data for use in student experiments in neurophysiology and animal behavior, using low-cost techniques and video digitization. (K.L.)

WHO-110 (March '85)

At the International Chemical Congress of the Pacific Basin Societies (PAC-CHEM '84) in Honolulu, December 1984, the following papers were presented:

D. Lunney, R. C. Morrison, D. Sowell, R. T. Mills (Chemistry Department, East Carolina University, Greenville, NC 27834): transportable talking STD-BUS data-acquisition computer for visually impaired science-students.

R. C. Morrison, D. C. Sowell, D. Lunney (address above): a scheme for converting infrared spectra to recognizable auditory patterns.

I. Singh (Department of Physical Science, Mohawk College, Hamilton, Ont. L8N 3PZ, Canada): microcomputer instrument communication using an RS-232C interface.

I. Singh (address above): computer-chemistry interfacing courses at Mohawk College.

K. Maeda, Y. Koyama, H. Rokusha (Electro-Technical Laboratory, 1-1-4 Umezono, Sakamura Ibaraki-ken, Japan): a personal mass-spectra data-base in a microcomputer system equipped with floppy Winchester and optical disk systems.

K. Kanohta, Y. Katagiri, T. Hakoda (Institute of Hygenic Sciences, 1-18-1 Setagoyaku, Tokyo, Japan): a massive proton-NMR spectra file search by a microcomputer.

H. Nakano, O. Sangen (Himeji Institute of Technology, Shosha, Himeji 671-22, Japan): drawing of molecular models with personal computers.

Y. Takahashi, T. Miyashita, H. Abe, S. I. Sasaki (Toyohashi University of Technology, Department of Material Science, 11 Hibarigaoka Tempaku, Toyohashi 440, Japan): an interactive molecular display system using computer graphics.

A. Mihkelson (School of Chemistry, Sydney University, Sydney NSW 2006, Australia): computer-assisted instruction applied to remedial teaching in first-year university chemistry. (K.L.)

WHO-111 (March '85)

Anyone interested in getting started in simulation of chemical systems should take a look at the following two bibliographies of information sources in computer-based simulation:

C. A. Pratt, "Going Further: A Compendium of Conferences, Organizations, Books and Software for Simulationists" Byte, March 1984 9(3) 204-208.

"Catalog of Simulation Software" Simulation 1984 43(4) 180-192: a bibliography of micro- mini- and main-frame simulation languages and simulation systems. (K.L.)

WHO-112 (March '85)

The June 1984 issue of Byte has a group of papers on the theme of educational computing. One paper is of especial interest "Designing a Simulated Laboratory" by N. Peterson (Learning Tools, NE 1050 Alfred Lane, Pullman, WA 99163) Byte June 1984 9(6) 287-296: discussion of an excellent CAI system with color video graphics and simulation in cardiovascular physiology. (K.L.)

WHO-113 (March '85)

The February 1985 issue of Byte has a group of papers on the theme of Computing and the Sciences. Of particular interest to chemists are the following:

K. Okamura, K. Aghai-Tabriz (Applied High-Technology Laboratory, North Dakota State University, Fargo, ND 58105): "A low-cost data-acquisition system" Byte Feb. 1985 10(2) 199-202.

E. E. Aubanel, K. B. Oldham (Chemistry Department, Trent University, Peterborough, Ont. K9J TB8, Canada) "Fourier-Smoothing without the Fast Fourier Transform", Byte Feb. 1985 10(2) 207-218.

E. J. Kirkland (School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853) "Viewing molecules with the Mackintosh", Byte Feb. 1985, 10(2) 251-259. (K.L.)

WHO-114 (March '85)

William Marling (English Department, Case Western Reserve University, Cleveland, OH 44106) has written an interesting paper on "Grading Essays on a Microcomputer", College English Dec. 1984 46(8) 797-810. While not directly chemical, it should be of value to anyone concerned with computer-based grading. His comments on the practical aspects of microcomputer use are interesting, especially as summarized in "Marling's Rules of Computer Use, the winnowings of three years in the devil's threshing yard". (K.L.)

