Computers in Chemical Education Newsletter

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Committee on Computers in Chemical Education
G. Scott Owen, Chairman/Department of Chemistry, Atlanta University, Atlanta, GA 30314
Donald Rosenthal, Editor/Department of Chemistry, Clarkson College of Technology, Potsdam, NY 13676

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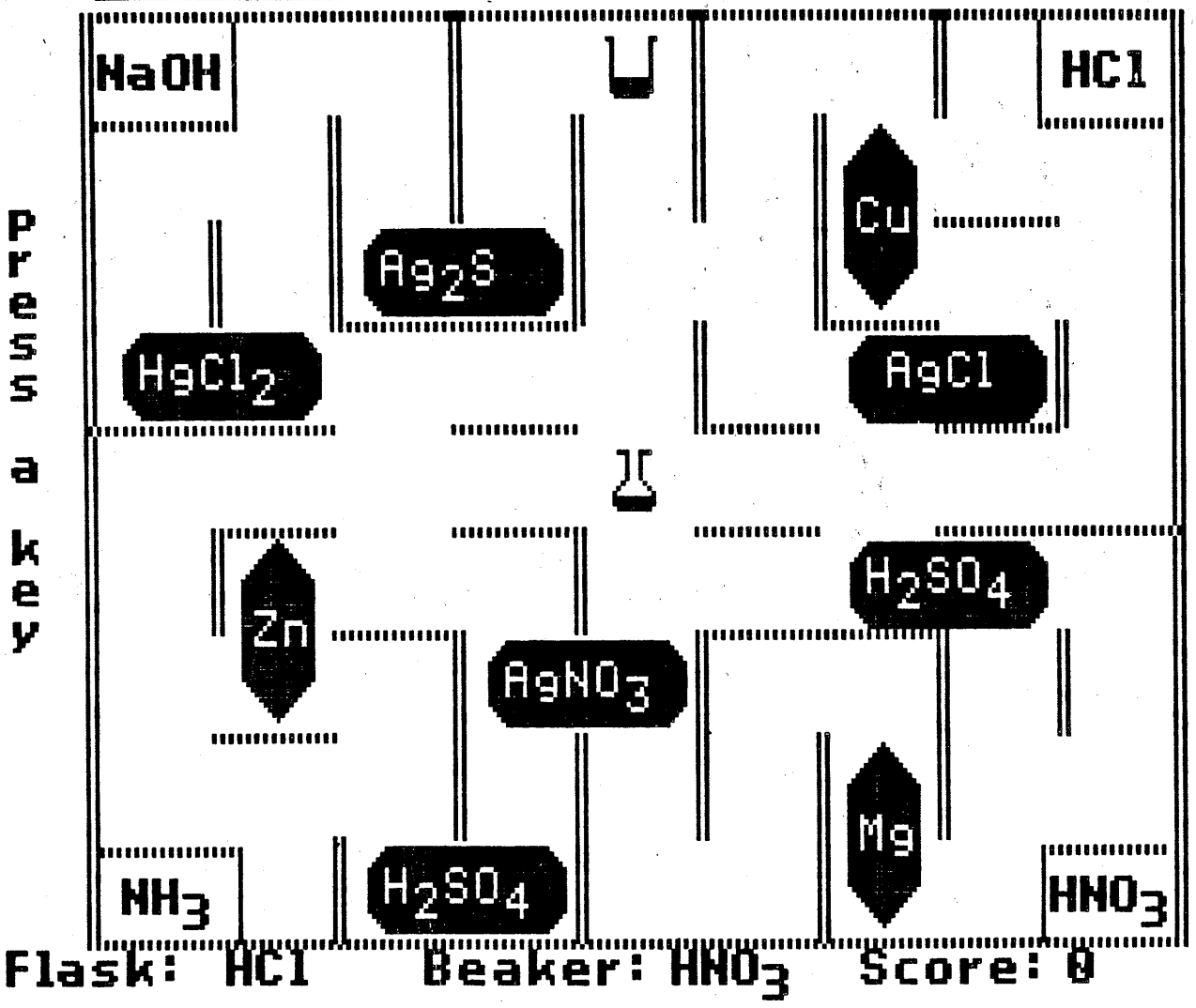

ON THE COVER

My request for graphics material for future Newsletter covers resulted in a considerable number of submissions. I would like to thank all of you who responded. There are ample materials for several future issues.

The cover for the present issue was supplied by Susan W. Rollinson (849 Lou Avenue, Clifton Forge, VA 24422), and was obtained from a screen dump of Stan Smith's CHEMAZE program (available from COMPress, P. O. Box 102, Wentworth, NH 03282). Sue indicates that few commercial programs have provisions for dumping text or screen graphics to a printer and that she gets screen dumps from "protected" programs by a "brute force" method. She hopes that this does not prompt publishers to further "lock-up" their programs. Her system consists of an Apple II with an Epson MX-80 printer (with "Graftrax") and a Grappler + interface.

Sue explains that booting a new disk does not destroy the contents of RAM, but just resets pointers and overwrites a small portion of RAM (the "Hello" program). The procedure for obtaining the screen dump is:

1. Obtain the figure you want on the screen of the monitor.
2. Remove the program or game disk.
3. Insert slave disk, APPLE DOS 3.3.
4. Press RESET to perform a "coldstart" (this will put DOS directly into upper RAM).
5. RUN one of the following Applesoft BASIC dump programs:

HI-RES DUMP

This program is used to obtain simple screen dumps.

```
100  REM PRINT HI-RES SCREEN
110  REM S.W. ROLLINSON, 1983
120 :
130 :
140  INPUT "PAGE 1 or 2?";Z$
150  IF Z$ = "1" THEN P$ = "G": GOTO 170
160  IF Z$ < > "2" THEN 140
165 P$ = "G2"
170  INPUT "DOUBLE SIZE?";Z$
180  IF Z$ = "Y" THEN P$ = P$ + "DR": GOTO 250
190  IF Z$ < > "N" THEN 170
200  INPUT "ROTATED":Z$
210  IF Z$ = "Y" THEN P$ = P$ + "R": GOTO 250
220  IF Z$ < > "N" THEN 200
230 :
240 :
250  PRINT CHR$ (4);"PR#1"
260  PRINT CHR$ (9);"80N"
270  PRINT CHR$ (9);P$
280  PRINT CHR$ (4);"PR#0"
290  END
```

EXAMINE · VALT

```
 50  REM EXAMINE VALT. FILE
 60  REM MOLECULAR ANIMATOR
 70  REM S.W. ROLLINSON, 1983
 80 :
 90 :
100  D$ = CHR$ (4):I$ = CHR$ (9):B$ = CHR$ (2)
110  DIM A$(60),C$(60),AN$(60),DI$(60),BL$(60)
115  INPUT "NAME OF STRUCTURE FILE:";N$
120  PRINT D$;"OPEN VALT.";N$
140  PRINT D$;"READ VALT.";N$
145  INPUT X
150  FOR J = 1 TO X
160  INPUT A$(J),C$(J),AN$(J),DI$(J),BL$(J)
170  NEXT J
180  PRINT D$;"CLOSE VALT.";N$
200  PRINT D$;"PR#1"
210  PRINT I$;B$
220  PRINT B$;"80N"
222  PRINT B$;"10L"
225  PRINT N$;" FILE"
230  FOR J = 1 TO X
240  PRINT J;I$;A$(J);I$;C$(J);I$;AN$(J);I$;
          DI$(J);I$;BL$(J)
250  NEXT J
260  PRINT D$;"PR#0"
270  END
```

Sue is hoping to develop stereo drawings to show the three-dimensional aspect of molecules using J. Jeffrey Howbert's "Molecular Animator" (available from COMPress) and a stereo viewer. This will be accomplished by printing molecules drawn from slightly different perspectives. It is necessary to re-bott the "Molecular Animator" for each picture.

FINAL MESSAGE FROM THE OLD CHAIRMAN

The CEEE has just held it's election for a new chairman. Both of the candidates, Paul Cauchon and Bill Halpern have been very active in CCCE affairs and either one would have been an excellent choice. The winner of the election was Paul Cauchon (Science Department, Canterbury School, New Milford, CT 06776) and he will serve as the chairman for the next two years.

*G. Scott Owen
Department of Chemistry
Atlanta University
Atlanta, GA 30314

COMMENTS FROM THE EDITOR
by Don Rosenthal*

This issue of the Newsletter represents a combined December 1983 and March 1984 issue (Volume VI, Number 4 and Volume VII, Number 1).

The number of issues of the revitalized Newsletter distributed has increased from about 500 for the March 1981 issue to 2000 for the present issue. The average number of pages in each issue has grown. Given these changes the cost of producing and mailing an issue has increased dramatically. Initially, back issues were routinely mailed to anyone requesting them. Now, to reduce costs, a dollar is requested to cover costs of mailing and Xeroxing. (The supply of many back issues has at this time been exhausted and Xerox copies are being mailed.) Those living outside the U.S. are presently being asked to make a voluntary contribution to cover the cost of mailing. The cost of producing and mailing the Newsletter is being subsidized by funds provided by the Division of Chemical Education to the Committee on Computers in Chemical Education, by C.C.C.E. income generated from workshops and the biennial meetings and by generous contributions from Project SERAPHIM. While some discussion of instituting subscription charges has occurred, we are reluctant to do this.

