these programs and sample data files, as well as a similar set of programs for a Beckman DBG UV/vis spectrometer, send a blank disk and a check for $10 to George Lisensky at the address above.

Microcomputer-Controlled Cyclic Voltammetry

Robin J. Ontko, Raymond N. Russell, and Paul J. Ongren[5]
Earlham College
Richmond, IN 47374

Cyclic voltammetry is both a powerful tool in analytical chemistry and an attractive experiment for teaching a number of concepts in electrochemistry, as pointed out by a number of recent articles in THIS JOURNAL (*5–8*). This note describes construction of a simple CV system using a microcomputer both for control of the cycling voltage and for reading the response current. This system has been used for CV experiments in analytical and physical chemistry courses. It has also provided lab experience with interfacing and some basic electrochemical instrumentation principles in more advanced courses.

The essential components of the system are a conventional three-electrode potentiostat and an Apple II microcomputer with an Interactive Microware ADALAB™ interface

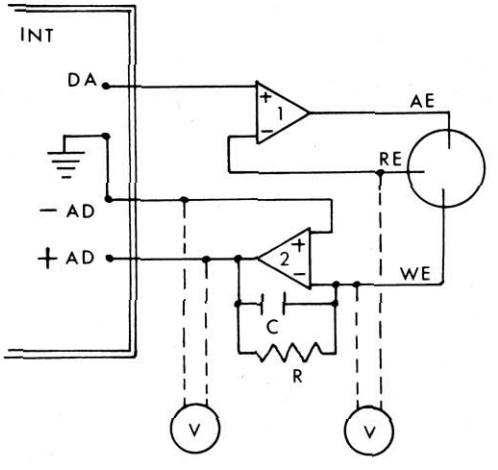

Figure 8. Circuit layout for the CV system. INT: Interface connectors (DA: digital-to-analog output; AD: analog-to-digital input). Op amp 1: voltage follower for driving voltage; op amp 2: current amplifier section. AE: auxilliary electrode; RE: reference electrode: WE: working electrode; C: 47 pf; R: 4.7 KΩ; V: optional voltmeters.

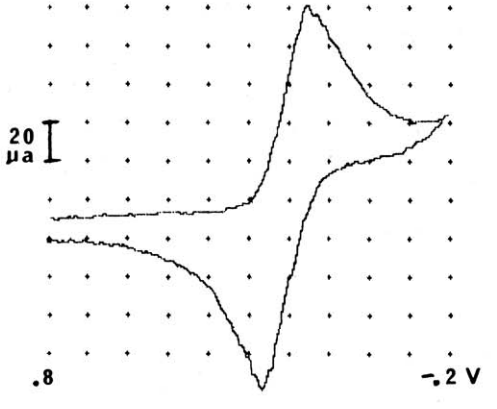

Figure 9. Screen dump of CV plot for m$M$$K_3[Fe(CN)_6]$ in 1 $M$$KNO_3$ (cf. ref. *7*). Initial hold time: 20 s, cycle time: 22 s. Scale values added.

card for D/A and A/D conversion.[2] A diagram of the circuit is shown in Figure 8. A reference SCE electrode, a Pt wire auxillary electrode, and a ~4 mm^2 Pt surface electrode were assembled to fit into a 30-ml beaker equipped with bubbler and magnetic stirrer. The amplifier circuits were constructed following Diefenderfer (*9*) using inexpensive 741 operational amplifiers. The 4.7-K resistor in the current amplifier section was chosen to lessen the chance of too large a signal entering the interface board, whose design limit is ±12 V. This can be replaced with a variable resistor to increase the range of the instrument. For convenience, the circuit was assembled on an Op Amp 2 Designer breadboard (E&L Inc.), which also served as the ±15 V power supply. The voltmeters, dashed in as options, are strongly recommended both as a quick indicator that the desired voltage cycle is actually appearing across the working and reference electrodes, and as a monitor on the current amplifier output voltage. Inexpensive digital voltmeters were used for this purpose.