WHO-115 (March '85)

Consult "The Reader's Guide to Micro Computer Books" by M. Nicita and R. Petrusha (1983, Golden-Lee Books, Brooklyn, NY 11238; 409 pp) for ratings and reviews of more than 400 books on microcomputers, microprocessors, operating systems and applications software. (K.L.)

WHO-116 (March '85)

Harper and Row have announced publication of a text on the preparation of CAI software by Ruth K. Landa, "Creating Courseware: A Beginner's Guide", April 1984, Harper & Row, New York, 350 pp. (K.L.)

WHO-117 (March '85)

It's easy to get bogged down in a morass of details when implementing CAI systems, so it's helpful to stand off and think about the general issues once in a while. The following three review papers are strongly recommended as background reading for anyone interested in teaching with the computer:

J. Nievergelt (Institut für Informatik, Eidgenössische Technische Hochschule, Zurich Switzerland) "A Pragmatic Introduction to Courseware Design" Computer (IEEE) Sept. 1980, 7-21: this excellent survey of the history and present practice of CAI is chiefly memorable for its excellent balance and common sense; it deflates the excessive claims of some CAI enthusiasts,

gives sound advice to authors on good (and bad) CAI practices, and presents a basic bibliography of CAI.

F. Hayes-Roth (Teknowledge, Inc., 525 University Ave., Palo Alto, CA 94301) "The Knowledge-bared Expert System: A Tutorial" Computer (IEEE), Sept. 1984, 11-28: this review explains the application of artificial-intelligence techniques to the solution of complex problems in an interactive mode. Although it would be possible to advance the quibble that such systems are not 'educational' in the narrow sense (they are certainly not drill-and-practice systems), I believe very strongly that expert systems do very much the same thing that a teacher does in solving a student's problems by question-and-answer techniques. I think that the future of CAI lies in the application of such expert-system techniques to teaching.

B. Woolf, and D. D. McDonald (Department of Computer Science, University of Massachusetts, Amherst, MA 01003)" Building a Computer Tutor: Design Issues": this paper analyzes the structure of student-tutor dialogues and explores the applications of artificial intelligence and expert system principles to CAI. It is a natural supplement to the Hayes-Roth paper mentioned above. (K.L.)

WHO-118 (March '85)

The Software Catalog is published twice each year by Elsevier Science Publishing Company, Inc. (52 Vanderbilt Avenue, New York, NY 10017: 1-800-223-2115). The Microcomputers edition was published in Winter 1985 (ISBN 0-444-00883-7) and is about 1700 pages in length. The catalog contains information on more than 14,000 commercially available program packages for most of the major microcomputers. The directory costs $75 and was produced from the Menu/International Software Database. A description of each program package, its source, price, application and compatibility is contained in a 909 page software section. This is the main section of the catalog. There are six indexes which refer back to this section. There is a computer system index which indicates which programs will run on any given computer. Also, there are operating system, programming language, microprocessor, subject and application, keyword and program name indexes. The subject and application index is divided into the following categories:

Commercial - including accounting, mailing lists, spreadsheets, word processing, (10.7 pages) and many other sections.

Educational - administration, CAI (62.5 pages), CMI (9 pages), counseling, library management and miscellaneous.

Industrial; Personal; Scientific - including chemistry; Professions/Industries - including chemical industry; and Systems.

This catalog could be useful in helping to identify packages for your computer. In introductory sections the catalog contains some information on commercially available data bases, local area networks, and a quick reference guide to LOTUS 1-2-3. (D.R.)

