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ABSTRACT

Selections from volume 4 (numbers 1-4) of the Task Force on Computers in Chemical Education (TFCCE) Newsletter are presented. Number 1 includes an introduction to and objectives of the newsletter and TFCCE, a report on computer-related activities in the chemistry department at Eastern Michigan University, a list of TFCCE members, a discussion of a newsletter section focusing on reader questions/answers related to hardware/software problems ("Queries") and information on locally developed or commercially purchased software/hardware ("Who Done It?"), and a listing of sources of computer assisted instruction (CAI) materials. Number 2 includes descriptions of CAI program distribution centers, sources of CAI materials, a modular instrumental analysis course, and computer uses at Canterbury School (CT). Number 3 includes a letter describing elements needed in programs, guide to CAI, report on computer use in chemistry at University of Texas (at Austin), data analysis using computers, and listing of secondary sources of literature on microcomputers. Number 4 includes discussions of use of computers in chemical education at University of Michigan and computer graphics, a summary of a conference on computers in education, a book review ("16-Bit Microprocessors"), and a listing of primary sources of literature on microcomputers. In addition, numbers 2-4 contain "Hardware/Software Queries" and "Who Done It?" sections. (JN)

COMPUTERS IN CHEMICAL EDUCATION NEWSLETTER

Published by the ACS Division of Chemical Education
Task Force on Computers in Chemical Education
G. Scott Owen, Chairman/Department of Chemistry, Atlanta University, Atlanta, GA 30314 David Rosenthal, Editor/Department of Chemistry, Clarkson College of Technology, Potsdam, NY 13676

Volume IV Numbers 1-4/ 1981

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Volume IV Number 1/March 1981

MESSAGE FROM THE CHAIRMAN

Welcome to the first edition of the new TFCCE Newsletter. We hope to publish the Newsletter quarterly. The objectives of the Newsletter (as well as the TFCCE) are to help keep Chemical educators abreast of new relevant hardware and software developments; to provide a forum for discussion of issues of common interest, to provide help and direction to newcomers (and oldcomers) to the field, and anything else which might be pertinent. The continued existence of the Newsletter will be partially dependent upon contributions from the readers.

There are several capabilities which we would like to see developed. One of these is to create a database of different users, their systems and applications. This would facilitate the interaction between users. For example, I have an APPLE II system (used for instrument interfacing and general programming) and I just obtained an S-100 bus system. Both of my systems will be running UCSD-Pascal and I am interested in communicating with others with similar systems. So please fill out the questionnaire in this newsletter so that we can begin to organize this database. Probably many of us now have the capability to use our small systems to talk to each other. I would like to explore the possibilities of using "electronic mail" to facilitate software and information exchange.

Another useful function of the Newsletter would be for hardware and software reviews. For example, I bought the ASM/65 assembler from Programma International, Inc. After creating and assembling a program on my APPLE I couldn't find a description of how to save the assembled code. Reasoning that nobody would possibly sell an assembler that couldn't save the assembled code I called Programma. They informed me that, yes, there was a "problem" with that assembler and they gave me a telephone number of the author (in Nevada). I called a couple of times but couldn't reach him so I gave up and bought a new assembler (SC-II).

On the other hand, I just bought a wonderful intelligent terminal program for my APPLE (DATACAPTURE 4.0 by Southeastern Software, 6414 Derbyshire Dr., New Orleans, LA 70126). This program allows me to easily create text offline and send it or to receive text from another computer. If, in receiving a large text file there is a memory overflow, the program will send a stop control character to the other computer, write the text out to disk, then continue receiving text - all automatically! Another very useful feature is the ability to define special characters which the APPLE normally does not have. This has always been a problem for me since I use the APPLE to communicate with PDP-11's which use the rubout/delete key (not available on the APPLE) to delete characters. With this program I defined control/R to be rubout/delete. I strongly recommend this program to anyone who uses their APPLE as an intelligent terminal.

COMPUTER-RELATED ACTIVITIES IN THE DEPARTMENT OF CHEMISTRY

EASTERN MICHIGAN UNIVERSITY

by John W. Moore

Students and faculty in EMU's chemistry department have access to a variety of computing facilities. We have the following hardware: several remote terminals, including a daisy-wheel printer supported by graphics software for timesharing on a DEC system-10; a 48-K Apple II Plus with disk, serial and parallel I/O, a communications interface, and a TEKSIM chip to simulate a Tektronix graphics terminal; two S-100 buses; Z80-based microcomputers operating under CP/M or UCSD Pascal with CRT graphics, a digital plotter, dot-matrix printer graphics, an A/D converter; and seven Commodore PETs. The PETs were just obtained this fall with funds from an NSF CAUSE grant.

Several faculty members and a number of students have been involved in computer related projects during the past few years. Ron Collins has worked with undergraduates Steve Duff and Dan Johnson on PRBGEN, a program that interacts with computer-illiterate faculty to obtain information that is then used by PRBGEN to write programs that print simple exam and homework problems. Nina Contis has written an extensive set of CAI lessons using CATALYST/PIL. These are used for remediation in introductory courses. Nina is also developing a course on computer-instrument interfacing that will employ our PETs and S-100 system. I still maintain the Computer-Generated Repeatable Test System that has been distributed to over 50 other universities, and am currently working on micro CGRT using an S-100 system. I continue to be interested in computer graphics of the sort used to illustrate the general chemistry text co-authored with Bill Davies and Ron Collins. (Bill is now at Hampden-Sydney.) I have worked with undergraduate Patrick Harrington to develop a graphics package for the DTC 300/S Daisy-wheel terminal. Working with graduate student Robert Williams and NSF-URPP undergraduate Kalle Gehring (from Brown University) extensive graphics software for the S-100 systems have been produced. One program has been interfaced to Ken Hick's stopped-flow apparatus. Ken's student, Sharon Pittenger (also NSF-URPP, from EMU), is currently verifying the accuracy of the stopped-flow system and developing an advanced undergraduate experiment based on it. Working with undergraduates John Estell (University of Toledo), John Vidolich, and Brian Carter, I am currently producing instructional programs for the PETs and Apple, maintaining the department's extensive set of canned programs for the DEC-10, expanding the data-analysis capability of the stopped-flow system, and producing a chemical adventure game that teaches descriptive chemistry.

TASK FORCE ON COMPUTERS IN CHEMICAL EDUCATION (TFCCE)

The Task Force was established by the ACS Division of Chemical Education to promote and publicize the use of computers in chemical education. Regional and national workshops and programs are planned, organized, and facilitated by the Task Force. This Newsletter is published under their auspices. The present members of the Task Force, their educational affiliation, and areas of specialized interest are:

William Bajcz, Huron Valley Lakeland High School, Midland, MI 48640.

R. Daniel Bishop, School of Ozarks, Point Lookout, MO 65726.
CAI on microcomputers.

Gary L. Breneman, Eastern Washington University, Cheney, WA. 99004.
CAI on microcomputers.

William M. Butler, University of Michigan, Ann Arbor, MI 48109.
CAI on microcomputers.

James D. Carr, University of Nebraska, Lincoln, NE 68588.
On and off-line evaluation of kinetic data.

Paul A. Cauchon, Canterbury School, New Milford, CT 06776.
Teacher-training workshops, interactive exercises and simulations.

James Choate, West Springfield High School, West Springfield, MA 01089.

R.W. Collins, Eastern Michigan University, Ypsilanti, MI 48197.
Computer generated exams and problems.

George Culp, University of Texas, Austin, TX 78712.
Design and development of CBI.

Raymond E. Dessy, V.P.I. and State University, Blacksburg, VA 24060.
Microprocessors, interfacing, and laboratory applications.

Clare T. Furse, Mercer University, Macon, GA 31207.
Microprocessors, interfacing and laboratory applications.

John Gelder, Oklahoma State University, Stillwater, OK 74078.
Computer simulation and graphics.

George A. Gerhold, Western Washington University, Bellingham, WA 98225.
CAI, microcomputers and computer literacy.

Henry Griffin, University of Michigan, Ann Arbor, MI 48109
Microcomputers in undergraduate instruction (emphasis on simulation), process control.

William P. Halpern, University of West Florida, Pensacola, FL 32504
PASCAL, BASIC for microcomputers.

H. Fred Henneike, Georgia State University, Atlanta, GA 30303.
Microprocessor; interfacing and laboratory applications.

M. Lynn James, University of Northern Colorado, Greeley, CO 80631.
Computers in high school and general chemistry.

K. Jeffrey Johnson, University of Pittsburgh, Pittsburgh, PA 15261.
CAI, computer assisted test construction, computer managed instruction, simulation and data reduction.

Charles E. Klopfenstein, University of Oregon, Eugene, OR 97403.
Laboratory automation and graphics.

Alfred H. Lata, University of Kansas, Lawrence, KS 66045.
CAI.

Mark L. Lyndrup, Montclair State College, Upper Montclair, NJ 07043.
Microprocessors, interfacing and laboratory applications.

Daniel Macero, Syracuse University, Syracuse, NY 13210.
Microprocessors, interfacing and graphics.

John I. McLeod, Morris Brown College, Atlanta, GA 30314.
CAI for general chemistry.

John W. Moore, Eastern Michigan University, Ypsilanti, MI 48197.
CAI, graphics, simulation, S-100 hardware, UCSD Pascal, CP/M.

G. Scott Owen, Atlanta University, Atlanta, GA 30314.
Microprocessors, interfacing, graphics and simulation.

Gilbert Pollnow, Univesrity of Wisconsin-Oshkosh, Oshkosh, WI 54901.
Numerical methods, graphics, interfacing with Tektronix 4051 and DEC MINC-11.

Kenneth L. Ratzlaff, Northern Illinois University, DeKalb, IL 60115.
Interfacing.

Thomas H. Ridgway, University of Cincinnati, Cincinnati, OH 45221.
Microprocessors, interfacing and laboratory applications.

William W. Schweikert, Deerfield Academy, Deerfield, MA 01342.
DEC system management.

Oliver Seely, Jr., California State College - Dominguez Hills, Carson, CA 90747.
Computer assisted test construction.

Stanely G. Smith, University of Illinois, Urbana, IL 61801.
CAI with PLATO and microcomputers, and graphics.

Leonard Soltzberg, Simmons College, Boston, MA 02115.
Graphics.

Charles L. Wilkins, University of Nebraska-Lincoln, Lincoln, NE 68588.
Laboratory computers, pattern recognition, optimization methods, graph theory.

W.V. Willis, California State University, Fullerton, CA 92634.
Data reduction from experiments, programming for analytical chemistry, computer assisted test construction.

QUERIES AND WHO DONE IT?

Some members of the Task Force have suggested that sections of the Newsletter be used as a means of exchanging information between readers. The QUERIES section would be used as a place for reachers to ask for help with hardware or software problems. For example, John Moore has an old IMSAI 8080 processor board plus some peripherals and wants to know if it can be made to work without the IMSAI front panel. He would like a copy of any documentation which anyone has (he has none).

The WHO DONE IT? section would contain information on hardware and software which readers have developed or obtained commercially and they believe would be of general interest. For example, Al Lata reports that the 3-D Graphics System by Bill Budge easily creates three dimensional shapes and permits their manipulation. Al has created a tetrahedron and rotated it about all three axes. This software is available from Top of the Orchard Software and will run on the APPLE.

Kenneth L. Ratzlaff (Department of Chemistry, Northern Illinois University, DeKalb, IL 60115) has agreed to handle hardware for both sections of the Newsletter. Henry Griffin (Department of Chemistry, University of Michigan, Ann Arbor, MI 48109) will handle software. Material which is returned with the enclosed questionnaire will be forwarded to Ken or Henry. Alternatively, material can be sent directly to them.

Material for the WHO DONE IT? section should include your name, address, and phone number and a brief description of the software or hardware as well as the names of the computers with which it can conveniently be used. Where commercial software or hardware is identified, please give name and address of the supplier and the cost. For software indicate the programming language and the format in which it can be supplied (nine track tape, cassette, floppy disk, listing, etc.). Be sure to include any charges you wish to assess. In the event that possible suppliers of "free" software, schematics and instructions do not wish to bother, we will arrange for its distribution. A small distribution fee would be assessed to cover costs and help to subsidize this Newsletter.

In order to insure consideration for publication in a particular issue of the Newsletter, items should be sent a month and a half before the month of publication. Publication is slated for March, June, September, and December. Decisions on when and if items are published will depend on the number of items received and the judgment of the section editors (Ken Ratzlaff and Henry Griffin).

SOURCES OF C.A.I.

Any teacher interested in introducing computer assisted instruction as an aid to students can ignore what everyone else has done and develop each of the programs himself. However, this is a time consuming process. Estimates appear in the literature which indicate that it takes from 50 to 150 hours to write and perfect programs which students might use for an hour. Many of us who plan to introduce massive doses of C.A.I. into courses have preferred to determine what's available, obtain those programs which appear to be of interest and write additional programs which fill in the gaps.

Information on C.A.I. programs is available in practically every issue of the Journal of Chemical Education. A "Selected Bibliography of Computer Programs in Chemical Education" for the period 1967-79 which refers to programs cited in the Journal of Chemical Education was prepared by Warren T. Zemke and is available from CONDUIT for $2 (Box 388, Iowa City, IA 52244). More recent programs are identified in some of the articles in the Computer Series edited by John W. Moore (e.g. J. Chem. Educ., 58 46 (1981)). References to programs described in this and other journals can be found in Chemical Abstracts (generally in the subject index under computer applications or computer programs). However, not all programs are described in journals.

There are a number of bibliographies which can be of assistance in locating programs. One of the best of these is the "Index to Computer Based Learning", Anastasia C. Wang, Editor, Instructional Media Laboratory, University of Wisconsin-Milwaukee, P. O. Box 413, Milwaukee, WI 53201. The 1978 edition of this work contains 2997 citations to programs available in a variety of subject areas. There are 283 citations to programs in chemistry. Each citation refers to one or a number of programs and contains a detailed description in terms of twenty-four characteristics. All citations are indexed by subject matter, programming language, central processor, instructional strategies, source and category of computer activity (CAI, CMI, etc.). This reference work is available in microfiche or hard copy (three volumes).

Another less comprehensive bibliography which provides some additional references particularly to programs developed in England is entitled "Computers in Chemistry Teaching: A Bibliography and Index of CAL Packages" by N.J. Rushby, London University (England), Imperial College Computer Centre, July, 1979. This bibliography of 33 pages is available on microfiche from ERIC Document Reproduction Service as ED 176-806. (ERIC microfiche documents are available in many libraries.)

Some of these programs are available at little or no cost from individuals who have written or gathered programs. One of the best organized efforts of this kind for those who use BASIC is that by the Center for Information Processing, California State University-Fresno, Fresno, CA 93740 (Dr. Jack A. Chambers, Director). They publish "The ABCs of CAI". (The fifth edition is due to appear in April.) This publication may be obtained by writing Dr. Chambers. In addition to considerable general information on CAI sites, references and organizations, there is a detailed description of over 100 programs which are available and can be obtained by using a form contained in the book. These programs are in a variety of subject areas. There were about twenty-three chemistry programs in the fourth edition. All programs are written in BASIC PLUS and run on a DEC PDP 11/45.

K. Jeffrey Johnson (Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260) has developed a large number of computer programs for use in instruction. These include

(1) 55 CAI tutorial-drill lessons written in the CATALYST/PIL authoring language (and not readily transferable unless you are able to run CATALYST/PIL, a language developed at Pittsburgh).

