Computers in Chemical Education Newsletter

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Committee on Computers in Chemical Education
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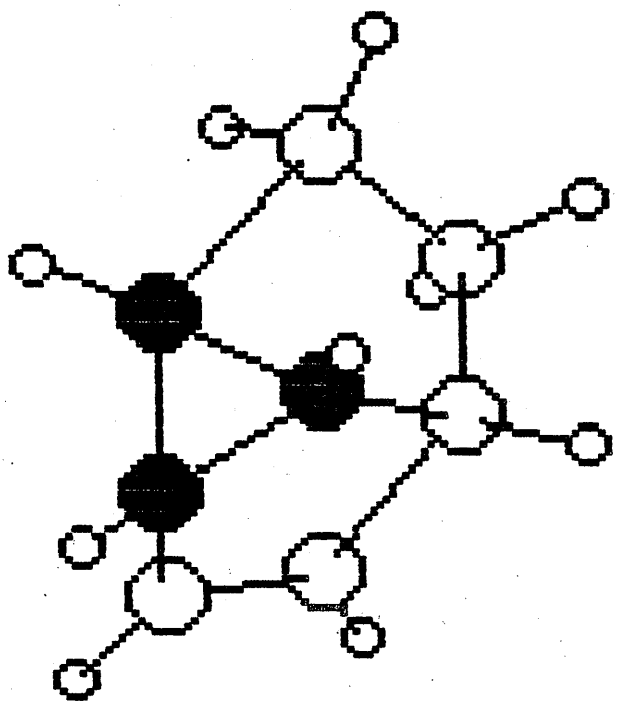
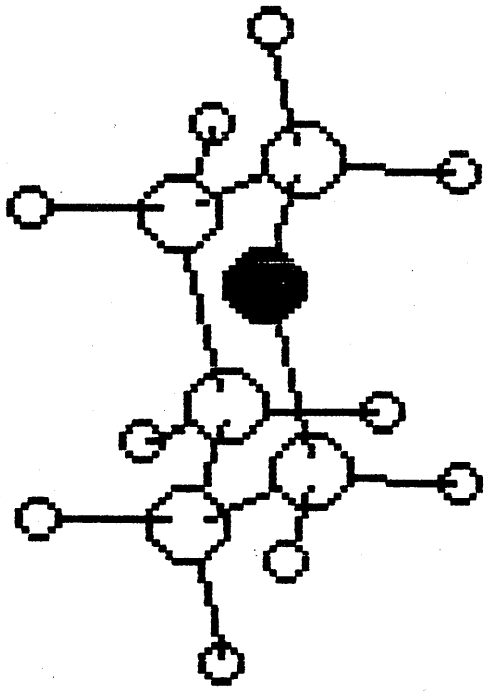


BENZENE-ETHYLENE PHOTOADDUCT



TETRAHYDROPYRAN

ON THE COVER

The two figures displayed on the cover were obtained by J. Jeffrey Howbert from screen dumps of his MOLECULAR ANIMATOR program from an Apple II to an Epson MX-80 dot matrix printer using plotting software of his own design. (The headings were added and are not part of the screen dump.) The MOLECULAR ANIMATOR is available from COMPress, P. O. Box 102, Wentworth, NH 03382. It runs on an Apple II+ with 48k under DOS 33. The program handles up to 60 atoms and provides three display modes - stick only, ball only and stick-and-ball. The last two modes use hidden-line algorithms that enhance the three dimensional effect. The program has high-speed free-running animated rotation (3 to 30 frames per second depending on the number of atoms) about the x, y or z axis (controlled by single key presses). Also, scaling and speed of rotation can be controlled. An editor for creating new shape files allows the user to work in Cartesian or internal coordinates. There are about 35 pages of documentation. The documentation includes three tutorials that introduce the parts of the program in a systematic fashion.

MESSAGE FROM THE CHAIRMAN

Among the correspondence in my "never-to-be-thrown-away" file is a letter I received from John Moore in January 1978 which began "...you have been nominated as a prospective member of the ACS DivChemEd Committee on the Role of Computers in Chemical Education (CRCCE)". After several years as a self-styled proselytizer regarding the wonders of academic computing, I realized that I was not alone and there existed within the Division of Chemical Education a very dynamic group that shared similar goals. Now, a short six years later, it is indeed an honor and a privilege to assume the chairmanship of this same committee whose membership includes so many pioneers in a field that is offering all of us the opportunity to become far more creative in teaching chemistry than we could ever have anticipated only a decade ago.

As originally conceived, the Committee on Computers in Chemical Education was charged with the task of "collecting, evaluating, and disseminating information about computers in chemical education." I do not see that our mission has changed significantly. What has changed, of course, is the number of people whom we must reach, as well as the nature and diversity of the information to be disseminated. With over 32,000 high schools, colleges and universities teaching chemistry, and an estimated 90% possessing academic computing capabilities, our task is indeed a vast one. But we have not been sitting still....recognizing the immediate and pressing need to carry the information to the teachers wherever they are in the most direct manner possible, we have begun supplementing our biennial 3-day workshops with a series of one day hands-on orientation sessions featuring a collection of about 200 state-of-the-art programs. During the past eighteen months this software has traveled over 30,000 miles from New England to the midwest to the Pacific coast, reaching over 600 teachers at 25 different locations. I believe this is one of our most successful and important projects. Looking forward to continued cooperation with Project SERAPHIM, I intend to expand the one day workshops as much as possible. The 1984-85 schedule of workshops is already taking shape; if you would like to host one in your locale, please contact me for further information.

Of course, our other principal method of disseminating information is this Newsletter. I would like to encourage all of you to make use of it as a forum for the exchange of ideas by contributing in some way. Share your experiences by responding to one of the Software or Hardware queries....write a brief article describing a special way in which you have used a particular piece of software or hardware in a uniquely effective manner....submit an anecdote concerning "unusual" things that you and/or your students are doing with computers.