I would like to urge all readers to join the Division of Chemical Education as a member or an affiliate. Annual dues are $5 and a membership form has been included in this issue. Also, a subscription order form for the Journal of Chemical Education is included in this issue. This Journal features the computer series edited by John Moore and other articles of interest to chemical educators at all levels.

The Biennial Conference scheduled for the University of Connecticut in August should be of considerable interest to computing enthusiasts. Two computer symposia and several workshops are available. A computer graphics exhibit and software contest will be held. Additional information and contest forms are available elsewhere in this issue. A birds-of-a-feather session is planned to discuss the work of the Committee, the Newsletter and Project SERAPHIM. Personally, I'd like suggestions from you about what could be done to improve the Newsletter. It is hoped that many of you will attend.

As announced in the preceding article, Paul Cauchon has replaced G. Scott Owen as Chairman of the Committee on Computers in Chemical Education. I would like to thank Scott for his assistance and advice in helping to make the Newsletter possible. He has provided considerable material for the Newsletter. Scott has done a great deal to promote the vigor of the Committee.

Paul Cauchon has been active in developing the highly successful C.C.C.E. Workshops for High School Chemistry Teachers. He has participated in many workshops and contributed articles and information to the Newsletter. All this in addition to teaching at Canterbury School and running Programs for Learning.

With this issue of the Newsletter, Ken Loach succeeds Henry Griffin as editor of the Software QUERIES and WHO DONE IT? sections of the Newsletter. I would like to thank Henry on behalf of the Newsletter for his efforts since March 1981. Ken Loach teaches analytical chemistry and computer science courses at SUNY College at Plattsburgh (Plattsburgh, NY 12901).

Congratulations to Ken Ratzlaff who has been elected Chairman-Elect of the A.C.S. Division of Computers in Chemistry. Ken edits the Hardware QUERIES and WHO DONE IT? sections of the Newsletter. Information on membership in the COMP division can be obtained from Daniel J. Macero, Department of Chemistry, Syracuse University, Syracuse, NY 13210. Dan and Ken are both C.C.C.E. members.

I would like to include an extensive list of summer meetings, workshops and courses in the June Newsletter. Please send all pertinent information to me by May 1st.

*Department of Chemistry
Clarkson University
Potsdam, NY 13676

COMPUTER INTERFACING WORKSHOPS
by G. Scott Owen*

I am going to be writing a small grant application to the ACS to develop a traveling computer interfacing workshop for the C.C.C.E. The workshop will be similar to the one given by myself and Bill Nonidez (University of Alabama at Birmingham) in Atlanta last fall. It was a two-day workshop using the Interactive Structures A113 ADC boards, Apple II computers, and function generators.

The grant application will be for the necessary peripherals (ADC, DAC, function generators, etc.) to equip ten Apples for such a workshop. I plan to develop the course and then the C.C.C.E. will ship the equipment around to others who would then give the course in their own region.

The proposed course would focus on the use and choice of ADC's and DAC's. Data acquisition programming, both in a high level language and assembler would be covered. Other miscellaneous topics would be sampling rates, signal conditioning, and a brief introduction to digital filtering techniques (both real time and post run).

Anyone with additional ideas about the course content (remember this is only a two-day course) and especially anyone who would be interested in teaching the course in their own region, please contact me.

*Department of Chemistry
Atlanta University
Atlanta, GA 30314

FOOD FOR THOUGHT

Like all other automatic gadgets, computers unfortunately also have a definite numbing influence on the human mind. Just as the car has made walking most unpopular among some members of the new generation, computers have made some research people lazy. Such people often prefer to give the calculations to the computer at once rather than to spend a little time and effort in attempting to discover whether human ingenuity can so simplify them as to make a computer unnecessary. The unreasoning faith in computers is best exemplified by the statement of a high school principal to the worried father of a boy who was not doing too well in mathematics. "Don't worry," he said, "by the time your son is out of school, all mathematics will be done by computers." It is sobering to remember that computers must still be given orders by men and that to this day 20% of the computing time is spent in "debugging" the computer - in simply discovering the unavoidable mistakes that the computer makes because of incomplete or unclear orders received from the men who run it.

Mario G. Salvadori
Mathematics, the Language of Science, 1980

COMMENTS ON HARDWARE DEVELOPMENTS IN CHEMISTRY

by Kenneth L. Ratzlaff*

The subject matter placed under the broad heading of Computers in Chemical Education can be separated into two categories. The first, and probably more important to this readership, is the subject of "Teaching Chemistry Better by Using Computers", and the second is the subject of "Teaching Better Chemists About Using Computers". The former often relates to lower level students, and the latter topic is nearly always reserved for upper level or graduate students. Some observations about trends in computer use in chemistry may well be useful.

First, a few comments about the computers being used in chemical laboratories: these comments are based on the instrument show at the 1984 Pittsburgh Conference. On the floor there were many companies using personal computers as the controller for their instruments. On the other hand, there were computers being designed expressly for the laboratory/professional user.

In the former category, I was impressed by the extent to which Apple and IBM PC computers dominated: typically used in chromatography to control pumps and massage data. Other personal computers on the floor included a few S-100/CP-M machines and some more sophisticated applications using DEC machines. Unfortunately, although the term "user-friendly" was often bandied about, there was a conspicuous absence of that quality: non-descriptive menus, poor error recovery, cumbersome command sequences, and a lot of "it can't be done" explanations. Few instrumentation houses have caught up with the quality of WordStar and similar packages.

What about the newer computers? Although 16-bit personal computers have gone the 8086/8088 route, scientific computer companies, Hewlett-Packard, Perkin-Elmer, Instrumentation Laboratories, and IBM Instruments, are all using the Motorola 68000. (One small company did point out, and correctly so, that their 8086 computer with an 8087 co-processor was the most powerful micro on the floor.) Software for all of these machines is somewhat slow in developing. In any case, commitment has been made to the 68000 for scientific computers, and this should hold up as Motorola produces support chips.

The previous two paragraphs probably have little relevance for applications akin to CAI in the freshman lab. Here other factors dominate: software availability, cost, and capability for communication with an operator/student. (Note that software comes first; unless we want to study about computers or indulge in specialized activities, a useful procedure is to select the software and then purchase a computer on which to run it.) The development of networks and the "mouse" will have significant impact on lower level applications.

In the teaching environment, networks will bring back the advantages of the time-shared computer without its disadvantages. Picture a room filled with 20 inexpensive Commodore 64's (computer and color monitor for less than $500 each). A relatively simple network, with a central 64 with fast hard disk, could load programs into the sattelite computers as fast as local floppies could, but also could maintain log of computer use and store results from student sessions. At $50 per machine for interfacing and about $4000 for the hub, the total drops to well under $1000 per machine.

Operator/computer interactions found in most systems is awkward. The question should be asked, how do we make the computer more "user-friendly"? One way is to improve the method of interaction: reduce the use of the keyboard and replace it with a light-pen or, better yet, a mouse. The mouse, first developed for the Xerox Star, is getting more press in its application in the Apple Lisa and Macintosh. It is a hand-held device which is used to control a cursor position by rolling it about on a table surface. The skill develops very naturally. The result is that the operator, whether secretary or student, readily interacts directly with the information; the computer facilitates rather than complicates this process. And that means more education takes place.

*Department of Chemistry
University of Kansas
Lawrence, KS 66044

AN APPLE FOR YOUR IBM PC—THE QUADLINK BOARD

by G. Scott Owen*

The Apple II computer presently dominates the Chemistry CAI software scene. Approximately 85% of Chemistry CAI programs run on the Apple. Those considering the purchase of a microcomputer must decide whether to restrict themselves to a machine with somewhat limited capabilities (the Apple) but lots of software or to purchase a more powerful machine (like the IBM PC) with very little software currently available.

One solution to this problem is to buy an IBM PC and put an Apple in it. This is now possible because of an IBM PC board called the QUADLINK developed by the QUADRAM Corporation (4355 International Blvd., Norcross, GA 30093, 404-923-6666). QUADLINK is essentially a complete Apple computer on a single board and allows you to run both Apple and PC software.

INSTALLATION

The installation of the QUADLINK board is a little more difficult than the usual add-in PC board because the cables for the floppy disk drive, video display, and speaker must first go to the QUADLINK and then to the PC. Installing the board requires taking the other boards out of your PC (unless you have fingers like RUBBER MAN), hooking up the cables and then reinstalling all of the boards. This actually sounds worse than it is as it only takes about 15 minutes.

The software installation is quite simple, you first execute a program called QUADLINK.EXE (this can be done automatically on boot up by using an AUTOEXEC.BAT file). Then a second disk is inserted (called the FILER) and booted up in Apple mode. From then on to switch from the PC to the Apple and vice versa merely requires a CTRL-ALT-I (to go from the Apple to the IBM) and a CTRL-ALT-A to go the other way.