(2) A Computer Assisted Test Construction System (CATC) consisting of 450 FORTRAN subroutines covering 29 topics normally covered in general chemistry courses. A sampling of these questions can be found in a book (K.J. Johnson and L.M. Epstein, "General Chemistry Examination Questions", Fourth Edition, Burgess, Minneapolis, 1979).

(3) 25 FORTRAN function evaluation, simulation and data reduction programs. Some of these are cited in the book, K.J. Johnson, "Numerical Methods in Chemistry", M. Dekker, New York 11980. All these programs run on a DEC 1099 (two PDP 10's in a dual processor configuration).

Jeff will provide any of this material for a $25 tape-handling fee.

At Clarkson we have about 112 BASIC CAI drill and practice programs which are used by students taking general chemistry. Twenty-six of these programs were obtained from Richard T. O'Neill (Xavier University, Cincinnati, OH 45207) and were developed with support from N.S.F. and the Exxon Foundation (obtained by Harold Weinstock, Department of Physics, Illinois Institute of Technology). The programs are intended for use as part of 22 learning modules covering topics in general chemistry. There are student manuals and teacher's guides which are part of the modules. These guides and manuals can be purchased from Professor Weinstock. Also, many are recently available on microfiche from ERIC Document Reproduction Service (ED 182-119 to 182-130). These programs have been described by Cynthia K. Jameson (J. Chem. Educ., 54, 238 (1977)).

Fifty-four programs were obtained from Donald O. Peterson (Gallaudet College, Washington, D.C.). Twenty programs were purchased from Programs For Learning (see below). Five were written at Clarkson and the remainder were obtained from various other sources. All programs are in VS BASIC and run on an IBM 4341. Approximately 88 programs may be obtained in "standard" tape format (9 track, 1600 bpi, EBCDIC or ASCII, no label, each block contains 10 logical records of 80 characters (card image) with single tape marks after each program and double tape marks at the end of the tape). The tape will contain a catalog, describing each of the free and purchased programs (purchased programs are not supplied). A tape containing these programs may be obtained for a $30 tape-handling fee (if interested write Donald Rosenthal, Department of Chemistry, Clarkson College, Potsdam, NY 13676).

The National Resource for Computation in Chemistry (Lawrence Berkeley Laboratory, Bldg. 50D, University of California, Berkeley, CA 94720) has issued a software catalog (Vol. 1, February 1980, LBL-10811), which lists mostly FORTRAN programs and subroutines with applications in graphics, chemical kinetics, macromolecular science, numerical methods, physical organic chemistry, quantum chemistry, statistical mechanics, crystallography and various software tools. Most of these programs were written with research applications in mind, but many are of potential value in advanced courses. These programs were written to run on a CDC 7600, but will run on other large computers. Most of these programs are available at no charge. Those interested should contact the Program Librarian at the above address.

There are a number of other sources from which programs can be purchased:

(1) Dr. Daniel Bishop, Custom Comp., P. O. Box 125, Branson, MO 65616. CAI general chemistry software for TRS-80 and APPLE.

(2) Dr. William M. Butler, Chemistry Room 1094, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109. Programs are available for PET, APPLE II, and TRS-80 Level II at $40 for each cassette containing four programs. Two cassettes presently available.

(3) Paul A. Cauchon, Programs for Learning, Inc., P. O. Box 954, New Milford, CT 06776. Over 50 chemistry programs are available in packages of 9 to 12 programs for $100 per package. BASIC programs can be supplied which will load and run on a variety of micro, mini, and macrocomputers. Also available is the text "Chemistry with a Computer" which contains 176 pages and 28 program listings.

(4) Dr. George Gerhold, MICROPI, 2445 Nugent Lummi Island, WA 98262. Common PILOT CAI authoring language is available in assembler at $275 for CP/M, North Star DOS or TERAK, $295 for HELIOS II, $195 for TRS-80, or $475 in PASCAL source code. A variety of courseware is available written in COMMON PILOT.

(5) Dr. Oliver Seely, Jr., Department of Chemistry, California State University - Dominguez Hills, Carson, CA 90747, indicates the SOCRATES package which provides test generation, item bank editing and building, scoring and item statistics is available to institutions using a CDC Cyber 170 (NOS operating system) by contacting the California State University-Dominguez Hills Foundation at the above address.

(6) CONDUIT (P. O. Box 388, Iowa City, IA 52244) distributes programs in ANSI FORTRAN and various levels of BASIC. Microcomputer versions of certain packages are available for the PET, APPLE, and TRS-80. Programs are available in chemistry and a variety of other disciplines. Prices vary from about $30 to $85 per package.

(7) Minnesota Educational Computing Consortium, 2520 Broadway Drive, Lauderdale, MN 55113 (612-376-1118). Several hundred instructional programs most of which are written in BASIC for the CDC Cyber 73 or ROM Applesoft for the APPLE II microcomputer. Programs are mostly applicable to primary and secondary education. A version of the PILOT CAI authoring language is available. The cost is about $15 per program, or $100 for the complete library of CDC Library programs. Diskettes for the APPLE II are $30.

(8) The Quantum Chemistry Program Exchange (Department of Chemistry, Room 204, Indiana University, Bloomington, IN 47405) has collected a number of computational programs primarily written in FORTRAN for research using large computers. Some of these programs can be useful in advanced chemistry courses.

Programs which will load and run on your computer without requiring any translation have much to recommend them. I have spent considerable time translating programs from one version of BASIC to another. Other C.A.I. users have translated programs from one programming language to another, so they could conveniently be run on their systems. It would be useful to develop "free" large libraries of programs available on different micro, mini, and macrocomputers which would be available at a nominal tape or diskette handling charge ($10 to $50). For example, if you were interested in running the 88 programs we are using at Clarkson on a micro, mini, or macrocomputer which does not run VS BASIC, you would have to translate these to another version of BASIC. If another user wanted to do the very same thing on a computer like yours, he could undertake the same translation process. However, it would make much more sense for him to obtain the programs from you so that they would load and run. If a sufficient number of users of different computers and different language were willing to make their "free" libraries available, this would greatly facilitate program transfer. This Newsletter could assist in this process by publicizing software availability. Those having significant amounts of software who are willing to make it available to others should indicate this on the questionnaire.

Software QUERIES

The March issue of the Newsletter contains a summary, "Sources of C.A.I.", of programs available for chemistry at various levels. Such programs are a useful start toward building an effective CAI component in undergraduate courses, but a little reflection will show that if existing programs were sufficient, CAI would be rather static and uninteresting. In fact, the continuing development of programs (software) is the underwater portion of the iceberg which supports the visible, spectacular advances in "hardware".

Some current developments in hardware were reviewed in the RESEARCH NEWS section of the 1 May 1981 issue of SCIENCE. The article emphasizes the jump in computational power which can be expected for 32-bit microprocessors, but the brief comments on software costs are very significant. The programs needed in 1975 to make an 8-bit processor function in a piece of equipment might have cost $20,000 to develop. The comparable cost for a 16-bit application in 1980 was about $450,000. Another decade jump in costs can be expected for the 32-bit devices unless some measures are taken to simplify program development. We invite readers to use this section to address the broader software problems and not limit their communications to questions of the "short answer" type.

Perhaps the most important of the general problems we must address is the transportability of programs. This theme underlines some of this month's queries and will be discussed in a systematic manner after we have gathered some descriptive information on the matter.

SQ1 (June 1981)

Burroughs B6000/7000

-Source of BCPL or Algol 68 compiler for Burroughs advanced systems

-Burroughs users who would like to exchange information and software useful in chemical computing.

K.W. LOACH (Chemistry and Computer Science Dept., SUNY College, Plattsburgh, NY 12901)

SQ2 (June 1981)

(NOS or RSTS/E operating system)

-Program for computerized class gradebook in BASIC, COBOL, FORTRAN, PASCAL or C Languages.

W.V. WILLIS (Chemistry Dept., California State Univ., Fullerton, CA 92634)

SQ3 (June 1981)

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-Tutorials on interpretation and presentation of scientific data for beginning students in physical science at the college level.

W.V. WILLIS (see SQ2)

SQ4 (June 1981)

**

-Any CAI package dealing with environmental pollution.

W.V. WILLIS (see SQ2)

Send queries and responses to Henry C. Griffith, Department of Chemistry, University of Michigan, Ann Arbor MI 48109, (313) 764-1438. You may wish to respond directly to those submitting queries, but please send copies of responses to me for possible inclusion in future issues of the Newsletter. Include your telephone number as well as your mailing address.

Hardware QUERIES

All hardware queries should be directed to Dr. Kenneth L. Ratzlaff (Director, Instrumentation Design Laboratory, Malott Hall, Kansas University, Lawrence, KS 66045). Dr. Ratzlaff will answer some of the queries himself and refer others to readers of the Newsletter. The success of this section of the Newsletter will depend upon obtaining Queries and Answers from the readers. If you disagree with an answer which is given, send Dr. Ratzlaff your reasons and these will be published.

HQ1 (June 81)

A. Barry Cox (Department of Chemistry, Jacksonville State University, Jacksonville, AL 36265) writes that his department is just beginning to use microcomputers and he has some experience with the 6800 CPU. His goal is to develop a course in computer interfacing at the bus level and he asks for suggestions about what type of hardware to use.

A HQ1 (June 81) by Ken Ratzlaff

This query addresses the problem of upward compatability of microprocessor tools. Having learned about using microprocessors at the bus level with a Motorola 6800 CPU, it would be convenient to stick with it for higher-level applications.

Professor Cox correctly points out that few, if any, chemists use the 6800. The reason is only secondarily related to the inherent capabilities of the 6800. Rather, it results from the fact that only two lines of microprocessors have survived in microcomputers suitable for chemistry applications: the 6502 (in the APPLE and PET) and the 8080/Z80 line (TRS-80, Altos, S-100). Chemistry applications need development software and that software has reached the highest level for the Z80, followed closely by that made available for the Apple and its 6502.

What does one then do with his experience with the 6800? There are three possibilities:

a) Recognize that the basic concepts are common to all and choose a new machine on its own merits. (For a lab/teaching computer which should be bus-oriented, an Apple or S-100 machine would be good).

b) Choose a microprocessor as closely related to the 6800 as possible but which still has good software support; the 6502 (in an Apple) would be that choice.

c). Sacrifice a bit in the diversity of hardware and software options available for Apple, S-100, and LSI-11 computers, and pursue the use of 6800-based microcomputers. Two vendors that specialize in this area are TSC, Box 2570, West Lafayette, Indiana 47906, and SWTPC, 219 W. Rhapsody, San Antonio, Texas 78216.

WHO DONE IT?

This section of the Newsletter contains information on useful hardware and software which readers have developed or obtained commercially. Information on software should be sent to Dr. Henry Griffin, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109. Information on hardware should be sent to Dr. Kenneth Ratzlaff, Director, Instrumentation Design Laboratory, Malott Hall, Kansas University, Lawrence, KS 66045. If in doubt, send a copy of your letter to both Henry and Ken.

Be sure to include your name, address and phone number, a brief description of the software or hardware, and the computer used. Where commercial software or hardware is identified, please give the name and address of the supplier and the cost. For software indicate the programming language and the format in which it can be supplied (nine track tape, cassette, floppy disk, listing, etc.). Be sure to include any charges you wish to assess.

WHO-1 (June 81) Professor Frank A. Settle, Jr. (Department of Chemistry, VMI, Lexington, VA 24450) has sent information on Project SIINC (Scientific Instrumentation Information Network and Curricula) an NSF funded project which provides computer-based dissemination of education materials for users of chemical instrumentation. A module on gas-liquid chromatography has been prepared (Task Force Director, Professor Harold McNair, VPI & SU, Blacksburg, VA). Modules on gas chromatography/mass spectrometry (Director, Professor Frank Karasek, Waterloo University, Waterloo, Ontario, CANADA); and atomic absorption (Director, Theodore Rains, Analytical Chemistry Division, National Bureau of Standards, Washington, D.C.) are in preparation. Additional modules on high performance liquid chromatography, inductively coupled plasma emission spectroscopy and priority pollutants are being planned. Persons wishing to access the modules from their own terminals and who are willing to evaluate the modules may become project associates. The only expense to the user is the telephone charges. Project associates will be sent a copy of the users guide. If you would like more information, write Professor Settle who is Project Director.

WHO-2 (June 81) Richard Wilhelmy (Department of Chemistry, Clarkson College of Technology, Potsdam, NY 13676) has found the ST-80D program (Lance Micklus, Inc., 6 South St., Milford, NH 03055—cost $80 and available through many hobby computer outlets, e.g. Hobbyworld Electronics, Inc., phone: 800-423-5387) works very well in converting a disk drive TRS-80 Level II with at least 16K of memory into a smart terminal. The program permits the terminal to talk to a timesharing computer (in this instance an IBM 4341) and can be used for transferring files to or from the other computer. The software can be used to transfer data from one TRS-80 to another. The software has reprogrammed some keys to perform different functions. The user can create translation tables from the keyboard to convert data from one system to another when some incompatibilities exist (32K of memory is required). The baud rate can be simply changed. The software has several other features which may be useful. To run the program a modem, at least one disk drive and a Radio Shack RS-232-C board in the expansion interface is required. According to the instructions supplied the software has been successfully used in communicating with a SIGMA/6, DECSYSTEM 20, HP2000 and a CDC system. A related program ST80UC can be used with the TRS-80 Level II 4K casette system (cost $25).

Scott Owen mentioned in the March Newsletter that DATACAPTURE 4.0 by Southeastern Software does similar things for the APPLE. Anyone who has identified similar software for other microcomputers, please drop a note to Henry Griffin.

C.A.I. Program Distribution Centers

In the last issue of the Newsletter I mentioned the desirability of establishing C.A.I. Program Distribution centers which would maintain and distribute libraries of "free" C.A.I. programs, and a catalog of such programs. Those wishing to obtain programs could write to the center and obtain the entire library for a modest fee. This fee being intended to defer some of the costs involved in maintaining and distributing the programs and catalog. The success of this venture depends upon those having "free" programs being willing to donate these to the distribution center. The name and author of the program would be identified in the source listing and the catalog.

Professor Patricia C. Flath, Paul Smith's College, P.O. Box 45, Paul Smiths, NY 12970 has offered to maintain a repository of programs written for the TRS-80 Model I in Level II BASIC. She presently has twenty to thirty programs. We would hope this number would grow through contributions. The library can be provided either on floppy disk ($30), cassette ($10 per cassette) or selected listings ($1 per listing). Those submitting programs will receive appropriate discounts. Please send your programs as soon as possible. Write directly to Dr. Flath if you desire additional information about the TRS-80 programs.

It would be desirable to establish similar distribution centers for the APPLE, PET, and other other micro, mini, and macrocomputers. Please write me at Clarkson, if you are willing to establish a distribution center along lines like those described above. Indicate what computer and other facilities you would have available.

More About Sources of CAI

In the last issue of the Newsletter information was provided about various sources of CAI. In this issue I would like to update some of the information provided and indicate additional sources of C.A.I. as revealed in the questionnaires which were returned.

Anastasia C. Wang has notified me that the 1981 edition of the "Index to Computer Based Learning" has been published and is available on a set of eight microfische cards (at $15 per set) or four paperbound volumes (at $48 per set). The new edition contains 1450 pages and information about 4868 computer based learning programs from 418 different sources. Write Education Communications Division, University of Wisconsin-Milwaukee, P. O. Box 413, Milwaukee, WI 53201 for more information.

