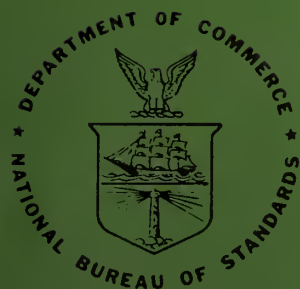


NBS

TECHNICAL NOTE

407

**Applications of a Time-Sharing Computer
in a Spectrochemistry Laboratory:
Optical Emission and X-ray Fluorescence**



**U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards**

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Applications of a Time-Sharing Computer in a Spectrochemistry Laboratory: Optical Emission and X-ray Fluorescence

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APPLICATIONS OF A TIME-SHARING COMPUTER IN A
SPECTROCHEMISTRY LABORATORY:
OPTICAL EMISSION AND X-RAY FLUORESCENCE

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ABSTRACT

A time-sharing computer system employing the Dartmouth College Basic compiler has been in use in this laboratory for more than two years, and it has been applied to both routine and non-routine calculations. Descriptions are given of the computer system and its associated programming language and commands. Typical applications and advantages and disadvantages of the system are discussed. An appendix contains descriptions of 13 programs thought to be of interest to other optical and x-ray spectrochemistry laboratories. Examples of input and output are given with each of these programs.

Key Words:

Analytical chemistry, calculations, computers, emission spectroscopy, programming, spectrochemical analysis, time-sharing computer, x-ray spectroscopy.

I. INTRODUCTION

The application of computers to data reduction and handling in spectrochemical analysis has been shown (see, for example, references [1], [2]) to provide significant savings in time and cost in certain situations. In addition, computer reduction of data may permit much more extensive calculations to be made than are otherwise feasible. This increased computation facility can give improved results and can even make analyses possible which would otherwise not be done by spectrochemical methods.

Until recently, a laboratory employing computers had a choice limited to making use of a central computer laboratory or installing a computer. The first option often involves delays of as long as several hours between submission of data and receipt of the results; such delays are most objectionable when the analyses form a part of a control loop and during research on computing methods. The second option provides for extremely rapid processing of data, particularly when a spectrometer is attached directly to a computer, but it requires a considerable capital investment as well as maintenance costs.

Specialized central computers provided with multiple remote terminals have become well known in the form of reservation services such as those in use by airlines and hotel chains, military systems like SAGE, the New York Stock Exchange quotation system, and systems in stores to handle orders, billing, and stock control. General-purpose, remote-terminal systems, are a more recent development (3, 4, 5, 6). With these systems, data can be transmitted and output can be received at a terminal in the laboratory, thus saving the time normally required to carry this information to and from the computer laboratory.

The information may be processed by the central computer system on a batch basis, or the system may employ time-sharing or multiprocessing, either of which will give very nearly as fast processing of data as if the user had his own computer.

Several general-purpose, time-sharing systems are now in operation. Some of these are owned by companies, universities, and government laboratories for the use of their own personnel. Other installations, called "computer utilities," are operated by computer manufacturers and service bureaus, and make the remote-terminal service available to any user on a contract basis.

This report describes more than two years' experience with a time-sharing system in a spectrochemical laboratory. The system and its programming language and operation are described, examples are given of some applications, and the advantages and disadvantages of the system for spectrochemical applications are summarized. An appendix contains descriptions of a number of programs which may be of use to other spectrochemical laboratories.

The Spectrochemical Analysis Section has been making use of computers for data reduction since 1955, and in 1956 it had installed the first digital spectrometer readout providing data in a form suitable for input to a computer. Until recently, computer applications in this laboratory were restricted to the larger jobs, such as homogeneity testing in the process of preparing standard reference materials. With the availability of the time-sharing service, computer use has been extended to many more computation tasks, as is described in this report.