The QUADLINK has full access to all of your peripherals (at least the display screen, the printer, and the disk drives) and will turn your IBM 360 K double density drives back into 140 K Apple drives. As an added goody, if you have the IBM PC monochrome adapter you can't do IBM PC graphics but the QUADLINK allows you to do Apple graphics, in monochrome of course. If you have the IBM PC color graphics board then you get excellent Apple color graphics.

The main question for chemistry users is will the QUADLINK run our Chemistry CAI programs. QUADRAM states that the QUADLINK will run 99% of all Apple II software, but being a pessimist, and knowing that most of the Chemistry software is copy protected and uses special Apple "tricks", I wanted to see for myself. Well, the good news is that it works fine. I got into Apple mode, put Stan Smith's Organic series disk (from COMPRESS) into drive A:, typed PR#6, and it started up with no problem.

I didn't test all possible Chemistry programs but I did test several that used shape tables, machine language routines and special Apple features like page flipping. As some of you may know, the location of the page flipping software switches are one of the few differences in the Apple II and IIe. The QUADLINK appears to emulate the II rather than the IIe. The QUADLINK board executed every program I tried which includes the following: the COMPRESS Organic series, Gordon Barrow's Physical and General Chemistry programs, and the Pascal MOLEC program by Jim Currie and myself.

In summary, the QUADLINK board is an excellent investment for someone who wants the features of an IBM PC but also wants to use Apple software. There are some copy protection schemes that will baffle the QUADLINK (actually it is the disk drives - some Apple copy protected disks use a half track scheme which the Apple disk drives can read but the IBM PC drives cannot).

Since I only tested the programs which I have, I would suggest that you check out the QUADLINK on your own programs. The list price for the board is $680 but it is available from mail order firms for much less. For example, one company that I have dealt with, Conroy-La- Pointe (800-547-1289), lists the QUADLINK at $485.

*Department of Chemistry
Atlanta University
Atlanta, GA 30314

WHO DONE IT?

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

WHO-61 (March '84)

T.C. O'Haver (University of Maryland, Chemistry Department) is doing some interesting work in the computer-simulation of analytical instruments (Anal. Chem. Nov. 1983, 55(13) 1326A-1328A). Instrumental simulations could allow students to gain some knowledge of unobtainable instruments or allow the exploration of extreme sample or instrument conditions. It is easy to imagine extension of this work to the simulation of instrument faults and failures and their diagnosis. Is anyone else working in this area? (K.L.)

WHO-62 (March '84)

There was an interesting article on the use of an oscilloscope as a readily available computer display (A.Rittanthane and T.M. Dougherty, American Laboratory, Oct. 1983, 42-54). The software is in 6502-assembler. (K.L.)

WHO-63 (March '84)

J. Rusling (University of Connecticut, Chemistry Department, Storrs, CT 06268) has been teaching students chronoamperometry, chronocoulometry and voltammetry using a PAR170 and a PAR174A electrochemical system interfaced with a TRS-80 microcomputer for data-reduction and display. (K.L.)

WHO-64 (March '84)

Microcomputer (July 1983) had a couple of article on inexpensive interfacing projects. The first (p. 86) was of a VIC20 to an ASR33 teletype and the second (p. 88) was of a VIC20 to an ordinary cassette-recorder as opposed to the specialized Commodore cassette recorder). (K.L.)

WHO-65 (March '84)

P.A. Wong (Andrews University, Chemistry Department, Berrien Springs, MI) has been doing sampled AC polarography with data-acquisition and processing on a SYM-1 microcomputer (6502 microprocessor). (K.L.)

WHO-66 (March '84)

D.C. Webster (American Laboratory, February 1982) has been using a Sinclair ZX81 as an inexpensive controller for an automatic titrator. His article has fairly full details of the interface hardware and of the machine-code and Basic software. (K.L.)

WHO-67 (March '84)

The Journal of Educational Computing Research has just begun publication (Baywood Publishing Co., 120 Maine St., P. O. Box D, Farmingdale, NY 11735; first issue January '84). It will publish original work in the development, application and outcomes of educational computing. (K.L.)

WHO-68 (March '84)

A number of computer companies are offering substantial discounts to colleges and universities willing to guarantee the purchase of a sizeable number of computers. Apple DEC, IBM and Zenith have all done this.

Apple's new Mcintosh which sells for $2,500 is being offered for $1,000 to 24 schools which can pass this price on to students, faculty and other staff members. Each school has agreed to purchase at least two million dollars worth of Apple products during the next three years and to share with one another any software or design modifications developed for the Macintosh. The 24 schools are Boston College, Brigham Young University, Brown University, Carnegie-Mellon University, University of Chicago, City University of New York, Columbia University, Cornell University, Dartmouth College, Drexel University, Harvard University, University of Michigan, Northwestern University, University of Notre Dame, University of Pennsylvania, Princeton University, Reed College, Rice University, University of Rochester, Stanford University, University of Texas at Austin, University of Utah, University of Washington and Yale University. These schools were selected by Apple partly based on projects they intend to develop on the Mcintosh. At Drexel every entering student will be required to

purchase a Macintosh (see September 1983 Newsletter). At the University of Michigan every one of its 6,000 engineering students will use the Macintosh for their $100-per-term computer user's fee. After four year, they can take the machine with them. (This is similar to Clarkson's scheme where $200 is added to tuition each semester--see March 1983 Newsletter).

The Macintosh has a 32-bit Motorola 68000 microprocessor; 128k of random access memory; a 9-inch diagonal, high-resolution, black and white screen, one 3 1/2 inch disk drive, a separate keyboard and a mouse. Ports connect the computer to external accessories. A printer, additional hardware and all software are available at additional expense.

Evaluations of the Macintosh appear in the February 1984 issue of Byte magazine (Vol. 9., #2, page 30) and in the April issue of Creative Computing (Vol. 10, #4, page 38).

Hardware QUERIES

Send Hardware Queries, rebuttals, and information to Ken Ratzlaff, Instrumentation Design Laboratory, Chemistry Department, University of Kansas, Lawrence, KS 60045 (413-864-3754).

Software QUERIES

Software Queries and answers should be sent to Ken Loach, Department of Chemistry, SUNY College, Plattsburgh, NY 12901.

SQ13 (March '84)

SUNY Plattsburgh has recently acquired a Perkin-Elmer 3600 microcomputer (M6800 microprocessor) interfaced to a PE783 IR spectrophotometer. Are there any PE3600 users interested in the exchange of PE3600 software and information? Does anyone have experience in PE3600 assembler programming or in the interfacing of non-Perkin-Elmer peripherals with the PE3600? If there are a sufficient number of responses, I'll investigate the possibility of forming an informal PE3600 user's group (Ken Loach, Chemistry Department, SUNY College, Plattsburgh, NY 12901).

SQ14 (March '84)

Where do you get your chemical computing information? Chemical Abstracts General Subject Index indexes it under only three headings: Computer Applications, Computer Programs, and Computers. There are no sub-headings. The CA coverage of chemical computing appears to be inadequate because most computer-related information of interest to chemists still appears in non-chemical sources.

I have recently been exploring the data bases on the Dialog system. Searches of the CA Search data base yielded little of interest. The Inspec data was more useful (based on 603 sources abstracted by the Institute of Electrical Engineers). Inspec is also available in the BRS data base system. Even more relevant was the Microcomputer Index data base (based on 530 sources). The only obvious drawback of the M.I. data base is that it is very new (only back to January 1983).

Please let us know of your experiences with these or any other systematic sources of information in chemical computing.

SQ15 (March '84)

Where is there information about translating Apple and TRS-80 programs into Commodore Basic and vice versa. Also, how can graphic features used by the Apple be converted to the Commodore? Particularly of interest are the translation of Apple HPLOT TO and HGR commands (Thomas J. Stuart, 23 Bonnett Avenue, Larchmont, NY 10538).

SQ16 (March '84)

Karl Konrad (Department of Chemistry, Southwestern Adventist College, Keene, TX 76059) is interested in chemistry software written for the Heath H-100 microcomputer and would like to hear from those who have software and are willing to share.

PROCEDURES AND GUIDELINES FOR EVALUATION OF EDUCATIONAL SOFTWARE**

by Dr. M. Lynn James*

OVERALL STANDARD: Does The Software Do What I Want It To Do And In A Way That I Want It Done?

PROCEDURES:

1. Obtaining Software to Evaluate: When software of interest comes to your attention, contact the publisher or their field representative to determine if samples are available for review. Frequently the field representative can make arrangements for samples to be sent to you or can bring a complete set of the software and demonstrate it or loan it to you for a short period of time. If such arrangements cannot be made, some software vendors will send materials "on approval", others require prepayment, but have generous return policies; while some require prepayment and allow returns only for defective disks. Inasmuch as the quality of software can only be determined effectively by reviewing it directly, the latter approach is risky.

2. Preparing to Review the Software: Read through the documentation first to make certain that you have the proper hardware to run the software and to learn of any instructions needed for using it. Doing this can save considerable time and frustration.

3. Reviewing the Software: It is wise to evaluate software from different perspectives. Such an approach should consider the wide range of student abilities. An intelligent student with a good background in chemistry and one very much at ease with computers may react differently from the student with limited abilities and background in chemistry who is totally unfamiliar with computer operation. Since chemistry software is generally designed to supplement regular courses, it is important that it be user friendly. One should make sure that any ancillary materials provided to the student are adequate. The review of software by students is very helpful in making an overall evaluation.

