COMMENTS FROM THE EDITOR

The two Seventh C.C.C.E National Computer Workshops held last summer were a great success. In this issue of the Newsletter George Sheats reports on the Workshops held in Potsdam. The overall evaluation by participants was very favorable. George helped to organize and ran the software exhibit and exchange. Harry Pence organized a computer book exhibit. In handling the registrations it became very obvious that there is considerable need for affordable workshops on computer interfacing. At an early stage, almost half the registrants opted for the one on interfacing. By April we had to close registration for the workshop at 24. I believe we could have obtained 50 registrants for this workshop even in a place as remote as Potsdam, NY. The Eighth C.C.C.E. National Computer Workshops will be held in Bozeman, Montana this summer and will include a microcomputer interfacing component. There is a genuine need for many more workshops of this type. We would be pleased to publicize any such workshops in the Newsletter. Just send the information to me.

The spring ACS Meeting in New York City (April 13 to 18) will contain many papers of interest to high school, college and university teachers. The preliminary program will be published in Chemical and Engineering News in mid-January and the final program will be published in February.

Professor Raymond Dessy (a member of the C.C.C.E.) will receive the ACS Award for Computers in Chemistry at the meeting. A one day symposium in his honor will be sponsored by the Division of Computers in Chemistry tentatively on Wednesday, April 16. On Thursday a symposium on Applications Software for Lecture and Laboratory Courses is planned for the Division of Chemical Education. This all day symposium will consider eight areas in which substantial commercially available applications software exist - word processing (D. Rosenthal - Clarkson University), software for computer interfaced instruments (R. E. Dessy - VPI & SU), data base management software and data bases (R. C. Graham - West Point), spread sheets (P. C. Flath - Paul Smith's College, and D. M. Whishnant - Wofford College), numerical methods (A. L. Smith - Drexel University), statistical methods (S. N. Deming - University of Houston), graphics and plotting (V. I. Bendall - Eastern Kentucky University) and electronic bulletin boards and networks (T. Russo - Bayonne High School and J. W. Moore - Eastern Michigan University). Each speaker will give some idea of the kind of software which is available. What the software can do and what it can not do. How it is being used and can be used by teachers and students in elementary and advanced courses. What future developments are likely to occur. Those attending who have used some applications software in innovative ways in teaching are invited to make brief comments during the 5 minutes available at the end of each topic. A form is included on the last page of this Newsletter requesting information concerning the extent to which you and your students use commercially available applications software. We would like to present some of this information either in the symposium or in the Newsletter.

Other sessions sponsored by the Division of Chemical Education include a symposium on Chemometrics, and general papers on computing (Wednesday afternoon and Friday morning). A symposium on Personal Computers in Analytical Chemistry is being sponsored by the Division of Analytical Chemistry.

CONDUCTOMETRIC TITRATIONS USING A GENRAD 1658 DIGIBRIDGE AND A DEC MINC-11/03 COMPUTER

by (Gil)bert F. Pollnow*

Some of the important features and applications of the DEC MINC-11 have been described in the June 1982 issue of the Newsletter by the author, and in a chapter of the book "Computer Education of Chemists" edited by Peter Lykos (Wiley-Interscience 1984). The MINC is still an exemplary laboratory computer, but by present standards is over priced and DEC discontinued its production last July. However, DEC's announced policy is to continue to support it with service for ten years. Some complete new systems are still available for approximately one third ($8000) of the original price from American Diversified Computer Products and Services, Inc., Haverhill, MA. In the seven years of use at UWO, it has proven to be extremely reliable and trouble-free.

The GenRad 1658 Digibridge ($3350 + $650 for GPIB) is a smart digital impedance meter and limit comparator which incorporates the latest microprocessor technology. It can be used to measure capacitance, inductance, or resistance at either 100 or 1000 Hz. Measurement results are clearly shown with decimal points and units, which are automatically presented to assure correctness. Display resolution is 5 full digits for C, L, and R (4 for D or Q). The overall basic accuracy is 0.1 percent. A frequency programmable bridge (Model 1689, 12 Hz to 100 kHz) with a basic accuracy of 0.02 percent, and the GPIB currently sells for $5850.

