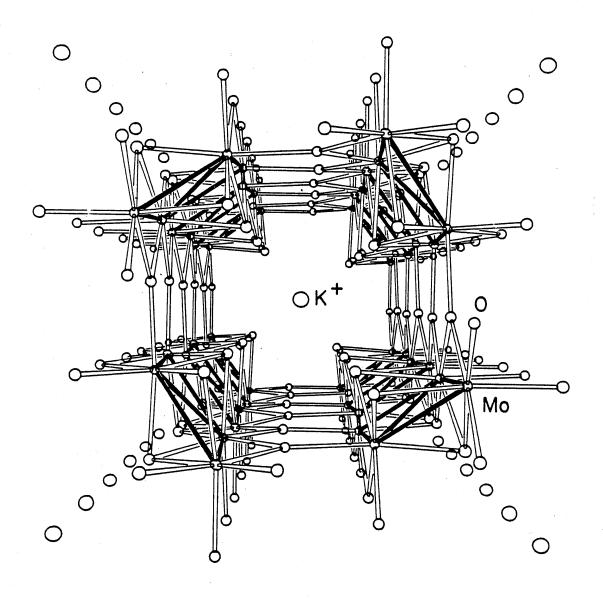
Computers in Chemical Education Newsletter

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Another small group consisting of representatives of each of the four subgroups prepared materials such as a suggested time schedule, checklists, forms, and sample flyer to assist presenters in the preparation and management of the workshops.

The package was tested by a second group of teachers who convened at Canterbury School in Connecticut immediately after the 8th Biennial Conference at Storrs. The details concerning the structure of these support packages are being finalized at this writing and will be described in the next issue of the Newsletter. What this all means, of course, is that the number of one-day workshops for high school teachers will increase dramatically during the next year, as each participant has agreed to give at least two. To make sure things work, the scheduling of workshops will be divided between two coordinators representing, eastern and western states. These coordinators will be identified in the next Newsletter. If you are interested in hosting a workshop this year, do not delay submitting a request. These workshops are certainly one of the most important projects of the Committee, judging from the reception they have been receiving.

EASING INTO INTERFACING

As noted above, laboratory instrument-computer interfacing appears to be one of the topics having considerable appeal at workshops and conferences on computers in chemistry. My own experience in this area is severely limited. There are obvious advantages to simultaneous data collection, processing and display. However, the development of software that makes all this possible for those of us who do not have the time or expertise to fashion our own has not proceeded at the same rate as the "traditional" applications such as CAI, drill-and-practice, simulations, etc. I do not believe this will be the case for long, as evidenced by discussions at EMU, Storrs and other conferences along with articles in the Newsletter concerning the ease with which one can interface and the potential applications of such techniques in the general chemistry lab at both the secondary and college level.

Early this summer, my interest in interfacing was greatly enhanced when I discovered the OHAUS "Brainweigh" B300, an electronic, top-loading, centigram, digital display balance with an RS-232 interface. A software package is available for this instrument that makes it truly simple to display objects on an Apple-driven monitor. Alternatively, a bar graph of the masses of a collection of up to 15 objects, or a time plot of changing mass can be displayed. Although I have not as yet had a chance to use the system in an actual teaching situation, there are many applications for a unit that can be set up quickly and that can measure a quantity that students can relate to immediately. For example, instead of talking about deliquecense or efflorescence, the change in mass can be shown dynamically by placing samples of appropriate substances on the balance. We can then explore questions such as "How will the growth/decay curve change if we pulverize the material?" "Will twice as much get heavier twice as fast?" A sample of cotton can be soaked with different solvents and the rate of evaporation related to such factors as molecular weight, vapor pressure, etc. Conservation of mass demonstrations can be brought to life in a variety of ways.

The programs in the Ohaus software package are in BASIC, and unprotected, thereby making it easy to adapt them to different applications.

The hardware is not inexpensive - the balance costs \$975, the supporting software package costs \$155 and it is necessary to have a serial card and a real-time clock in your Apple to make it all work. But since the balance itself and all of these 'extras' have additional uses, justifying the expenditure may be a bit easier. In any event, I think there is a lot that can be done with this system. More specific information is available from Jack Gardner, OHAUS Scale Corp., Florham Park. NJ 07932, 1-800-526-0659.

I plan to devote a good bit of attention to exploring appropriate uses of this equipment during the coming academic year and I'd be delighted to receive suggestions from anyone about demonstrations and/or experiements in which continuous on-line processing of mass data would be useful.

ON THE COVER

Dr. Charles C. Torardi of the Central Research and Development Department, E.I. duPont deNemours & Co., Wilmington, DE 19898 submitted a graphics representation of a compound with which he has worked. The figure gives a view down the c axis of K2M08016 (related to the mineral hollandite). Planar metal-metal bonded tetranuclear molybdenum atom clusters are present. In the figure, Mo-Mo bonds are represented by black solid lines and Mo-O bonds by open lines. Potassium ions occupy sites in channels that run parallel with the c axis.

The figure was obtained using the Oak Ridge Thermal Ellipsoid Program on a DEC 11/60 computer and a Hewlett-Packard 7221T plotter.

MESSAGE FROM THE CHAIRMAN

Earlier this year I was privileged to participate in two SERAPHIM sponsored events of significance orchestrated by John Moore at Eastern Michigan University. Both were highly successful, being characterized by a constant exchange of ideas and intellectual ferment, producing feasible suggestions to accomplish specific tasks.

The first was the Powow in May where past, present and future roles of computers in chemical education were analyzed by a diverse and dynamic assemblage, representing a wide range of experiences and viewpoints, particularly in terms of just how far computers can and should be expected to permeate pedagogical pursuits. Altogether, about 40 chemistry educators, research chemists, computer programmers, learning-theory experts, and representatives of computer-related companies participated. Dick Cornelius sparked considerable discussion when he introduced "GEORGE" (as in "Let ** do it"), a problem-solver designed to take students a quantum leap beyond the pocket calculator. The hardware picture of today, tomorrow and the near future was presented by Bill Butler and Scott Owen emphasized the fact that what we do with machines in the next decade depends primarily on our imagination and our ability to define what it is we really want to accomplish in our classrooms. As Stan Smith put it, "The world is over-populated with programmers who know how to make machines do anything, but who don't know what they want them to do." A summary of the symposium appeared on pages 34 and 35 of the June 25th issue of C&E News. Here it was reported that "Some of the recommendations fell into the 'pie in the sky' category, although computer technology has a history of bringing pie down to Earth, often in a surprisingly short time." Numerous specific recommendations emerged from the three day session, some of which may be implemented even by the time you are reading this - the CHYMNET conferencing network, for example. A more complete report will appear in the October issue of the Journal of Chemical Education (as computer series #55).