II. THE COMPUTER SYSTEM

Figure 1 is a block diagram of the computer system discussed in this report. The system and software (5) were developed at Dartmouth College by a group headed by Professors John G. Kemeny and Thomas E. Kurtz. It makes use of two computers, a master and a slave, a large disk memory, a number of remote terminals, up to 40 of which can be served by the system simultaneously, and auxiliary input-output devices and magnetic tape memory, all commercially available equipment. The remote terminals may be at any location that can be reached by good-quality telephone lines.

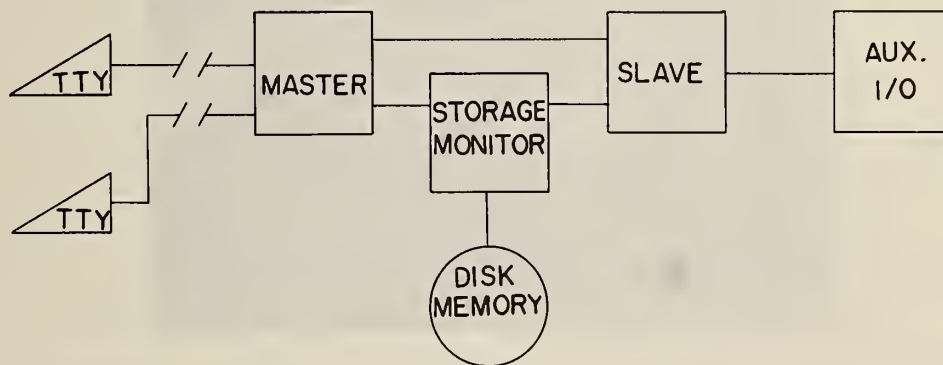


Figure 1. Block diagram of time-sharing computer system.

The functions of the master computer are communication with the terminals and control of the system. The calculations are done on the central processor unit (slave computer), and the disk memory serves for temporary and permanent storage of programs, data, and other information. The contents of the disk memory are copied daily onto a magnetic tape; if the disk memory fails, it can be reloaded with information no more than one day old. The auxiliary input-output devices are used for initial loading of the disk, and for batch operation of the computer at night or during periods of light use of the time-sharing system.

Figure 2 shows the remote terminal in this laboratory; it is a standard teletypewriter (Teletype Model 33ASR) which is rented from the local telephone company. Programs or data may be entered on the keyboard or from a punched paper tape which is fed into the tape reader. The punched paper tapes may have been prepared in advance on the same teletypewriter, or they can be prepared automatically by suitable readout equipment on instruments in the laboratory.

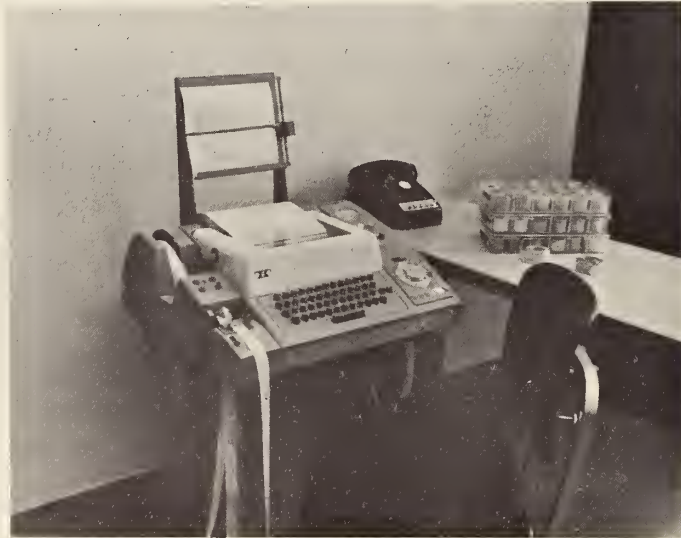


Figure 2. Teletype terminal for communication with time-sharing computer.