4. Performing the Evaluation: It is helpful to obtain a written evaluation especially if one is choosing from among competing software or if a time lapse will occur between evaluation and ordering of the software. A variety of checklists are available for this purpose. One such form specifically designed for use in chemistry is the one prepared under Project SERAPHIM to act as criteria for reviews of instructional software for the Journal of Chemical Education (see p. 12-14 of the December 1982 Newsletter). Some individuals, however, may find a form designed by themselves to meet specific local needs more valuable. Check lists of either type can not only aid in making a decision regarding quality of the software but can be helpful in convincing others of the desirability of acquiring it. Guidelines for formulating such an evaluation form are listed below.

GUIDELINES:

PROGRAM CONTENT

--Is the Content of the Material Suitable for Your Students?

--Does the Content of the Materials Fit with Your Curricular Goals?

--What Value Does the Content Convey?

--Is the Content Contained in the Materials Accurate?

--Is the Content Educationally Significant?

--Are the Goals and Objectives of the Materials Explicitly or Implicityly Clear?

PEDAGOGY

--What is the Nature of the Feedback the Program Provides to Students?

--What Assumptions About Learning and How Students Learn are Built into the Software?

--Does the Software Permit Modification to Meet Individual Student Needs?

--Is the Software Package Self Contained, or Does It Require Teacher Intervention?

--Can the Program be Used with Various Types of Class Arrangements (Individual, Small Group, Whole Class)?

--Does the Program Tap a Variety of Learning Modes (Visual, Aural, Numerical, Verbal)?

PROGRAM OPERATION

--Is the Program Free of Bugs and Breaks?

--How Does the Program Handle User Errors?

--How Much Control Does the User Have Over the Program Operation?

--Are Directions in the Program Itself Clear and Acceptable?

--Is There Good, Clear Documentation for the Teacher?

--Is There Good, Clear Documentation for the Students?

--How Well Does the Program Use Graphics, Sound, and Color Capabilities?

--Are Screen Displays Effective?

STUDENT OUTCOMES

--How Easy is the Program for Students to Use?

--Is the Program Interesting to Students?

--Does the Program Make Appropriate Use of Limited Computer Resources?

--Do Students Enjoy Using the Programs?

--How Well Do Students Learn What the Program Is Intended to Teach?

--What, If Any, Unintended Learning Results From Using the Program?

--How Effective is This Program Compared with Noncomputer Instruction in the Same Area?

Adapted from Peter Coburn, et al., "Practical Guide to Computers in Education", Addison-Wesley Publishing Co., Reading, MA, 1982, Chapter 5.

*Department of Chemistry
University of Northern Colorado
Greeley, CO 80639

**This material was made available to participants at the Sixth Biennial Computer Workshop held at the University of Kansas in August 1983.

BOOK REVIEW

Alan Smith (Chemistry Department, University of Southern Maine, Portland, ME 04104) is Editor of the Book Review section of the Newsletter. Anyone willing to review books for the Newsletter or wishing to suggest books for review should contact Alan.

WORD PROCESSING FOR SMALL BUSINESSES

by Steven F. Jong
Group Technology, Ltd., P.O. Box 87
Check, VA 24072
1983, 190 pp., paper $11.95 plus $1 shipping
ISBN 0-672-21929-8
Reviewed by D. Rosenthal*

This book describes word processing and the factors to consider in selecting a word processor for specific applications. The book assumes the reader has little or no familiarity with word processors or computers, but is also of possible interest to those who are somewhat knowledgeable about such matters. While the title implies small business applications, the contents should interest most chemists who wish to learn about word processors and perhaps wish to buy a word processor system.

The book consists of seven chapters. Chapter 1, entitled "You Too Can Profit from Word Processing" states that word processing is the most popular application of microcomputers, that a business letter costs $14 to $18 to produce and that word processing will reduce the cost of document production by one-third and the time involved by two-thirds. The four primary questions the book answers are (1) What can word processing do for you?, (2) What can't it do?, (3) What should you know before you buy?, and (4) What will it cost?.

Chapter 2 briefly describes typical hardware components (the display, screen, keyboard, printer, interfaces, disks and disk drives, memory and the CPU), and their characteristics. Some of these devices are illustrated through pictures. Chapter 3 describes word processing software and discusses in some detail the possible features of editors, formatters and printer control. The chapter includes consideration of hyphenation, spelling, mail-merge packages and user-friendly features like help facilities, menus, manuals, tutorials and courses. It points out that a particular software and hardware system will not have all of these features.

Chapter 4 describes hardware and Chapter 5 explains what software was available at the time the book was written. Part of this information is obsolete. Some of the hardware is no longer being manufactured and some new systems are now available. One or two pages are devoted to each item of hardware or software described. Tables summarize the features of much of the hardware and software.

Chapter 6 contains useful hints on selecting a system to suit your needs. It discusses the pros and cons of using microcomputers versus minicomputers for word processing. The author suggests making two lists, one of system requirements and the other of features that are desirable but not essential. Possible systems should be evaluated in terms of these requirements and desirable features. The minimum features deemed essential are: a fully assembled system having dual disk drives, a 12-inch monitor with 80 characters per line and 24-line capability, upper and lower case characters, a full office keyboard, plus shift, ESC, CTRL and cursor keys, at least 48k of memory, a letter quality printer, warranty and service contracts. The system must allow for growth; the software must capture all keystrokes must feature disk buffering; it must have word wrapping capability (that is, be able to split the line automatically by inserting a carriage return at the appropriate spot), character deletion/insertion capability; besides, the software must perform at least some on-screen formatting. Chapter 6 enumerates additional desirable features. The author indicates the steps that you should take in evaluating a system prior to purchase. The most important precept is that you must use and test the printer you want with the computer and software you propose to acquire before purchasing. This book gives a specific prescription on how to benchmark a system being considered for purchase.

The last chapter of this book (Chapter 7) predicts what's ahead for microcomputing: prices will come down; hardware and software will become more powerful and user-friendly.

One appendix contains seventeen general references. More than half relate to short articles in computer journals. The second appendix contains a glossary of terms.

The information contained in this book can be of value to anyone considering the purchase of a word processing system who does not already know very much about word processing and who is seeking advice.

*Department of Chemistry
Clarkson College of Technology
Potsdam, NY 13676

March 1984

PAL:
EXPLORATIONS IN COMPUTER BASED INSTRUMENTATION
AN INTERFACING PACKAGE

by Robert F. Tinker
Cambridge Development Laboratory
100 Fifth Avenue
Waltham, MA 02154 $199.00
Reviewed by Brian Pankuch*

NEEDED: Apple II+, 48K, DOS 3.3

SUPPLIED:

HARDWARE is a PAL interface box, with a ribbon cable which connects the Apple game port to the PAL interface, two cables which connect light and temperature sensors back to the PAL interface. All the equipment is easily set up to allow either of the sensors to send its electrical signal back over the cable to the appropriate input on the PAL interface, which sends its output over the ribbon cable to the Apple game port.

Software comes on a diskette which can and should be copied. The programs supplied allow you to do experiments on:

1) Camera speed measurement - allows you to check exposure times.

2) Reaction times - an individual can check the time it takes them to cover or uncover the light sensor in response to a 'beep' from the Apple.

3) Pendulum timing - use a swinging weight to cut the light path from a light source to the light sensor and see the period after each pass of the pendulum on the screen.

4) Light $1/R^2$ - you can vary the distance between the light sensor and the light source and measure the distance with a meter stick. The distance between the sensor and the source will appear on the screen as calculated by the $1/R^2$ law.

5) Flicker fusion - you see what appears to be a point of light on the screen, the rate at which it is being switched on and off is slowed till you are aware of the on-off flicker, touch a key and the rate of the flicker is displayed.

6) Cooling Curve - take a heated substance, insert the temperature probe and a graph will be drawn of temperature vs. time on the screen.

7) Heart rate measurement - put your fingers over a source of light and the light sensor over your finger - you see your pulse on the screen. The Apple does some curve analysis, it puts x's of the points its using on the screen. It reports your heart rate or that the data was unsuitable. Also, this program was used to collect pendulum data to display the actual graph and measure the period of the pendulum.

8) Solar energy - use the temperature sensor to measure solar insolation.

The MANUAL is brief and to the point. There are a few places in which the manual is unclear, e.g. the way to attach the ribbon cable at the Apple game port isn't carefully explained. Since there are only two possibilities I tried both, found the correct direction and didn't even have any smoke coming out of the computer.

STRENGTHS:

Overall the package fits together well. The individual experiments are interesting. You get a genuine understanding for what is happening, as you make a change in the position of the sensor or in what it is measuring and the output on the screen changes. Most of the experiments are easy to set up and perform. Only the ability to measure temperature as a function of time is directly applicable to the usual chemistry experiments. However, I can think of a number of reactions which when placed between a light source and the light sensor would give an interesting graph of light intensity versus time.

WEAKNESSES:

One of the sensor cables came with a short in it; since you get two cables, check both with a multimeter before concluding your interface doesn't work. The reaction time experiment is probably the easiest to check yourself and the equipment with.