The second event, during the week of June 24 was a rather unique affair designed expressly for fourteen high school chemistry teachers. Instead of setting the traditional goal of orienting the participants in the use of computers in teaching chemistry, this week-long session aimed at training teachers to train other teachers. The plan was to first define the optimum format and then develop appropriate materials to be used in conducting one day workshops of the type currently being cosponsored by the CCCE and SERAPHIM (see information elsewhere in this issue).

The initial task to be accomplished involved prioritizing the multiplicity of topics which might be included in such a workshop. Ten possibilities were identified, discussed, and then rated, with four topics clearly emerging as "essential":

- Introduction to computers as instructional tools
- II. Evaluation of software through hands-on experience
- III. The use of computers in "support" roles such as word processing, spread sheets,
- IV. Computer/instrument interfacing

Recognizing that individually, any of the above could be the sole topic of a two or three day session, four subgroups were created to carefully analyze each topic and come up with a feasible approach for presenting it as only a segment of a one-day workshop. Once the approach was determined, handouts, software and other materials were assembled by each team to comprise a workshop "support package" to be provided to anyone who conducts a SERAPHIM-CCCE sponsored workshop.

Scientific Applications of the Apple Game Port Part II by Kenneth Ratzlaff*

In Part I of this series, which appeared in the June issue, the general approach to the applications of game ports was reviewed. In Part II, a number of potential applications will be described. In the third part of the series some experiments on the principles of data acquisition using game ports will be presented.

The Apple game port has two types of inputs: the paddle input and the button input. The paddle input is an Analog-to-Digital Converter (ADC) of a specialized type: the result of the conversion is proportional to the <u>inverse</u> of the input current. A linear result is obtained when a variable resistor is placed between it and a voltage source (Ohm's Law); in the case of an Apple II, a resistance of 0-150 k Ω between 5V and the input will generate readings between 0 and 255. The <u>button</u> input accepts a logic level encoded in "TTL" logic (approximated as OV = 'O' and 5V = '\frac{1}{1}).

Similarly, the annunciator outputs generate logic TTL levels which can be used to $\underline{\text{control}}$ external devices by turning them off or on.

In the following sections, a number of applications of these input and output units will be described. In many cases, the applications described have not been tested. The components that are required are available from Newark Electronics, 500 N. Pulaski Road, Chicago, IL 60624.

Analog (Potentiometer) Inputs

In this discussion, we will restrict ourselves to transducers (sensors) which are resistive and exhibit large changes in resistance. Three are naturals. The first is an ordinary potentiometer which is what the Apple paddle contains; the resistance is proportional to the rotary or linear position. The second is a thermistor whose resistance makes large changes with temperature. Finally, the photoresistor makes very large changes with light level. Most other resistive transducers, such as strain gages, make such small changes that a Wheatstone bridge is necessary to amplify the signal; the result is not easily handled by the paddle input.

<u>Potentiometers</u>. Potentiometers (pots) are used to measure <u>position</u>, a parameter less often measured in chemistry than in some other disciplines. However, some applications can be instructive.

The first and simplest example is a <u>pendulum</u>. Either the shaft or the body of a single-turn pot can be mounted in a stationary position; a rod with a bob is attached to the moving member. Since the full excursion of the pendulum will be about 120°, the pot should be selected so that angle will give 150 k Ω ; the closest commercial unit is 250 k Ω or 500 k Ω . Acquisition of readings as a function of time will produce the typical sine wave. Some attention must be paid to establishing a time base.

Potentiometers are used in weather monitoring. If the bob on the pendulum is replaced with a vane and a mechanism is constructed to position that vane properly with respect to the fluid (air) flow, the reading can be related to wind velocity. Pots exist which do not have stops; when rotation reaches full scale, the rotation can continue at 0Ω . Also, a vane attached to the shaft can sense wind direction.

A decade ago, ten-turn pots were used as transducers with strip-chart recorders. The string used to couple the pen with a servo motor was wrapped around the shaft of a ten-turn pot with an appropriately-sized Erector set pulley; the resultant resistance is proportional to the pen position.

Thermistors. Over a short temperature range, the resistance of a thermistor is inversely proportional to temperature. More exactly, the relationship is:

$$\frac{R_{o}(T_{1})}{R_{o}(T_{2})} = e^{\beta(1/T_{1}-1/T_{2})}$$

where the R_0 's are the resistance at the two temperatures T_1 and T_2 . A typical thermistor

(Fenwal GA45Pn, 50 $k\Omega$ at 25°C) exhibits the following resistances:

<u>T([©]C)</u>	$R(k\Omega)$
0	142
25	50
50	30
100	4.6

The proper thermistor for the temperature range is chosen by determining that the resistance corresponding to the lowest temperature does not exceed the range of the POT input. Conversion of the result to a linear scale is required, but that can and should be done in software. Two free sources of information on thermistors are the Thermistor Manual (Fenwal Electronics, POB 585, Framingham, MA 01701) and the Temperature Measurement Handbook and Encyclopedia (Omega Engineering, Box 4047, Stamford, CT 06907). Fenwal thermistors are available at reasonable prices from Newark.

Thermistors are extraordinarily versatile devices. The obvious application is for temperature monitoring. Since our simple configuration has no provision for offsets in the signal, it may be difficult to obtain sufficient sensitivity for such experiments as Heat of Solution; Harvey Blanck has set up a more sophisticated arrangement using an operational amplifier (see WHO-84) to generate an offset so that he can obtain a sensitivity of .002 °C! Our thermistor above will have a much smaller sensitivity.

Another method of obtaining an offset is shown in Figure 1. The offset is obtained

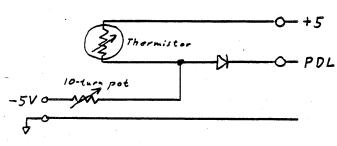


Figure 1

with a negative power supply. We can make some rough calculations (ignoring resistances in the Apple circuitry) by making the following calculations. To get a reading of about 85 on the Apple, we would need a resistance of 150,000 * 85 / 255 = 50,000. The current passed by that resistance is 5/(50,000) = .1 ma. Using a 5 k Ω thermistor at 25°, 5/(5,000) = .1 ma would flow. If we use a -5V power supply and a resistance of 5 k Ω , the thermistor current will be bucked out and the reading will be 255, but when the temperature increases by 1°C, the thermistor current will be about 1.1 ma and the net current will be .1 ma; the resultant reading is about 85.