We are planning a committee meeting sometime during the 8th Biennial Chemical Education Conference. Out of this will come a number of new directions and projects. If Storrs is in your summer plans, look for the announcements concerning this meeting and/or visit our Software Evaluation Center to let us know what kind of help you need! See you at Storrs...

COMMENTS FROM THE EDITOR

The success of this Newlsetter depends upon your learning something useful by reading it. As the editor, I attempt to gather together materials. Much of this information should come from you. For example, in most issues Queries are printed from the readers. Frequently, the editors of the Queries sections do not know the answers to these questions. If you as a reader have insights, please let us know. If you have items for the Who Done It? section or would like to write an article or review a book please write to the appropriate section editor or to me. Be an active rather than a passive reader. In Ken Ratzlaff's article "Scientific Applications of the Apple Game Port" he asks for information from readers who have developed applications or have ideas about how the game port can be used. This information will be included in Ken's second article which is scheduled to appear in the September issue. Ken will need to receive information from you early in July in order to meet the publication deadline.

A Birds-of-a-feather session for those interested in computers and computer-related activities will be held on Wednesday afternoon, August 8th at the 8th Biennial Conference on Chemical Education at the University of Connecticut. The exact time and place will be announced at the meeting. Those who will attend this session include Paul Cauchon (Chairman of the Division of Chemical Education's Committee on Computers in Chemical Education), Joe Lagowski (Editor of the Journal of Chemical Education and co-director of Project SERAPHIM), John Moore (co-director of Project SERAPHIM and Editor of the Computer Series in J. Chem. Educ.), Ken Ratzlaff (Chairman of the ACS Division of Computers in Chemistry and Editor of the Hardware Queries and WHO DONE IT? sections of the Newsletter), Ken Loach (Editor of the Software Queries and WHO DONE IT? sections of the Newsletter), other members of the Committee on Computers in Chemical Education and myself. This meeting will provide an opportunity for an exchange of ideas. Questions, suggestions, comments and criticisms will be welcome. We hope that those of you who come to the Biennial Conference at Storrs will attend.

The Seventh Biennial Computer Workshops sponsored by the ACS Chem Ed Committee on Computers in Chemical Education will be held at Clarkson University. Tentative dates are July 28th to August 1st, 1985. A committee is being organized to handle the advanced planning for this meeting. Discussions regarding the meeting will be held at the Conference. Anyone having suggestions for workshops, symposia, exhibits or other aspects of the planning should communicate with me prior to the Storrs meeting. (D. Rosenthal, Department of Chemistry, Clarkson University, Potsdam, NY 13676.) Further information on the meeting will be sent to all of you sometime in the fall.

The mailing label used with this issue of the Newsletter is different. This is because the tape which I inherited containing the original mailing list has been transformed into a data base which can be sorted by zip code, last name, first name, or in other ways. The format of the label or lists can be changed. In the process of transformation some capital letters were globally changed to small letters. The transformation process may have introduced some errors. If corrections are needed in your mailing label, please let me know.

A free subscription to the Newsletter can be received by anyone who fills out a pink form. Anyone wishing to receive more than one copy of the Newsletter is expected to pay $1.50 per issue for each additional issue received. Special rates are available for those who wish to distribute Newsletters at courses, workshops or meetings. Generally, there is no charge for Newsletters distributed at events which are sponsored by the Division of Chemical Education or the CCCE. Advance notice is required if a substantial number of copies is required.

The Personal Computer at Stevens Institute of Technology
by James M. van der Veen*

Stevens Institute of Technology began a program requiring every incoming student to own a Digital Equipment Corporation PC-350 in September 1983.

Stevens is largely a residential college of 1600 full-time undergraduates plus 1500 part and full-time graduate students located on a campus on the Hudson River overlooking midtown Manhattan. At present about 85% of the undergraduate students are in a unified engineering curriculum which allows some specialization in the junior and senior years in mechanical, electrical, chemical, and civil engineering. There is a science curriculum which has a mathematically oriented core followed by specialization in chemistry, chemical biology, physics, or mathematics. Next year there will be a new department in computer science drawing together separate programs already in existence for some time in the electrical engineering, mathematics, and system planning and management curricula. There are roughly 15 chemistry and chemical biology students in each graduating class. The chemistry program is approved by the A.C.S.

Stevens has historically had a strong emphasis on computer use starting with an IBM-1620 computer in the early 1960's and progressing through a UNIVAC 1105, IBM 360-Model 40, and since 1968, various models of the DEC System 10 and VAX computers. Four years ago, a separate Undergraduate Graphics Center was established with RAMTEK Color graphics terminals and a DEC 11/34 computer. In the Fall of 1982 all incoming Science and System Planning and Management students (80 in all) were required to own an Atari 800 computer. The introductory programming course focused on the development of numerical methods techniques, graphics, BASIC programming, and a collection of mathematical techniques in a personal library that could be used to assist in solving problems assigned in later courses. All the science students in this group took a course in computational physics in the sophomore year that expanded the concept of a library of useful routines. Experiments in data acquisition were also introduced. One limitation of the ATARI system was the lack of a FORTRAN compiler or interpreter and an Institute-wide curriculum requirement that all students learn and use FORTRAN. Uncertainty about the effect on student recruitment of an $800 increase in cost limited the choice of computers originally considered. (Tuition is currently $7400 per year.) However, student response was so positive that we decided to explore a system that would support FORTRAN, was disk based, and had graphics, an assembler, a 16 bit processor, and would allow for interfacing to laboratory experiments. After considering several different possibilities, a DEC Professional 325 was chosen with 256K core, two 400 Kbyte floppy disks drives, an interpretive FORTRAN and BASIC, a simple word processor and editor, graphics routines, and a monochrome graphics monitor. The processor was the 16 bit DEC 11/23 using the menu driven monitor called POS. The cost to students was $1800 (the list price was $4400) and included subsidies by Digital as well as Stevens. Students were charged the full $1800 on their first bill and had full title to the computer from the beginning. Additional financial aid, usually in the form of loans, was made available where necessary. The effect of this decision on recruitment seems positive. (There has been some drop in female applicants (normally 10% of the students) for undetermined reasons.)