WHO-119 (March '85)

The March issue of Communications of the ACM, 28(3) 269-279 (1984) features two articles of interest to educators. The first article contains the recommendations of a task force regarding a suggested curriculum for secondary school computer science. This article summarizes a report jointly approved by the ACM Education Board and the IEEE Computer Society Educational Activities Board in July 1984. Four courses are recommended for implementation at secondary school level:

1. Introduction to Computer Science I (a full year course),
2. Introduction to Computer Science II (a full year course),
3. Introduction to High-Level Computer Language (a half-year course),
4. Application and Implications of Computers (a half-year course).

Courses 1 and 2 are designed for students with a strong interest in computer science. Course 1 is a prerequisite for course 2. Satisfactory completion of these two courses should prepare a student for second year computer science in post-secondary educational institutions either directly or through the Advanced Placement Exam.

Course 3 is a course about programming in a high-level computer language (Pascal, LOGO, BASIC, structured BASIC and other languages are suggested as possibilities). This course is neither vocational nor a prerequisite to any other course.

Course 4 is oriented toward the student learning to use the computer and understanding the implications of computer applications. Students will acquire a broad view of the roles computers play and an appreciation for the influence computer use can have on social organization. Programming is not included in this course.

This article and the full report describe in some detail the objectives and content of these four courses.

The second article in this issue of Communications of the ACM describes a proposed curriculum for programs leading to teacher certification in computer science. This report was prepared by a task force working through the ACM's Elementary and Secondary Schools Committee. (D.R.)

WHO-120 (March '85)

The March issue of SIAM NEWS (Volume 18 #2) contains an article entitled "Statistical Analysis on Microcomputers" by John C. Nash (p. 4) and an article entitled "Pascal for Scientific Computation" by L. B. Rall. The second article describes the Pascal-SC compiler for use with a Z80 microprocessor and CP/M. (D.R.)

WHO-121 (March '85)

The March 1985 issue (Volume 12 #6) of The Computing Teacher contains a list of sixty colleges and universities each of which are offering at least nine quarter hours of computers in education summer courses. The name, address and phone number of the person to contact, the dates of the courses, admission requirements, computer equipment, names of the courses, credit hours and tuition costs are provided. (D.R.)

WHO-122 (March '85)

The Journal of Computers in Mathematics and Science Teaching is published four times each year (fall, winter, spring and summer) by the Association for Computers in Mathematics and Science Teaching (ACMST, P. O. Box 4455, Austin, TX 78765). The membership subscription rate is $18 for individuals and $36 for schools. A typical issue is 60 to 80 pages in length and contains about nine feature articles, five columns and nine departments (editorial, letters, update, software reviews, book reviews, new products, new books, program listings and a calendar). The Summer 1984 issue (Volume III, No. 4) contained a cumulative subject index. Eleven items were listed under chemistry. The Fall 1984 issue (Volume IV, #1) features an article by Michael H. Powers entitled "A Computer Assisted Problem Solving Method for Beginning Chemistry Students" (p. 13-19). Other articles included "A Computer Literacy Program for Prospective Elementary School Teachers", "Numerical Integration on a Microcomputer", "Using the Microcomputer to Teach About Nuclear Energy", "School Uses of Microcomputers: Report 5 from a National Survey", and some conference abstracts. The Journal contains material which is of interest to elementary and secondary school teachers as well as college teachers. (D.R.)

Software QUERIES and REPLIES

Software QUERIES and REPLIES should be sent to Ken Loach, Department of Chemistry, SUNY at Plattsburgh, Plattsburgh, NY 12901, (818) 564-2230. Hardware QUERIES and REPLIES should be sent to Jim Beatty, Chemistry Department, Ripon College, Ripon, WI 54971, (414) 748-8123.

SQ-26 (March '85)

Leo Geoffion (Skidmore College, Saratogo Springs, NY 12866) would like to hear from any microcomputer users (especially of IBM, DEC and Apple) who would like to join the Skidmore Computer Bulletin Board, and share information on microcomputer use in colleges. The Bulletin Board is intended to act as a forum for questions about the educational use of computers, reviews of software and discussion of personal computer problems.