The ±2-V input and output range settings of the ADALAB board are normally used. Output and input resolutions are 12 bit, including sign, so that there is no serious resolution problem for normal scan ranges of several tenths of a volt. The applied potential is controlled and the current response is read through a simple Basic program that uses a machine language routine, QUICKI/O™, to control the interface. A preliminary loop accepts a user-selected hold time to stabilize the system at the initial potential of a cycle. A second loop is then used to cycle the applied potential and to acquire 250 voltage readings from the current amplifier at equally spaced times. The applied potential necessarily changes in steps in this system rather than in continuous fashion. In order to approximate a continuous change best, these steps are kept as small as possible and the voltage is then incremented several times between readings of output current. The program calculates the magnitude of each step from the cycle time (user selected), the total time required for 250 input readings, the time required for each output change, and the total voltage change. A step size of 1 mV is typical for scans such as that shown in Figure 9. The part of the program necessary to obtain this type of data is about 30 lines long; a full program listing is available upon request.

In operation, the electrodes are immersed in the desired solutions and the control program is started to insure an applied voltage of 0 *before* the amplifiers are turned on. This avoids supplying an unpredictable voltage input and the possible consequence of a damaging voltage output. As an additional protection feature, the program also returns the drive voltage to zero if excessive currents are produced during a run. The typical CV screen plot shown in Figure 9 may be compared with previous publications in THIS JOURNAL (*6, 7*). The program does not plot the first three points of each scan since these often show relatively large current transients due to capacitance effects. While a grid has been added for ease of locating peak voltages and currents, the student must supply the voltage limits, and use computed peak current values to interpret the vertical scale. This particular system can also take advantage of available software to add a labeled and numbered grid if desired.[6]

Given a microcomputer such as an Apple II+ or IIe, and a good dc power supply, the principal additional cost of the system is the ADALAB board, about $500. For routine work, a commercially available unit such as the Bioanalytical Systems Model CV-1B provides advantages in terms of speed, sensitivity, stability, and convenience at a comparable cost. The present system, on the other hand, produces CV scans of reasonable quality, and in addition exposes students to laboratory interfacing and some principles of instrumentation.

[5] Author to whom correspondence should be addressed.

[6] Sciplotter II™ from Interactive Microware, Box 139, State College, PA 16804.

In our program, it is also advantageous to have the same computer and interface available for collecting data from other types of experiments such as emf titrations or gas chromatography. Given the principles of microcomputer control of the applied potential, as well as the capacity for reading the response signal, extension to other voltammetric experiments is an obvious possibility.

MOLDOT: Space-Filling Perspective Diagrams of Molecules

Steven Brumby
Australian National University
Canberra, A.C.T. 2601, Australia

The use of computers for molecular graphics is an active field of research, partly because the techniques are relevant to the design of drugs (*10–13*). The techniques are also available to teachers who may occasionally wish to emphasize aspects of a molecule's 3-dimensional character.

I have developed a program named MOLDOT for the IBM PC, which prints space-filling perspective diagrams of molecules using a dot matrix printer. Typical output is shown in Figure 10, where the program has been used to illustrate the intriguingly different structures of [2,2]metacyclophane and 2,11-dithia[3,3]methacyclophane[7], as determined by X-ray crystallography (*14*, *15*). The source code for the main program is in Basic, and assembly language subroutines are called.

A number of molecular graphics programs have been written for microcomputers (*16–24*). Some of these programs use the graphics display capabilities built into popular microcomputers. Other programs output their results using plotters. The program described here seems to be the first which uses a dot matrix printer for output.

The idea of representing a molecule as a collection of dots came from the impressive molecular graphics which have been achieved with calligraphic displays, when the van der Waals surface of the molecule is shown as uniformly distributed points of color on a dark background (*25*, *26*). In that method of displaying molecules, it is not usually necessary or desirable to eliminate the hidden surfaces. However, when one uses a dot matrix printer for output, it is desirable to eliminate the hidden surfaces, to prevent confusion and to give a satisfactory 3-dimensional impression.