During the summer of 1983 there was a flurry of developments including a decision that the interpretive FORTRAN was not acceptable. In order to support a compiler FORTRAN the system was upgraded to 512 Kbytes of memory, a 5 Mbyte Winchester drive was provided on loan, and a version of the DEC Tool-kit Software for the VAX was supplied. The Tool-Kit includes a FORTRAN compiler, BASIC, a sophisticated editor, a MACRO-11 assembler, and a library of FORTRAN callable graphics routines in addition to those included in BASIC. It uses VAX-like monitor commands in contrast to the menu drive POS system that comes normally with the Professional.

Our bowling alley was converted to a distribution center. Five hundred systems were purchased by freshmen. In addition, some 200 systems were ordered by other students, faculty and staff. After distribution, the same site was used as a repair center. Most problems were solved by switching boards. The more difficult cases were sent back to DEC.

Throughout the Fall term there were several major updates of system software and a decision was made to increase the 5 Mbyte disks to 10 Mbyte disks to make a more comfortable programming situation for FORTRAN and the Tool-Kit. None of these changes resulted in extra charges to the students. The standard student system for next year includes the 10 Mbyte disk (not on loan), Took-Kit software, 512-Kbyte memory, PC 350 rather than a PC 325, and the rest of the software mentioned above. The price will still be $1800 again involving substantial subsidies from Digital and Stevens. Over 1200 systems will be on campus by next fall. All systems will have the powerful WORD-11 word processing system. Although the student systems do not include printers, a laboratory containing several printers and PC-350's is available for making listings and for handing in assignments. Many students have acquired their own printers.

Most work with the PC's has been in a stand alone mode. With state aid we are acquiring a VAX 11/785 which can be used as a host for more efficient program development by faculty for distribution to students. Also, we are beginning exploratory work on networking a small group of PC-350's but that is very much in the initial phase. The 350 can be put in terminal mode and performs admirably as a graphics terminal for use in displaying views of molecules calculated on the host KL-10 by ORTEP or PLUTO. Hard copy pictures can be generated directly in raster form on the PC's printer or queued to the vector CALCOMP plotter interfaced to the main host computer. Although all students have accounts on the central campus computer, we have not encouraged students to use their systems as terminals as the congestion both of the phone system and of the central campus host would bring the whole operation to an abrupt halt. So far, few freshmen have ventured onto the central computer and we are naturally very curious how upperclass use of the KL-10 will change as the PC's percolate through the curriculum. The choice will be between a devoted powerful PC and a heavily loaded mainframe with a substantial research load.

One initially hidden cost of the personal computer plan was the necessity of rewiring all dormitories, designing a new furniture layout that would allow for adequate desk space for rooms containing two computers, and providing telephone wiring to each room which could be used for networking as those plans proceed. The networking could easily cost $4,000,000.

The development of computer use and applications throughout the curriculum has been procedding at a feverish pace. Because of the unified core taken by all students in both science and engineering programs, it has been possible to plan to make use of a hierarchy of commonly shared computer experiences. Both faculty and students are not enthusiastic about the use of computers for CAI. The emphasis has been to develop a user-friendly computer environment so that students and faculty will turn to the computer as the instrument of choice for solving appropriate problems. By having the computer easily at hand, it is hoped that the hostility that developed towards computers in batch oriented introductory programming courses and later unfortunate experiences with overloaded time-shared computer systems would not develop with the personal computers. Work is underway in over 25 courses throughout the curriculum to explore material and approaches that could make significant use of the 350. Initially, each student takes a programming course that includes BASIC, FORTRAN, graphics and the start of a collection of numerical techniques for use in later courses. Word processing use is encouraged. Work is in progress on developing a collection of IMSL-like subroutines that may be used for incorporation as subroutines in programs written to solve problems in a variety of courses. The mechanical engineering faculty is interested in the use of the 350 to prepare orthographic views of objects using raster and vector graphics. Work is in progress on software to make it possible to construct figures easily via computer.

In freshman chemistry we did not want to teach programming before the students had the introductory programming course. Our initial approach in August 1983 was to consider the NSF project SERAPHIM CAI software for the Apple II computer and to choose programs which could be converted to 350 BASIC, whose graphics could be adapted or duplicated, and which related to material in the general chemistry course. Eight programs were converted including RAST, ANIONS, DIPROTIC, HBA, THERMO, LOWREY, ABCKIN and WEAK. Several of Stan Smith's programs of potential interest could not be tried because they used ENBASIC which is a machine language specific (Apple II) course authoring language. A program which allows 2 and 3-D constructions of molecules from stencil elements was developed which could serve as a general slide making program. Dr. Malinowski is writing programs for simulating N.M.R. and mass spectral instrument response to be used in exploring use of some of the controls before students actually use the instruments. He is developing CAI introductions to the instruments in his laboratory. In addition, he has convereted his factor analysis programs from the Apple II to the PC-350.

Dr. Ermler's course in theoretical chemistry is taken by all science students in their junior year. He is working on adapting programs and a small data base for that course for use in some problem assignments particularly in chemical thermodynamics, statistical mechanics, quantum chemistry, and spectroscopy.

Several programs from Johnson's book, "Numerical Methods in Chemistry" have run successfully on the 350 using character graphics and I understand that Ken Jordan of the University of Pittsburgh has converted many of the programs to true graphics in color. These would mostly be useful in the junior and senior year.

Other applications in theoretical chemistry, kinetics, and especially in laboratory interfacing are being explored. A real time interface module for the PC-350 has just become available which will give access to RS232 and IEEE488 lines, as well as A/D and D/A channels.

We would be happy to share our experiences with the DEC Professional 350 and to learn of the efforts of others with this new machine. Also, we would like to share experiences with others who have, or are planning, a massive influx of small computers into the educational process.

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Molecular Orbital Calculations on Microcomputers

by G. Scott Owen*

I have been very enthusiastic about the potential cabability of the new generation of microcomputers (8086/8088) for number crunching tasks. This is because of the increased memory space available and because of the existence of the 8087 Numeric Data Processor. I felt that it was possible to perform mainframe type calculations on the IBM PC but until now this has been frustated by the lack of a good FORTRAN compiler.