NRCC (National Resource for Computation in Chemistry), which will be disbanded by the end of September, is no longer distributing software. Some of their programs have been released to the Quantum Chemistry Program Exchange (Department of Chemistry, Room 204, Indiana University, Bloomington, IN 47405) and the National Energy Software Center (Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439). This latter center has a catalog of over 780 programs in a variety of subject areas. Some of these programs might be of value in advanced courses.

Carolyn A. Werman (Department of Chemistry, Merrimack College, North Andover, MA 01845) has eight programs on concentration and will furnish free BASIC (PDP11) listings.

Paul Edwards (Chemistry Department, Mercyhurst College, Erie, PA 16546) has collected a number of programs for the Apple II Plus which are available on DOS 3.3-16 sector diskettes. Programs are available free except for the cost of the diskette.

William L. Switzer (Department of Chemistry, North Carolina State University, Raleigh, NC 27650) has a number of titration curve programs written in BASIC which run on the Apple II Plus. He is willing to make these available to others.

Lyle D. Wescott (Department of Chemistry, Christian Brothers College, Memphis, TN 38104) has developed programs entitled Nomenclature-alkanes, conformations-cyclohexane, organic qual and Lowry/Bronsted. All programs are available on cassette for the PET 3.0 ROM, 16K. ($10 per program, $30 for all four.) The last two programs are available on diskette for the Apple II (48k, $10 per program, $15 for both programs).

Ray L. Johnson (Hillsdale College, Hillsdale, MI 49242) has a number of programs for PET with MTUK visible memory system. Programs are in analytical chemistry-data acquisition and simulations. Listings are free if you send a stamped self-addressed envelope.

Richard W. Ramette (Carleton College, Northfield, MN 55057) has a number of BASIC programs on equilibrium and analysis written for the VAX 11/780.

Gerritt P. Bean (Department of Chemistry, Western Illinois University, Macomb, IL 61455) has programs which simulate NMR spectra (up to 6 spins), perform Huckel MO calculations, and simulate consecutive or competitive reactions available on TRS-80 floppy disk and compiled in FORTRAN.

James P. Birk (Department of Chemistry, Arizona State University, Tempe, AZ 85281) has twenty programs written for the TRS-80, Model I in Level II BASIC. These programs are suitable for use in any first year chemistry course. Available on cassette at a cost of $5 plus $1 per program.

G.L. Breneman (Department of Chemistry, Eastern Washington University, Cheney, WA 99004) has over 34 BASIC programs available for use in General Chemistry, Quantitative Analysis and Organic Chemistry. Some of these have been described in print (J. Chem. Educ., 52, 295 (1975); 55, 224 (1978); 56, 776, 783 (1979)). Listings are available from a Univac 90/80-02 ($5 for each program listing). Three acid-base simulations are available on a TRS-80 cassette ($10 per program). Floppy disk source programs are available for Apple II ($15 for the first program, $10 each additional program).

Richard T. O'Neill has 65 programs written in PDP 11/45 BASIC PLUS. Many of these are suitable for use in general chemistry, organic chemistry and other courses. Included are most of the programs described by Cynthia K. Jameson (J. Chem. Educ., 54, 238 (1977)) and additional programs written by Dr. O'Neill or obtained from other sources. The programs can be obtained for $30 on 600 foot 9-track ASCII tape by writing Rev. Ronald J. Fergusen, S.J., Director of Academic Computing, Xavier University, Cincinnati, OH 45207. The charge covers the cost of the tape, mailing and processing.

Any readers having programs which they are willing to make available to others should send the following information to me: type and number of programs, courses in which they could be used, programming language, system on which they currently run, form in which they are available (9 track tape, cassette, floppy disk, etc.) and cost, if any. Some information provided in the questionnaires was too scanty to warrant presenting. Some of the information provided above is not sufficiently informative, because insufficient information was provided to the editor. Any future announcements must be more detailed.

Teaching Instrumental Analysis with the Aid of the "MINC" Computer

by Dr. W. V. Willis*

The instrumental analysis course at C.S.U.F. is a modular course designed for chemistry majors in their senior year, graduate students, and practicing industrial chemists. Four one unit modules are offered in the spring semester each year and one or two in the fall, depending on demand. Students may take from one to four units per semester. Enrollees have completed general chemistry, organic chemistry, quantitative chemistry lecture, and one semester of physical chemistry as prerequisites.

Significant improvements result from this approach. Different faculty with particular specializations can become more involved since individual responsibility is typically one or two modules. New topics can be introduced as needed. The Computers and Interfacing module grew out of the recognition of the importance of including this topic in the chemistry curricula as well as particular faculty interest and minicomputer availability. A separate module on electronics and instrument design is being considered.

The modules currently offered are shown in Table I. The course does not attempt to integrate all of these methods, except to the extent to which trace analysis is emphasized with pre-designed experiments. Students are encouraged to define their own projects which might relate to a research problem or an on-the-job analytical problem. For example, student projects in polymer characterization have helped broaden the scope of the laboratory and increased awareness of the faculty to this important area.

The Computers and Interfacing module is offered as the first module. Students learn how to acquire and process signals. This includes carrying out simple signal processing procedures and data file manipulation. This allows them to carry out more sophisticated experiments later on.

The MINC Computer is a DEC PDP-11 lab-oriented dual floppy disk system currently configured with a signal preamplifier and A/D converter. Output is via a CRT, Model 43 teletype, or high resolution graphics plotter. The programming language is BASIC PLUS, with some added specialized commands for simplified data acquisition and display. Interfacing is quickly and conveniently done by using the recorder output of a spectrophotometer, for example, or the plotter output of a gamma ray spectrophotometer. (More sophisticated interfacing with computer controlled variation in experimental parameters is planned for an advanced module.) Students typically write software for real time proces--ing and CRT display of data from chromatographic, UV/VIS spectrophotometric, and potentiometric experiments, whereas virtual data files are used to store data from infrared, mass spectrometric, and activation analysis experiments. Algorithms for peak location and integration, spectral smoothing, and evaluation of statistics are frequently employed. A program library is maintained for demonstration and instruction, and as a resource for other students. We have found this format to be particularly useful in our department, and well received by our students and participating industrial chemists.

TABLE I

Description of the Modules

A	Computers and Interfacing - (DEC PDP-11 MINC system) BASIC language (introductory computer science programming course recommended prerequisite) analog/digital interfacing (UV/visible, IR, GC, MS, electrochemistry and radiochemistry applications).
B	Optical Spectroscopy - Ultraviolet/visible, infrared, atomic absorption, flame emission, fluorescence.
C	Nuclear magnetic resonance and electron spin resonance.
D	Separations - High performance liquid chromatography, gas chromatography, mass spectroscopy, GC/MS.
E	Electrochemistry - Potentiometry, polarography (dc, pulse, differential pulse, ac), chronopotentiometry, chronoamperometry, coulometry, cyclic voltammetry.
F	Radiochemistry - Synthesis of labeled compounds, isotope dilution techniques, radiotracer methods.

*Chemistry Department, California State University, Fullerton, CA 92634

Computers at Canterbury—A Case Study

by Paul Cauchon*

Canterbury School is a small independent college preparatory school located in rural Connecticut, with 300 students, 200 of whom are boarding, and a faculty of 32. Classes are small, averaging 12 to 16 students. The curriculum emphasizes English, mathematics, modern language, science and history, and the athletic program is typical of this type of school with all students involved in some sport each season. What is not so typical about Canterbury is the role of the computer in this traditional prep school atmosphere.

Computers first appeared in the curriculum in 1963 as a six week module in a physical science course. Students were introduced to various levels of languages, culminating with FORTRAN, using blackboard simulations and Yale's IBM 7090/7094 system. A time-sharing terminal was installed as soon as such a service became available (1965), but by 1972 prices on mini's had dropped to where ownership became economically preferable. It was at this point that the role of the computer radically changed. Until 1972 the computer terminal served only a fraction of the students through a one-semester course in programming. With the arrival of the PDP8 on campus, time constraints were lifted which resulted in both recreational computing and CAI becoming a reality. Micro's began to appear on campus in 1978 and at the moment hardware consists of the original PDP8 with a single teletype and magnetic tape, 2 PET's, a TRS80, and 2 Apple's, all with cassette and dual floppy disk drive.

To ensure maximum student usage of the facilities, the computer room is located in the heart of the academic center and operated on a completely open-door basis. All systems are available on a walk-in schedule from 7:30 a.m. to late each evening, seven days a week. Self-teaching guides to all machines are freely available to encourage hands-on experimentation.

Although the computers are maintained primarily for instructional purposes, games play a significant role in orienting students to the machines, and help them combat "terminal terror". Game tapes and disks are available afternoons and on weekends, frequently attracting a sizeable crowd of novices who have never touched a terminal before. It is an easy step from using games to running a CAI program.

Students are more formally involved with the machines in the two computer courses which are taken by about 25% of the population. One is a fairly rigorous introduction to problem solving and the other is simply labeled "Computer Literacy". Both stress hands-on contact.

Heaviest use of the terminals comes through the science department, chemistry in particular, where drill and practice exercises plus simulations supplement or replace a sizeable portion of conventional textbook assignments. On the average, at least one drill and practice program per week is assigned to chemistry classes, starting with metric units and chemical symbols in September through organic nomenclature and solubility product problems in May. Simulations include a titration, qualitative analysis and an ammonia synthesis. Such assignments are always made a week or so in advance to provide ample opportunity for students to run the programs as many times as needed to master the skill or explore the experiment. Most programs can be run on all of the machines, since they are all in BASIC and many students have developed a proficiency in moving software from one machine to another - a skill acquired by copying games out of books and magazines.

Student reaction to computer-based assignments has been overwhelmingly positive; they run the drill and practice programs at least three times, on the average, i.e. until they get a good score and feel confident about the material. Thus, they do at least three times as many problems as they would with the conventional textbook assignment. Competition to see who can get the most correct in succession springs up with the open-ended drills such as with chemical formulas or electron configurations Learning goes on in a dynamic, non-threatening environment. What more could one ask for?

It is a rare student who passes through Canterbury without encountering a computer in some useful context. Computers at this school are clearly recognized as important and effective tools for accomplishing the business at hand, which is learning, and this is how it should be.

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SEPTEMBER NEWSLETTER

I expect to distribute the September Newsletter so that it will reach you before the ACS meeting in New York on August 23rd. Any items to be included in the Newsletter should be received by July 16. QUERIES and WHO DONE IT? items should be sent directly to Henry Griffin or Ken Ratzlaff. Information on Workshops, Meetings, Conferences, and Courses as well as sources of C.A.I. should be sent to me.

I would appreciate receiving suggestions regarding the Newsletter. If you wish to remain or be placed on the mailing list and you have not already returned the renewal questionnaire, please return the appended pink questionnaire by July 16th.

Donald Rosenthal, Editor

Volume IV Number 3/September 1981

Letter from the Editor

In the last several issues of the Newsletter considerable emphasis has been placed on computer assisted instruction, graphics, hardware, interfacing and laboratory automation. These are areas of considerable faculty interest. If students are exposed to the results of such endeavors in the classroom, laboratory and terminal room, the student obtains appreciation of the many uses of computers. However, I believe one of the most useful things which students can learn about computers is how to program them. Not very much has been said about this in previous issues of the Newsletter. I intend to devote this column to this topic by describing my own experience and some of the problems and decisions which need to be made regarding the use of the computer and computer programs by students.

"Computer Programming for Chemists" was introduced as a required course for all freshman chemistry majors about ten years ago at Clarkson. By introducing programming in the very first semester, students could use their programming abilities in other courses, and by the time they are seniors they can develop considerable programming ability. Many students do become very proficient programmers. Many other students seem to have lost most of the proficiency they had by the time they are seniors. This latter result is not unexpected for the small number of students who simply develop a dislike for computers and computing, and avoid both like the plague. However, the faculty must share some of the responsibility for the lack of development of computing proficiency. The computer makes it possible to easily perform calculations which would otherwise be prohibitively time consuming. This is one reason the computer is such a valuable tool to a practicing chemist. In the classroom and the laboratory students should be able to easily perform calculations which would not be feasible without the computer. We expected that instructors would make use of this new capability. Mostly, they did not. Most chemistry textbooks do not require or even recommend the use of the computer. It is almost as if the computer did not exist.

It can be argued that such problems could not be worked by many students, since they do not have ready access to a computer. At Clarkson, and I suspect at many other schools, student access to computing facilities is not a problem. It may also be argued that in most courses students have enough to do without becoming bogged down in writing long, time-consuming programs. This is a valid argument. However, I am not advocating assigning complicated programs. The programs could be quite simple and for a reasonably proficient programmer might take less time than what is presently required to solve comparable problems.

One of my former colleagues taught a laboratory course for which he had developed computer programs for almost every experiment. Students were expected to use each program and to turn in the listing and output with each final report. I believe that in many instances students were using the computer without really understanding what they were doing. In my opinion, it is worthwhile and desirable to use certain canned programs, particularly those involving certain numerical and statistical methods. I believe that every chemistry department should make such programs available to their students. The programs I believe should be available are:

(1) A program which calculates the average, standard deviation, random error (using the t-test) and is capable of rejecting an outlier.
(2) A program which performs linear least squares calculations and calculates the slope and intercept (where $y = mx + b$) and the standard deviation of these parameters as well as the standard deviation from regression.
(3) A similar program to (2) for polynomial regression.
(4) A program which can find the desired root(s) of any equation ($f(x) = 0$).
(5) A program which will solve simultaneous equations.
(6) A program which can perform numerical integration.
(7) A program which can perform numerical differentiation.

Microcomputers can easily be programmed to provide each of these programs. Most large computers have programs like these in their scientific subroutine packages. Listings of such programs are available in many standard reference works, and from many program libraries.

While I have written with particular reference to Clarkson undergraduates, I know that similar conclusions are valid for students from many other colleges and universities.

Those of you who teach required junior or senior level courses should ask your students to write a relatively simply program. Try and ascertain how much difficulty the students had in performing this task. The results may be surprising.

At Clarkson we are addressing this problem by requiring the students to write programs in sophomore, junior and some elective chemistry courses.

If you disagree or agree with what I've written and have something to add, please write. I would be pleased to publish your comments on this or any other matter.

Elements of Good CAI

by Dan Bishop*

At a recent workshop, I had the opportunity to present a list of suggested guidelines to be used in evaluating educational software. Most of the participants at the workshop were interested in purchasing hardware and software to be used in the elementary school classroom. It occurred to me that the same set of criteria which I proposed to them would be applicable to educational software at any level. Furthermore, the list can also serve as a useful set of rules for the instructor who is actually writing programs for classroom use. To be sure, it is a rare program which exhibits all of the qualities set forth here. But by using specific critiera to judge or compare programs, authors and users alike should be able to raise the quality of the software available to the educator. It is with that goal in mind that I share the following with you.

1. The computer itself should be "invisible" to the student. Unless we are actually teaching computer science, the logistics of setting up and using the computer should be of little concern to the student. Certain basic instructions are inevitable, but the computer system should be set up and the programs written in such a way that the student can operate the program with very little knowledge of the computer itself.

2. The program should make ample use of prompts so that the student always knows what action is expected of him. A common prompt such as "PRESS RETURN TO CONTINUE" should be used with abandom. A "menu" displaying the options available to the student at specific points in the program is very important. A sample menu which I have found to be generally very useful follows:

```
PRESS THE KEY CORRESPONDING TO YOUR CHOICE:
      (0) End the Program
      (1) View a Worked Example
      (2) Work a New Problem
      (3) See the Solution to the Last Problem
```

3. The program should make ample use of the RANDOM function to provide variety in BOTH the problems presented AND in the responses given following the student's answer. A program that always responds with "THAT IS CORRECT" or with "THAT IS WRONG" becomes dull more quickly than one in which a dozen responses appear for each case. Furthermore, the responses can be quite varied and humorous. Students seem to be willing to take more guff from the computer than most of us as instructors would dare to give out!