Information sent from the terminal to the master computer is stored on the disk memory. When the operator has transmitted all necessary information to the computer, he types the command RUN. His program and data are then placed in a queue for time on the central processor. Each user who has typed RUN is allotted a few seconds of time on the central processor. If this allotment of time is not enough to finish the calculations, the partially complete program is stored on the disk memory while other users are given their turns, and it is then reentered into the slave computer. This process is repeated as often as is

necessary to complete the calculations. The average program requires less than 10 seconds of computing time and is completed by the computer in less than a minute, although a longer time may be required for transmission of the results, depending on the length of the output.

The results of the calculations are also stored on the disk memory, and they are then picked up by the master computer and transmitted to the terminal. Printout starts as soon as a part of the results is available, so that the operator may well have received the first printout before the calculations are complete. This makes it possible for the operator to intervene in the calculations, as will be described below.

With up to 40 users in contact with the system it might seem that any one user must wait for a considerable time for a calculation to be entered into the slave computer. In practice, much more time is spent by each user in entering information or receiving output than is required for the calculations. Thus, only a few users require calculations on the slave computer at any one time, and the overall effect is to give each user nearly as rapid response as if he had his own computer.

Programs need not be transmitted each time they are to be used. Each program is assigned a name by the user, and when it has been entered the first time the command SAVE will cause the program to be stored permanently on the disk memory. When the program is to be used again, it can be called up by a simple sequence of commands. Material stored on the disk can be removed by the command UNSAVE. A stored program can be modified; the changes will not be stored permanently unless the command SAVE is typed after changes are made. Thus, the user can try various modifications without hazard to the stored program.

Saved programs are stored on the disk memory in the BASIC language (see below) and are converted to binary machine language (compiled) each time they are run. The binary form of the program is stored temporarily on the disk memory each time an incompletely processed program is moved out of the slave computer to permit another user a turn. Conversion of the program from BASIC to machine language on each run makes possible frequent changes of the program. The BASIC compiler in the system is efficient enough so that even the longest program is compiled within a few seconds, and the delay is hardly seen by the user.

III. THE PROGRAMMING LANGUAGE AND SYSTEM COMMANDS

One difficulty in the routine application of computers has been the need for detailed instructions, or programs, in binary form for the computer. In order to simplify programming, a number of languages have been developed so that the instructions can be written in letters and decimal numbers, usually in a form resembling algebraic expressions with the alphabetic characters arranged to resemble English words. The computer makes use of a compiler program to transform these programs into binary form.

The programming language most often employed for scientific calculations has been FORTRAN, which has several versions. While a number of scientists have learned to write programs in FORTRAN, it is more common practice to have the programs prepared by a professional programmer. The scientist must explain his problem and perhaps a method of solution to the programmer. This is sometimes difficult in practice, and the use of a programmer introduces an extra person between the scientist and his calculations. Although it is often desirable to have the program written by an experienced programmer, in many cases the scientist can write it in less time and at a lower cost.

The time-sharing system described in this report uses a programming language called BASIC, which was also developed at Dartmouth College (7). BASIC is a relatively simple language, lacking the complexities of most other programming languages while retaining their most essential computation features. It has proven to be remarkably easy to learn. With such an easily learned language, the scientist can prepare his own programs and he can later modify them to change the input format, the output format, or the nature of the problem. Also, a computer program provides a method of transferring exact information on

computational methods between scientists, provided that both the sender and the receiver of the information know the same programming language.

It is not the purpose of this report to describe the BASIC language; complete information can be found elsewhere (7). Appendix I illustrates the 17 types of statements which make up this language and the 11 types of statements which have been added for matrix algebra. Inspection of Appendix I will show that the designations of the BASIC statements are straightforward, making them easy to learn. For example, the very important arithmetic assignment statement has the form $LET X = Y+Z$; when the computer reaches this statement it will replace any numerical value which may be stored in a memory location assigned to the variable X with the sum of the values of the variables Y and Z. It must be recognized that the statement need not be an algebraic equality, but may have such forms as $LET X = X+1$; in this case, the value stored for the variable X will be increased by one.