Thermistors are also used to measure heat transfer by placing them in a self-heating mode. If the current through the thermistor can be increased, the thermistor will resistively heat itself (this is also a danger in any thermistor application). If the environment of the thermistor insulates it, the resistance will drop, but if the heat can be carried away by the thermistor environment, the resistance will increase. Two simple applications are use as a liquid level sensor and as an air speed indicator. Both can potentially be implemented with a 4 k Ω thermistor using a higher excitation voltage and a larger offset.

Photoresistors. The resistance of a cadmium sulfide photoresistor varies greatly with the light level, but it is, alas, too non-linear for quantitative spectroscopy applications. However, there may be some useful applications for which the linearity is only of secondary consequence. Consider the spectroscopic detection of a titration endpoint. In finding the point of inflection, the nonlinearity is not important. The optical arrangement will require some care to ensure that the proper proportion of light from the source reaches the detector. Also, the classic iodine clock reaction could be automated in some cases, photodiodes and phototransistors can be used with the POT input.

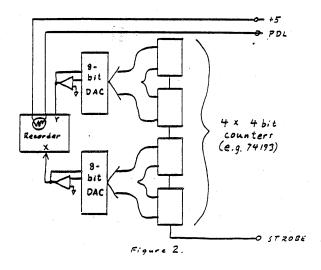
David Jordan (SUNY-Potsdam) sent a copy of an article about image processing (Ronald Peelen, Sky and Telescope, page 177, February 1984; see the editor's note in particular). The article outlines the construction of a drum and scanning unit used to scan a photograph with a quantitative photodetector, measuring the reflected light at each position to be displayed on the screen. The editor suggests the use of the photoresistor connected through the game port. The photoresistor might be rastered over the image by an X-Y plotter or digital plotter with the photoresistor in the pen position. The plotter can be controlled through the serial port to position the detector over any specified location on the paper. If an analog X-Y plotter is easier to obtain, the strobe output could be used to feed a counter which generates values for a pair of digital-to-analog converters (see the block diagram in Figure 2).

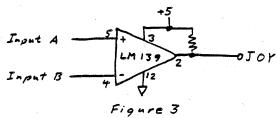
Physiologists have used photoresistors to measure heart rate. A red light-emitting diode (LED) is positioned to shine onto one's hand; the photoresistor detects the scattered light. Small changes in the amount of light scattered by the tissue occur with each heartbeat. However, the positioning of the components is critical, if the device is to operate satisfactorily.

SINGLE BIT DIGITAL INPUTS

How may the pushbutton inputs be used? If considered 1-bit analog-to-digital converters, a variety of applications is suggested. First, there are those phenomena which are either in position or out of position, such as the end of the travel of a stop syringe in a stopped-flow apparatus or a foot pedal to give a command to the computer when the operator's hands are full. The switch is connected between 5 volts and the pushbutton input, and these switches come in a host of configurations.

With any transducer, the signal either is or can be converted to a voltage between 0 and 5 volts; an integrated circuit comparator (such as a National Semiconductor LM139 in Figure 3) will output a '0' or '1' depending on which of the two inputs is greatest.

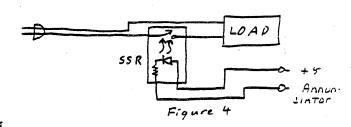




SINGLE-BIT OUTPUTS

Annunciator outputs are convenient for controlling switches. Sometimes, an instrument will include a "TTL" logic-level input to turn a function on or off, and the annunciator output can be connected directly to it. Sometimes, a modification of an instrument can be made. In many cases, the pushbutton on the instrument is comfigured to be a TTL input to the instrument's microcomputer. Then the annunciator output can be wired to that input so that when either one goes to ground ('0') level, the button function is actuated; and the computer can actuate any function now actuated by a pushbutton.

AC power is very easy to turn off and on from the annunciator output by the use of a Solid State Relay (SSR). The SSR is turned on when an internal LED shines onto an internal phototransistor, so the annunciator need only turn on the LED. The (+) terminal of the SSR module is connected to +5 volts, and the (-) terminal is connected to the annunciator; the LED goes on when the annunciator output is at ground level. Again, Harvey Blanck has an example in which a power supply is controlled from computer logic using an SSR. SSR's come in a variety of sizes to switch currents of a few milliamps to 100 amps.



OTHER GAME PORT I/O

Some computers, for example the Commodore-64, can handle many more bits of digital inputs which accept data in parallel. The Commodore has two connectors, each of which has 5 digital input bits marked JOYO, JOYI, JOY2, JOY3, and BUTTON. With 10 input bits, one can easily read data that are encoded in parallel such as the output of a panel meter. Another contribution from Harvey Blanck (WHO-85) illustrates how it can be done. Unfortunately, the Commodore game port has no output lines; either the parallel port that is provided or the cartridge slot may be easier to use for some applications.

Seed That Apple RND Generator! by Darnell Salyer*

Do your programs use the random number generator of the Apple? Have you "seeded" the generator to be sure the <u>same</u> series of random numbers is not used during each execution on your freshly activated microcomputer?

Writers of many computer assisted instructional programs for chemistry, including commercially available programs, have not taken measures to see that random number selection begins at a randomly chosen place in the fixed sequence of numbers accessed by RND(n). The oversight is quite likely if a program written for some other computer is modified for use on the Apple.

If an instructional program uses RND a variable number of times, as for example in branched tutorials which depend on user's answers or responses, a repetition of the sequence of random numbers used in the program will not be so readily apparent except when all responses are correct or all are incorrect.

If a CAI program calls for random numbers a fixed number of times regardless of the number of correct or incorrect responses, and if RND is not seeded, then a student user would see the same examples, unknown number, molecular weights or other data values, comments, "readings" in instrument simulations, graphics features, etc. each time he/she sits down at the microcomputer, turns it on, and runs the program. In like manner, two or more users would see identical CAI items upon first executions of a program.