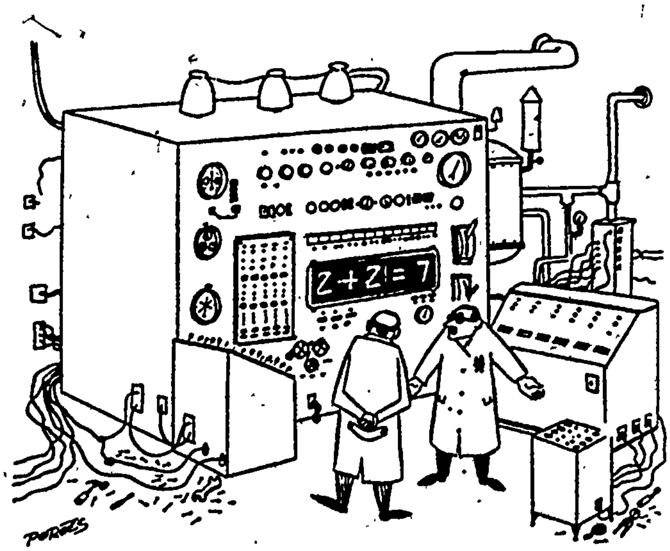
4. As indicated by the menu above, all tutorial programs should include a subroutine that shows exactly HOW the particular problem presented should have been worked. The actual numbers used in that problem should be used in the solution subroutine. Furthermore, the same subroutine can then be used with the "worked example" option.

5. The program should be written to take advantage of the full capabilities of the specific computer on which the program is being run. Since each microcomputer on the market today uses totally unique approaches to graphics, this means that the better programs are those that are written to be run on a specific microcomputer. Programs that are written in such general terms that they are easily translated for use on many different computers tend to lose much of the excitement and interest which are generated with appropriate use of graphics. It has been my observation that some of the major software suppliers have overlooked this important point.

6. Most important of all, the program should have a clearly defined educational objective, and that objective should be clearly met by the material presented in the program. The use of the computer should neither obscure nor distract from the attainment of these objectives.

The microcomputer is, after all, merely a modern tool to help us achive our goal of facilitating the learning process for our students. If it can provide the variety necessary to increase our students' attention to the subject material, and perhaps provide some entertainment along the way so that they will become less easily distracted from their studies, then we will have made a wise choice in our software.

*Custom Comp
Microcomputer Systems/Software Service
P. O. Box 429
Buena Vista, CO 81211



Porges American Legion

"Well . . . back to the old drawing board!"

The Use of Computers by Chemistry Students at the University of Texas at Austin

by George H. Culp*

The use of computers in instruction at the University of Texas at Austin was pioneered in the late sixties by Dr. J.J. Lagowski, Department of Chemistry. Since that time general instructional computing use has grown to encompass the majority of all academic departments and involves more than 30,000 student accounts campus-wide.

Within the Chemistry Department instructional computing use continued in much the same philosophical vein as when we started some 15 years ago: as a supplement or adjunct to traiditional methods of teaching. Computers (including dual Cyber 170/750's, a DEC-20, a NOVA 4 and 32 TRS-80 microcomputers) are used primarily for problem solving, drill and simulation. Tutorial dialog and testing applications are in use to a lesser degree.

One of the primary uses of instructional computing within the department is associated with the introductory laboratory course. The enrollment in this course varies between 900 and 1200 students each semester. The course is typical of introductory laboratory courses, consisting of about 15 experiments performed in weekly 4-hour laboratory sessions. However, before interacting in the real laboratory environment, students are required to use a PRELAB program for each experiment. These programs, written in BASIC and available on both the NOVA and TRS-80 computers, examine the students' ability on the experimental background, concepts, strategy, calculations, etc. for the week's assignment. When completed successfully, students are permitted to enter the laboratory to perform the experiment. After completion, students return to the computer terminals to interact with REPORT programs which analyze the results of their data collection and score their performance accordingly. Instructors have on-line access to student records associated with both PRELAB and REPORT use.

Additional use on the Cyber and the DEC systems occurs regularly each academic year. In the period September 1, 1979 to August 31, 1980, fourteen classes involving more than 2300 student accounts ran over 8000 jobs on these systems. For the most part, these jobs were problem-solving or data analysis applications using Fortran programs written by the students. The average cost per terminal-connect hour was \$2.25. To date departmental use this year has shown an increase of approximately 10% in student accounts and jobs.

Readers may contact either Dr. J.J. Lagowski, at the Department of Chemistry or Dr. George H. Culp, for further information.

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Austin, TX 78712

AUGUST 23-28: ACS National Meeting, New York, NY.
The symposium on "Interpreting Complex Chemical Data: Teaching Chemometrics" (Monday morning and afternoon) some of the other symposia sponsored by the Division of Computers in Chemistry and the breakthrough lecture "Chemistry and the Microcomputer Revolution" by Raymond Dessy (Monday afternoon) may be of special interest. An informal TFCCE gathering will be held at the CHED Hospitality Center located in the Sheraton City Squire Hotel (on 7th Avenue between 51st and 52nd Streets) on Tuesday or Wednesday afternoon. Check for exact date and time at the CHED Hospitality Center or outside the Sheraton Centre, Royal Ballroom A on Monday. Anyone may drop by to discuss the work of the Task Force on Computers in Chemical Education, the Newsletter or anything else.

MARCH 28-APRIL 2, 1982: ACS National Meeting, Las Vegas, NV.
The symposium on "Teaching Chemistry with Simulations and Games" welcomes contributions from anyone who uses such techniques and has found them to be effective. Demonstrations are encouraged. If you are interested in participating, contact Dr. John W. Moore, Department of Chemistry, University of Wisconsin, Madison, WI 53706 (608-263-2424). Deadline for receipt of abstracts is November 1, 1981.

JULY 11-16, 1982: 6th International Conference in Chemical Research and Education, Washington, DC area. Topics to be included are chemical synthesis, structure elucidation, structure/activity relationships, theoretical chemistry, chemical graph representations, pattern recognition, factor/cluster analysis, computers in the labs, computers in the classroom, chemical graph searching, and U.S. Government activities in the field of computers in chemistry. Attendance will be restricted to 150 participants. For further details contact Dr. Stephen R. Heller, Chairman, 6th ICCCRE; EPA,MIDSD,PM-218; 401 M Street, S.W.; Washington, DC 20460 (202-755-4938).

AUGUST 8-12, 1982: 7th Biennial Chemical Education Conference, Oklahoma State University, Stillwater, OK. For further details write to Dr. Dwaine Eubanks, c/o Department of Chemistry at the above address.

Some Points to Ponder

Quotations cited from an article entitled "PL/1 in Good Style" which appeared in the May 1981 issue of the "SIGDOC Newsletter" (ACM):

> "If you have a choice between being clear and being clever, be clear! If for some obscure reason you absolutely must be clever, be sure to clearly comment your cleverness."

> "THINK!! The computer is an idiot machine; don't be an idiot programmer."

Hardware QUERIES

HQ2 (September '81)

Professor David C. Hampton of Wartburg College called to find out if there were others with experience in converting analog information to digital and entering it into an Apple.

A HQ2 (September '81) by Ken Ratzlaff

We will begin by presenting several approaches to this problem, mentioning advantages and drawbacks. For the next issue, reader input would be helpful in order to assess the various possibilities. Chemistry is an experimental and increasingly instrumentation-oriented discipline. The effect of small computers on instrumental measurements has already been revolutionary, and a similar effect on the teaching of experimental chemistry will come when direct information input from instruments and/or sensors is commonly understood and implemented.

There are four general approaches to this problem: (1) tapping the instrument's own digital panel meter, if present, to acquire the data through a parallel interface port; (2) purchasing a digital voltmeter with a parallel digital output feature and attaching it to a parallel interface port; (3) constructing an interface on a blank circuit board; (4) obtaining a board with an analog-to-digital converter.

The first two are roughly equivalent. Panel meters and digital voltmeters are quite similar, converting at 2-30 Hz. The digital output may either be fully parallel or multiplexed. The fully parallel output presents 4 pins for each digit plus a pin for the "1" digit, a pin for the sign, and another for over-range indication; this requires 19 bits for a 4½ digit (+/-19999) meter. Since digital input ports typically accept only a byte, (8 bits), a multiplexer circuit controlled by the computer's output port is necessary; this circuit requires only 3 or 4 IC's. We have used this route in interfacing several Cary 118's to various computers. If the output is multiplexed, the BCD representations of all the digits are presented sequentially on the same 4 pins with additional pins indicating or controlling the digit being represented. We have used this type of interface when working with a Cary 219. Many instruments and voltmeters have an (expensive) option for an IEEE-488 standard output; the protocol for this output is quite complex since it allows many computers and instruments to communicate over the same data path. However, this power comes at a price: the computer port is also complex both to build and to support with a software driver. The PET does come with an IEEE-488 port, and SSM Microcomputer Products produces the A488 board for Apple which contains both the hardware and the drivers in firmware to support it.

The advantages of using voltmeters or panel meters are that well-engineered and versatile units (often with auto-ranging) are readily available, and the interface to a parallel port is relatively straight-forward. The disadvantages are that the conversion rate might be too slow, and the conversion from BCD to binary may be tedious in software (it can be done in hardware with several 74185 IC's, but this usually violates the "Don't do in hardware what can be done in software" axiom of computer interfacing).

The third method requires two key ingredients: a little skill at wire-wrapping or access to someone with 30 minutes to demonstrate the procedure, and components including a blank Apple prototyping board, some common IC's, and an ADC. Some details were discussed in J. Chem. Ed., 58, 470 (1981) (although unforgiveably) the author reversed the terms INPUT and OUTPUT in Figure 4). New ADC's are now available which can make this interface very simple; if readers are interested, this column can consider specific circuits in future.

Finally, a commercially-available ADC board can be used. Unfortunately, there is insufficient commercial interest in this area. When considering those boards that are available, several specs should be considered. First, what is the conversion rate? Most commercial units for Apple are slow, converting at only 2-30 Hz; however, this rate is very often sufficient, and the conversion methods involve integration of the signal so that they are relatively immune to electrical noise. Furthermore, all of the programming can be accomplished without machine language subroutines, even in BASIC. Faster ADC's, 1-30 KHz, will usually require a machine language driver, and the fastest ADC's, > 30 KHz, will usually require complex Direct Memory Access circuitry.

Second, what is the resolution? Many ADC's have only 8 bit (1/256) resolution which is generally insufficient; 10-12 bit units are common, and 14 or 16 bit units are available at very high cost. Third, what is the output code? For no good reason, some manufacturers use BCD converters which require time-consuming routines for conversion to binary. Fourth, what clocks or timers are available to establish a time-base? Finally, are multiplexers or programmable amplifiers available? The former allow software-controllable selection of a single analog input from a variety of inputs, and the latter provides software-controllable selection of the voltage gain. Some form of voltage gain is often necessary since ADC's typically require inputs in the 0-1 volt or 0-10 volt ranges whereas instruments typically provide 10-100 mv full scale.

With that information as background, in the next issue we would like to follow up with a list of vendors for Apple ADC boards, their specs, and where possible, the experiences of readers with all types of analog inputs. A current list of vendors follows:

1. California Computer Systems, 250 Caribbean, Sunnyvale, CA 94086 408-734-5811.
   3½ digit BCD, 400 ms.

2. Mountain Computer, 300 El Pueblo, Scotts Valley, CA 95066 408-438-6650.
   16 channel multiplexed, 8 bit, 125 KHz.

3. Interactive Microwave, P. O. Box 771, State College, PA 16801 814-238-8294.
   12 bit, variable range, 20 Hz, with DAC's and clock.

4. TecMar, Inc., 23600 Mercantile Road, Cleveland, OH 44122 216-464-7410.
   16 channel, 12-16 bit, 30-125 KHz.

5. Interactive Structures, 112 Bala Ave., Box 404, BalaCynwyd, PA 19004 215-667-1713.
   16 channel, 12 bit, programmable gain, 50 KHz.

Please send your queries, rebuttals, and information to Ken Ratzlaff, Instrumentation Design Lab, Chemistry Department, University of Kansas, Lawrence, KS 66045. 913-864-3754.

New Methods of Kinetic Data Evaluation Using Laboratory Computers

by James D. Carr*

In 1979, two research groups in the University of Nebraska's Chemistry Department, installed Horizon Northstar microcomputers in the laboratory for the collection and evaluation of stopped-flow spectrophotometric data. After some experience with traditional computational methods greatly speeded by the use of the computer, it became clear that much more elaborate computations could be done, essentially in real time, to solve more complex chemical problems. Two examples of this will be cited here.

Professor Sheldon Schuster and his students are studying many aspects of the chemistry of ATP. A specific reaction under investigation is the enzymatic hydrolysis of ATP as shown in eq. 1.

$$ATP + H_2O \xrightarrow{Mg^{2+}} ADP + H_2PO_4^- + nH^+ \qquad (1)$$

This reaction is monitored by coupling the proton release to a colorimetric indicator, specifically phenol red. As protons are released, the red color of the basic form of phenol red is rendered colorless and the absorbance change is monitored. Difficulty arises because of the different pKa values of ATP, ADP, and H_3PO_4 and the pH dependent binding of Mg^{2+} to these species. All these factors cause the value of n in eq. 1 to vary as a function of pH. Also, pH changes the course during the reaction. The relationship between absorbance and concentration of ATP is therefore not at all simple. Eq. 2 shows the relationship of concentration of hydrogen ion released to concentration of ATP hydrolyzed at constant magnesium concentration.

$$\left(\frac{\partial[H^+]}{\partial[ATP]}\right)_{pMg} = 1 + \frac{\frac{[H^+]}{K_{1ATP}} + \frac{[H^+][Mg^{2+}]}{K_{1ATP}K_{MgHATP}} + \frac{2[H^+]^2}{K_{1ATP}K_{2ATP}}}{1 + \frac{[Mg^{2+}]}{K_{MgATP}} + \frac{[H^+]}{K_{1ATP}} + \frac{[H^+][Mg^{2+}]}{K_{1ATP}K_{MgHATP}} + \frac{[H^+]^2}{K_{1ATP}K_{2ATP}}} - \frac{\frac{[H^+]}{K_{1ADP}} + \frac{[H^+][Mg^{2+}]}{K_{1ADP}K_{MgHADP}} + \frac{2[H^+]^2}{K_{1ADP}K_{2ADP}}}{1 + \frac{[Mg^{2+}]}{K_{MgADP}} + \frac{[H^+]}{K_{1ADP}} + \frac{[H^+][Mg^{2+}]}{K_{1ADP}K_{MgHADP}} + \frac{[H^+]^2}{K_{1ADP}K_{2ADP}}} - \frac{\frac{[H^+]}{K_{2P}}}{1 + \frac{[Mg^{2+}]}{K_{MgP}} + \frac{[H^+]}{K_{2P}}} \qquad (2)$$

This equation when combined with Beer's Law and the known colorimetric and acidic properties of phenol red can be used to obtain a plot of moles of ATP hydrolyzed vs. time. The reaction mechanism can be deduced from this plot. This work is described in detail in ref. 1.

LITERATURE ON COMPUTER-RELATED TOPICS

I. Abstracts

Locating articles, books, theses, reports, computer programs and information on meetings requires a search of different literature sources from those chemists frequently use.