This problem has now been solved with the arrival of the new MICROSOFT FORTRAN 77 compiler. This compiler supports the 8087 and also supports the large amount of memory available for the IBM PC. With this compiler, each named COMMON block can occupy up to 64 K bytes of space.

We (actually my student, Jannetta Bowden) have implemented the QCPE program CNINDO on the PC. In its current version the program will perform CINDO/INDO calculations on molecules of up to 20 atoms and 50 orbitals. The program requires a minimum of 256 K bytes of RAM. It executes fairly rapidly and the results are identical to our VAX 11/780 implementation. Some representative execution times are given below(these are "wall clock" times, i.e. they include the time for the file input and output and not just CPU time):

MOLECULE	ATOMS	ORBITALS	TIME (min:sec)
Methane	4	8	0:55
Acetone	8	20	6:42
Butane	14	26	8:02
Cyclohexane	18	36	16:30
Ribose	20	50	45:03

All of the above times are with the 8087 NDP (our current version of the FORTRAN libray for use without the 8087 doesn't work - we have a bad copy.) I would suspect that without the 8087 the times would be an order of magnitude larger. We are currently working on a version that would allow up to 40 atoms and 90 orbitals. This will probably require about 384 K bytes of RAM and a 90 orbital calculation would take about 4 1/2 hours. I haven't tested it but the program will probably run on many of the IBM PC compatible machines.

If you are interested in this program please send me $20 and I'll send you a disk containing the FORTRAN source program, the compiled Fortran program, documentation and a set of sample input data.

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Scientific Applications of the Apple Game Port
by Kenneth Ratzlaff*

Part I. The Basis of the Measurement

Understanding the fundamentals of data acquisition and control is an important part of learning about the use of small computers in chemistry. Data acquisition typically involves an analog-to-digital converter subsystem to digitize voltage levels, the typical output of scientific apparatus. Although sometimes different analog levels are provided as output for control, control usually involves simply turning some device on or off or delivering a pulse.

In a series of articles in this Newsletter, I would like to indicate how data acquisition and control can be taught at moderate equipment costs using game ports. Alternatively, analog-to-digital converter subsystems and parallel port boards could be used but this would typically add $500 to the cost of each computer system. Such additional costs are justifiable when a particularly important interface problem demands it, but the principles of data acquisition and control can be adequately taught using the game port.

In this article, I will introduce the components of the game port. In the next issue, I want to gather together some of those applications that have been made. In a final article, I will introduce some experiments which introduce the fundamentals of data acquisition.

The Apple II Game Port

The Apple game port is accessed by a DIP connector on the main board of the computer. The socket is an ordinary integrated circuit socket, so you need a cable which is terminated with a DIP connector, available from Radio Shack and many hobbiest mail order concerns. The pins of this socket are defined as follows:

1	+5 volts	7	Potentiometer 2	12	Annunciator 3
2	Push button 0	8	GROUND	13	Annunciator 2
3	Push button 1	9	----	14	Annunciator 1
4	Push button 2	10	Potentiometer 1	15	Annunciator 0
5	STROBE*	11	Potentiometer 3	16	----
6	Potentiometer 0				

The +5 volt pin can supply up to 100 ma to your external device to light lamps or LEDs, etc.

The two pushbutton inputs are simple standard TTL inputs which are used in two typical ways. First, they were designed to detect a switch closure; if an ordinary mechanical switch is connected between the input and ground, the input will read a logical 0 when the switch is closed (the input is shorted to ground) and a logical 1 when the switch is open. If the device under study has a TTL-compatible output, connection of it directly to this input is possible.

The status of a pushbutton input is determined by programming. (In BASIC a function PEEK (49249) or PEEK (49250) provides information on the status of push button 0 and 1, respectively.

The four annunciator outputs are TTL outputs which can be used to deliver pulses or logical conditions to other TTL circuits, for example, to start various operations. Also, they can be used to control mechanical or solid-state relays, turn on power transistors, and in general turn almost anything on and off (except maybe back-row freshmen).

The annunciator outputs are turned on and off by writing statements which will access their addresses; the access may be either to READ (PEEK) from the port or to WRITE (POKE) to a port. For Annunciator 0, the statement I = PEEK(42940) will turn the output off; the statement I = PEEK(42941) will turn it back ON. For Annunciators 1-3, the corresponding address pairs are 49242/49243, 49244/49245, and 49246/49247.

The potentiometer input is a very special type of analog-to-digital converter input. Its operation is controlled by the computer, and we will not go into the method of conversion here since one method of using it is to use the PDL command in BASIC.

The result of a conversion is directly proportional to the resistance between the input and 5 volts. The maximum result (255) is delivered when that resistance is greater than or equal to 150 K Ω and the result will be zero when the resistance is zero. Therefore, the paddle input can be used as an ADC when the transducer (sensor) makes a large change in resistance.

The most obvious sensor is the paddle or a similar potentiometer. A single or multi-turn pot can be used to sense angle or, with a pulley, linear position. Since linear position can be related to a lot of things (force, speed, flow-rate, pressure, weight, etc.) with mechanical converters, this input could be quite versatile.

There are also several solid-state transducors which make a great change in resistance with change in a physical phenomenon. These phenomena include temperature, light-level and pulse-width.

Part II, the Next Installment.

Before the next issue, I need to hear from persons who have developed an application or an idea for an application using the game port. Of course, Apple IIs are not the only computers with game ports; many of the same capabilities are in Commodore 64's, VIC's, Atari's, etc.

I will construct a "bits and pieces" section on the topic using the following information:

Type of data acquired or device controlled;
Hardware (including source where that is important);
Circuit diagram where it is not obvious.