Although dialects of Basic for minicomputers such as the Digital PDP 11/70 and for some micros, e.g. Radio Shack TRS-80, typically provide that a statement such as RANDOM or RANDOMIZE will achieve the seeding for an accompanying RND statement, that same provision was not made for the Apple. Unfortunately, this is not made clear in most of the Basic reference manuals this writer has seen. The Atari produces nonrepetitive sequences with RND (\emptyset) while RND(-TI) for Commodore machines takes its seed from an internal timer. The assertion that "every time" RND is used with any positive argument a new random number from \emptyset to 1 is generated is incorrect at least with respect to initial start-up. It should also be understood that simply changing the positive values for dummy argument \underline{n} of RND(\underline{n}) makes no difference since all give the same sequence upon initial use.

In an appendix of one widely used manual for the Apple, the intrinsic subroutine executed by CALL -756 is described very briefly. This will place a number between 1 and 255 in specified memory locations 78 or 79. The call executes as an input and the "seed" is placed when the program user strikes a key. Since most programs will usually contain early input statements, such as those asking for "press return" after directions, the call may easily be added to serve as the input.

1110 PRINT "PRESS RETURN WHEN READY TO CONTINUE";

1120 CALL -756

1130 FOR XX = 1 to PEEK (78): TA = RND(5): NEXT XX

For the Apple II+ a seed may be obtained from (78) or (79) even without the call, as long as the program has had one or more inputs prior to peeking. In such cases line 1130 alone gives entry to the random number sequence at one of 255 different places. A seed number of values is essentially thrown away and the next value would be the first used by the main program. The seed may be adjusted arithmetically.

In addition to CALL -756 another short machine language program was recently described which seeds the Apple RND and requires a keystroke. 3

Other means of seeding:

- a) If a program has required entry of a student name, the date, time, numbers or other information, the seed may be taken from an appropriate ASCII or VAL statement.
- b) If game paddles are in use a PDL(n) value may be read and used.
- c) A separate small auxiliary file containing a seed could be used with the program. The program opens the file, reads the number, increments the number, writes it back into the file and closes. Also, such a file could provide a record of program usage.

The seed obtained by any of these procedures is then used in some manner, as in line 1130 above, before the main program uses RND(n) for the first time. Diskettes with a menu for program selec-

tion such as those of the Seraphim project may have the generator seeding provision places in the menu to facilitate any program selected.

Sometimes it may not be possible to add the call and/or needed lines, especially if a program is copy protected or unlistable. It may be possible to execute seeding statements in immediate mode or with a short program from the same or another diskette, and then, without turning the computer off, RUNning or BRUNning the main program or the menu.

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- 1. Mansfield, Richard (ed.), "Zones of Unpredictability", in COMPUTE!, 5(11), 146-47 (1983).
- Poole, Lon et al., Apple II User's Guide, Appendix D, Osborne/McGraw Hill, 1981.
- 3. Isaacson, Mark, "The Missing Applesoft Random Number", in The Apple Orchard, 4(6), 76-77 (1983).

SERAPHIM-CCCE HIGH SCHOOL TEACHER WORKSHOP SERIES

The workshops have two basic objectives:

-To illustrate how microcomputers can be of use to a chemistry teacher

-To provide an opportunity to preview representative samples of commercially available software.

This is accomplished with a collection of software and supporting materials which currently includes all the SERAPHIM disks plus 150 commercial programs from 15 different publishers.

The guidelines for organizing a workshop are as follows:

PROJECT SERAPHIM and the CCCE will provide:

- A set of software and supporting printed materials.
- Publicity in national publications.
- A qualified workshop leader, when none is locally available.

The host institution is responsible for providing:

- A minimum of 10 Apple computers for every 20 participants.
 One large screen (23-25") color TV/monitor for every 15 participants with proper connectors to mate with the Apple output.
- An overhead projector and screen.
- Adequate meeting rooms to accommodate both the demonstration and the hands-on parts of the workshop.
- An assistant who is familiar with the hardware and facilities.
- Controls to make sure that copyrighted materials are NOT COPIED.

The cost of the workshop is \$10 per person with a minimum charge of \$200. If necessary, the workshop organizer can assess an additional fee to cover local costs (for refreshments, lunch, etc.). The CCCE will pay all shipping costs and expenses incurred in providing a workshop leader. For further information and application forms, contact Paul Cauchon at Canterbury School, New Milford, CT 06776, (203) 355-3452.

Hardware QUERIES

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

Software QUERIES and REPLIES

Software queries and replies should be sent to Ken Loach, Department of Chemistry, SUNY College, Plattsburgh, NY 12901, (818) 564-2230.

For a long time, chemists have had to make do with general purpose computer languages and software, written without the chemist's needs in mind. A pleasing feature of mid-80's computing is the growing number of lab-related high-level software systems now coming on to the market.

We need help in evaluating these packages. If any of you have any experience with the following systems (or any others of interest to chemical educators) please tell us of your experiences. Brief notes of full reviews will be welcomed.

SQ23 (Sept. '84)

Laboratory Technologies Corporation (328 Broadway, Cambridge, MA 02139) displayed their REAL-TIME Lab Notebook utility at the recent Pittsburgh Conference. REAL-TIME is a data-analysis package, suitable for instrumental interfacing. It is used in conjunction with Lotus 1-2-3, the widely used spread-sheet data system. The package can be used for data analysis, storage, transformation, statistical analysis and report generation. It is currently available for the IBM-PC (256 k memory) and will be available in other versions. Does anyone have any experience with this utility? (K.L.)

SQ-24 (Sept. '84)

Elsevier Science Publishers (52 Vanderbilt Ave., New York, NY 10017) introduced their new line of laboratory-oriented software packages at the recent Pittsburgh Conference. They are implemented in various languages (several Basics and UCSD Pascal) for several micros (HP, Apple and IBM, so far). Each is intended for teaching or application of modern data-analysis methods, with emphasis on optimization and non-parametric statistics. CHEOPS allows optimization of general experimental conditions by either of two simplex optimization methods. CLUE classifies analytical datasets by hierarchical clustering techniques, so that samples can be classified as to their degree of similarity. BALANCE compares paired data-sets, with interactive guidance toward choice of the most suitable statistical test. INSTRUMENTUNE-UP uses simplex optimization to guide the adjustment of multi-control instruments to their best operating conditions.

All of the above packages are supplied with fully documented source-code, allowing inspection of the algorithms and the possibility of source-code modification. Does anyone have any experience with any of these packages? (K.L.)