A. "Chemical Abstracts" does reference some sources of useful information. Much of interest can be found in the General Subject Index under Computer Applications or Computer Programs. The keyword Education frequently helps to locate articles in chemical education under these more general headings.

B. "Computing Reviews" is a review journal published by the ACM (Association for Computing Machinery). All articles, books and other publications are classified into one of a number of categories. Some of the categories which are likely to be of interest are: (1.3) Introductory and Survey Articles, (1.5) Education, (3.1) Applications Natural Sciences (3.13 is Chemistry and 3.32 is Computer Assisted Instruction), (4) Software, (5) Mathematics of Computation, (6) Hardware, (8.1) Simulation and Modeling, and (8.2) Graphics.

The "ACM Guide to Computing Literature" is published annually and serves as an index to "Computing Reviews" but also includes some literature not cited and reviewed.

C. "Resources in Education" (RIE) and "Current Index to Journals in Education" (CIJE) are published by The Educational Resources Information Center (ERIC). RIE contains abstracted citations to non-journal literature. CIJE contains annotated references to journal articles. Much material of interest can be located in the subject indices under Computer Assisted Instruction, Computer Managed Instruction or other computer designations. Over 800 libraries and resource centers subscribe to the ERIC microfische collection which includes most documents cited in RIE.

Microfiche and paper copy of RIE documents can be ordered from the ERIC Document Reproduction Service. One to five fiche (up to 480 pages) costs 91¢. One to 25 pages of paper copy costs $2.00.

To illustrate the kind of literature abstracted let me describe three documents cited in the May 5, 1981 number of RIE. The first (ED 196 431) is entitled "School Microware: A Directory of Educational Software" which was published by Robert Haven, Dresden Associates, Dresden, ME. This 52 page document published in September, 1980 lists over 500 programs/packages which run on the APPLE, PET or TRS-80 and are available from commercial sources. Each program/package is described and the grade level for which the package is suitable is indicated. Twenty-five chemistry programs were identified. The commercial sources and their addresses were given. ED 196 709 is an NSF grant report entitled "Technical Problems in Implementing University - Level CAI in Mathematics and Science" by Arvin Levine, Lee Blaine and Patrick Suppes of the Institute for

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Mathematical Studies in the Social Sciences, Stanford University. This report describes VOCAL (Voice Oriented Curriculum Author Language) which is in the development stages. This study represents an attempt to develop and evaluate the use of computer synthesized speech in CAI. ED 196 417 entitled "Simulating CBE on Paper: A Small Step Backwards" by Lisa P. Brenner - Rush University and the University of Illinois College of Medicine. This NIH grant report compares the relative learning effectiveness of lessons taught by PLATO CAI versus lessons taught from paper copies of material derived from the PLATO lessons. The report concludes that students appeared to learn as effectively from the paper versions as from the on-line lessons.

The student manuals and teacher's guides (which contain program listings) of the modules described by Cynthia K. Jameson (J. Chem. Educ., 54, 238 (1977)) are referenced in RIE and available on microfiche from ERIC (ED 182-119 to ED 182-130).

D. "Computer and Information Systems Abstracts Journal" is an international publication of the world literature which abstracts periodicals, government reports, conference proceedings, books, dissertations and patents. Abstracts are classified under the main headings computer software, computer applications, computer mathematics and computer electronics. Chemistry, computer assisted instruction, computer graphics and education are some of the subject index categories of interest. CAI, CATC and CML are some of the items to be found in the Acronym and Nomenclature Index.

E. "Computer and Control Abstracts" covers topics like (1.1) and (2.2) education and training, (11) mathematical techniques, (40) numerical analysis, (50) computer hardware, (60) computer software, (70) computer applications.

Subject index topics of possible interest include chemical analysis, chemistry computing, computer aided instruction, computer graphics, computer interfaces, computerized instrumentation, computerized spectroscopy and education.

F. "Scientific and Technical Aerospace Reports" (STAR) represents a major component of the NASA information system covering aeronautics, space and supporting disciplines. Abstracts of reports, translations, patents, dissertaions and theses are included. NASA cited documents are available on microfiche in many libraries. Many of the other documents are available in hard copy or microfiche from the National Technical Information Service (NTIS). In the annual subject index documents of interest can be found under computer assisted instruction, computer graphics, and computer programs. Three citations in 1979 Subject Index found under computer assisted instruction are: (1) N79-25775- "Computers and the Learning Society"- 700 pages - summarizing the results of hearings before a subcommittee of the 95th Congress which described the utilization and impact of computer technology on various modes of learning. (2) N79-20782- "The Educational Effectiveness of Graphic Display for Computer Assisted Instruction," - a report of the Army Research Institute for the Behavioral and Social Sciences which reviewed the literature on instructional graphics and concluded that assumptions about the inherent value of graphics for instructional purposes are unsubstantiated by empirical evidence. (3) N79-24676 and 24677- "LHC-PILOT User Guide and System Guide" - 78 and 43 pages, respectively. Describes a version of the CAI authoring language PILOT which has been implemented on a Data General Minicomputer. (4) N79-33900- "Aspects of Effective Authoring Systems and Assistance: Recommendations for Research and Development" - 36 pages - a contract report by Karl L. Zinn (University of Michigan) and Alfred Bork (University of California, Irvine) - deals with the authoring process and related problems in CAI.

Part II of this report will appear in the next issue of the Newsletter and will consider journals, newsletters and other primary literature sources.

DECEMBER NEWSLETTER

Any items to be included in the December Newsletter should be received by November 1st. QUERIES and WHO DONE IT? items should be sent directly to Henry Griffin (software - Department of Chemistry, University of Michigan, Ann Arbor, MI 48109) or to Kenneth Ratzlaff (hardware - Instrumentation Design Laboratory, Chemistry Department, University of Kansas, Lawrence, KS 66045). Information on workshops, meetings, conferences, and courses should be sent to me.

I would appreciate receiving any suggestions regarding the Newsletter.

Donald Rosenthal, Editor

NEWSLETTER MAILING LIST

The mailing list has been updated for this issue of the Newsletter. If you are not on the mailing list and would like to be, please write me indicating that you have seen the September 1981 issue and would like to be placed on the mailing list for the December issue.

Donald Rosenthal, Editor
Computers in Chemical Education
Newsletter
Department of Chemistry
Clarkson College of Technology
Potsdam, NY 13676

Volume IV Number 4/December 1981

THE USE OF COMPUTERS IN CHEMICAL EDUCATION AT THE UNIVERSITY OF MICHIGAN

by William M. Butler and Henry C. Griffin*

Students begin to use computers in their chemistry courses during the first year -- principally in the laboratory course for general chemistry. The basic philosophy and implementation of this application of Commodore PET/CBM microcomputers is described elsewhere (see J. Chem. Educ., 56, 543 (1979)). The same type of microcomputer is used in quantitative analysis (for curve fitting and statistical analysis with programs written by the teaching staff) and instrumental analysis (control of and data acquisition from a gas chromatograph). A transition toward programming, as opposed to running someone else's programs, is made in physical chemistry laboratory. A similar transition for hardware (using machine language instructions and devising input and output) is made in a junior-level course in the principles of chemical instrumentation. In addition to these uses of microcomputers, about half of our chemistry majors take a course in programming concepts from the Department of Computer and Communication Science. For this course students use the University's central computer through the Michigan terminal system (MTS). Also, MTS is used to analyze data (such as to extract molecular parameters from HCl-DCl spectra) in the physical chemistry laboratory course. Finally, 20-30% of the chemistry majors use computers (micro, mini, or maxi) in senior research work.

The general chemistry computers are used by about 2500 students per year. The software for the laboratory course emphasizes simulation and graphics:

- a titration with an animated buret,
- characterization of a first order reaction,
- measurement of thermochemical properties,
- identification of an organic unknown from physicochemical properties,
- ranking of redox reagents, and
- interpretation of transitions in one-electron atoms.

Over the past several years the number of PETs in the freshman chemistry facility (the "PET SHOP") has increased to its present level of 38. This includes 23 of the older (small keyboard), 8 KByte PETs. The 15 newer PETs have been expanded to at least 16 KB (16 KB of RAM costs $19 plus labor for solder installation) to allow for larger programs. The mixture of machines causes some problems in selecting programs. Currently the older machines are loaded by cassette and remain loaded with a particular program for many days. The newer machines can be loaded one at a time from floppy disk, and more frequent program changes are reasonable. We have in hand, but have not yet implemented, a network which would connect all of the newer PETs to a 1 MB dual floppy disk system and allow loading of any of our chemistry programs by menu selection. Currently we are class testing a set of extended drill-and-practice programs designed to help students having difficulty with basic chemical concepts and processes. Effective use of these programs will require rapid changes in programs and extended facility hours (currently about 35 hours per week).

The equipment in the PET SHOP represents an investment of about $22,000. We have not analyzed the cost of software, but it is probably at least as much. We have looked for and found some programs written elsewhere (such as from Jim Beatty at Ripon College) which fit into our curriculum. Note particularly that students do not write programs for general chemistry; they have been written by staff members. Many students, including freshmen, can write BASIC programs and could refine their skills with our computers. At present this use is forbidden because of the difficulty in reloading the instructional programs. Most of our programs disable the "stop" interrupt so that they cannot be erased by the students.

Although we have several programs which would be appropriate for introductory organic chemistry (including those written by Professor Lyle Wescott during his leave from Christian Brothers College), we do not have enough computers to serve the 800-900 students in those courses. However, students in an upper level organic qual course have found such programs very useful.

The upper level courses are sufficiently small that the main barrier to using computers is effort needed to write the software. Where the intent is to teach programming, the barrier is for the student. Writing programs takes a lot of time, and less than half of the 80 students who take physical chemistry laboratory during a year select the computer experiment from a set of choices. (Essentially all students in the course use programs provided on MTS for data analysis.) The computer facility used by the physical chemistry students is available to all upper level undergraduates and graduate students in the department. The facility consists of seven 16K-32K PET computers, a printer, two Apple IIs, a digital plotter, modems, a Nova 2 and high-resolution plasma display, and disk storage. It is used primarily by undergraduates in work related to other courses, including undergraduate research.

Most of the seniors who receive credit for a research project (25-30 per year) use instruments which include dedicated minicomputers. Although the processes carried out in these research instruments are much more sophisticated than the simulations used in regular courses, there is little emphasis on the computers as programmable devices.

The central computer will always be the major machine for computing in our department. However, few undergraduate activities require the power of a large mainframe and microcomputers will become progressively more significant in the curriculum.

*Department of Chemistry, University of Michigan, Ann Arbor 48109

MICROCOMPUTER GRAPHICS
by John W. Moore*

For the past year and a half my students and I have been developing a high-quality microcomputer graphics system at Eastern Michigan University. This system is based on the S-100 bus and includes the following hardware: IMSAI mainframe and power supply, Cromemco ZPU processor and TU-ART I/O boards, 64K Seattle Products RAM, Tecmar A/D Convarter, Cambridge Development Laboratories high resolution black-and-white graphics with video monitor, IDS 440G "Paper Tiger" dot-matrix printer, and Houston Instruments DMP-2 digital plotter. Graphics software has been written in UCSD Pascal and Z80 assembly language under the UCSD p-System. Our graphics package has been used to good advantage in the process of interfacing a stopped-flow kinetics apparatus to the microcomputer, and we are currently working on an interactive graphics program that allows the user to enter and edit scientific text and scientific graphics by means of a keyboard and light pen.

At present the graphics package can accomplish the following functions: draw and erase (draw in black) vectors on the video monitor; draw vectors on the plotter; plot characters (alphabetic and numeric) on the monitor or plotter; plot points corresponding to each data pair in an array on monitor or plotter; scale a data array; draw and label axes; determine the pen position; determine or change the position of the origin of the screen or plotter coordinates; draw regular polygons on monitor or plotter; clear (to white or black) or scroll the monitor screen; read the screen coordinates of a light pen; and dump the contents of the monitor screen to the IDS 440G dot-matrix printer. The last-mentioned device produces hard copy graphics more quickly than the plotter, but the resolution is less than half as good. The graphics routines for our microcomputer have been patterned on those in the Calcomp-based system used on the DEC-10 computer at Eastern Michigan University.

Software for the package consists of two main files and a data file that contains information necessary to generate the sequence of vectors to plot each character. One of the main files contains 19 Pascal procedures and 2 functions. These include all necessary software to control the plotter and most of the routines for screen graphics. The other main file consists of 11 assembly-language routines that provide low-level and higher-speed control of the CDL graphics interface. These routines were written by undergraduate student Kalle Gehring during a 10-week NSF Undergraduate Research Participation Program in the summer of 1980. As an example of the resolution provided by the video monitor and the Paper Tiger, see the figure at the end of this article. This was generated using the graphics package and the short program given below. The same figure could have been drawn on the plotter (and indeed was, to provide a cover for Kalle's report) by changing the fifth line of the program to "plots(plotter);" and removing the "clear(black);" statement. On the plotter the resolution is twice as good.

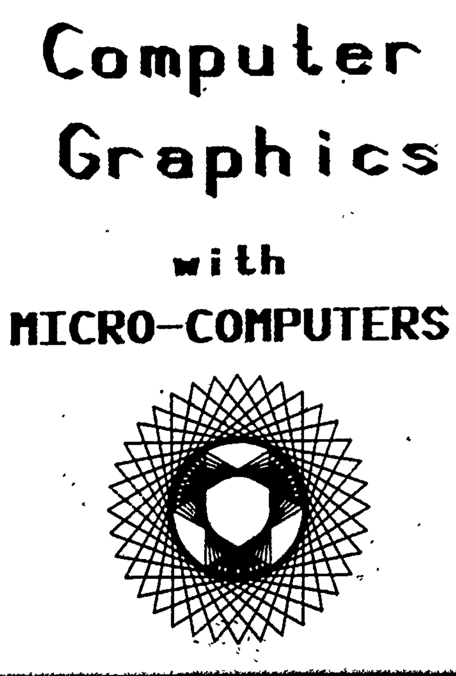
All-in-all we are very happy with our graphics hardware and software. For its price ($1200) the Houston Instruments plotter does an amazing job; new and better models have since become available, at somewhat higher prices for smarter or multi-color plotters. After an initial start-up problem when our light pen did not work, and once we learned how to guarantee proper initialization of the graphics boards on the first try, the CDL graphics interface has performed yeomen service. Our only complaint is that horizontal lines flicker due to the interlaced refresh of the screen. This and the price of just over a thousand dollars are a small price to pay for a 512 x 640 pixel display that can be expanded to include gray scales or full color, is I/O mapped so that it occupies no memory space in our 64K machine, and provides reasonably speedy animation of simple objects, using a Pascal program. We find that screen dumps to the Paper Tiger provide good enough hard copy for all but publication-quality drawings (see figure below). Consequently the plotter is used much less than we had anticipated, and the printer is used for more than just program listings.