The general-purpose interface bus (GPIB) option provides full "talker/listener" and "talker only" capabilities consistent with the IEEE-488 Bus standard. Incidentally, the IEEE-488, ANSI MC1.1, and IEC 625-1 standards are all synonymous with the GPIB standard which was first introduced by Hewlett-Packard in 1965. A separate connector also interfaces with component handling and sorting equipment. System configurations with the GPIB bus may be either in the form of a star, a daisy chain, or a combination of the two. The unique connector allows connections to be made piggyback since each has both a male and female part. Data transmission rates are in the 500 kbyte to 1 Mbyte/sec range giving the GPIB a throughput of 4 to 8 Mbps. Some 4000 instruments from 500 different manufacturers are estimated to be currently utilizing the GPIB bus.

By virtue of a patented new measurement technique in which a microprocessor computes the desired impedance parameters from a series of 5, 8, or 16 voltage measurements, no user calibration adjustments of the 165B bridge are ever required. Even the sine wave test signal used to measure the impedances starts with a digital signal 256 times the selected test frequency, F, (100 or 1000 Hz). Binary dividers count down from 256 F, providing 128 F, 64 F, 32 F, ...2 F, F. This set of signals is used to address a ROM which contains a 256 step approximation to a sine function. The ROM output (as an eight-bit binary number) is converted by a D/A converter to a sine wave, which is then smoothed by filtering before going to the conductance cell.