Each line of the program and of the data must begin with a line number. The line numbers can be from 0 to 99999 and need not be successive. If the lines are entered out of order, the computer will rearrange them by line number. If two or more lines are given the same number, only the last to be entered will be retained. This feature of the system permits easy correction or modification of a program or data. To make such a change, the operator types the number of the line to be changed followed by the new information. A line can be erased by typing only its number.

BASIC has 10 built-in functions, including geometric functions (sine, cosine, tangent, arctangent), logarithm, square root, etc. Thus, the statement $LET X = LOG(Y)$ will cause the variable X to be assigned a value equal to the natural logarithm of the variable Y.

An important simplifying feature of BASIC is that the programmer needs to pay little attention to the format of the input data or of the output. Numbers can be of various lengths (up to nine digits), with or without a decimal point, or expressed as a number plus an exponent ($5E-3 = 0.005$). In input, numbers are separated by commas; spaces may be added between numbers for neatness and for ease of proofreading. However, the programmer need not specify in the program the form and length of the input numbers, as in FORTRAN. Output is limited to two formats. One allows for up to five columns on a page, with 15 spaces per column, while the other permits closer packing of the output numbers but will not easily give neat columns of results. This feature of BASIC is sometimes a disadvantage, since it may be difficult or even impossible to get the output in the desired form. Most often, however, the available formats are adequate, and can be designated in a much simpler manner than the output format in FORTRAN.

In addition to the programming statements, there are several system commands which are used to control the computer system from a terminal. The commands RUN and STOP begin the running of a program and stop it before the calculations are completed. A running program can also be stopped by pressing the BREAK button on the teletypewriter. The command TAPE informs the master computer that a program or data are to be transmitted through the tape reader. The commands OLD and NEW indicate that the operator wishes to move to a different program. The computer replies by causing the teletypewriter to print OLD (or NEW) PROBLEM NAME --, the operator replies with the name of the next program he wishes to use. If he had typed OLD, the computer will locate the stored program on the disk memory and make a copy of it in the working area of the memory. If the operator had typed NEW, the computer will prepare to

receive a new program and will then reply READY. A list of stored programs can be received by typing the command CATALOG.

No terminal can call up programs initially loaded from another terminal; thus, interference from other users is prevented. There is an area of memory called the "library" which contains programs of general interest, such as those for various types of statistical calculations. These can be called up from any terminal by typing the name of the program followed by three asterisks. Individual users can modify these programs according to their own needs, but cannot permanently alter the forms stored in the "library." They can, however, save altered "library" programs in their own areas of the memory. The ready availability of such programs in the "library" has been helpful to us; some of our programs are based on "library" routines.

The EDIT commands permit the operator to alter selected portions of a saved program. For example, the command EDIT DELETE followed by line numbers will selectively remove portions of a program, leaving the rest untouched.

When the command RUN is typed, the computer will provide output if possible, or it may reply with one or more error messages. Some error messages point out mistakes in the program or data. For example, ILLEGAL FORMULA IN 590 informs the operator that line 590 of his program has a formula containing an error making it impossible for the computer to carry out a calculation. Other error messages indicate that a problem has arisen in a particular calculation. One such message may be DIVISION BY ZERO IN 620, showing that the denominator of an equation in line 620 has the value of 0 in this case. The computer will assign the largest number it can to the result of this

calculation (about 6×10^{76}) and will continue the calculation.