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Notes and Comments—A Bit of Serendipity
by Paul Cauchon*

Not long ago, I acquired an SX-64, the portable version of the popular Commodore-64. The obvious advantages of size and convenience were what led me to make the purchase, however, I was a bit apprehensive about working with the 5" schreen, since I am already wearing tri-focal glasses (bi-focals with a narrow window of visibility designed to focus at normal computer-screen distances). Two years after turning in my bi-focals, I still have not fully adjusted to the "computer lens", and continue to engage in awkward optical and cranial gymnastics during keyborad sessions, particularly when trying to distinguish eights from zeroes, or tracking a listing as it scrolls past. Well imagine my surprise when, after about an hour of testing (playing with my new machine) I suddenly realized that the screen was actually easier to read than either the full size PET or Apple monitors. Now, after several hours of serious coding, I am convinced that the small screen does not pose the kinds of visual problems I had envisioned. In fact, its just the opposite!

Quite simply, the reduced screen size enables me to view all 25 lines of text through my narrow 'seeing-slit' at a comfortable distance and from a relaxed position. I'm not sure it will work that way for all my fellow tri-focalists, but if you've been holding off buying convenience for fear of ruining your eyes even further, you might want to reconsider.

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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 and REPLIES

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

SQ14 (March '84) Reply: On Chemical Abstracts indexing of computer-related abstracts by John T. Dickman (Chemical Abstracts Service, P. O. Box 3012, Columbus, OH 43210).

"I, too, would be interested in responses to your question of where users obtain their chemical-computing information. Applications of a technology may creep into a broad discipline more or less unannounced and then suddenly be recognized. I would be interested in learning of some of the non-chemical sources of computer related information of interest to chemists. We are always on the lookout for new or additional sources."

He appends a copy of a section of the 1984 Index Guide, showing that in addition to the headings Computer Applications, Computer Programs and Computers, C.A.S. also uses the headings Calculation, Automation, Control, Control apparatus, Process control and dynamics Information science, Process optimization, Process stimulation, Algorithm, Cathode-ray tubes, Optical imaging devices and Memory devices.

My personal (and editorial) feeling is that these headings are now insufficient and somewhat out-of-date. I suggest that the additional headings (or sub-headings) Minicomputer, Microcomputer, Software, Peripheral, Interface, Simulation, Converter, A/D and Converter, D/A should be adopted by C.A.S. for indexing chemically-related computer information. Any other suggestions? (K.L.)

SQ15 (March '84) Reply: On translation of Apple or TRS-80 Basic to Commodore Basic and vice versa. W.D. Hobey (Chemistry Department, Worcester Polytechnic Institute, Worcester, MA 01609).

1) A good place to start is The Basic Conversions Handbook for Apple, TRS-80 and PET Users by D.A. Brain et al. (Radio Shack, $6.) Unfortunately, graphics translations are often difficult although the book gives hints on this.

2) There was a fold-out Basic-to-Basic Conversion Chart for a number of micros in the British periodical Personal Computer World (date unknown).

SQ17 (June '84):

Carleton Stinchfield (Greefield Community College, Greenfield, MA 01301) is looking for a Compucolor User's Group, and for a convenient source of Compucolor supplies.

SQ18 (June '84):

John Henderson (Chemistry Department, Jackson Community College, 2111 Emmons Road, Jackson, MI 49201) asks is there any way to incorporate chemical structure diagrams into text created with a word processor (such as the Applewriter) on an Apple IIe?

SQ19 (June '84):

G. Avitabile (Department di Chimica, Via Mezzacannone 4, Napoli, Italy 80134) asks are there any good sources for guidelines on transportability of software between micros? (for a partial answer, see SQ15 reply above). Does anyone have any experience in the translation of English-based software into other language-bases?

SQ20 (June '84)

James E. Ekhaml (Chemical Engineering Department, Trident Technical College, P. O. Box 10367, Charleston, NC 29411) is working with 60 DEC Rainbows and would like to contact anyone familiar with their application to the teaching of chemistry or chemical unit operations.

SQ21 (June '84)

Brother James Spooner (Holy Family High School, 801 Rogers Ct., Ashland, KY 41101) wants to know if anyone has experience with software or computer-interfaces from Human Relations (Media) Software of Pleasantville, NY?

SQ22 (June '84)

Ma. del Carmen Clemente Jul (Escuela Technica Superior de Ingenieros de Minas, Rios Rosas 21, Madrid-3, Spain) is looking for a Fortran compiler for the DEC Rainbow 100, and for information on interfacing instruments and devices for data acquisition and experiment control with the Rainbow.

WHO DONE IT?

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

WHO-69 (June '84)

Charles Summers (Chemistry Department, Parkersburg High School, 2101 Dudely Avenue, Parkersburg, WV 26101-3492) is using Pets and Apples in teaching chemistry and physics, and has experience in interfacing 6502 micros (e.g. to a photoresistive diode detector for pendulum and inertial measurements). (K.L.)

WHO-70 (June '84)

Collegiate Microcomputer has recently begun publication (Collegiate Microcomputer, Rose-Hulman Institute of Technology, Terre Haute, IN 47803). It is a refereed journal devoted to "all aspects of microcomputers in Higher Education". The fourth issue (Vol. 1 (4), Spring '83) had a useful article by Bill Durham et al.of the U. of Arkansas on the construction of an instrument interface for a Commodore 64 (with full circuit diagrams).(K.L.)

WHO-71 (June '84)

Mini-Micro Systems (April 19, 1984) contains a comprehensive tabular digest of the operating characteristics and list prices of a wide range of mini- and micro-peripherals (disks, disketts, modems, printers, tapedrives, and terminals) from about 50 manufacturers. (K.L.)

WHO-72 (June '84)

Byte (April '84) has an interesting set of five articles on various aspects of micro-interfacing for instrument control and data acquisition. There is also a useful article on how to set up a Vic 20 or Commodore 64 as a terminal-emulator (for a mainframe computer) with full ACSII capabilities, including all carriage-control characters. (K.L.)

WHO-73 (June '84)

Computers and Electronics (March '84) has an article on inexpensive X/Y plotters with summaries of operating and constructions principles and lists of hardware and software suppliers. (K.L.)