It is sometimes helpful in making sense of moderately complicated van der Waals surfaces if a skeleton of lines representing the bonds is superimposed on the diagram, as in Figure 10. The user of the program may determine whether such a skeleton will be drawn. It is also possible to draw the skeleton without the van der Waals surface. This can be helpful when selecting suitable angles by which a molecule is rotated before being drawn, since a skeleton of bonds without a van der Waals surface is generated very rapidly. When the van der Waals surface is drawn, execution is relatively slow, even when the program is executed in its compiled form: for example, Figures 10a and 10b required about 20 and 16 min, respectively. Execution times do not depend strongly on the number of atoms, but rather on the total number of dots, whether hidden or visible. A parameter proportional to the separation between the dots on the molecule's surface must be supplied by the user during execution, and this parameter has an important influence on the execution time.

Run times could probably be improved significantly if the program were rewritten with greater use of integer, rather than floating-point, arithmetic. Another approach would be to employ an 8087 coprocessor to speed up the floating-point arithmetic.

[7] This topic was suggested to me by Y. H. Lai.

A single-sided MS DOS formatted disk with files comprising source code, executable programs, and data files, plus explanatory notes and details of the method of computation, is available from Project SERAPHIM. The package requires an IBM, or IBM-compatible, PC with at least 192 K bytes of memory. Logitek, IBM, and Microline printers have been used successfully, but any dot matrix printer with a bit image mode in which the horizontal and vertical spacings between the dots are the same should be suitable. Control codes for the three printers mentioned are recorded on the disk and can be accessed by the main program. For users of printers with different control codes a utility program is provided which can be used to record the required control codes on disk.

Inexpensive Computerized Experiments

John W. Moore and Paula Miles
Eastern Michigan University
Ypsilanti, MI 48197

Malcolm Rasmussen
Australian National University
Canberra, A.C.T. 2601, Australia

Kenneth Hartman
Ames High School
Ames, IA 50010

Patricia Barker
Minisink Valley High School
Slate Hill, NY 10973

We have developed several laboratory exercises that make effective use of an inexpensive thermistor probe (*27*) and colorimeter (*28*) that can readily be interfaced to the game ports of several microcomputers (*29*). In addition we have designed adapter boxes (*30*, *31*) that bring the necessary signals from the game ports to the outside of the computer and standardize the process of connecting sensors to different types of computers, and we have developed software to collect and analyze data for each type of computer. Thus, for example, when Apples and Commodore-64's are used in the same laboratory the directions given to students can be the same for all computers, and the sensors can easily be disconnected when the experiment is complete.

Detailed directions and instructor's notes are currently available from Project SERAPHIM for nine experiments. Thermistor Calibration (*32*) involves collection of temperature/thermistor-reading data, least-squares analysis to fit the data to a nonlinear equation, and evaluation of the sensitivity and accuracy of the thermistor over different ranges of temperature. Heats of Reaction (*33*) uses the calibrated thermistor to measure increases in temperature upon adding acid to base or base to acid in a coffee-cup calorimeter. Collecting data by computer allows this experiment to be done as a titration where ten approximately 5-ml aliquots of acid (or base) are added to a 50-ml aliquot of base (or acid). The data can then be analyzed by Job's Method to determine the stoichiometry as well as the heat of the reaction. The computer permits rapid data collection, allowing the experiment to be done in roughly half the time normally required; also, immediate data analysis indicates possibly incorrect points and encourages students to repeat any questionable experiments.

Photochromic Kinetics (*34*) uses the computer-interfaced colorimeter to obtain absorbance versus time for the fast thermal decay of a photochemically generated reagent. Mercury dithizonate is irradiated with bright visible light using an overhead or slide projector and then allowed to decay