Figure 3 illustrates the sequence of operations employed in entering a program and receiving output from it. Transmissions from the computer other than the program output have been underlined. The program in this illustration is TABLE, an example of a very short, but useful, program. TABLE will generate a table of X as a function of Y. The semicolon at the end of line 0 suppresses the carriage return and line feed so that the print statement on line 10 will come on the same line of output. The print statements on lines 20 and 40 cause blank lines in the output, making the form neater. Lines 50 to 90 constitute an iterative loop which will, in this instance, cause the calculation and output to be made 10 times for 10 successive values of Y. To use the program for any other function, the operator changes only a few lines. In addition to generating tables, the program can be used to find the value of Y for a given X, when the form of the function does not permit an easy explicit solution. The operator can change line 50 in successive passes to narrow down the region of Y values searched. In the example, if it was desired to find the value of Y for $X = 0.5$, the operator would, on the second trial, change line 50 to

```
50 FOR Y = 60 TO 70 STEP 1.
```

With this procedure, the value of Y can be found to several significant figures in a few minutes at the terminal.

HELLO

USER NUMBER--M11190

*** ON AT 9:12.

SYSTEM--BASIC

NEW JOB JLD--NEW

NEW PROBLEM NAME--TABLE

READY.

TAPE

READY.

```
0 PRINT "TABULATION OF : ";
10 PRINT "X=EXP(-MU X DEPTH/COS(THETA)) . "
15 PRINT "DEPTH=10 MICRONS, ABSORBER=FE, RADIATION=CU K . "
20 PRINT
30 PRINT "THETA", "X"
40 PRINT
50 FOR Y=0 TO 90 STEP 10
60 LET T=Y/57.29578
70 LET X=EXP(-311.1*.001/COS(T))
80 PRINT Y,X
90 NEXT Y
99 END
```

RUN

WAIT.

TABLE 9:13 CEIR 12/15/67

TABULATION OF : X=EXP(-MU X DEPTH/COS[THETA]) .
DEPTH=10 MICRONS, ABSORBER=FE, RADIATION=CU K .

THETA	X
0	.732641
10	.729133
20	.718158
30	.698216
40	.666235
50	.616322
60	.536762
70	.402687
80	.166701
90	0

TIME: 0 SECS.

BYE

*** OFF AT 9:14.

Figure 3. Example of use of the time-shared computer system. Transmissions from the computer other than program output are underlined.

IV. THE INPUT STATEMENT

In normal computer usage, the scientist submitting a program and data can exercise only those controls and decisions that are built into the program. In the time-sharing system, it is possible to cause the computer to pause during the running of a program and wait for additional instructions. This is done by including in the program an INPUT instruction; when the computer reaches this instruction it will stop the processing of the program and move the compiled program and intermediate results to the disk memory, print a question mark, and wait for the operator to enter additional information on the keyboard of the teletypewriter. For example, a program might include the following statements:

```
510 PRINT "DO YOU WANT MORE OUTPUT, YES (1) OR NO (0)";  
515 INPUT Q  
520 IF Q=1 THEN 530  
525 STOP  
530 . . . . .
```

When the computer reaches line 510, it will print the words indicated, followed by a question mark, and then pause. If the operator enters the number 0, the processing of the program will be stopped at line 525. If the operator enters the number 1, the statement in line 520 will cause the computer to move over the STOP statement and go on to additional calculations and/or output as indicated on lines 530, etc.

The INPUT statement can also be used to allow the operator to select among several alternative branches built into the program, based on his evaluation of output received up to that point. Another use of the INPUT statement is to allow the operator to select a desired value for a variable. In these ways, the operator can work along with the computer.

He can use his judgment to make decisions which could be extremely difficult to write into a program, while the machine rapidly performs the detailed mathematical calculations. An example of this use of the computer system is given below, in the discussion of the programs CODEBC and CFIT2.

V. APPLICATIONS OF THE SYSTEM IN SPECTROCHEMISTRY

Several programs applicable to optical emission and x-ray spectrometry are indicated by brief summaries and examples of input and output in Appendix II. We will consider here a few examples of the programs in some detail. These apply to (1) fitting analytical curves and reading out concentration results for samples, and (2) calculations required in photographic photometry.