My temperature probe is dissolving! Or rather the tape it's wrapped with is. I tried using naphthalene for cooling curve experiment and the probe didn't like it at all. I should be able to rewrap it but beware. I've used the whole system for demonstrations and several times wished I could erase the entire screen at a single keystroke. We also found the rate program would not run; it turned out that an invisible CONTROL C was embedded at the end of the name in the directory. We renamed the program without the CONTROL C and the program works satisfactorily.

Using the program to measure heartbeat is elusive and not very reproducible, but fun enough to be worth playing with. In a few places the manual tells you to do one thing and the program something a bit different. For instance, you are told to use three waterbaths to calibrate the temperature sensor; after setting them up you only use two.

OVERALL EVALUATION:

Compared to any other interfacing kit I've seen, this is by far the easiest and most interesting to use. If you have been lucky enough to meet Dr. Tinker in one of his many workshops, you will be happy to find the same cleverness and thoughtfulness throughout the package. I'm going to send a copy of this review to Cambridge Development Laboratories. With a little quality control the above weaknesses should disappear by the time you read this. The package without the above problems is easy to use, and provides you with intriguing possibilities.

*Department of Chemistry
Union County College
1033 Springfield
Cranford, NJ 07016

COMPUTERS IN CHEMISTRY AT THE UNIVERSITY OF WATERLOO

by Chung Chieh*

There have always been many applications of computers in chemical research, particularly in theoretical chemistry, crystallography, and spectroscopy. Some schools have acquired mainframe computer facilities for use in undergraduate instruction. Recently, we have established a microcomputer network dedicated for use in chemical education. This network consists of eight IBM Personal Computers all connected to one master controller IBM-PC, which has one floppy and one hard disk drive; however, it is expandable to 32 slave computers. The network was developed by the Department of Computer Service (DCS) at the University of Waterloo. The network software was written by J.F. Bolce and C.E. Pilkington, whereas the network interfacing was developed by A. Weerheim. Two of them (J.F.B. and A.W.) were involved in developing a similar network for the Physics Department before the IEEE-488 board became available. The group responsible for development of the network named it JANET standing for Jerry-Adrian NETwork or Just Another NETwork. Since JANET is a rather nice name, we choose to name our network the Chemistry JANET.

The hard disk in the master has a storage capacity of 17 megabytes. The disk is partitioned into many virtual disks. These virtual disks can be system disks, such as IBM-DOS, NETWORK COMMANDS, FORTRAN, APL, PASCAL, WORD-PROCESSING, course disks which hold specific software for certain courses, private disks for faculty members or students to do their work, and student disks assigned for courses. Some disks contain software, which is in a public library, other disks can be accessed only by those having a password to them.

Every IBM-PC in the network is a work station, which performs like a stand-along PC, but the users never have to worry about finding the right disk to insert into the proper drive. A user at a work station can access a maximum of 4 disks. Disk A can be a system disk, a course disk, or a boot disk, whereas disk B is the user's own disk which is accessed in write mode. Disks C and D can be accessed as one of the languages or programs in the public domain.

At the time this article was submitted the system was in operation for only a few weeks. Initially, we set up a few demonstration accounts (no password required) to encourage anyone interested in the system to try it. One of the demonstration programs provides real plots of the Van der Waal's equation. He, Kr, N_2, CO_2, and H20 were chosen as examples. These plots look rather nice on the screen, but they can also be printed out on the EPSON dot-matrix printer.

The advantages of a network like JANET is that many users can share softwares without having to be bothered with the managing of many floppy disks. It is ideal for a chemistry department like ours. I would like to exchange programs as well as ideas with other institutions or colleagues so that I can build up a rich library of software for the education of chemists.

*Department of Chemistry
University of Waterloo
Waterloo, Ontario
Canada, N2L 3G1

WORKSHOPS, MEETINGS, CONFERENCES & COURSES

Please send information to Donald Rosenthal, Editor. Describe the program, include location, sponsoring group, dates, costs, who to contact for further details (name, address, and phone number). Information should be sent as far in advance as possible. Information on summer programs should be sent before May 1st.

March 26 - 29: "Personal Micromputer Interfacing and Scientific Instrument Automation", VPI and State University, Blacksburg, VA 24061.

Hands-on workshop with each participant wiring and testing interfaces constructed using STD bus cards. Directed by David E. Larsen, Dr. Paul E. Field, Dr. Jonathan A. Titus and Dr. Christopher Titus. Registration fee $495. Contact Dr. Linda Leffel, C.E.C. at the above address, (703-961-4848).

April 7: "C.C.C.E. Workshop for High School Chemistry Teachers", St. Cloud University, St. Cloud, MN 50301.

An all-day session devoted to demonstrations, discussion and hands-on evaluation of software. For further information contact Judy Strong

April 8 - 13: ACS National Meeting, St. Louis, MO.

General papers, symposia and poster sessions. See the February 27 issue of C & EN for the final program. Registration fee $90 (for ACS members) and $155 (for non members). Contact George M. Bodner, Department of Chemistry, Purdue University, West Lafayette, IN 47907, (317-494-5313).

April 17: "C.C.C.E. Workshop for High School Chemistry Teachers", Buhl Science Center, Pittsburgh, PA.

An all-day session devoted to demonstrations, discussion and hands-on evaluation of software. Co-sponsored by the Society for Analytical Chemists of Pittsburgh and the Committee for Computers in Chemical Education (C.C.C.E.). For further information contact Rita Bastiani (412-921-0173).

April 28: "C.C.C.E. Workshop for High School Chemistry Teachers", Manhattan College, Riverdale, NY 10471.

An all-day session devoted to demonstrations, discussion and hands-on evaluation of software. For further information contact Brother Leo Michiels (212-920-0204).

May 31 - June 2: "College Chemistry Canada", 11th Conference, John Abbott College, Montreal, Quebec, Canada H9X 3L9

Speakers include Derek Davenport, Leslie Davis, Stephen Hanessian, Dudley Herron, David Humphreys, William Marshall and William Mooney. Workshop on microcomputers and review of available software. Discussions on pedagogical strategies for reaching the underprepared student. Contact Barbara De Lorenzi, P.O. Box 2000, Ste. Anne de Bellevue at the above address, (514-457-6610, Ext. 399).

May 31 - June 2: "Personal Micromputer Interfacing and Scientific Instrument Automation", VPI and State University, Blacksburg, VA 24061.

Hands-on workshop with each participant wiring and testing interfaces constructed using STD bus cards. Directed by David E. Larsen, Dr. Paul E. Field, Dr. Jonathan A. Titus and Dr. Christopher Titus. Registration fee $495. Contact Dr. Linda Leffel, C.E.C. at the above address, (703-961-4848).

June 13 - 15: "6th Annual National Education Computing Conference" (NECC '84) in Dayton, OH.

Sessions and related activities are planned for both experienced and new computer users. Pre-conference workshops are scheduled for June 11 and 12. Contact Lawrence A. Jehn, Computer Science Department, University of Dayton, Dayton, OH 45469

July 15 - 17: Workshop on "Enhancement of Creativity in Chemistry Using Microcomputers" at Michigan Technological University, Houghton, MI 49931.

The workshop will focus on modification of a simple program, project development, program development and peer review. For more information contact Dr. Larry Julien, Department of Chemistry and Chemical Engineering at the above address.

August 1 - 3: "The Computer: Extension of the Human Mind", University of Oregon, Eugene, OR 97403. Sponsored by the Center for Advanced Technology in Education.

The third annual computer and instructional technologies conference will focus on the needs of the individual who is responsible for school and district level use of computers and other emerging instructional technologies. General and small interest group sessions will be supplemented with vendor exhibits and film-video theater related to computer technology in education. Pre- and post- conference workshops will be conducted on the educational uses of computers and will feature hands-on opportunities for those with varied levels of computer expoertise.

Registration fee $95. There is an additional fee for workshops and academic credit. Contact Summer Conference Office, College of Education at the above address

August 5-10, 1984: "Eighth Biennial Conference on Chemical Education" sponsored by the ACS Division of Chemical Education at the University of Connecticut, Storrs, CT 06268

Morning and evening sessions will feature symposia, poster presentations and contributed papers. Symposia on "Computers for Personal and Classroom Use" and "Computer Literacy" are planned. Workshops and serendipity sessions will be held in the afternoon. Computer graphics and instructional computer program contests and displays are planned. College and high school chemistry programs.

Tentative costs include registration fee $75 in advance ($90 on-site) plus $15 per family member, lodging $16/day (double), $24/day (single), meals $13.25/day. Contact Dr. John Tanaka at the above address.

August 26 - 31: ACS National Meeting, Philadelphia, PA

General papers, symposia and poster sessions. April 15 is the deadline for submission of abstracts. Contact Adrienne Kozlowski, Department of Chemistry, Central Connecticut State University, New Britain, CT 06050, (203-827-7439).

September 6 - 8: "Personal Micromputer Interfacing and Scientific Instrument Automation", VPI and State University, Blacksburg, VA 24061.

Hands-on workshop with each participant wiring and testing interfaces constructed using STD bus cards. Directed by David E. Larsen, Dr. Paul E. Field, Dr. Jonathan A. Titus and Dr. Christopher Titus. Registration fee $495. Contact Dr. Linda Leffel, C.E.C. at the above address, (703-961-4848).