Communication between the MINC and the Digibridge is by means of character strings, as illustrated in the brief program below, and as described in more detail in the second reference above.

```
100 REM PROGRAM  [RLC4] TO READ GEN RAD 1658 DIGIBRIDGE VIA IEEE-488 BUS
110 DISPLAY_CLEAR \ IEEE_BUS_CLEAR \ ALL_INSTR_CLEAR \ SET_TERMINATORS(10)
120 C=3 \ N=2
130 SEND("D2S0C0F1L1R4M2X4E1",C)
140 FOR I=0 TO N
150 TRIGGER_INSTR(C)
160 INSTR_TIME_LIMIT(0)
170 RECEIVE(C$,,C)
180 R=VAL(SEG$(C$,10,15))
190 E$=SEG$(C$,5,6)
200 IF E$=' O' THEN  \ F1=1 \ GO TO 230
210 IF E$='kO' THEN  \ F1=1000 \ GO TO 230
220 IF E$='MO' THEN  \ F1=1.00000E+06 \ GO TO 230
230 PRINT R,E$,F1*R
240 IF I=N THEN 260 \ PAUSE(10)
250 NEXT I
260 END


10.024       O          10.024
1.0006       kO         1000.6
.03259       MO         32590
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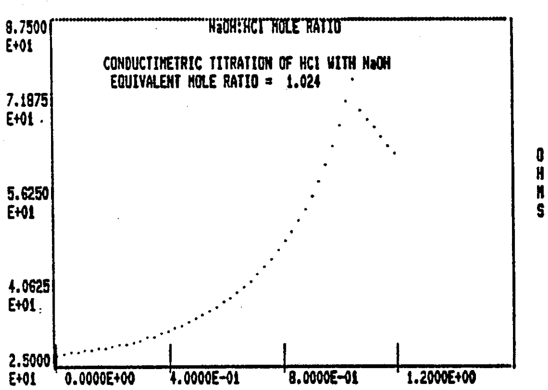
The MINC programmed instruction: SEND ("charaCter string", address) sets the instrument functions. This is followed in the program by the instruction: TRIGGER_INSTRUMENT (address) which actuates a measurement. The results of the measurement are returned to the computer by the programmed instruction: RECEIVE (character string,,address). The 17 character string which is received, is searched for the information of interest using the SEG$ (string label, first position, last position) operator. If numeric values are required, the VAL operator converts the string segment to its decimal equivalent. Other portions of the string are searched for labels which characterize the auto gain and measurement mode and must be utilized to multiply, by the correct multiple of ten, the previously generated number.

The conductometric titrations were carried out using a specially constructed dipping type pair of platinized Pt electrodes sealed, with epoxy resin, into a common support. Measurements were programmed to be taken 5 seconds after each addition of titrant, with continuous and vigorous stirring using a magnetically coupled Teflon coated bar. Control parameters of the Digibridge were programmed as follows: medium speed, parallel equivalent circuit, 1 kHz frequency, average of ten readings, and auto-ranging mode. A cell constant of 0.450/cm was calculated from manual measurements using a 0.0200 N KCl solution. The titration cell was supported in a controlled constant temperature bath at 25.0°C for all measurements.

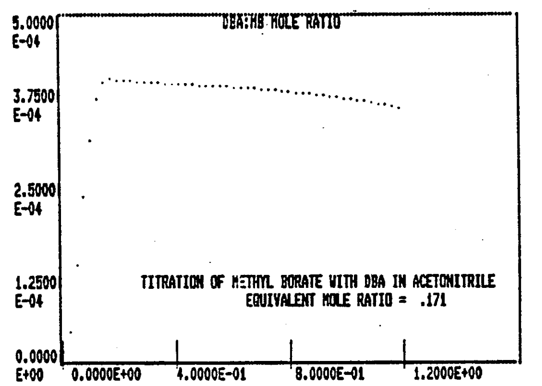
Prior to starting the titration of interest, the normality (or molarity) of both solutions (titrant and titrand), volume of titrand, calibration constant for the buret (ml/sec), and number of increments to be added for the complete curve are entered in the program.

Titrations were carried out utilizing a Sargent-Welch (Model C) constant rate buret (50 ml), with the volume of each increment of titrant being determined from an earlier calibration, under computer control via the D/A and clock modules. The mechanical volume counter on the buret was found to be consistently inaccurate relative to the computer calculated and measured volumes actually delivered, despite its apparent readout precision of 0.01 ml. Gordos solid state relays (GA5-4D25) which can be triggered by the 5 ma output of the D/A module formed the interface to the buret 115 V supply line. Temperature was monitored by means of a calibrated thermistor connected to the pre-amp module, which on the MINC is internally connected to a corresponding channel of the A/D converter.

Progress of the titration was continuously monitored on the CRT and the Okidata printer, both of which displayed the volume of titrant added, conductance in mhos, temperature in degrees C, mole ratio of the reactants, and the derivative of the conductance with respect to the mole ratio of reactants. In earlier versions, the titrations were monitored by simply plotting the resistance against the volume of titrant added. Since this program was developed for research purposes in non-aqueous solvents (acetonitrile), it was found more useful to plot the conductance in mhos vs the mole ratio of reactants. In either case, the change in sign of the slope can be used to precisely determine the equivalence point. The data are stored in sequential files for subsequent use prior to graphing. Copies of the CRT are obtained from a dedicated Tektronix 4632 video, silver-paper based, copier. Shown below are two titration curves, which are self-explanatory.



MOLARITIES: .100 NaOH, .100 HCl; Pt ELECTRODES, 1KZ, MED, PAR, AVE, 24.0 C



0.0996 M MB, 0.0991 DBA, Pt ELECTRODES, 1 KZ, MED, PAR, AVE, 25.0 C

In introducing these techniques, the student first utilizes the bare-bones program, shown above, and another one to gain familiarity with the Digibridge and the MINC by having the latter take a series of ten measurements on a manually operated precision decade resistance box at regularly spaced time intervals, and then plotting the resistance as a function of the time. With this experience and a discussion of the GPIB instructions involved, the extension to other applications is readily apparent.

The program can be readily adapted to determining the equivalent conductance as a function of concentration of strong and weak acids or bases, and true thermodynamic equilibrium constants extrapolated to zero concentration, as in the physical chemistry laboratory course. A separate publication of those results is planned.

A copy of the listing is available from the author upon request.

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