WHO-74 (June '84)

CAL News is a newsletter published by the CEDAR Project (Imperial College Computer Center, Exhibition Road, London SW7 2BX, England). It gives information on computer-based learning projects, CAL research and forthcoming events in the United Kingdom. (K.L.)

WHO-75 (June '84)

Chemometric Newsletter is the bulletin of the Chemometrics Society (Secretary: Dr. Robert Meglin, Director, Analytical Laboratory, University of Colorado-Denver, 1100 14th Street, Denver, CO 80202). The Newsletter publishes news and abstracts in the field of chemical data analysis, pattern recognition and chemical statistics. The March '84 issue (number 11) is a systematic Survey of Chemometric Publications of 1983 with 311 abstracts in the following fields: General, Automation & Interfacing, Calibration, Computing, Control & Optimization, Curve-Fitting and Resolution, Data Handling, Education, Factor Analysis, Information, Parameter Estimation, Pattern Recognition, Resolution & Sensitivity, Spectral Analysis, and Statistics. In general, chemometric studies tend to use computer methods heavily and should be of interest to chemical educators. (K.L.)

WHO-76 (June '84)

R.A. Adams has published information on more than 100 current microcomputer journals in "An Annotated Bibliography of Microcomputer Periodicals" 1982 (ERIC Reproduction Service Ed 226 720, 35 pp, available on microfische). (K.L.)

WHO-77 (June '84)

Computer Graphics is published by the ACM Special Interest Group on Graphics. A special issue was published in February 1984 which contains the specifications for a proposed American National Standard Graphical Kernel System (GKS). GKS was designed to handle all the capabilities required for most graphics applications without becoming unduly large or complicated. It was designed to be user friendly. The system is device independent - able to work with a wide range of different output and input devices without modification of the program structure. The system should be capable of implementation in most standard programming languages and with most operating systems. The interface with FORTRAN 77 is considered in much detail. If implemented, GKS should facilitate the transportability of graphics from one system to another. (D.R.)

WHO-78 (June '84)

The Fall 1983 issue of the SIGUCC NEWSLETTER (Volume 13(3), pages 12-15) contains an article on "Microcomputers as a University Resource" by Aaron H. Konstam. In this article microcomputer networks are compared to traditional timesharing systems as a supplier of academic computing power. It is concluded that the microcomputer network can supply computer power more cheaply, more efficiently, and in many cases, can provide better computing resources. Microcomputers are easier to teach about and use. Some advantages of using timesharing systems are mentioned. The Winter 1983 issue (Volume 13(4)) contains several related articles. "Networked Microcomputers: New Challenges for Computing Center Management" and "Microcomputers for Academic and Administrative Use at the Rochester Institute of Technology" give some additional insights about the use of microcomputers. (D.R.)

WHO-79 (June '84)

The Spring 1984 issue of the SIGUCCS Newsletter contains an article by J.S. Sobolewski, D. Hoskins and T. Nguyen entitled "Planning and Funding Academic Computing" (Volume 14(1) 5-10). This article analyzes data from a 1982 survey of 189 four-year college and university computer centers. Information is presented on the level and distribution of funding for academic computing, the services that are typically provided and the process used by the institution to achieve long-range planning. Survey results are summarized in nine tables. Separate data are compiled and tabulated for public and private institutions. Minimum, maximum and average values of quantitative replies are tabulated. Over 75% of the schools surveyed had computer centers providing both academic and administrative computing. An average of $74 per student is spent each year on academic computing. About 46% of the computing center budget is spent for instructional computing, 16% for research computing and 49% for administrative computing. An average of 2.3% of the total school budget is spent on the computing center; 1.3% is spent on academic computing. 46% of the computing center budget is spent on staff, 43% on hardware, communications and maintenance and 11% on supplies. Information on student access to computing, hardware availability, and other data are included in the article. (D.R.)

WHO-80 (June '84)

The Winter 1984 issue of SIGCUE Bulletin contains an article by Moshe Cohen entitled "Exemplary Computer Use in Education" (Volume 18(1), 16-21). Two elementary schools, two middle schools, and two high schools were selected for detailed study. All schools were located in or near San Diego, CA. The facilities and programs at each of the schools were quite different from each other. The article contains references to other studies of computer use in schools. (D.R.)

WHO-81 (June '84)

The Winter 1984 issue (Volume 11(1)) of the Journal of Computer-Based Instruction is one of two special issues on educational reserach and computer-based instruction. These two issues will consider educational computing in terms of learning theory, instructional theory and computer-based instruction. The articles in this first issue are "The Minnesota Adaptive Instructional System: An Intelligent CBI System" by R.D. Tennyson, D.L. Christensen and S.I. Park; "Empirically Based Procedures for Designing a Response-Sensitive Sequence in Computer-Based Instruction: An Example from Concept-Teaching Strategies" by O. Park; "Research on Drill and Practice Strategies" by P.R. Merrill and D. Salisbury and "A Discussion of the Attributes, Role, and Uses of CAI Materials in Foreign Languages" by R. Rashio and D.L. Lange. (D.R.)

WHO-82 (June '84)

ACCESS - The Journal of Microcomputer Applications is published bimonthly by LEDS Publishing Co., Inc. (P. O. Box 12847, Research Triangle Park, NC 27709). Single issues are $4.00, $21.00 for six issues. The Journal contains articles on numerical analysis, statistics, graphics and engineering or scientific applications. Source listings of programs most of which are in BASIC are frequently included. Some of the articles in the March/April issue (Volume 3(2)) include "A Comparison of Two Basic Compilers for the Apple II Computer", "Some Considerations in Adapting FORTRAN Programs to CBASIC for Use on Microcomputers", "Monte Carlo Techniques: Part I Integration", "Data Entry Program for the IBM-PC", "Linear Equation Solver" using Gaussian elimination with partial pivoting, scaling and iterative improvement, "Gauss-Seidel Iterative Method for Large Matrix Systems". All of these articles contained BASIC programs source listings except for the first two which had no listings and the last which contained a FORTRAN listing.