October 28 - November 1: "Second International Congress on Computers in Science", Washington, DC sponsored by Science Magazine and Scherago Associates.

The conference will emphasize the use of the workstation by the scientist. Talks in a number of areas including computer aided molecular design, workstation hardware, artificial intelligence, databases, laboratory automation and robotics. There will be poster sessions, workshops and a vendor exhibition. Prospective authors should contact Ed Ruffing, Scherago Associates, 1515 Broadway, New York, NY 10036 (212-730-1050). Conference chairman is Dr. Stephen R. Heller, EPA, PM-218, Washington, DC 20460 (202-382-2424).

CONTEST FOR INSTRUCTIONAL COMPUTER PROGRAMMERS

Project SERAPHIM, an NSF-DISE-sponsored project for disseminating instructional modules in chemistry, will hold its third instructional computer program contest in conjunction with the Eighth Biennial Conference on Chemical Education in Storrs, Connecticut, August 5-10, 1984. A prize of $200 will be awarded to the author of the instructional program judged best by participants in the conferences, and prizes of $100 will be awarded for the best program written by an author in each of four categories: (1) secondary school teacher, (2) two-year college teacher, (3) four-year college teacher, (4) student. Programs may deal with any aspect of chemistry at any level from high school to graduate courses. All programs entered must be able to run on at least one of the following microcomputers: Apple II, Atari 800, Commodore PET 4000 series, Commodore 64, Radio Shack TRS-80 Model I or III, Radio Shack Color Computer, and IBM Personal Computer. All authors must agree to release their programs for distribution by Project SERAPHIM, whether or not the program wins a prize, and programs may not contain any copyrighted code that would prohibit their distribution by SERAPHIM.

Criteria used in judging the programs will be the same as those used in writing software reviews for this Journal (see the December 1982 issue for more details). All attendees at the biennial conference will be eligible to review programs and will be asked to complete program evaluation forms for all programs they interact with. The forms will be tabulated by Project SERAPHIM staff, and the winners will be announced in this Journal in the fall.

To enter the contest, complete an entry form and submit it by July 13 to: Dr. John W. Moore, Project SERAPHIM, Department of Chemistry, Eastern Michigan University, Ypsilanti, MI 48197. Programs on floppy diskettes must be received at the above address by July 27 in order to be distributed to the judging sites on time. If documentation is needed in order for a program to be used appropriately, that too must arrive by July 27. Copies of the review criteria, entry blanks, and other information can be obtained from the address above at any time.

(NOTE: see pgs. 15 and 16 of this Newsletter.)

MEMBERSHIP FORM

To become a member or an affiliate, please check the appropriate box:

☐ I am a Member of the ACS and wish to become a Member of the Division of Chemical Education. Annual dues $5.

☐ I am not a Member of the ACS and wish to become an Affiliate of the Division of Chemical Education. Annual dues $5. (Affiliates have all the membership privileges except voting and holding elective office.)

☐ I wish to join ACS and also become a member of the Division of Chemical Education. Annual dues $5 plus current ACS annual dues. (You must meet ACS membership requirements. The Division receives a BONUS if you join national ACS through the Division.)

☐ Please send me an ACS membership application.

Name _____

Address _____

_____

City _____ State _____ Zip _____

Send this form, completed, to:

Wilmer J. Stratton, Treasurer
Department of Chemistry
Earlham College
Richmond, IN 47374

CCCEN

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CCCEN

PROJECT SERAPHIM, NSF-DISE ACS OFFICE OF HIGH SCHOOL CHEM.

1984 INSTRUCTIONAL COMPUTER PROGRAM CONTEST ENTRY FORM

Name of program: _____

(Use separate form for each entry. Duplicate if necessary.)

Level and subject area: (Circle number or numbers of all suitable areas)

1. High School Chemistry	2. General Chemistry	3. Organic Chemistry
4. Analytical Chemistry	5. Inorganic Chemistry	6. Physical Chemistry
7. Biochemistry	8. Environmental Chem.	9. Polymer Chemistry
10. Industrial Chemistry	11. Remedial Math	12. Numerical Methods
13. Statistical Analysis	14. Other (specify) _____	

Language: (circle one or more)

21. BASIC 22. FORTRAN 23. Pascal 24. Other (specify) _____

Hardware: (circle type on which your submitted disk will run)

31. Apple II/II+/IIe	32. Atari 800	33. Commodore PET 4000
34. Commodore C-64	35. TRS-80 Model I or III	36. TRS-80 Color Computer

Specify required features of hardware (e.g., 48K Apple II with game paddles): _____

Operating system and/or any special software required: _____

Name of author: _____

Brief description (20 words or less) of program:

_____

_____

_____

Address of author: _____

_____

Category: ___ Student ___ H.S. Teacher ___ 2-yr. College ___ 4-yr. College

I agree that should Project SERAPHIM wish to distribute the program named above the Project may do so. I certify that this program is original and does not contain copyrighted, patented, or other material that would preclude its distribution by Project SERAPHIM.

_____ _____
(signed) (date)

Mail this ENTRY FROM to: John W. Moore, Department of Chemistry, Eastern Michigan University, Ypsilanti, MI 48197; (313) 487-0368; (313) 487-0106 (messages only)

DEADLINE FOR RECEIPT OF ENTRY FORM: July 13, 1984.

1/18/84

1984 INSTRUCTIONAL COMPUTER PROGRAM CONTEST

WHO CAN ENTER?

Anyone who has written an original computer program for instruction in chemistry and is willing to have the program distributed by Project SERAPHIM.

WHAT PRIZES ARE OFFERED?

$200 for best program by any author
$100 each for best program by:

- A student
- A secondary-school teacher (supported by ACS High School Office)
- A two-year college teacher
- A four-year college teacher or any other author

WHAT KINDS OF HARDWARE ARE SUPPORTED?

Apple II
Atari 800
Commodore PET 4000 series
Commodore 64
IBM Personal Computer
Radio Shack TRS-80 Model I or III
Radio Shack Color Computer

WHAT CRITERIA WILL BE USED IN JUDGING?

Ease of Use: Documentation; Operation; Error handling: Flexibility
Subject-Matter Content: Accuracy; Completeness; Need for better treatment; Safety consciousness
Pedagogic Value: Innovativeness; Soundness; Comparison with alternative approaches
For more details, see Project SERAPHIM Criteria for Reviews of Instructional Software

WHO WILL THE JUDGES BE?

Attendees at the Eighth Biennial Conference on Chemical Education (Storrs, Connecticut, August 5-10, 1984) who interact with three or more of the programs. Final tabulation of judges evaluations will be made at SERAPHIM headquarters in September 1984.

WHEN IS THE DEADLINE FOR ENTERING?

Entry Form must be received by **July 13, 1984.** We suggest you send a copy of the back of this page, keeping the original for your records.

Program (on floppy diskette) and any written documentation you want the judges to evaluate must be mailed to John W. Moore at the address below to be **received by July 27, 1984.**

MAIL TO:

John W. Moore
Department of Chemistry
Eastern Michigan University
Ypsilanti, MI 48197
(313) 487-0368; (313) 487-0106 (messages only)

SOFTWARE LIST

Instructional Computer Programs--Chemistry

Computers in Chemical Education Newsletter UPDATE #2*

January 1984

Prepared by

Project SERAPHIM, NSF-DISE

John W. Moore, Director

J. J. Lagowski, Co-Director

Project SERAPHIM
NSF Development in Science Education
Project Headquarters:
Department of Chemistry
Eastern Michigan University
Ypsilanti, MI 48197
(313) 487-0368; 487-0106

* NOTE: This is an *update* of the Project SERAPHIM Software List that appeared in the June 1983 Newsletter with an update in September 1983. To obtain the *complete* 54-page Third Edition, send $5 to Project SERAPHIM.