Calculations normally done graphically are usually programmed for the computer by a curve fitting procedure. Such a procedure is straightforward when the equation of the curve is known. However, analytical curves from spectrographs and spectrometers can have a variety of shapes, and must be empirically fitted. In addition, not all of the analytical data on the standards will necessarily fit on a smooth curve. This can be caused by an erroneous reading for one of the standards; when unusual materials are being analyzed, it may be necessary to include some standards which are not well characterized. When graphical methods are used, the analyst applies his experience and educated judgment to decide on the shape of the curve and whether any points are to be excluded. It is extremely difficult to program the computer to perform such judgments.

The programs CODEBC and CFIT2 perform the functions of fitting analytical curves and reading out results for samples. The computer makes least-square fits of polynomial equations to the data for the standards, starting with the first degree and continuing to as high as the eleventh degree if there are enough data. At the option of the operator, the program will fit either reading vs. concentration or log reading vs. log concentration. The first output of the program is a list of degree of polynomial

and, for each degree, an index of determination and the standard error of Y. An INPUT statement causes the processing of the data to pause at this time, while the operator decides what degree of polynomial is to be used. When this information has been entered, the computer gives the coefficients of the equation fitted to the data and, at the option of the operator, a list of the following information on the standards: input intensities, input concentrations, calculated concentrations, and the absolute and percent differences between the input and calculated concentrations. The operator may decide, on the basis of this information, that one or more of the standards do not fit well on the curve; in this case the operator may interrupt the program, edit the input data, and restart the program at the beginning. If the operator has not interrupted, the computer will convert each instrument reading for each sample to a concentration. The two programs diverge at this point. Only CODEBC provides a list of concentrations found for each run on each sample. Both programs provide the average concentration found for each sample (if there were two or more runs) and the standard deviation (if there were three or more runs). CODEBC also has provision for receiving input data on the standards in terms of concentration ratios, rather than concentrations. In this case, the output for the samples includes both the concentrations and the concentration ratios.

Another type of calculation that has normally been carried out graphically is the conversion of microphotometer readings on photographic plates to relative intensities. Several functions of the microphotometer readings have been devised in the past which give a nearly linear relation between the function and the relative exposure, thus simplifying the calibration process. The Seidel transform,

$S = \log \left(\frac{1}{T} - 1 \right)$, where T is the transmittance, is most often used and gives a nearly straight line for many but not all photographic emulsions. Several other transforms have also been developed. Some of these yield better results by inclusion of an adjustable constant whose value is determined empirically or by calculation.

When a straight-line relation between a function of the transmittance and the logarithm of the exposure can be found, only the slope of the line needs to be known. Since only relative intensities are normally measured, the intercept of the line can be assigned any convenient value. The process of emulsion calibration is thus reduced to finding the slope of a line, rather than the more complex procedure of fitting a curve.

The program KAISER has been developed to take advantage of this observation. It employs the Kaiser (8) transform: $K = A \log \left(\frac{1}{T} \right) + (1-A) \log \left(\frac{1}{T} - 1 \right)$, where A is an adjustable constant. Kaiser derived an equation for finding the proper value of A from transmittance values for two pairs of lines of known relative exposures. The value of A found from this equation has a large standard deviation, and the program provides for the calculation of as many as 100 values of this constant in order to arrive at a more reliable estimate from the average. When the best value of A has been found, individual slopes are calculated from the pairs of transmittance readings for two steps of the sector or filter. An average slope and its standard deviation are then calculated, and any individual slopes differing from the average by more than three times the standard deviation are rejected. The output of the program includes values for A and for the slope of the line, as well as statistical data on each. The program also provides for checking of the input data against the calculations, with rejection of "wild" data

that might affect the average values. The program includes two INPUT statements to permit the operator to control the amount of output.