WHO DONE IT?

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

WHO-84 (Sept. '84)

A typical 4 1/2 digit panel meter (Non-Linear Systems PM-450) was interfaced to a VIC-20 using the joystick interface lines by Harvey Blanck (Department of Chemistry, Austin Peay State University, Clarksville, TN 37044). The circuit is general enough to be used with most instruments that have BCD outputs. (K.R.)

WHO-85 (Sept. '84)

An interface for a heat of solution experiment using a VIC-20 has very high sensitivity (.002°C) and precision control of the heater. Harvey Blanck (see address in WHO-84) uses a thermistor in a Wheatstone bridge with a differential amplifier to amplify the signal before digitization through the paddle input; by increasing the size of the output resistor, the circuit could be adapted to the Apple. A bit on the user port controls a solid-state relay to control a power supply for the heater. (K.R.)

WHO-86 (Sept. '84)

J. Schwarz had a review of CAI languages and systems in the first issue of the new periodical "Machine-Mediated Learning". This new publication deals with all aspects of instructional machinery and is aimed at managers and researchers in CAI and related fields (published by Crane, Russak and Co., 3 E. 44th St., New York, NY 10017). (K.L.)

WHO-87 (Sept. '84)

"Analytical Instruments and Computers" is a new controlled circulation periodical. Anyone wishing a free subscription should apply to: Bob Loeffler, Cleworth Publishing Co., Analytical Instruments and Computers, One River Road, Cos Cob, CT 06807. (K.L.)

WHO-88 (Sept. '84)

Douglas I. Relyea (Crop Protection Synthesis, Uniroyal Chemical, Nagatuck, CT 06770) gave a recent ACS NERM paper on his TRS-80 MOLGEO system for molecular geometry calculations and displays. Molecular coordinates for up to 50 atoms can be translated into molecular graphics with rotational and stereo transformations as needed. (K.L.)

WHO-89 (Sept. '84)

Frederick L. Lisman (Fairfield University, Fairfield, CT 06430) gave an ACS NERM paper on the Fairfield University chemistry department's CHEM-COURSE system. It is written mainly in APL for the DEX20, and makes use of the DEC Gigi terminal and the Regis graphics language. (K.L.)

WHO-90 (Sept. '84)

Bhaisav Toshi (SUNY College, Genesco, NY 14454) gave an ACS NERM paper on his APL system for CAI in physical chemistry and mathematics. His use of CAI stresses the provision of powerful calculation capabilities to the student and makes clever use of color-coding and screen-position coding in the screen-display. (K.L.)

WHO-91 (Sept. '84)

Professor D.F. DeTar (Department of Chemistry, Florida State University, Tallahasee, FL 32306) invites authors to submit papers to "Computers and Chemistry" on research-level aspects of chemical computation; including algorithms, new hardware and software, and evaluations of existing hardware and software. The periodical publishes many matters of interest to chemical educators (but does not deal with strictly pedogogical chemistry such as testing preparation, grading and CAI). (K.L.)

WHO-92 (Sept. '84)

James J. Filliben (Center for Applied Mathematics, National Bureau of Standards) has developed the "Dataplot" language and interactive system for the statistical analysis and graphical presentation of experimental data. Dataplot is available through the National Technical Information Service (NTIS) and can be run on most mainframes and superminis and with a wide range of graphics terminals and plotters. (K.L.)

WHO-93 (Sept. '84)

David Balaban, Julia L. Wang and Jack W. Frazer (Lawrence Livermore National Laboratory, P.O. Box 808, L-311, Livermore, CA 94550) have developed a data analysis system called "Dmodel" (Analytical Chemistry, 1983, 55, 900-904). This system is functionally a subset of "Dataplot" (see WHO-90, above), but was developed independently of it. "Dmodel" is sufficiently small to run on any PDP11 or LSI11 mini- or microcomputer. (K.L.)

WHO-94 (Sept. '84)

T.P. Walters (Chemistry Department, St. Olaf College, Northfield, MN 55057) presented a paper on data-telemetry with a personal computer at the Spring ACS Meeting in St. Louis. (K.L.)

WHO-95 (Sept. '84)

The Spectroscopy Society of Pittsburgh operates an audio tape-cassette library with over a 1,000 cassettes and 30 films on different topics. The library has recently acquired all the computer software available from SERAPHIM. They are considering adding other computer software. These materials can be borrowed by schools, colleges, laboratories and others in the scientific community. In addition to materials which should be of interest in many different chemistry courses their approximately 90 page catalog lists materials relating to computing including the Prentice-Hall Media slide-cassette Introduction to Microcomputers (in 3 parts), Computer Programming Basic (in 3 parts), Computer Programming (5 parts), Introduction to Computers and Data Processing (in 4 parts) and Handling and Processing Information (in 5 parts). All materials may be borrowed. The user must pay return transportation costs. Write to Edwin S. Hodge, SSP Film and Tape Library, 3133 Glendale Avenue, Pittsburgh, PA 15227, (412-882-6636) for further details. (D.R.)

WHO-96 (Sept. '84)

The July 1984 issue of SIAM NEWS (vol. 17(4), p. 8) contains an article on the IBM Project at Carnegie-Mellon. Several thousand personal computer workstations each between 20 and 100 times more powerful than current home computers are scheduled to be in place by 1986. Seven thousand should be installed by 1990. The objective is to fully integrate computing into undergraduate and graduate curricula. The workstations will eventually be part of a network which will provide shared central storage, electronic mail, data and program sharing, document transfer and connection to the university's mainframe computers and national networks. Each personal computer workstation will be a 32-bit processor capable of executing one million instructions per second and will have one million bytes of random access memory, a virtual memory operating system, high-resolution bitmap graphics, graphical input, audio output, video display and keyboard. (D.R.)

WHO-97 (Sept. '84)

The May/June issue of Access (Vol. 3(3), p. 24-34) features an article by Robert T. Kintz entitled "Turning Your Computer into a CAT: Signal Averaging on a Microcomputer". The article contains listings of the assembly language and BASIC programs used by the author with his Ohio scientific microcomputer. Also, this issue of Access contains on p. 41-44 a description and BASIC listing of a program which calculates the molecular weight and percent elemental composition of a compound, when the molecular formula is entered. (D.R.)

WHO-98 (Sept. '84)

The July issue of Communications of the ACM (Vol. 27(7), p. 638-648) contains an interview with Andres van Dam entitled "Computer Graphics Comes of Age". This article summarizes major advances in computer graphics over the past 25 years. (D.R.)