Title	Subject*	Hardware	Oper. Sys.	Author
Apple Programs				
Marquardt Non-Linear Least Squares Fitting	12 13	Apple II, 48K, 1 disk PET or VIC)8K	DOS 3.3	Carl Trindle U of Virginia
BAL EQN NAMING	1-2	Apple II, 48K, 1 disk	DOS 3.3	D. Masterman Jackson Hole H.S.
GRAPHITTI	1 2 11	Apple II, 48K, 1 disk printer optional	DOS 3.3 Applesoft	S. Kador W. Churchill H.S.
EQUIL TIC-TAC-TOE	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	D.J. Olney Lexington H.S.
WAQUAL	1 2 8	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	John K. Estell
MOLARITY	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	M.A. Dees Wauwatosa H.S.
pH (7 programs)	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	M.A. Dees Wauwatosa H.S.
PCC1 PCC2 ST1	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	Rev. J D. Wheeler Rockhusst Coll
STEREOCHEM	3	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	W.E. Godwin U Arkansas, Monticel
GAS LAWS	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	V. Tannenbaum
DALTON	1 2	Apple II, 48K, 1 disk game paddle	DOS 3.3 Applesoft	V. Bendal H. Powell E KY Univ
SULFURIC ACID	1 2 10	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	E. Dalton J. Newman B Green St

APPLE PROGRAMS

Supplier**	Cost***	Description of Program
SERAPHIM Apple Disk #5 PET Cassette #3 PET 8050 Disk #1 Category III	$4.00-disk $5.00-cassette	Performs non-linear least squares analysis using the Marquardt algorithm. Four pages of documentation.
SERAPHIM Apple Disk #14 Category III	$4	Drill and practice on balancing equations, mass-mass problems, and naming elements and compounds.
SERAPHIM Apple Disk #13 Category III	$4	A tool that students can use to produce well organized data tables and graphs. Can also be used to combine and summarize data collected by an entire class.
SERAPHIM Apple Disk #13 Category III	$4	Tic-tac-toe game in which questions about aqueous equilibria must be answered correctly in order to occupy a square.
SERAPHIM Apple Disk #13 Category III	$4	Simulates a wastewater treatment plant. Students must choose the fractions of waste that will receive primary, secondary, and tertiary treatment. Effect on pollution level of a river is shown.
SERAPHIM Apple Disk #12 Category III	$4	Generates problems on calculating molarity of solution given amount of solute and volume of solution or calculating amount from volume and concentration, etc. Checks sig. figs.
SERAPHIM Apple Disk #12 Category III	$4	A series of programs on pH from integer pH through buffer solutions and titrations. Titration curve has buret and beaker to show how titration is done.
SERAPHIM Apple Disk #12 Category III	$4	Generates problems on % composition of compounds, mole-mole stoichiometry.
SERAPHIM Apple Disk #12 Category III	$4	Drill and practice on identification of chiral centers, R-S notation. Three sections single center, no mult. bonds single center, mult. bonds two centers, no mult. bonds.
SERAPHIM Apple Disk #13 Category III	$4	Tutorial on gas laws.
SERAPHIM Apple Disk #11 Category III	$4	Students add gas to a closed container with a blowout value that requires a specified pressure. Can be a game (most points for closest to blowout pressure) or an experimental simulation. Requires ideal-gas calculations.
SERAPHIM Apple Disk #11 Category III	$4	Tutorial on sulfuric acid manufacture and simulation of sulfuric acid plant. Allows user to experiment with reaction conditions to obtain best economics of production.

Apple Programs

Title	Subject*	Hardware	Oper. Sys.	Author
CHEMISTRY GAMES	1 2	Apple II, 48K, 1 disk	DOS 3.3 Applesoft	E. Dalton J. Newman 8 Green St
OCTANE TUTORIAL & GAME	1 2 8	Apple II, 48K, 1 disk Atari 800, 48K 1 disk	DOS3.3, Asoft Atari BASIC	Susskind, Donahue, Pascual
SOLUBILITY	1 2	Apple II, 48K, 1 disk Atari 800, 48K 1 disk	DOS3.3 Asoft Atari BASIC	Susskind, Pascual, Moore
MILLIKAN	1 2	Apple II+ 48K 1 drive game paddles	DOS 3.3	Dr. Robert C. Rittenhouse
QUANTUM-2	2 5 6	Apple II+ 48K 1 drive	DOS 3.3	Dr. Robert C. Rittenhouse
CHEMAZE	1 2	48K Apple II, 1 disk	DOS 3.3, Applesoft	Stanley Smith and Ruth Chabay
Molecular Animator	1 2 3 5 7 9	48K Apple II, 1 disk	DOS 3.3, Applesoft	J. Jeffry Howbert
Introduction to Crystallography	5 6	48K Apple II, 1 disk TRS-80 Mod I or III, 1 disk	DOS 3.3, A-soft TRS DOS	David Y Curtin
Organic Qualitative Analysis	3	48K Apple II, 1 disk	DOS 3.3, Applesoft	James Johnson
Polymer Chemistry	3 6 9	48K Apple II, 1 disk	DOS 3.3, Applesoft	H. Gibson J. Pochan S. Smith

Supplier**	Cost***	Description of Program
SERAPHIM Apple Disk #11 Category III	$4	Three chemical games: hangman animal order the elements (a periodic table game).
SERAPHIM Apple Disk #15 SERAPHIM Atari Disk #1 and #2 Category III	$4 Apple $8 Atari	Tutorial on gasoline, octane rating, engine knock and compression ratio, gasoline additives. Game involves simulated cross-country drive for which gasoline must be blended to match characteristics of car.
SERAPHIM Apple Disk #15 SERAPHIM Atari Disk #1 and #2 Category III	$4 Apple $8 Atari	Game in which one or more students are dealt hands of cards that represent ions in aqueous solution. Points are scored by combining cards to form ppt. or evolve gas from solution.
Chemistry Department, Walla Walla College, College Place, WA 99324	$10	Graphically simulates Millikan's oil droplet experiment to facilitate collection of data and calculation of the fundamental charge.
Chemistry Department, Walla Walla College, College Place, WA 99324	$20	Generates dot-density and surface plots of electron densities for planar cross-sections of atomic orbitals. Includes orbitals up through 3d's.
COMPress, P.O. Box 102, Wentworth, NH 03282	$40	Pac-Man-like game that requires knowledge of inorganic solution chemistry. Available as part of the COMPress general chemistry package by the same authors.
COMPress, P.O. Box 102, Wentworth, NH 03282	$75	Allows you to construct and manipulate molecular structures of your choice. Designed to rotate at various speeds around all three axes. Allows for adding, deleting, or modifying atoms. Sample molecules included.
COMPress, P.O. Box 102, Wentworth, NH 03282	$100 (2 disks) b-ups $10/disk	Provides an introduction to organic chemical crystallography. Includes: Crystal Geometry Crystal Symmetry Space Groups.
COMPress, P.O. Box 102, Wentworth, NH 03282	$75 (1 disk) b-ups $10/disk	Tests students' abilities to identify organic compounds. 25 unknowns included on disk. Each unknown contains one of the following: unsaturation, alcohol, phenol, aldehyde, ketone, amide, ester, carboxylic acid, amine, aromatic, or sat. hydrocarbon
COMPress, P.O. Box 102, Wentworth, NH 03282	$500 (7 disks) b-ups $15/disk	Introductory level course covering the major concepts aplying to polymers. Disks are: Introduction to Polymers Nomenclature of Polymers Structure of Polymers Mol. Wt. of Polymers — Chain-Growth Polymerization Step-Growth Kinetics — Polymer Quiz

SOFTWARE LIST

Title	Subject*	Hardware	Oper. Sys.	Author
Apple Programs				
Test Generator	1 2 3 4 5 6 7 8 9 14:tool	48K Apple II, 1 disk	DOS 3.3, Applesoft	Thomas B. Wiggers
Atari Programs				
OCTANE TUTORIAL & GAME	1 2 8	Apple II, 48K, 1 disk Atari 800, 48K 1 disk	DOS3.3, Asoft Atari BASIC	Susskind, Donahue, Pascual
SOLUBILITY	1 2	Apple II, 48K, 1 disk Atari 800, 48K 1 disk	DOS3.3 Asoft Atari BASIC	Susskind, Pascual, Moore

Supplier**	Cost***	Description of Program
COMPress, P.O. Box 102, Wentworth, NH 03282	$50 (1 disk) b-ons $10/disk	A flexible tool that allows you to create an extensive file of test questions in a variety of formates: Multiple choice Matching True-false Fill in the blank You can organize questions by topic, chapter or any other way, add or edit questions.
SERAPHIM Apple Disk #15 SERAPHIM Atari Disk #1 and #2 Category III	$4 Apple $8 Atari	Tutorial on gasoline, octane rating, engine knock and compression ratio, gasoline additives. Game involves simulated cross-country drive for which gasoline must be blended to match characteristics of car
SERAPHIM Apple Disk #15 SERAPHIM Atari Disk #1 and #2 Category III	$4 Apple $8 Atari	Game in which one or more students are dealt hands of cards that represent ions in aqueous solution. Points are scored by combining cards to form ppt. or evolve gas from solution.