Availability of graphics has made our interface to an Aminco-Morrow stopped-flow kinetics apparatus much friendlier to the user than it would otherwise be. Percent transmittance versus time data collected via the Tecmar A/D are displayed immediately on the graphics screen, just as they would be on the storage oscilloscope formerly used for data collection. The user, prompted by the system's console terminal, has the option of saving (to disk) or rejecting the data in the most recent kinetic run. Several %T vs time curves can be kept on the screen at once, and the user can retain or erase the most recent one. Analysis of data is interactive. The system displays the data and the user indicate with the light pen the smallest and largest time values between which data will be analyzed. This is a real advantage when some side reaction causes deviation from first-order kinetics after several half-lives. Data collected after the effect of the side reaction has become appreciable can be ignored. Once least-squares analysis has been performed, a first order or second-order plot is made on the screen so that the user can judge immediately the quality of the data. At any stage in the data-analysis procedure the screen image can be dumped to the Paper Tiger, providing hard copy that the user can study at leisure. In effect the CDL screen graphics display has replaced the storage oscilloscope on which data were previously collected. Programming of the stopped-flow interface was done by Robert Williams, an M.S. candidate at EMU.

Readers who are interested in the software described above can obtain program listings and a graphics manual by sending $2 to cover the cost of duplication and mailing. I can also supply programs on a single-density 8" floppy diskette, USCD Pascal format, soft sectored IBM 3740.

The program on the right produces an 8½x11 version of the figure below:

```
program cover-sheet;
uses graphics;
var i; integer;
begin
plots(monitor);
clear(black);
for i := 1 to 5 do begin
    symbol (4,2,5,0,5,'with',90);
    symbol (5,0,0,5,'MICRO-COMPUTERS',90);
    scroll (2/63);
end;
for i := 1 to 20 do begin
    symbol (1+i/252,0.5+i/126,0,75,'Computer',90);
    symbol (2,5+i/252,0.75+i/126,0,75,'Graphics',90);
end
for i := 1 to 12 do polygon (7.5,3.5,2,3,i*10);
for i := 1 to 122 do begin
    setcolor (black);
    polygon (7.5,3.5,1,3,(i-5)*7);
    setcolor (white);
    polygon (7.5,3.5,1,3,(i)*7);
end;
dump(down);
end.
```



Computers in Education
by Stuart L. Whitehurst*

WCCE 81. (International Federation for Information and other Developments Processing)

The third World Conference on Computers in Education opened in Lausanne Switzerland on July 27. Some 1300 participants from all parts of the world had gathered to attend conferences and panels for what turned out to be five very hectic days. (I would never have thought anything was more tiring than teaching!)

More than 150 speakers and panelists, plus a reasonable number of exhibitors from N. America and Europe were ready to lead us in to the promised land of the 21st century, where the teacher will be free to animate and direct resources which the student will have at his disposal.

The ubiquitous APPLE and its rapidly growing rival ATARI fought for the star attraction spot in the exhibition section; it must be admitted however, that the more sober MICRO PLATO system from CONTROL DATA completely stole the show for many. What more could we ask for as teachers than -

Touch activated screen
Graphic display
Special alphabet capability
Animation
Special easy to use lesson developer?

Perhaps color would have enhanced its appeal even more. Here's to the day when our "APPLES" and "TRS 80's" will have these capabilities for even less than they cost now.

Conference sessions and panels were interspersed throughout the week between 8:30 - 17:30 daily. It was necessary to make a very careful choice of meetings to attend. However, excellently prepared conference preprints were available right from the start which facilitated this task. Conferences were in the following general areas -

1. Information and the various disciplines.
2. Computer Assisted Learning and other direct uses of computers in education.
3. The impact of new technologies.
4. Social impacts including the changing roles of teachers.
5. National policies and models for computer education, with special reference to the needs of developing countries.
6. Aims, policies and curricula for informatic education.

For science teachers in general and chemistry teachers in particular there was not much that was new. This reflects the advance that chemistry teaching using computers has over many subjects such as languages, art, and music. These three areas were quite well explored during the sessions. Of a dozen or so papers given in the science field an interesting one concerning environmental studies in England was given by a representative of the Advisory Unit for Computer Based Education, Hatfield, U.K. Aims of the unit are -

1. To develop an awareness of the scope and nature of the impact of motorways upon the environment.
2. To learn about aspects of motorway construction which are used to minimize environmental impact.
3. To provide an introduction to some of the ideas planners use to assess environmental impact.
4. To provide students with an opportunity to discuss environmental planning with their peers.
5. To develop an awareness of the range of considerations involved in planning environmental factors, cost, and engineering problems.

Another interesting paper in the chemical field aimed at the university level student of organic chemistry was given by F. Moreno Mayor of the U. Politecna de Madrid, Spain. This program involved the student in identifying an organic compound of known molecular formula; the computer provided spectroscopic information as requested by the student.

A major item of interest to chemistry teachers was the paper given by Keith A. Shaw of the Department of Chemistry, Sheffield City Polytechnic, Sheffield, England. His paper described some attempts to develop and use computer assisted learning (CAL) material at the high school level in the U.K. in the areas of simulation, modelling, academic games, case studies and the electronic blackboard approach. Many participants immediately recognized the programs about which he spoke as being from the Chelsea College (Schools Council) Science packages; this was not surprising as he has written many of them. At the risk of boring readers who may already be familiar with the Chelsea packages, I will briefly run over the types of applications developed and mention developments which are foreseen. In exploiting computers as a learning resource, chemistry teachers have developed five types of applications to date:

a) simulations of laboratory experiments and industrial processes,
b) exploration, evaluation and modification of mathematical models,
c) academic games,
d) computer based case studies, and,
e) the electronic blackboard concept.

The material developed has usually been designed with one or more of the following methods of use in mind -

a) to assist in the initial teaching of a topic,
b) as extension and/or enrichment material,
c) as remedial or reinforcement material to help in the consolidation of knowledge and concepts.

The simulations and games (about ten of them) go together very well with the mainly "drill and practice" material from Programs For Learning. There is very little overlap of material, and with judicious choice of programs an effective student learning and practice aid for the senior chemistry student can be produced.

In the past, Chelsea's programs had been developed for mini and main frame computers, consequently, no use had been made of "graphics". It would appear that a series of units are under development using the ability of "micro's" to display information pictorially, through their high and low resolution graphics facilities. Included in this will be the presentation of graphs, bar charts and animated sequences. Good quality graphics (i.e., a resolution of at least 350 x 150 dots) will be required. These packages will fall into the category of electronic blackboard utilization. The control of the development and presentation of an idea may most appropriately be controlled by the teacher using the micro computer as a visual aid.

Given the inability of the microcomputer manufacturers to provide GOOD educational software, it is up to teachers to produce it. To do this we will need many more thousands of teachers with computing awareness and ability (and incidentally more time). What is happening at present to make more "computing teachers?" Summer computing courses for teachers are multiplying rapidly in all parts of the world. An open university project will soon see the light of day in England; one of the aims of which is to introduce interested adults including teachers to the world of computers and computing. The Open University is a means whereby any adult can follow a course of university level study in practically any discipline to degree level using distant-learning resources. This involves watching TV programs, listening to radio programs, following correspondence courses and summertime in-service training during vacations.

The overall aim of the project is to design and develop a modular course which will provide access to in-service training in micro-electronics in the school for those for whom there is currently no adequate provision. Another one of the aims is to provide those involved in education with the opportunity to acquire basic knowledge and skills which will enable them to start to:

a) use microcomputers to support their own teaching and administrative activities,
b) implement the changes necessary to incorporate into the curriculum either new teaching practices or new subject material resulting from the availability of microelectronics,
c) prepare their students for the changes which microelectronics will bring both to their lives and to society,
d) understand the limitations of microelectronics based technology so that they will not try to use it inappropriately or give misleading information to their students.

The target audience will be primarily teachers in schools in which there are 9-18 year olds. There will be modules at three levels:

level 1: Awareness
level 2: Basic knowledge and skills
level 3: Classroom experience

Each module will represent about 30 hours of study, and a complete course would normally correspond to studying a linked set of four to six modules.

An additional aim of the course is to promote widespread good practice in the use of microelectronics by teachers, so as to improve their effectiveness in performing their teaching and administrative tasks, and to stimulate and encourage effective curriculum development in the area of microelectronics in schools. The course will include the following six modules:

1: An introduction to Microelectronics in the School,
2a: Educational Software - Creating a Program,
2b: Educational Hardware - Controlling a Device,
3a: Microcomputers in Action in the Classroom,
3b: Using Microelectronics in the Classroom,
4: Impact of Microelectronics in School and in Society.

IT SHOULD ALL BE PRETTY EXCITING!

Not to be left out, the British Broadcasting Company (B.B.C.) is to launch a major new project in the field of computer literacy in January 1982. The aim of the project is to introduce interested adults to the world of computers and to provide the opportunity for viewers to learn through direct experience how to program and use a microcomputer. The project is built around a ten part TV series, and includes a book, a linked microcomputer system complete with users guide, a range of application programs and an associated course in programming in BASIC provided by the National Extension College, a corresponding course organization based in Cambridge.

To come back to my earlier allusion to "the promised land of the 21st century", there are many people willing to point the way, but in the end it will be our responsibility to find our own way there.

*Currently a teacher of Chemistry at the International School of Geneva, Route de Chene, Geneva, Switzerland

On Software

Don Rosenthal's "Letter from the Editor" in the September issue of the Newsletter sought to open discussion on some important aspects of the use of computers in education. I was particularly struck by his report on the attempt to produce computer literacy for freshmen at Clarkson. "We expected that instructors would make use of this new capability. Mostly, they did not." These statements had a very familiar tone and seemed applicable far beyond the specifics of computers. How often do we fail to use (and thus reinforce) our students' skills in mathematics, physics, English, etc.? These discontinuities can occur even in a rather traditional chemistry curriculum. I do not want to get into that issue now; my point is that the last half of Don's letter gives very reasonable goals for computers in an undergraduate program -- and the primary emphasis is on software.

The Clarkson example emphasizes computers as devices for numerical manipulation (data reduction, statistical analysis). An equally, if not more, important use within the scope of this Newsletter is aid to instruction. One lesson Stan Smith reports from his experience with Plato at the University of Illinois is that there is a minimum level for effectiveness of any instructional form in a curriculum. One data-reduction program or one videotape presentation per term may be a distraction, a negative influence. I wonder whether the goal of a little bit of computing throughout the curriculum is below the effectiveness threshold. Don't we need to use computers regularly in order that the familiarization time not be excessive with each use?

It seems to me that this idea of startup costs is particularly applicable to writing programs. I would be unhappy if one of my students wrote a program of any complexity without checking it with test data. Obtaining the test data might be equivalent to solving the problem by hand, so there may be little incentive for a student to write the program. I think that Don was addressing this point when he said that textbooks ignore computers. Only when our coursework includes the types of problems which are more easily solved by programming and using computers than by hand will the use of computers expand naturally. Note clearly that we would be knowingly inserting barriers to students who lack computer skills.

The existence of a critical mass for computer software in undergraduate instruction is a major concern of mine. The two regular Newsletter features, Queries and Who Done Its, do not address this issue. I believe that Queries are important in showing the types of problems we teachers are facing, but no one item is apt to attract broad interest. Therefore, I propose to treat them as "want ads" with the expectation that interested parties will get together through their own devices. The Who Done It, which can include answers to Queries, can contribute to identifying elements in an effective set of programs, but this medium falls short of showing when critical mass has been reached. Therefore, I invite critical reviews from users of software who have found a sufficient set of materials for one or more courses. These reviews could convince others that "now is the time to move." I have heard that several authors are writing packages of programs for general chemistry. We should have more information in the next Newsletter.

Software queries and answers should be sent to Henry Griffin, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109.

SQ5 (December 1981)

For: Apple II
Item: - Software modules to simplify creating high resolution graphics from Applesoft.
- Management system to record test scores, etc. and to keep track of student progress.
- Any software for use in lower division courses in chemistry. (This item can be taken as an expression of interest in finding programs which have not been distributed widely.)

W.R. BORNHORST (Grossmont College, 8800 Grossmont College Drive, El Cajon, CA 92020 [714] 465-1700)

SQ6 (December 1981)

For: Apple II PLUS
Item: - Software to analyze kinetics data suitable for physical chemistry experiments.

S.L. BURDEN (Department of Chemistry, Taylor University, Upland, IN 46989)

SQ7 (December 1981)

For: Apple II
Item: - Is there a quick and easy way to put lower case letters, subscripts, and superscripts in the video display? These features are needed for chemical notation.

R.L. THORP (Chemistry Department, Vestal High School, Vestal, NY 13850)

SQ8 (December 1981)

For: Any system
Item: - Has anyone used EXPER SIM for simulations in physical sciences?

BENJAMIN IRVIN (Chemistry Department, St. Andrews College, Laurinburg NC 28352 [919] 276-3652 x352)

(EXPER SIM is designed to teach measurement or experimentation in social sciences. It might have interesting applications in descriptive chemistry. Please send information for inclusion in a future Newsletter. HCG)

Hardware QUERIES

Send hardware queries, rebuttals, and information to Ken Ratzlaff, Instrumentation Design Laboratory, Chemistry Department, University of Kansas, Lawrence, KS 66045, phone: (913-864-3754).

A HQ2 (September '81) Continued

In the last issue (September, 1981) we considered the various available options for passing information in and out of Apple computers in analog form. I asked for some experiences and/or more information, and I want to pass along that which was received.

Dr. William Bradford of Oakland University (Rochester, MI) uses Howlett-Packard 47310A A/D converter systems which have an IEEE 488 interface port and elected to obtain IEEE 488 interface boards to interface the converter to this Apple. His first experience was with the California Computer Systems Model 7490 board; however, neither he nor the CCS representative were able to make it work, so that idea was abandoned. His distributor exchanged it for a Mountain Computer 16 channel A/D-D/A (8 bit) board which operates quite well. Mountain Computer equipment is exceptionally well-documented and gets consistently good reviews.

This leaves the question of what to do with the HP A/D's. Another source of interface boards not included on last month's listing is SSM Microcomputer Products (2190 Paragon Drive, San Jose, CA 95131). Their A488 board includes all necessary software in PROM and appears to be quite powerful. However at $475, it is not cheap.

Professor John Zimmerman (Wabash College, Crawfordsville, IN) has also had a bad experience with a CCS product. The performance of the Model 7470 is below that required for almost any lab application; its conversion rate is barely over 2 Hz, and the data is BCD encoded with routines available to convert it only to character strings.

Since the last issue, an announcement has been received for an add-on system for the Apple called the "ISAAC" from Cyborg (342 Western Ave., Boston, MA 02135 (800-343-4494)). This package includes A/D (16 channel or 8 channel differential, 12 bit, 40 KHz, variable input range), 4 D/A converters (12 bit), 16 bit parallel I/O, 16 bit counter/timer, distribution panel, test kit, LABSOFT programming language (Applesoft BASIC + 40 new commands for use with lab peripherals and graphics) and manuals. For such a package, you would expect to pay, and indeed you do: $3950 without the Apple or its other peripherals. However it looks like a good easy-to-install and use system for the research lab.

I have in my files information on boards from these other manufacturers, and the following is a review of that data:

Interactive Structures, Inc., 112 Bala Ave., Box 404, Bala Cynwyd, PA 19004 (215-667-1713).

AI13 12 bit A/D Converter with 16 channel input, 8 voltage ranges (199 mv to 10 V), 20 microsecond conversion time, $550.

Hardware QUERIES (continued)

AI02 8 bit A/D Converter with 16 channel input, 0-5 volt input, 70 microsecond conversion time, $299.
A003 8 bit D/A Converter, 2-8 channel, 10 volt range, $195-$437.

Interactive Microware, Inc., P. O. Box 771, State College, PA 16801 (814-238-8294).

APPLAB interface card including: a) 12 bit A/D converter, 50 ms conversion time, jumper-selectable input ranges; b) 12 bit A/D converter, jumper-selectable output ranges; c) 8 bit parallel I/O; d) three counters, a 32 bit countdown timer and two 16 bit timer, counters; e) driver, demonstration, and diagnostic software on disk compatible with Applesoft, $495.