The values of A and the slope from KAISER form the input to the program INTEN2, together with microphotometer readings which are to be converted to relative intensities. INTEN2 provides for a number of alternate calculations. For example, a photographic plate may have been characterized by a single calibration, or up to ten calibrations may have been made for various wavelength intervals. If a step sector or filter was used, it may have as many as six steps, and the step factor may be two -- as is most common in this laboratory -- or some other value. A background correction may or may not be made. INTEN2 is written to cover all of these alternatives. Furthermore, it is not necessary for the operator to state explicitly which of these alternatives applies. The computer will make this decision from an inspection of the input data, using information inherent in the data. For example, when both line and background transmittance values are given to provide for background correction, there will be twice as many input numbers as when only transmittance values are given; any number larger than 1000 must be a wavelength; a number below ten may be a step number, but it cannot be the transmittance of the background.

KAISER and INTEN2 combined would be too long a program for this computer system, but only a small amount of data must be carried over from the first program to the second. In some cases, it is necessary to carry over much more extensive data from one program to the next. The sub-routines WRITE1, WRITE2, and WRITE4 provide for output of one to four selected variables in the proper format for re-

entry into another program. The operator starts the tape punch at a time indicated by the printed output of the subroutine, and the data are thus recorded on tape.

The few examples given above and in Appendix II show only applications of the computer system to routine calculations. Except where operator judgment is required, as in CODEBC and CFIT2, batch-loading computers would be equally satisfactory in many cases. The time-sharing computer is especially valuable for non-routine calculations. For these "odd jobs," the BASIC language permits very rapid writing of programs, and time-sharing operation, because of its rapid response, speeds up the process of debugging. In this way, the computer system can take over many computations now performed more laboriously on desk calculators. Often, an operator can sit at the keyboard and quickly evaluate the effect of changing a variable or the form of an equation.

There are apparently no very large computer systems now available to run programs in the BASIC language, so that when very long programs or very extensive data are available it will be necessary to write programs in some other language such as FORTRAN. The time-sharing computer system can be very helpful even in this case. Programs can be written in BASIC and tested on the time-sharing system with small batches of data in order to evaluate proposed methods of calculation. When the methods have been worked out in this way, a FORTRAN program can be prepared to perform the same calculations. This method of programming permits much faster development of new types of machine calculation than would otherwise be possible.

VI. LIMITATIONS OF THE SYSTEM

The time-sharing system which is described in this report is not a very large machine, and a major part of the core of the computer is taken up by system programming. Thus, there is only limited space available for programs and data. The program and data combined cannot take up more than about 6200 spaces (letters, numbers, etc.). Even with a very short program, there can be no more than 1280 numbers in the data. These limitations restrict the use of the system to relatively short problems, but in practice these include most of the calculations required in a spectrochemical laboratory. At times, long calculations can be divided into shorter segments, as was done for the process of calibrating a photographic emulsion and converting microphotometer readings to relative intensities.

A second disadvantage of this time-sharing system is that the rate of data transmission is limited, by the teletypewriter, to 10 characters per second. This is a serious disadvantage only when very large amounts of output are required. In normal computer operation, it is the usual practice to take as output all data which might conceivably be of value, even though only a small fraction of this is regularly required. In the time-sharing system it is convenient to ask for only the essential output, since additional PRINT statements can be added when more information is needed. In some cases, it has been convenient to include INPUT statements in the programs to allow the operator to control output easily.

These limitations are not inherent in time-sharing. It is probable that larger machines, with improved systems programming, will remove these difficulties in the near future. There is, however, another limitation which is inherent in time-sharing. Because time on the slave computer

is shared with other users, the time at the terminal will always be much longer than the computation time. Most programs require only a few seconds of time on the slave computer, and for these time-sharing introduces no difficulties. A few experimental programs have been run which required a minute or more of time on the slave computer, and which required five minutes or more of terminal time. These probably do not represent an optimum use of the system. Even so, the time-sharing system did provide results in less time than would be needed to carry the data to a central computer laboratory for processing on a batch-loaded computer.