APPLE

ATARI

SOFTWARE LIST

Title	Subject*	Hardware	Oper. Sys.	Author
Commodore PET Programs				
Marquardt Non-Linear Least Squares Fitting	12 13	Apple II, 48K, 1 disk PET or VIC >8K	DOS 3.3	Carl Trindle U of Virginia
TR6: Phase Transitions in Pure Compounds	6	PET 16K	BASIC 3.0	Daniel McConnell East Mich Univ
NICE PLOTTING ROUTINE	14:general tool	PET 16K MTU graphics	BASIC 3.0	John Vidolich East Mich Univ
Nomenclature Alk Conformations	2 3	Commodore PET 4000 series, 32K	Basic 3.0	Lyle Wescott Christ. Brthrs Coll
Unknown Id (for organic qual.)	3	32K Commodore PET, 1 disk drive and printer	CBM DOS	Michael W. Rapp U Central Ark.
Curve and Plot	14:general tool	PET MTU graphics	BASIC 3.0	Vahid Matidi East Mich Univ
HABER				R. Edens and K. Shaw
RKINET: Reaction Kinetics				A. W. B. Aylmer-Kelly
VIC-20 Programs				
Marquardt Non-Linear Least Squares Fitting	12 13	Apple II, 48K, 1 disk PET or VIC >8K	DOS 3.3	Carl Trindle U of Virginia

COMMODORE PET PROGRAMS/VIC-20 PROGRAMS

Supplier**	Cost***	Description of Program
SERAPHIM Apple Disk #5 PET Cassette #3 PET 8050 Disk #1 Category III	$4.00-disk , $5.00-cass ette	Performs non-linear least squares analysis using the Marquardt algorithm. Four pages of documentation.
SERAPHIM PET 8050 Disk #1 PET Cassette #3 Category III	$4.00	Calculates data needed in order to plot a phase diagram for a single component.
SERAPHIM PET Cassette #3 PET 8050 Disk #1 Category III	$4.00	A subroutine to allow simplified plotting of data on the PET screen using MTU high-resolution graphics hardware and software.
SERAPHIM PET Cassette #2 PET 8050 Disk #1	$4.00-disk , $5.00-cass ette	Drill and practice on naming of alkanes and on the conformations of cyclohexane.
SERAPHIM PET Cassette #3 PET 8050 Disk #1 Category III	4.00	Student solves up to 30 unknowns (from text by Lehman or Shriner) and turns in printed record to instructor.
SERAPHIM PET Cassette #3 PET 8050 Disk #1 Category III	$4.00	Does linear and exponential least-squares analysis on your data Plots the data in high resolution.
CONDUIT The University of Iowa P.O. Box 388 Iowa City, IA 52244	$40 b-ups $10 manuals $1.50	Information not available from CONDUIT
CONDUIT The University of Iowa P.O. Box 388 Iowa City, IA 52244	$40 b-ups $10 manuals $1.50	Information not available from CONDUIT
SERAPHIM Apple Disk #5 PET Cassette #3 PET 8050 Disk #1 Category III	$4.00-disk , $5.00-cass ette	Performs non-linear least squares analysis using the Marquardt algorithm. Four pages of documentation.

Title	Subject*	Hardware	Oper. Sys.	Author
TRS-80 Programs				
STOICHIOMETRY (in Spanish)	1 2	TRS-80 Model I or III 16K	TRS DOS 2.2	Guido Concha
QUANT PROGRAMS (in Spanish)	2 4	TRS-80 Model I or III 16K 1 drive, printer	TRS DOS 2.2	R. Infante-Mendez
CHEM1 CHEM2 CHEM3 CHEM4	3	TRS-80 Model I or III 16K	TRS DOS 2.2	R.D. Sands Alfred University
Introduction to Crystallography	5 6	48K Apple II, 1 disk TRS-80 Mod I or III, 1 disk	DOS 3.3, A-soft TRS DOS	David Y Curtin
LEAST SQUARES	4 6 9 13	48K TRS-80 Mod III 2 disks	TRS DOS	Vernon R. Miller
HABER				R. Edens and K. Shaw
RKINET: Reaction Kinetics				A. W. B. Aylmer-Kelly
IBM-PC Programs				
CYCLOHEXANE STEREOCHEM	3	IBM PC with 64K, 1 disk, color/graphics adapter	PC DOS, IBM BASICA	T.P. Forrest G.A. Dauphinee
RACOON	3 6	IBM PC 64K 1 disk color/graphics adapter printer plotter optional	PC DOS	P.F. Schatz U Wisconsin-Madison
HALEQN DRILL	1 2	IBM PC with 64K, 1 disk, color/graphics adapter	PC DOS, IBM BASICA	Hal Bender Clackamas CC
MAXWELL	2 6	IBM PC with 64K, 1 disk, color/graphics adapter	PC DOS, IBM BASICA	J.C. Whitmer W Washington U

TRS-80 PROGRAMS /IBM-PC PROGRAMS

Supplier**	Cost***	Description of Program
SERAPHIM TRS-80 Disk #3 Category III	$4	Stoichiometry problems. All prompts are in Spanish.
SERAPHIM TRS-80 Disk #3 Category III	$4	Ten programs for quantitative analysis laboratory. (See J. Chem. Educ., Sept. 1983, p. 733.) All prompts to students are in Spanish.
SERAPHIM TRS-80 Disk #1 Category III	$4	Shows substitution addition, reduction, elimination, oxidation, neutralization, rearrangement, & displacement reactions of paraffins, olefins, acetylenes, alkyl halides, alcohols, ethers, aldehydes, ketones, amines, nitro cpds, acids, salts, etc.
COMPress, P.O. Box 102, Wentworth, NH 03282	$100 (2 disks) bi-ops $10/disk	Provides an introduction to organic chemical crystallography. Includes: Crystal Geometry Crystal Symmetry Space Groups.
Dept of Chem. Roanoke College Salem, VA 24153	$50	Linear least squares to fit data to 19 equations rearranged to linear form. Menu driven, stores data on disk.
CONDUIT The University of Iowa P.O. Box 388 Iowa City, IA 52244	$40 bi-ops $10 manuals $1.50	Information not available from CONDUIT
CONDUIT The University of Iowa P.O. Box 388 Iowa City, IA 52244	$40 bi-ops $10 manuals $1.50	Information not available from CONDUIT
SERAPHIM IBM Disk #3 Category III	$4	Demonstrates ring inversion, proper orientation of bonds to ring substituents. Drills on cis and trans isomers of dimethyl cyclohexane.
SERAPHIM IBM Disk #3 Category III	$4	Given data on chemical shift and coupling constants RACOON simulates NMR spectra. Spectra can be plotted on the graphics screen and/or a digital plotter and/or graphics printer.
SERAPHIM IBM Disk #3 Category III	$4	Drill and practice on balancing chemical equations. Students enter coefficients and are told whether they are correct. Little tutorial help. Equations can be changed by instructors who know a little BASIC.
SERAPHIM IBM Disk #3 Category III	$4	A graphics tool for plotting Maxwell-Boltzmann distribution function for ideal gases. Intended to be used with texts or assignments. Allows several graphs on same set of axes. (T or M.W. can be varied.)

TRS-80

IBM-PC

COMPUTER GRAPHICS CONTEST GUIDELINES

FOR THE BIENNIAL CHEM ED MEETING AT THE UNIVERSITY OF CONNECTICUT

AUGUST 5TH TO 10TH, 1984

(1) All entries are to be submitted in one of the following categories:
  (a) Microcomputer Graphics
  (b) Minicomputer and above Graphics

(2) A first prize of $25 will be awarded in each category. A second prize of $10 and three additional prizes of $5 will be awarded in the microcomputer category. The number of additional prizes in category (b) will depend upon the number of submissions.

(3) The original figure as obtained from a printer, plotter, or screen photograph is to be submitted. Preferably, each figure is to be on an 8.5" x 11" page and under no circumstances should it be larger than 17" x 22". Appropriate entries will be displayed at the Biennial Meeting.

(4) Each entry is to have the following information below the figure as submitted:
  (a) Title
  (b) Name and address of submitter
  (c) Category (a or b)
  (d) Hardware - computer; printer,plotter or camera
  (e) Software required - programming language and other special software required. Size of program written by submitter.

(5) Each entry will not be returned and may be used by the Computers in Chemical Education Newsletter.

(6) Those submitting entries are encouraged (but not required) to submit the program which generated the graphics material. If submitted, the listing may be published in the Computers in Chemical Education Newsletter (at the discretion of the editor).

(7) An entry form is to accompany each submission. This form will contain a statement indicating the graphics material is original, the information contained in this application is correct and the author gives his permission for the figure to be used by the Computers in Chemical Education Newsletter.

(8) All entries are to be submitted to Professor Donald Rosenthal, Department of Chemistry, Clarkson College of Technology, Postsdam, NY 13676 by July 1, 1984. (Phone 315-268-2389 or 315-265-9242)

(9) The entries will be judged by a Committee. The decisions of the judges will be final.

(10) The subject matter of all entries must be relevant to chemical education or chemical research. At the discretion of the Committee entries which are not appropriate may be rejected.

COMPUTER GRAPHICS CONTEST

BIENNIAL CHEM ED MEETING AT THE UNIVERSITY OF CONNECTICUT

AUGUST 5TH TO 10TH, 1984

ENTRY FORM

Title of Graphics Submission: _____

Name(s) of author(s): _____

Address: _____

_____

_____

_____

ZIP

Phone : ( ) _____

Graphics Category (check one only):
___ Microcomputer Graphics
___ Minicomputer and above Graphics

Hardware:
Computer _____

Core Requirements _____ K bytes

Printer, Plotter or Camera _____

Other Hardware Requirements _____

Software:
Programming Language _____

Operating System _____

Special Software _____

Size of Program Used to Produce Submission _____

I certify that this submission is original, not copyrighted by others and the information contained in this form is correct. The content of this submission is relevant to chemical education or research. The Computers in Chemical Education Newsletter has my permission to use the figure should it wish to do so.

_____
Signature of author(s)

Mail this entry form together with an original copy of the figure to Professor Donald Rosenthal, Editor, Computers in Chemical Education Newsletter, Department of Chemistry, Clarkson College of Technology, Potsdam, NY 13676 by July 10, 1984. (Phone 315-268-2389 or 265-9242)

An appropriately filled out copy of this form must accompany each submission. Duplicate this form if additional copies are required.