TecMar Inc., 23600 Mercantile Rd., Cleveland, OH 44122 (216-464-7410)

TM-AD211 A/D converter subsystem, 12 bits (14 bit and 16 bit options available), 30 KHz (40, 100, 125 KHz options available), 16 channel or 8 channel differential inputs, programmable gain option (uses ANALOGIC subsystem), $495-$1787 depending on options.

TM-DA101 D/A converter subsystem, 12 bits, 2 channel, 8 bit parallel I/O, jumper-selectable output range, $295. Companion board available for filtering, current gain, etc.

<u>HQ3 (December '81)</u>

Dr. Ronald Rich, Bluffton College, Bluffton, OH, asked about word processing systems that give maximum capability in handling scientific documents; he reported that he had heard that WordStar, the most popular word processing software system, when used with a Diablo printer would not print all of the characters on the Diablo print wheel.

<u>A HQ3 (December '81)</u>

This is a topic which requires the suggestions and comments of readers. Regarding WordStar, I checked with Mr. Ronald Proesel of MicroSolutions (139 Sacramento, Sycamore, IL 60179) who says that correct operation of WordStar will provide access to every character on the Diablo Scientific print wheel; however, I did not see examples.

Aside from purchasing dedicated word processing computers, two possibilities for scientific word processing are the WordStar software/daisy wheel printer approach which should handle most needs, and using a graphics printer (Epson, MPI, etc.,) with the fonts including subscript, superscript, and greek characters generated in the software. To my knowledge, the latter has not been implemented. However, I have heard that people in mathematics are working on this as the basis of a manuscript submission system for their primary journals; I was told that even figures would eventually be part of the manuscript stored on magnetic media. Experiences or suggestions anyone?

WHO DONE IT?

Summary by Ken Ratzlaff

WHO-3 (December '81)

Computer-Controlled Titrator with High Resolution Graphics Display

Controls a constant rate buret and logs data with simple locally-constructed interface. Plots titration curve as data is collected. Computes and plots in different colors the first and second derivatives and Gran plots. Prints end point values and plots curves on printer. Delivery of titrant can be slowed down beginning at a user-selectable pH or mv value and delivered one drop at a time until the endpoint is reached.

Computer Hardware: Apple II, Paper Tiger 480
Instrumentation: Sargent Constant Rate Buret, Orion 701 pH meter.
Documentation & Software: Prof. Stan Burden, Department of Chemistry, Taylor University, Upland, IN 46989, $25 including diskette.

WHO-4 (December '81)

Computer Controlled Nitrate-Ion Selective Electrode Analysis System

Logs data from both standard and unknown solutions. Readings taken at user-specifiable intervals until a user-specifiable constancy is achieved for each standard or unknown to compensate for electrode drift. Points logged from standards are displayed in color graphics as they are logged. The standard data is fit with a cubic equation and both the data points and the fitted curve are plotted (in different colors) in high resolution graphics for visual display of calibration curve. The equation is solved using the Newton-Raphson technique and the millivolt readings obtained from each unknown. The corresponding concentration is printed out.

Computer Hardware: Apple II, Paper Tiger
Instrumentation: Orion 701 pH meter or Keithley 179 Instrumentation with IEEE 488 interface.
Documentation: As for #1.

WHO-5 (December '81)

Computer Analysis of Data for Phosphate Analysis Using Fluoride Ion Selective Electrode and Gran Plots of Back Titration of Lanthanum with Fluoride.

Data entered manually; software computes and prints out Gran plots and computes concentration of unknown. Essentially eliminates manual plotting of Gran plots and reading results from them.

Computer Hardware: Apple II, printer
Documentation: $8 including diskette from S n Burden (see #1).

NOTE TO READERS: Please share your accomplishments with our readers by sending short descriptions of your work to this column. Each future submission should contain a) a short description, b) a list of computer hardware required (the computer, storage medium, memory, other boards, printer, plotter, etc.), c) software packages required by the user but not included (operating system, languages, graphics packages, etc.), laboratory instruments required, e) type of documentation available including cost, ium (disk format if applicable), and your name and address.

Summary by Henry Griffin

WHO-6 (December '81)

James G. Macmillan (Department of Chemistry, University of Northern Iowa, Cedar Falls, IA 50614) has developed a carbon NMR simulation for Apple II systems with 48K RAM and a disk (DOS 3.2.1 or 3.3). The program is written in Applesoft BASIC. It calculates carbon chemical shifts for alkanes based on empirical equations (Lindeman and Adams, Anal. Chem., 43, 1245 (1971)). The alkane is specified by responses concerning bonded atoms. Chemical shifts are tabulated and the spectrum is displayed. A second mode of operation involves random selection of an unknown by the computer. The author has not specified a charge for the program, but some arrangement to cover the cost of a disk can be anticipated.

WHO-7 (December '81)

Vinay Kumar and John I. McAndrews (Department of Physical Sciences, Northern Kentucky University, Highland Heights, KY 41076) and Jon W. Mauch (Madeira High School, Madeira, OH 45243) have written Applesoft programs to aid in analyzing titration data. The basic program PLOTTER accepts data in either pH of mV values, displays the data for possible corrections, calculates and displays first and second derivatives, and displays the plots in color graphics. The expanded program PLOTTER (REV. JM) provides hardcopy of data, calculated values, and graphs with a suitable printer. (The authors used an IDS-440 printer with graphics option interfaced through an A2 B0002 parallel printer card.) Single copies of listings of either program are available free from Kumar. For the program on diskette, send $10 (money order or cashier's check) to J.W. Mauch.

WHO-8 (December '81)

PaperMate by Michael Riley: The potential for using microcomputers for "wordprocessing" is responsible for much of the projected spread of these machines into small businesses during the next year or two. Of course, none of the computers can be used for wordprocessing without programs designed for this purpose (and suitable peripherals, such as disk units for file storage and "letter quality" printers). In the traditional wordprocessing machine, the programs are based on firmware and are not accessible to the user for modification. In essence the programs are like the operating system in a computer. When general purpose microcomputers are used for wordprocessing, in principle the user can modify the software to fit particular needs. The range of complexity of available programs matches the broad range of computers, but even for a given computer many different programs can be used. In general the more expensive ones are not accessible to the user either because they contain significant amounts of undocumented machine code or because the programs are protected against copying. PaperMate shows that a full feature program need be neither expensive nor inflexible. PaperMate is available for $30-$40 from A B Computers (115 E. Stump Rd., Montgomeryville, PA 18936; (215-699-5826)). It is written in BASIC for the PET/CBM computers and makes effective use of screen editing functions provided by those computers. Features of the program include SAVE and LOAD of text from disk or tape, adaptation to various printers and PET ROM's, justification and tabulation (of monospaced type), formating (margins, line spacing, lines per page, page headings and footings), insertings for form letters, and others. It does not have "find" or "find and replace" commands.

PaperMate has been modified by Henry Griffin (Department of Chemistry, University of Michigan, Ann Arbor, MI 48109) for use in the general chemistry office. His modifi-

WHO-8 (continued)

cations provide imbedded commands for the Centronics 737 printer to give subscripts, superscripts, underlining, and changes between type styles. Check a recent A B Computer ad for current price. Write Professor Griffin for a listing of modifications which permit writing chemical notation.

WHO-9 (December '81)

L.A. Hull (Department of Chemistry, Union College, Schenectady, NY 12308 offers an Applesoft program for 3-D display of line drawings of molecules. He finds provision for rotations, including bond rotations, and displacements to be particularly useful for illustrating organic structures. Data for several common organic molecules are included in the package. A diskette (DOS 3,3 Apple II Plus) and description cost $25.

WHO-10 (December '81)

Doug Green (Cortland Jr.-Sr. High School, Cortland, NY 13045) offers animations of five phase changes. The programs give high resolution displays with large text, are menu driven, and have sound effects. They run on Apple II or Apple II+ with DOS 3.3 and has been used with 9th grade physical science and high school chemistry students. Cost: $15 for the programs and disk, $10 on your disk.

WHO-11 (December '81)

C.F. Hammer (Department of Chemistry, Georgetown University, Washington, D.C. 20057) has three programs QUINS (quantitative, UV, visible, infrared and NMRO, MOFO (molecular formula determination using mass spectral, proton or C-13 NMR data or more than one of these techniques), and LABDET (label determination from mass spectral data). All are in FORTRAN IV, Version 2.5 and run on a PDP 11/23 under the RT-11 operating system. Those wishing the programs must provide an RL01 disk or single density RX01 floppy disk.

WHO-12 (December '81)

D. Salyer (Rm. 337, Moore Bldg., E. Kentucky University, Richmond, KY 40475) has twenty-four review programs on topics usually covered in introductory chemistry. Each program contains multiple choice questions and problems. The programs are written in BASIC PLUS and will run on a PDP 11/70. There is no charge for sample listings.

WHO-13 (December '81)

D.M. Whishant (Northland College, Ashland, WI 54806) has ten programs which involve laboratory simulations and provide support for general chemistry laboratory experiments. The programs are written in microsoft Level III BASIC and run on a TRS-80, Model I with 32k. Send a cassette or floppy disk.

WHO-14 (December '81)

The Lister Hill National Center for Biomedical Communications has developed an extended version of the C.A.I. authoring language CORE PILOT '73 called LHC 8080 PILOT. This version of PILOT is written in assembly language and PL/M and operates under the CP/M operating system and requires a minimum of 48k of memory (64k recommended). LHC 8080 PILOT has many extended features including n-dimensional numeric functions, extended matching, and dynamic construction and execution of statements. The software includes a built-in editor. All distribution will be handled by the National Technical Information Service (NTIS), U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161. The order number for the executable LHC 8080 PILOT package is PB82-114943. The cost is $30 and the program is supplied on an eight inch soft sectored IBM 3740 format floppy diskette. The distribution package includes a 100 page User's manual. The version supplied on the diskette uses port number assignments which are probably incompatible with your hardware. One small section of source code must be patched into the code section to customize it to the users specific configuration. (Information supplied by Roy A. Standing, LHC, National Library of Medicine, Bethesda, MD 20209.)

WHO-15 (December '81)

Dresden Associates, P. O. Box 246, Dresden, ME 04342 is publishing "School Microware Directory". The 1981-82 Directory consists of two issues. The September 1981 issue listed over 1200 software products from over 100 companies available for the Apple, Atari, PET and TRS-80. The April 1982 issue will include 300 more programs. All software is classified as being instructional or administrative. The instructional software is classified as to subject (60 subject categories) and grade level (K-12). Programs are listed by subject and grade level and by hardware system. The cost of each program and address of the suppliers are included. An index by program name and subject is included. The cost for one year (two issues) is $25. An examination copy of the 1980 Directory (500 programs) is available from Dresden Associates for $4 (it is available on microfische through ERIC Document Reproduction Service as ED196 431 for 91¢. The 1980 Directory can be found in many libraries and resource centers which serve as ERIC microfische repositories.) The 1980 Directory lists 25 chemistry programs.

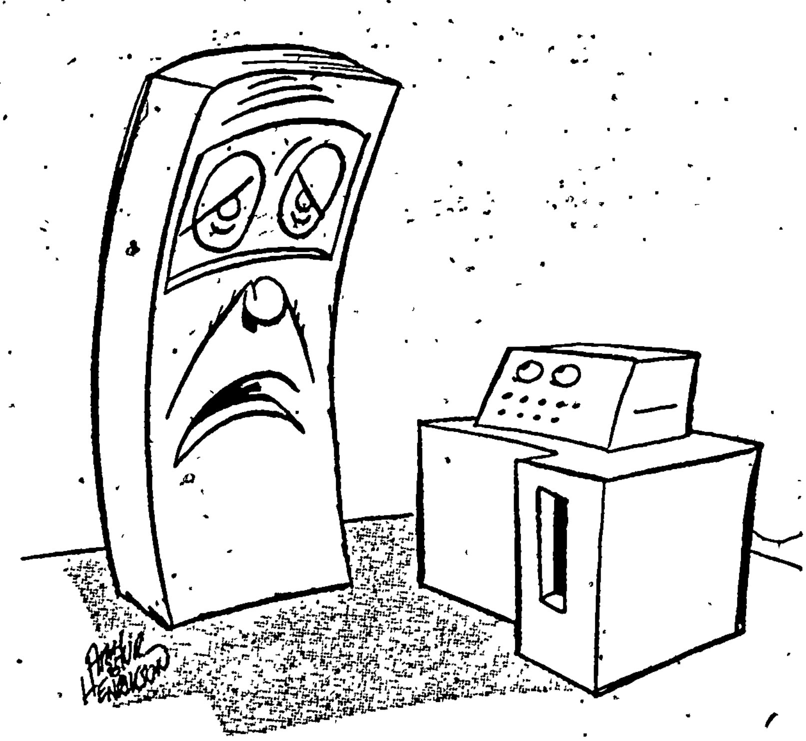
WHO-16 (December '81)

The NIH-EPA Chemical Information System (CIS) consists of a collection of over seventy chemical databases linked together by a number of programs for interactive searching through these databases. Over 228,000 chemicals having over 657,000 names are represented. Information on mass spectra, C-13 NMR spectra, x-ray diffraction, acute toxicity and water toxicity data are available. Also, there are some data analysis programs including statistical analysis and mathematical analysis algorithms. The system is available 24 hours each day via interactive terminals through Telenet. The $300 per year subscription fee is waived for educational institutions and public libraries. These organizations are allowed a monthly discount of $100 towards their connect time usage. This free allowance does not include telephone network charges and certain other charges. The system has been described in a number of publications (including S.R. Heller and G.W.A. Milne; Anal. Chim. Acta, <u>122</u>, 117-138 (1980); J. Chem. Inf. Comput. Sci., <u>20</u>, 204-211 (1980)). For more information contact C.I.S. Project Information Sciences Corp., 2135 Wisconsin Ave., Washington, D.C. 20004 (800-424-2722).

NSF has recently announced funding of a major project in the DISE program. The principal investigator is John W. Moore and co-principal investigator is Joseph J. Lagowski. The project will set up procedures for soliciting, evaluating, publicizing, and disseminating instructional modules, many of them computer based. It will draw upon other NSF-funded projects in chemistry, chemical engineering, materials science, physics, and mathematics, as well as on individual chemists or groups of chemists for instructional modules. These modules will be reviewed and tested in classrooms or laboratories, and reviews by actual users of the modules will appear in the Journal of Chemical Education. Areas of special interest for preparation of instructional modules are industrial chemistry and polymer chemistry.

In addition to preparing and distributing modules, the project will attempt to improve authors' skills. Workshops (based on those already organized by the Division's Computer Task Force) for both novice and advanced authors of computer-based instructional materials are planned. The first of these will occur in conjunction with the Seventh Biennial Conference on Chemical Education at Oklahoma State University next August. The project will also explore the feasibility of distribution of the materials it produces via nationwise time-sharing networks, allowing potential users to obtain modules essentially instantaneously, to read reviews from or contribute criticisms of modules to an electronic bulletin board, or to obtain updates and corrections to existing modules via a local telephone call.

Persons who wish to obtain more information about the project, who are interested in volunteering as reviewers, or who may have computer programs or other modular materials to contribute should contact: Dr. John W. Moore, Visiting Professor (until June 1982), Department of Chemistry, University of Wisconsin, Madison, WI 53706; (608) 262-0215.



Henrickson — Data Management

"I feel miserable. All day long they've been feeding me raw data."