WHO-99 (Sept. '84)

The September 1984 issue of Scientific American is a special issue on computers and contains many general articles of interest. (D.R.)

BOOK REVIEW

Alan Smith (Chemistry Department, University of Southern Main, Porland, ME 04104) has served as Book Review editor since December 1982 and contributed a great deal to the success of this section. Because of the pressure of other activities, Alan has asked to be relieved of his duties as editor. I am pleased to announce that Dr. Harry E. Pence (Department of Chemistry, State University College, Oneonta, NY 13820) has agreed to serve as editor beginning with the December issue. Anyone willing to review books for the Newsletter or wishing to suggest books for review should communicate directly with Harry. (D. Rosenthal)

The Fifth Generation—Artificial Intelligence and Japan's Computer Challenge to the World by Edward A. Feigenbaum and Pamela McCorduck Addison-Wesley, 1983, 288 p., \$15.95

One Jacob Way, Reading, MA 01867

ISBN 0-201-11519-0

Reviewed by Brian Pankuch*

I don't know about you, but the idea of artificial intelligence has never been particularly appealing to me. Perhaps because many articles and books consist of long winded arguments on whether systems can or will be able to 'think". Being fortuitously snowbound, thanks to an unseasonable snowstorm, I found myself quickly engrossed in this very readable book. Feigenbaum is a leading computer researcher and McCorduck an experienced science writer in this field. Their collaboration is hard to put down.

For instance, the movement from general theories on learning to using specific knowledge bases in real applications is described. What is the difference between a data base and a knowledge base? An example of a data base is a compilation of the known facts on a given molecule, versus a knowledge base which would include the data base plus all you learned in graduate school, specialized courses, from journals, from actual practice and experience on molecular structure. The knowledge base would be much more complete, not just facts, but how to use the facts.

Use of a knowledge base with appropriate programming gives an expert system. In use these expert systems have given medical diagnosis comparable to that of a specialist and above the level of a nonspecialist physician. One system created at Stanford, DENDRAL, infers chemical structure and data and provides details of molecular structure which exceeds the human designer's capability.

The systems seem to work best on projects which require large amounts of specific know-ledge. These systems which use the appropriate information to solve a problem can save a lot on the cost of data collection and analysis. At their best, they function as an intelligent assistant and can explain lines of reasoning taken or why certain paths were not taken. They seem to work well where a lot of reasoning is needed.

I found the approach taken by a knowledge engineer, the person who is the kingpin in putting the expert system together, particularly interesting. First a specialist in a given field must be convinced to spend a lot of time with the knowledge engineer. Both work together on a substantial problem in the specific field. Often the specialist first gives the textbook version of the solution. The expert system written on this basis generally doesn't work well. Next the knowledge engineer watches how the specialist actually manipulates the data - not how he says he does it, how he actually does it. This is where the difficult part, the heuristic part, (where to go by the book and where to ignore the usual) comes in.

The knowledge engineer's job is so difficult and critical that many believe it must be automated if expert systems are to succeed in general.

Where does the Japanese challenge come in? The Japanese have a ten year plan to build a fifth generation computer which includes these expert systems and the ability to be programmed in a natural language. Other Japanese challenges have certainly displaced workers in autos and electronics, but resulted in a more efficient marketplace with a wider choice of products for consumers. Is this challenge different?

The authors argue persuasively that the results of this race are much more important and will drastically affect leadership in the information society to come. Or perhaps more important, they and we may be the ones to lose our jobs this time. In the future, our country could lose one of the few areas of excellence we have left. Some interesting statistics: Japan has five times the engineers, 1/20 the lawyers, 1/7 the accountants as the U.S. on a per capita basis.

To put the book in perspective, I tried to interest my better half in reading it, but the immediate demands of changing plans for her Brownie troop took precedence. A ten year competition is hard to take seriously; the Brownie troop is much more immediate. All views on sweeping national and world forces and future events are certainly arguable, but this is an interesting book to read. I recommend it highly.

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

> MS-DOS and PC-DOS User's Guide by Peter Norton Robert J. Brady Co., 1984, 250 p., \$15.95 Routes 197 & 450, Bowie, MD 20715 Reviewed by Harry E. Pence*

Microsoft's microcomputer disk operating system, MS-DOS, is not only widely used on IBM-PCs under the name PC-DOS but is also a common operating system on many of the other 8088/8086 based personal computers. The new versions of MS-DOS, such as DOS-2.0 and DOS-2.1, include many new features that have improved the power and flexibility of DOS but have also made it more complicated for the novice to learn. This book is intended to teach the fundamentals of DOS and also to suggest ways in which the system can be employed most effectively.

Norton's book has been designed to satisfy a broad range of DOS users. It discusses not only the IBM version of the operating system, but also the alternative forms of the various commands that are found on other IBM compatible personal computers, such as Columbia, Compaq, etc. In addition, commands that appear only in the 2.x versions of DOS are placed in bold-faced type, to accommodate readers who are still using older DOS versions such as 1.10 or 1.25.

Norton utilizes the analogy of an office worker's desk very effectively to introduce the basic concepts which are needed to understand DOS. The disk storage is explained as being like a filing cabinet, the computer memory like the desk top, etc. These explanations are very clear and important ideas are reinforced by cartoons, some of which are rather clever. Unfortunately, I did not find the book encourages the type of hands-on approach that I prefer. Even though the author suggests that the reader should try various techniques on the computer, the text does not provide the type of assistance that is normally needed by someone who is working with a computer for the first time.

In the Introduction, the author promises that the book will not only describe how to get started with DOS but will also provide practical advice about how to use a personal computer and what types of software are best to buy. Peter Norton is an experience computer consultant who is well known both for the Norton Utilities software package for the IBM-PC as well as because of his many articles in computer magazines, and so his opinions deserve careful consideration. He covers topics such as how to choose software, copy protection, advantages of hard disks over floppies, and the best programming language to use. Most of his suggestions are not profound, but they should provide helpful guidance to someone just beginning to work with a computer as well as some interesting food for thought for all users.

The book offers an excellent coverage of some of the advanced features of DOS. Potentially one of the most useful sections of the book is the discussion of batch files. Batch files can replace a number of DOS instructions with a single command, and so they are a convenient way to save a great deal of typing. More important, they can be set up to provide some protection against incorrect commands that can cause the loss of data. There is good discussion of some of the new UNIX-type features, such as re-direction, filters, and pipelines. Norton provides a description of EDLIN, the DOS text editor, that should be quite adequate for most purposes. However, he suggests that readers should use a better editor than EDLIN.