Volume 2 issue 10 contains an article entitled "The Chemists Helper" which describes and includes a BASIC listing of a rather sophisticated program which will calculate molecular weight and percent composition if the molecular formula is entered. Sample input and output are shown for (C4H9)4C, C6H5COCH3 and C(C(C(CH3)3)3)4. Also, this issue of ACCESS contains an article on "Numerical Accuracy of Least Squares Computer Programs" with some test data to be used in evaluating a program which can perform a least squares fit of the equation Y = B0 + B1 * X1 + B2**2 + ... The article contains a listing of a BASIC program which uses modified Gram-Schmidt orthogonalization. (D.R.)

WHO-83 (June ' 84)

The Computing Teacher is the Journal of the International Council for Computers in Education and is published nine times each year August to May. A one year subscription costs $21.50. It is intended for persons interested in the instructional use of computers at the pre-college level. "The journal emphasizes teaching about computers, teaching using computers, teacher education, and the impact of computers on curriculum."

In the March 1984 issue (Volume 11, No. 7) David Moursand proposes that 2% of a school district's budget be allocated for instructional computing. The average U.S. school allocates $2,500 per student per year. 2% of this would be $50 per student per year. If half this amount were used for the purchase of hardware, one $1,000 computer system could be purchased for every forty students each year. Assuming a four year lifetime for the computer, after four years there would be one computer for every ten students. Currently there is a U.S. average of one machine per 120 students. With one machine per 10 students, every student should have about half an hour of computer access each day. The remaining $25 per student would be used for software and materials, in-service education, computer coordinators and for other purposes.

Generally, in each issue there are sections entitled Letters to the Editor, What's New Software Reviews, Book Reviews, Computers in the Teching of English Computers in Science Ed, The Logo Center, and Classified Ads. In addition, there are typically a dozen or more feature articles. The March issue had articles on (1) "Use Logo Graphics in a BASIC Program"; (2) "Computer Demonstrations for your Benefit". Readers are advised to ask to see demonstrated the features they require and are given fuidelines on how to evaluate a system, (3) A Guide to Producing Educational Software"; (4) "The Rat and the Maze" is a programming problem involving two dimensional arrays. A listing of a BASIC program which solves the problem is given. (4) "Charting a Summer Course" lists fifty-five colleges and universities which are offering at least nine quarter hours of computers in education summer courses. (5) "Computer Competencies for School Administrators"; (6) "Helping Students with Recursion: Teaching Strategies" Part III: Teaching Students About Embedded Recursion; (7) "Public Domain Software Listings" - An updating of software collected through the efforts of SOFTSWAP is included in this article. Program disks can be copied at no charge, or ordered by mail ($10/disk). Fifty-two Apple disks, six Atari disks, two IBM disks, and eight PET disks are among the software presently avaialable. Previous listings appeared in Volumes 9(8) and 10(9). Ann Lathrop (San Mateo County Office of Education, 333 Main Street

Redwood City, CA 94063) is in charge of the SOFTSWAP project.

LOGO software is available from the Young People's Logo Association Software Exchange, 1208 Hillsdale Drive, Richardson, TX 75081. Ten Apple disks (or tapes), one Atari disk, three Commodore disks, six MIT disks and six TI disks are available and their contents are listed. If you submit a working program, you may select any tape or disk from the catalog. YPLA will copy the programs onto a tape or disc. A blank disk or tape and return postage must be included. Alternatively, $10 can be sent for any tape or disk in the catalog. Information on eleven other sources of public domain software is included.

The December/January issue (Volume 11(5)) featured a number of articles on LOGO. (D.R.)

BOOK REVIEWS

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.

With this issue, we are pleased to publish two reviews by a new reviewer, Dr. Harry E. Pence. Harry is Professor of Chemistry at the State University of New York College at Oneonta, Oneonta, NY 13220. He is an inorganic chemist by trade, and is interested in instructional uses of computers, especially in general chemistry. He programs in FORTRAN, BASIC and Pascal, and is beginning to explore the caverns of C. We think that readers will find these reviews to be interesting and informative.

PASCAL PROGRAMS FOR SCIENTISTS AND ENGINEERS
by Alan R. Miller
SYBEX, 374 pages, 1981, $17.95
Reviewed by Harry E. Pence

Pascal is strongly recommended as a teaching language by many computer scientists and enthusiastically endorsed by columnists in some computer magazines. However, chemists who set out to learn about chemical applications of this language may encounter some frustrations. Although there are many Pascal textbooks, few of them deal with problems of interst to chemists, and the sample programs in chemistry books are usually written in FORTRAN or BASIC. Miller's book provides an excellent opportunity to learn more about Pascal while also developing a "toolkit" of scientific programs that may be used for either teaching or research.

This book was developed from a course in computer methods for engineering students taught at the New Mexico Institute of Technology, and the list of topics covered is very impressive for what I presume is a one semester course. An elementary knowledge of Pascal is assumed, and it is helpful to have one of the standard Pascal textbooks at hand for reference. The author intends the material to be read sequentially, so that the techniques introduced initially, such as random number generation, sorting, plotting, and matrix manipulations, are used in later programs. This can make it somewhat difficult to run an isolated program for a specific application, but it does make the topic development very logical and understandable.

Miller presents an extensive discussion of computational methods, including topics such as numerical integration, the Newton-Raphson Method, linear and nonlinear curve-fitting, and the solution of simultaneous equations. He not only suggests several different approaches for each of these techniques but also points out some of the complications which may arise. The text includes roughly sixty-five complete Pascal programs that demonstrate these various techniques. The discussion of the various subjects is quite clear, but as might be expected from the number of topics covered, the coverage of the mathematical background is sometimes rather brief. Those who wish a more extensive mathematical treatment can either consult the books mentioned in the bibliography or else go to one of the more mathematical references, such as A.C. Norris' book on computational chemistry.