BOOK REVIEW

"16-BIT MICROPROCESSORS" by Christopher A. Titus, Jonathan A. Titus, Alan Baldwin, W. N. Hubin, Leo Scanlon, from Group Technology, Ltd., P. O. Box 87, Check, Virgina 24072 703/651-3153 $ 14.95

A few years ago there was a substantial distinction between minicomputers and microcomputers. Often the defining differences were the word length (mini's had 12-32 bit words compared to the micro's 4-8) and the number of chips in the Central Processing Unit (micro's had 1, mini's had more). Somewhere in between was the LSI-11 CPU which was the low-end PDP-11 mini or a high-end micro. Later, people began to realize that the difference was less in how the CPU was constructed and more in how it was used (mini's have operating systems and high-level languages, etc.). The performance of the 8-bit machines was still substantially below that of the PDP-11's, NOVA's, and HP's.

The latest microprocessors are blurring the distinctions in CPU's even further. Several single-chip sixteen-bit microprocessors are already established and are vying for dominance. Some of these will never achieve importance in laboratory computers just as some eight-bit processors never did. The determining factors include not only the professor's ability (architecture, speed and instruction set), but also the marketing skills of the companies who design the computers; software developers will follow with software when they detect that a certain processor will have a significant market share. Clearly we prefer the most powerful processor to be employed in the best-designed computer, and for it to have the best software support.

The purpose of this book is an aid in making the first evaluation, that of the CPU's performance. Six sixteen-bit microprocessors are considered, the Intel 8086, the Zilog Z8000, the DEC LSI-11, the Texas Instrument 9900, the Motorola 68000, and the National Semiconductor 16000. An introductory chapter deals with the basic concepts of microcomputers before the architecture of the CPUs are described in one chapter each. Each microprocessor is also evaluated for four tasks or benchmarks: a bubble sort (ordering a group of integers according to their value), a string search (matching a test string to a larger string of several words), multiplication and division (by finding the square roots of several integers) and a lookup (using a table to find the sine of an angle). The results are presented in a table below. For each of the benchmarks, the assembly language program is provided and the execution times are determined (except for the 16000). The results are fascinating; for every test, the Z8000 (at 10 MHz) was the fastest followed by the 8086 or 68000 (at 8 MHz). The LSI-11 lagged well behind and the 9900 trailed distantly. It should be pointed out that the latest LSI-11 family member, the 11/23, generally executes about 2.5 times faster than the member tested. Also the 16000, not tested, has many features which will probably allow it to out-perform the others by a significant margin.

At this point the usefulness of this book probably ends for those who do not intend to design from scratch their own computer system; for chemists generally, we need only to conclude that the Z8000, 8086, and 68000 will generally out-perform the LSI-11's and 9900's. We must still consider the availability of a well-engineered product with good software support.

Book Review (continued)

Here at KU, we have decided to enter the sixteen bit area with the 8086 in spite of its slight limitations demonstrated in the benchmarks. In brief, this was because (1) IBM's choice of that family has given a substantial stimulus for software development, (2) Intel has designed (8087) and I/O (8089), and (3) well-engineered products for the S-100 (IEEE 696) bus, to which we are already committed, are available now.

There are probably two reasons for using this book: first, to research the primary sixteen bit microprocessor offerings in order to determine which is best suited for the application for which one is to design a new computer, or second, to get a general feel for the comparative merits of the new microprocessors. I enjoyed the book. It is easy-to-read, not overly filled with jargon, and devotes most of its space to information truly of interest to the assembly language programmer. However, reachers must be cautioned not to choose a microprocessor based only on the architecture and benchmark information since in many or most cases software availability will be the factor which determines the success or failure of a computer to handle an application.

BENCHMARK RESULTS

	Bubble Sort	String Search	Mult/Div (Average)	Lookup (Sine)
8086 (8 MHz)	2.1 s	.235 ms	.171 ms	.024 ms
Z8000 (10 MHz)	1.6	.095	.061	.012
LSI-11	10.5	.979	.457	.149
9900	33.	2.25	.770	.320
68000 (8 MHz)	2.0	.424	.104	.018

Reviewed by Ken Ratzlaff, Instrumentation Design Lab, Chemistry Department, University of Kansas, Lawrence, KS 66045.

Publishers and authors wishing to have books reviewed should send review copies to Donald Rosenthal, Editor, Computers in Chemical Education Newsletter, Department of Chemistry, Clarkson College, Potsdam, NY 13676. Readers who are willing to review books should write the editor.

Literature on Computer-Related Topics
Part II

Journals, Newsletters and Other Primary Literature Sources

In the first article in this series, published in the September issue (Vol. IV Number 3), seven abstracting journals were described: "Chemical Abstracts", "Computing Reviews", "ACM Guide to Computing Literature", "Resources in Education (RIE)", "Current Index to Journals in Education (CIJE), "Computer and Information Systems Abstracts Journal", "Computer and Information Systems Abstracts Journal", "Computer and Control Abstracts", and "Scientific and Technical Aerospace Reports (STAR)". These journals are useful in locating articles, books, theses, reports, computer programs, and other publications.

This article will discuss some of the primary literature sources. At the outset it needs to be said that there are many sources of useful information. Publications in this field reflect the explosive nature of developments. I will exclude explicit mention of users' groups, although these may be a very useful source of computer programs. Some of these users' groups and some manufacturers do an excellent job at making users aware of software which will run on their computers. In what follows I will list the publications, its address, cost, and some of the contents of a few recent articles.

A. "Journal of Chemical Education" is published once each month by the Division of Chemical Education of the American Chemical Society. The domestic subscription price is $15 per year for individuals and $30 per year for libraries, institutions and companies. The journal can be ordered from Journal of Chemical Education, Subscription Fulfillment Department, 20th and Northhampton Streets, Easton, PA 18042.

One very useful group of articles is the Computer Series edited by John W. Moore. To date, twenty-two articles have appeared in this series. The most recent is "Integration of Major Computer Program Packages into Experimental Courses" (October 1981, Vol. 48, No. 10, p. 796). The first article in this series "A Tool, Not a Gimmick - an Introduction to Computer Applications in Chemical Education" appeared in March 1979 (Vol. 56, No. 3, p. 140). Some articles in this series dubbed "Bits and Pieces" provide brief descriptions of software and hardware. (To date 7 of the 22 Computer Series articles are "Bits and Pieces". The most recent of such articles (September 1981, Vol. 58, No. 9, p. 690) included descriptions of "Interfacing an Apple II Microcomputer to a UV-Visible Spectrophotometer," "Preparation of Posters and Overhead Transparencies" with the Hewlett Packard 9872A digital plotter, "A Simple Hückel Molecular Orbital Computer Program Written in BASIC for Microcomputer Use", "PMR Spectroscopy on a PET", "Computer-Assisted Instruction in General Chemistry", "OPTSCAN and GRADE - Automated Grading and Record Keeping", "KEMGAM: A Chemical Adventure", and "Non-Linear Least-Squares Optimization of Parameters for First-Order Kinetics on Programmable Calculators." (The first 16 articles in the Computer Series together with a dozen full length descriptions of computer applications are available in paperback as "Interactions: Computing in the Journal of Chemical Education" for $9.75. This volume can be ordered from Journal of Chemical Education, 238 Kent Road, Springfield, PA 19064.)

In addition to the Computer Series there are many other articles describing computer applications. For example, the November 1981 issue (Vol. 58, No. 11, p. 904) contained an article entitled "Field Test Evaluation Report on Introduction to Polymer Chemistry" by K. Chapman and J. Fleming. This article summarizes the evaluation of a course on Polymer Chemistry delivered via the PLATO computer system.

B. "Journal of Computer-Based Instruction" is published quarterly by the Association for the Development of Computer-Based Instructional Systems (ADCIS). Personal subscriptions are $12 per year ($20 for institutions). The journal can be ordered from Gordon Hayes, Executive Secretary, ADCIS International Headquarters, Computer Center, Western Washington University, Bellingham, WA 98225. Recent articles of interest include: (1) "Publication Practices for Microcomputer Programs" by Constance Curtin, (May 1981, Vol. 7, No. 4, p. 123); (2) "Computer Assisted Instruction: Factors Affecting Courseware Development" by J.W. Sprecher and J.A. Chambers (November 1980, Vol. 7, No. 2, p. 47); (3) "Artificial Intelligence Approaches to Computer-Based Instruction" by W.S. Bregar and A.M. Farley (May 1980, Vol. 6, No. 4, p. 106); (4) "Active External Control: A Basis for Superiority of CBI" by A. Arner, C. Moore and S. Smith (May 1980, p. 115); (5) "CAI Readiness Checklist: Formative Author - Evaluation of CAI Lessons (November 1979, Vol. 6, No. 2, p. 47); (6) "The Future of Computers in Education" by P. Suppes (August 1979, Vol. 6, No. 1, p. 5); (7) "Intelligent Videodisc and the Learning Society" by A.R. Molnar (August 1979, p. 11)

C. "T.H.E. Journal" (P.O. Box 992, Acton, MA 01720), Technological Horizons in Education, is published six times per year, and is available free on a limited basis. Other subscriptions are $15 per year. In addition to articles there are Calendar, News, new publications, software/courseware, applications and new products sections. Articles in recent issues include (1) "How to Set Up an Electronic Bulletin Board" by T. Lukas (September 1981, Vol. 8, No. 5, p. 50); (2) "Networking: What are the Alternative Systems" (September 1981, p. 61); (3) "One State's Approach to Computer Literacy" by Alice M. Kirchner (May 1981, Vol. 8, No. 4, p. 43); (4) "Computers and Education: The Genie is Out of the Bottle" (February 1981, Vol. 8, No. 2, p. 34); (5) "Getting From Here to There: The Status of Instructional Computing in Higher Education" by James W. Johnson (November 1980, Vol. 7, No. 6, p. 48); (6) "Microcomputers and Videodisc: Innovations of the Second Kind" by A.W. Molnar (November 1980, p. 58).

D. "The Journal of Computers in Mathematics and Science Teaching" is published quarterly by the Association for Computers in Mathematics and Science Teaching (P.O. Box 4455, Austin, TX 78765). The journal is sent free to members of the ACMST. The cost of membership is $7 per year. The first issue of this new journal appeared in Fall 1981. The Journal intends to include (1) descriptive uses of computers to enhance instruction, (2) tutorials on the use of computers for instruction, (3) reseraech studies on teaching with computers, (4) lists of available software, (5) reviews of software, (6) announcements of conferences and events, (7) bibliographies of articles, and (8) book reviews. The first issue contained considerable information of interest to chemistry educators, and included the following articles: "Computer-Based Methods in Chemistry" by J.J. Lagowski; "A Microcomputer-Assisted Presentation of Atomic Orbitals" by J.A. Petrich.

E. "Byte - The Small Systems Journal" is published monthly by McGraw Hill. The domestic subscription rate is $19 per year. The journal can be ordered from Byte Subscription, P.O. Box 590, Martinsville, NJ 08836. In addition to articles each issue contains letters, education forum, books received, software received, language forum, technical forum, education forum and programming quickies sections. Recent articles include (1) "The Microcomputer as a Laboratory Instrument" by Daniel Cosgrove (November 1981, Vol. 6, No. 11, p. 84); (2) "Animation in Computer-Assisted Instruction" by R.R. Eckert (July 1981, Vol. 6, No. 7, p. 358). This article featured animated graphics and sound from an audio cassette tape controlled by the program. Each issue of BYTE has a central theme with several articles devoted to the topic. The November issue featured Data Base Management Systems. The September issue considered Artificial Intelligence. The August issue considered Smalltalk - A Language for the 1980s. This journal is very popular. Both local colleges have had to place recent issues on the reserve shelves in order to prevent their disappearance from the library.

F. "Dr. Dobb's Journal for Users of Small Computer Systems" is published 12 times per year by People's Computer Co., Box E, 1263 El Camino Real, Menlo Park, CA 94025. A domestic 1 year subscription costs $21. This journal describes software. The October 1981 issue (Vol. 6, Issue 10, No. 60) included: (1) "TEK 4010: A Tektronix Simulator" by Anthony B. Skjellum. This article describes how to run Tektronix software on microcomputers and includes an assembly language listing for the Z80; (2) "BASIC-FORTH" by C.H. Ting. This is a program which demonstrates the principles involved in FORTH. The article includes a listing in BASIC; (3) "The Conference Tree - Computer Conferencing on Personal Computers" by John S. James. The September 1981 issue (Vol. 6, Issue 9, No. 59) was a special issue on FORTH.

G. ACM Publications - The Association for Computing Machinery is dedicated to the development of information processing as a discipline and to the responsible use of computers in an increasing diversity of applications. The ACM has a number of different publications.

(1) "Communications of the ACM" is published monthly. A subscription is included in the annual membership dues of $28 ($9 for student membership), $42 for non-members (Association for Computing Machinery, 1133 Avenue of the Americas, New York, NY 10036). This publication has a good calendar of events, articles on computing practices, Reports and Research Contributions. Most of the articles are of general interest to computer scientists but only of occasional interest to chemical educators. The June 1980 issue (Vol. 23, No. 6, p. 332) contained an article entitled "Computer Assisted Instruction: Current Trends and Critical Issues" by J.A. Chambers and J.W. Spreacher.

Of considerably more interest are the publications of some of the over 30 Special Interest Groups (SIGS).

(2) "Sigcue Bulletin" (a publication of the ACM Special Interest Group of Computer Uses in Education). This bulletin contains articles, a bulletin board containing news items, and reviews of books, periodical articles and ERIC titles, and a calendar. In the April/July 1981 issue (Vol. 15, No. 2 and 3) the Bulletin Board contained information on (a) Dartmouth College's exploration of videodisc technology educational uses (p. 19), (b) an educational interest group being formed by those using T.I. computers (p. 21), (c) Stanford's new MA program in Interactive Educational Technology which will combine courses in computer science, educational psychology and curriculum theory and design (p. 22), (d) A Microcomputer Registry of elementary, middle, and senior high schools (p. 24). Some articles of interest include: "Preparing On-Line Quizzes by Bork (October 1980, Vol. 14, No. 4, p. 2), "Good Courses Involve Computers" by A. Bork (July 1980, Vol. 14, No. 3, p. 3), "A Survey on Computer Assisted Instruction at the University of Texas at Austin" by C.S. Cavin, E.D. Cavin, and G.H. Culp (April 1980, Vol. 14, No. 2, p. 13), "Documentation in Computer-Based Instruction" by G.P. Kearsley and S. Hunka (January 1979, Vol. 14, No. 1, p. 3).

(3) "Sigucc Newsletter" (a quarterly publication of the ACM Special Interest Group on University Computer Centers) distributed free to members of ISGUCC (annual dues are $7.50 for ACM members) subscriptions are $15 for non-members. (SIGUCC, c/o ACM Headquarters Office, see (1) for address). This Newsletter serves as a way to develop and improve facilities and services in higher education. Articles of interest in recent issues are: (a) "Creating High Computer Impact in a Small Liberal Arts College" by B.L. Houseman (Spring 1981, Vol. 11, No. 1, p. 9); (b) "Directions of Computing in Higher Education - Predictions from University Computer Center Directors: The Results of a Survey" by J.L. Moss (Fall 1980, Vol. 10, No. 3, p. 5); (c) "Computing Uses in Higher Education - Some Opinions" by J.L. Moss (Fall 1980, p. 10).

This article will be concluded in the next issue of this Newsletter. If I have not mentioned some of the publications you have found useful, write to me (the editor) and I will include your suggestions in the next issue.