Since this book seems to be rather clearly aimed at beginners, it is no surprise that not all of the advanced DOS techniques are equally well discussed. Topics related to hard disks are scattered throughout the book, rather than being grouped together in one or two places, and the explanations would be clearer if they included more specific examples to show how the techniques actually work. In certain circumstances, it can be very valuable to reconfigure the system, but Norton doesn't discuss how this can be done with the new versions of DOS.

Norton has written a clear description of the important features of DOS that will probably be useful to a broad range of computer users, but in order to achieve this breadth, he has sacrificed some specificity. The strongest features of the book are the use of everyday analogies to clarify basic concepts of DOS and the equally down-to-earth advice on how to set up a new computer system. If you are using PC-DOS 2.0 or 2.1 on an IBM machine, you may well wish to consider a book that deals specifically with your system, but if you cannot find a book that fits your situation, or if you are a beginner and wish to obtain a general understanding of how DOS works, this is a book that you should consider.

*Professor of Chemistry SUNY-Oneonto Oneonta, NY 13820

> PC ODS User's Guide by Chris Devoney Que Corporation, 1984, 330 p., \$12.95 7960 Castleway Drive Indianapolis, IN 46250 Reviewed by Harry E. Pence*

This book was designed with a specific purpose in mind: to teach a beginner how to use both basic and advanced features of PC-DOS version 2.0 on an IBM personal computer. Throughout most of the book, the author uses what I would consider to be a true hands-on approach. He explains what the reader should type in at the keyboard as well as what response is expected from the computer, using different type fonts to identify which is which. There is even an explanation of the common error messages at the back of the book to make it easier to correct mistakes.

Like many other authors I have read, Devoney urges all users to change to the new versions of DOS in the 2.x series. He suggests several reasons for this, including the increase in minifloppy disk storage, the greater convenience of the new commands, and the improved speed of disk operations. In addition, the newest software products will probably utilize the more powerful features of the latest DOS releases, and so will require the changeover.

Although this book is designed to teach DOS 2.0, it should be equally useful for the latest release, PC-DOS 2.1. As far as I can determine, the only difference between these two is that the new release fixes some bugs in the old version and also changes the disk reading procedure slightly to prevent data loss on PCjr's that use PC-DOS. No commands seem to have been added or deleted.

DeVoney covers all of the common DOS commands, including their most useful switches, and discusses all of the important advanced topics. The presentation is excellent throughout, and the topics are treated in a logical order. In particular, the discussion of the hard disk related commands, such as BACKUP, and RESTORE, are quite clear and include step-by-step explanations of the concept. This is also true in the treatment of hierarchical directories, where the example sets up and revises a multiple level directory. There is one error in this latter section, where an MK is written instead of an MD, but otherwise I found very few errors in the book.

In older versions of DOS, the only way to change the configuration of the operating system was by means of a special routine written in assembler. The new versions allow this to be done by simply changing the system configuration file, CONFIG.SYS. With this procedure, it is easy to increase the number of disk buffers for improved random disk access, to install a device driver to control peripherals, or to make other modifications. DeVoney discusses this technique and also the use of the MODE command to change the set-up of the computer. The choice of topics is very good, except that I wished that he had included some discussion of device drivers.

DeVoney has designed the book carefully so that it not only is good for learning the system but also serves as a good reference. Many types of information are summarized in easy to read tables, and approximately a third of the book is a summary of all of the PC-DOS commands. This is not simply a copy of the DOS documentation, but rather an expanded treatment of each command which includes probable error messages, a listing of switches, special rules, and useful notes.

This book is intended to do a definite job, and it accomplishes this task very well. Those who prefer a hands-on approach to learning about the computer and wish to learn specifically about applications of version 2.0 or 2.1 of PC-DOS on an IBM-PC should find this to be a worthwhile book.

*Department of Chemistry SUNY - Oneonta Oneonta, NY 13820

FOOD FOR THOUGHT

The electronic computer bridges all segments of our spectrum of change, raising — and solving — problems in each.

Its sociological effects will derive from its tremendous potential as a decision maker and from its application in the field of automation. It will free the productive processes of industry from dependence on the labor of human hands and the thought of human minds. It will solve problems; it will create others.

Could a computer be built, capable of weighing legal evidence, making it possible to circumvent the factor of human error? The idea is not so farfetched as it might appear. The computer has already been introduced into the administrative machinery of the income tax, where it has taken over some of the functions of judge, jury, and executioner. Fearful as we may be of its merciless analysis, we must admit its impartiality.

Extension of this idea leads me to suggest the coinage of a new word, cybernocracy, meaning government by computer. Imagine, if you can, a computer sitting in the White House, optimizing the political well-being of each of us. We would continue to vote every four years — not for one program as opposed to another, but for or against a change of programming, and whether to the right or to the left. All of which leads logically to a fascinating concept that might be called differential cybernocracy: a state of political Nervana where change is always possible but revolution impossible — unless someone pulls the plug on the computer!

B.D. Thomas Science and Society: A Symposium, 1965.

WORKSHOPS, MEETINGS, CONFERENCES & COURSES

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

- August 26 31: ACS National Meeting, Philadelphia, PA
 Symposia and sessions are planned on New Techniques in Data Acquisition, Computer
 Searching by Academic Chemists, Chemical Reaction Databases, and Computer Sotware
 Techniques in NMR, etc. See July 9th issue of C & E News for full program.
- September 6 8: "Personal Micromputer Interfacing and Scientific Instrument Automation", VPI and State University, Blacksburg, VA 24061.

 Hands-on workshop with each participant wiring and testing interfaces constructed using STD bus cards. Directed by David E. Larsen, Dr. Paul E. Field, Dr. Jonathan A. Titus and Dr. Christopher Titus. Registration fee \$495. Contact Dr. Linda Leffel, C.E.C. at the above address, (703-961-4848).
- September 16 21: "11th Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies" at the City Line Marriott, Philadelphia, PA.

 Symposia and sessions on Computerized Quantitative Infrared Analysis, New Software and Hardware Methods in Analytical Chemistry, Computer Aided Technology, etc. An ACS short course on Electronics for Laboratory Instrumentation by Malmstadt, Enke and Crouch precedes the conference (9-14 to 9-15). FACSS XI workshop on Personal Computers in the Analytical Laboratory by Leyden, O'Haver and Staab (9-17).