I have found this book to be very enjoyable, and one of my students who is currently working through it has expressed a similar response. The discussion is clear, the organization is good, and the programs are presented in a format that is easy to follow. The author reports that he has tested most of the programs on several different Pascal compilers. I have tried many of the programs, and the few cases where minor modifications were necessary to make them run may well be because our Pascal compiler is not one of the common commercial versions. In order to make the programs as portable as possible, the author has used only a fundamental set of Pascal commands. I regret not having the chance to see examples where some of the more elegant structures are used, but this regret is more than balanced by the fact that the programs run so well. I do wish that exercises had been provided, and I hope that this omission will be corrected in the next edition.

In summary, I have found much that I like in this book and very little that I dislike. Because of its clarity and organization, it should be useful to many different individuals having a broad range of computer experience. It is especially welcome to find such a readable book that covers so much valuable material on computational methods.

BASIC PROGRAMS FOR SCIENTISTS AND ENGINEERS
by Alan R. Miller
SYBEX, 318 pages, 1981, $15.95

FORTRAN PROGRAMS FOR SCIENTISTS AND ENGINEERS
by Alan R. Miller
SYBEX, 280 pages, 1982, $16.95
Reviewed by Harry E. Pence

Despite my personal interest in Pascal, there is no doubt that for many chemists the computer language of choice continues to be either FORTRAN or BASIC. While working on the review of Miller's Pascal book, I was pleased to learn that he had also written versions of his book in both of these other languages. Although I received copies of these editions too late to examine them extensively, they are both very similar to the original, and so I wished to mention them for the benefit of those who find the description of Miller's book to be interesting, but prefer to work in one of the more traditional computer languages.

In each case, the approach and list of topics covered is almost exactly the same as that in the Pascal book; however, there are a few significant differences. The most important change is the addition of problems at the end of each chapter. Although the number of exercises provided is still rather small (only a total of thirty), they should increase the usefulness of the books for both self-study and classroom instruction. As in the previous volume, the author has gone to great lengths to assure that the programs will run on a wide variety of different systems.

Unlike the situation in Pascal, there are a number of books available which provide scientific subroutines and programs in BASIC or FORTRAN. However, Miller's books do offer a clear well-integrated approach to a large number of useful computational techniques. Chemists who use BASIC or FORTRAN may well find these books to be a worthwhile addition to their libraries.

WORKSHOPS, MEETINGS, CONFERENCES & COURSES

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

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 under-prepared 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 10 - 15: "Microcomputer and Minicomputer-Interfacing and Applications" at Continuing Education Center, VPI and State University, Blacksburg, VA.

ACS Laboratory Short Course: Course revised to include lectures on local area networks, laboratory information systems, molecular design processing, electronic notebook, robotics in the laboratory, use of graphics, image analysis, voice I/O, expert systems and managing the electronic laboratory. Directed by Dr. Raymond E. Dessy. Course repeated September 16 - 21, December 9 - 14 and March 10 - 15, 1985. Contact Harold Walsh, ACS Educational Activities Office, 1155 Sixteenth Street, N.W., Washington, D.C. 20036, (202) 872-4508.

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

June 17 - 23: "Microcomputers in the Chemistry Curriculum", The Fifth Annual ACS Summer Institute for College Teachers at Syracuse University, Syracuse, NY 13210.

The course director is Dr. Daniel Macero (315-423-2686). The institute will feature classroom instruction on and hands-on laboratory experience with microcomputers and related devices. The institute is intended for chemical educators particularly college or university faculty. No prior knowledge of microcomputers is assumed, although some BASIC programming experience is beneficial. Topics to be covered include basic computer hardware, interfacing principles, microcomputer software, software development for chemical applications, data enhancement techniques, laboratory data management and information retrieval, graphical devices, computer networking, and examples of computerized chemical systems (titration,GC, polarography, and rapid scan spectroscopy). Tuition $395, meals $115, housing $89 per person for a double room, $121 for a single room. Contact Education Division, American Chemical Society, 1155 Sixteenth Street, N.W., Washington, DC 20036 (202-872-4508) for registration.

July 9 - 27: "The Computer as an Instructional Tool" at the Taft Center for Teacher Evaluation, Watertown, CT 06795.

Taught by Paul Cauchon. The course is designed for the teacher who has little or no background in computing and involves exploring the development and use of microcomputers as instructional aids. The first week is devoted to an introduction to BASIC programming. During the second and third weeks participants study and develop programs which apply to their own particular areas of interest. Cost is $300 per week for tuition, room and board. Graduate credit is available. Teachers may enroll for one, two or all three weeks. Detailed information is available from Edward M. North, Director at the above address (203-274-2516).

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 expertise. Registration fee $95. There is an additional fee for workshops and academic credit. Contact Summer Conference Office, College of Education at the above address (503-686-3460).

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 "Defining Computer Literacy for Chemists" are planned. Workshops on "Choosing a Microcomputer System: Hardware and Software", "Evaluating Computer Assisted Instruction Programs", "Chemical Demonstrations", "Structural Inorganic Chemistry", "Experiment Development" and "Grant Proposal Writing" will be held in the afternoon. Computer graphics and instructional computer program contests and displays are planned. College and high school chemistry programs. Costs include registration fee $75 before July 22nd ($90 on-site) plus $20 per family member, lodging $16/day (double), $24/day (single), meals $12.40/day. Contact Dr. John Tanaka at the above address. (203-486-2443 or 4223)

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

General papers, symposia and poster sessions. 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).

November 8 - 10: "Ed Comp Con - 84 Conference" sponsored by the IEEE Society at the Convention Center, San Jose, CA 95101.

CAI and educational uses of computers will be strongly emphasized. Deadline for submission of papers is June 15th. Submit to Professor D. C. Rhine, Suite 447, Styes Hall, Western Illinois University, Macomb, IL 61455 (309-298-1315 or 1452).

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)

COMPUTER GRAPHICS EXHIBIT

___ I wish to submit graphics materials for a Special Graphics Exhibit rather than the Computer Graphics Contest.
Provide information in the appropriate portions of the above contest form, but sign in the space below.

I certify that this submission is original, not copyrighted by others, and relevant to chemical education or research.

_____
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 1, 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.

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)

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