SQ-27 (March '85)

Pat Flath (Paul Smith's College, Paul Smith's NY 12970) would like to hear from anyone who knows how to connect a TRS-80 Model III or IV to a large TV screen for classroom demonstrations.

SQ-28 (March '85)

Pierre Dupont (CEGEP de l'Qutaouais, 333 boul. Cite des Jeunes, C.P. 5220, Hull, QE J8Y 6MS, Canada) is interested in hearing of any programs for CAI in instrumental chemistry.

One such program which is available involves an NMR simulation. This program was mentioned in the November issue of J. Chem. Educ. (61(11) 1003-1008). This program was developed by Paul Schatz (Department of Chemistry, University of Wisconsin, Madison, WI 53706).

Anyone who has not already done so should read the J. Chem. Educ. article mentioned. It is a summary of a conference in late May of 1984 on computer uses in chemical education, and it is exciting reading.

INTERFACING WITH A DMM

by Jim Beatty*

Interfacing an instrument to a microcomputer could be a major chore if one chooses to build an analog to digital converter and the necessary power supply. Building and testing of the A/D converter can be a useful educational experience. But, for a busy teacher at a liberal arts college or a research scientist, purchasing a digital multimer (DMM) with an IEEE-488 option is often more sensible.

The DMM approach can be economical and is versatile. A DMM is well protected from overloads and other potential abuse. There are no long delays encountered when waiting for parts. Connecting the DMM to a microcomputer is as easy as plugging in a disk drive. Test data can be collected within the first hour. A physical chemistry experiment introduced last year at Ripon College illustrates how useful and simple an interface can be. Explanations are given below for some of the decisions which were made.

The hydrolysis of tertiary butyl iodide in aqueous ethanol was selected because the reaction is too fast to be followed conveniently by classical methods (half-life of the order of 5 minutes) and it is slow compared to the sampling time of the DMM (2.5 readers per second) and associated equipment. The hydrolysis was followed by measuring the conductance of the solution using a dipping type conductance cell and a Yellow Springs Model 32 conductance meter. The YSI meter was selected because it had a 0 to 2 volt recorder signal directly proportional to the conductance reading. The solution was stirred using an air driven magnetic stirrer in a constant temperature bath. The reaction vessel was a graduated cylinder. A Keithley 179A 4 1/2 digit multimeter with an IEEE-488 option was connected to the recorder outputs of the conductance meter. A Commodore 8032 was connected to the IEEE output of the multimeter using a cable purchased with the meter. A BASIC program about one half page in length was used to collect and store the data in a disk file, and print out a back-up copy of the data.

The BASIC statements given below collect N data from the DMM at time intervals DT seconds apart.

```
100   REM DT = TIME INTERVAL IN SECONDS, N = NUMBER OF POINTS
110   DT = 30
120   N = 60
130   T(0) = 0
140   OPEN 1,24
150   FOR I = 0 TO N
160   REM TI IS COMPUTER TIME IN 1/60 SEC
170   IF TI/60 < T(I) THEN 160
180   INPUT # 1, V(I)
190   IF ST = 2 THEN 180
200   PRINT T(I), V(I), TI/60
210   T(I+1) = T(I) + DT
220   NEXT I
230   CLOSE 1,24
```

ST is the status bit in the above program. The program remains in a loop until data is received.

Students were advised to make a sample run and then to modify the program to take an optimum number of data points. The students were asked to modify a least squares program so that it would load the disk file and determine the order and rate constant.

There is a definite advantage in using an IEEE parallel bus over an EIA-RS-232C serial bus. The EIA serial bus requires the matching of Baud rates and everyone seems to use a different level of EIA. Keithley recently made available a 5 1/2 digit multimeter at roughly the same price as for the 4 1/2 multimeter I purchased.

A copy of the laboratory experiment may be obtained from the author on request.

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