 Preregistration fee is \$55. Workshops are extra. Contact Bruce Chase, E. I. du Pont, Experimental Station, CR&D 328/126, Wilmington, DE 19898 (302-772-4434).
- September 16 21: "Microcomputer and Minicomputer-Interfacing and Applications" at Continuing Education Center, VPI and State University, Blacksburg, VA.

 ACS Laboratory Short Course: Course revised to include lectures on local area networks, laboratory information systems, molecular design processing, electronic notebook, robotics in the laboratory, use of graphics, image analysis, voice I/O, expert systems and managing the electronic laboratory. Directed by Dr. Raymond E. Dessy. Course repeated December 9 14 and March 10 15, 1985. Contact Harold Walsh, ACS Educational Activities Office, 1155 Sixteenth Street, N.W., Washington, D.C. 20036, (202-872-4508).
- October 26: "Word Processing Packages Evaluation" sponsored by NERComP at Trinity College, Hartford, CT.

 Evaluation, critique and demonstration of word processing packages on personal computers. Registration fee \$60 for NERComP members. \$120 for educational institutions and non profit organizations. Contact NERComP, 439 Washington Street, Braintree, MA 02184 (617-848-6494).
- October 28 November 1: "Second International Congress on Computers in Science", Washington, DC sponsored by Science Magazine and Scherago Associates.

 The conference will emphasize the use of the workstation by the scientist. Talks in a number of areas including computer aided molecular design, workstation hardware, artificial intelligence, databases, laboratory automation and robotics. There will be poster sessions, workshops and a vendor exhibition. Conference chairman is Dr. Stephen R. Heller, EPA, PM-218, Washington, DC 20460 (202-382-2424).
- November 8 10: "Ed Comp Con 84 Conference" sponsored by the IEEE Society at the Convention Center, San Jose, CA 95101.

 CAI and educational uses of computers will be strongly emphasized. Contacr M. Dundee Maples, P.O. Box 525, Cupertino, CA 95015 (408-352-1402).
- April 28 May 3, 1985: ACS National Meeting at Miami Beach, FL Symposia and general papers. Abstract deadline is December 15th. General chemical education papers should be sent to Howard Moore, Florida International University, Miami, FL 33199. CHED meeting chair is Richard Steiner, Department of Chemistry, University of Utah, Salt Lake City, UT 84112; (801-581-6681). A symposium on Bachelor Degree Programs in Computational Chemistry is being organized in the Division of Computers in Chemistry by Dr. Peter Lykos, Illinois Institute of Technology, Chica-Chicago, IL 60616 (312-567-3430). Those in departments which have developed strong minors in computer science or computer engineering may wish to participate. Inquiries, titles and abstracts should be sent to Professor Lykos by November 1st.

The Biennial Workshops sponsored by the ACS Division of Chemical Education's Committee on Computers in Chemical Education and Project SERAPHIM will be held at two locations. One set of workshops will be held at Clarkson University in Potsdam, New York. The second set of workshops will be in Southern California. The planning for these workshops has not yet been completed. Registration forms and further information will appear in the December issue of the Newsletter.

The eastern meeting will begin at noon Sunday, July 28, 1985 and end at noon Thursday, August 1, 1985. Six workshops are being planned: Getting Started with a Computer; CAI Program Design and Development; Introduction to Pascal; Computer Graphics; Microcomputer Interfacing; and Electronic Spreadsheets, word Processing, Numerical and Statistical Methods. This meeting is being chaired by Donald Rosenthal, Department of Chemistry, Clarkson University, Potsdam, NY 13676 and a twelve member organizing committee has been established.

The west coast workshops will be held later in August 1985 and will be somewhat different in format from those in the east. This meeting is being co-chaired by Professor William V. Willis, Department of Chemistry, California State University, Fullerton, CA 92634 and Professor Oliver Seely, Department of Chemistry, California State College, 1000 E. Victoria Street, Dominquez Hills, CA 90747. In order to assit the organizing committee, those who are interested in attending the west coast workshops are asked to fill out and return a copy of the questionnaire presented below.

	WEST COAST COMPUTER WORKSHOPS QUESTIONNAIRE
1.	
	Computers in Chemical Education Workshop in Southern California in the week of (check one August 19, 1985 () or both):
2.	I am interested in obtaining hands on experience with the following computers (check all that apply):
	() IBM PC () Apple IIe, II ⁺ () Macintosh () PDP 11 () Columbia () Other (name)
3.	I would prefer a one, two, or three day workshop on the following topics (check all that apply):
	Topic 1 day 2 day 3 day
	Getting Started with Computers () () () Interfacing () () () Computer Assisted Construction (CAI) () () () Authoring Software () () () Graphics () () () Word Processing & spread sheets () () () Data Base Management () () () Molecular Design () () () Pascal () () () Other (name) () () ()
4.	I would also like to have the following activities at the workshop site: Poster sessions () Software demonstrations () Other
5.	I have attended other ACS Computer Workshops Yes () No ()
6.	I prefer: A. Concurrent workshop sessions on different topics () B. A sequential offering of individual workshops ()

PLEASE RETURN THIS QUESTIONNAIRE TO PROFESSOR WILLIAM V. WILLIS (address above)

SOFTWARE LIST

Instructional Computer Programs--Chemistry Fourth Edition

Prepared by

Project SERAPHIM, NSF Science Education

John W. Moore, Director

J. J. Lagowski, Co-Director

Elizabeth A. Moore, Project Manager

The Project SERAPHIM SOFTWARE LIST has been revised, enlarged, and indexed as of July 1984. It now lists nearly 300 programs, is over 90 pages in bulk, and has a bright orange cover. It is obviously too big to have as a "part" of the CCCE Newsletter. To obtain a copy, still at the bargain price of \$5, send a check in that amount and payable to Project SERAPHIM to:

Project SERAPHIM
NSF Science Education
Department of Chemistry
Eastern Michigan University
Ypsilanti, MI 48197

Persons with programs to be added to this list may do so by writing to the Project and asking for the form: Survey of Instructional Computer Programs in Chemistry.

(OVER...)

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Department of Chemistry; Eastern Michigan University;
Ypsilanti, MI 48197; (313) 487-0368; 487-0106.