This limitation of time-sharing computer systems may also be alleviated in the future by equipment-sharing computers, having the ability to carry out several calculations simultaneously.

VII. DISCUSSION

The material in this report can only suggest the impressive speed at which complex calculations can be performed on the time-sharing computer system. The rapid response of the system makes it possible to do jobs which would be prohibitive by graphical or desk calculator methods, or even with a machine in a central computer laboratory. When an instrument is set up for an analysis, it is possible to run a few standards and to do preliminary calculations with the results thus obtained to determine whether or not the analytical instrument is functioning properly. The delay of up to several hours encountered in most central computer laboratories would not be acceptable for this purpose.

The rapid response and ease of programming characteristic of the time-sharing system make the use of the computer attractive even for very small jobs, such as determining the average and standard deviation of a series of numbers. A few of the newer desk calculators, having multiple registers, can do such simple calculations as quickly as with the time-sharing system, but the older single register calculators are significantly slower in such calculations.

The data input format for the time-sharing computer system is somewhat different than for other computer systems, since it requires that each line of data start with a line number and the word DATA and that numbers be separated by commas. This format can be supplied by automatic readouts.

An emission spectrometer and an x-ray spectrometer in our laboratory are equipped with a completely automatic readout which provides the data in printed form and on paper tape with proper format for the time-sharing system. Switches on the readout provide for suppression of the word DATA and for replacing of the commas with spaces when other computer systems are to be used for the calculations. In addition, a microphotometer is equipped with a semi-automatic readout which follows each number with a comma, but which requires the operator to enter the line number and the word DATA at the start of each line.

VIII. ACKNOWLEDGMENT

We thank Mr. Joseph M. Cameron and Mr. Joseph Hilsenrath for helpful advice on the preparation of this report.

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Appendix I. BASIC Statements

Example of Statement	Function
LET X = Y + Z	Arithmetic assignment statement.
READ A, B	Read next two data points, and assign these values to variables A and B.
DATA 50.5, 11, 5E3	Input of data.
PRINT X1, X2	Print output; in this case the variables X1 and X2.
GO TO 55	Unconditional transfer of processing to statement on line 55.
IF X = Y THEN 55	Transfer of processing to statement on line 55 if stated condition is met.
FOR I = 1 TO 50 NEXT I	Repetitive computations as directed by statements between FOR and NEXT.
END STOP	Stop processing of program; END must be last statement in program. STOP may be used in body of program.
DEF FNA (X) = SQR (SIN (X) - 1)	Defines functions to be used later in program.
GOSUB 400	Transfer processing to a subroutine starting on line 400.
RETURN	Marks end of subroutine and return of processing to the line following the given GOSUB.
DIM A (100)	Sets aside space in memory; in this case for a list of up to 100 numbers assigned variable names A (1), A (2), etc.
REM THIS IS AN EXAMPLE	Remarks may be inserted in program to mark certain portions or to contain information for users.
INPUT Z	Data input; see Section IV.
RESTORE	Restore computer to start of data list; number used by next READ statement will be first on list.

Matrix Statements

MAT READ A (M,N)	Read a matrix M rows by N columns.
MAT PRINT A	Print a matrix.
MAT C = A + B	Add two matrices.
MAT C = A - B	Subtract two matrices.
MAT C = A * B	Multiply two matrices.
MAT C = ZER (M,N)	Introduce a zero matrix.
MAT C = CON (M,N)	Introduce a matrix of all ones.
MAT C = IDN (M)	Introduce an identity matrix.
MAT C = TRN (A)	Transpose a matrix.
MAT C = INV (A)	Invert a matrix.
MAT C = (K) * A	Multiply a matrix by constant K.

Note: Vectors may be substituted for matrices; e.g. MAT READ A (M).

Appendix II. Summary Description of Some Computer Programs
in the BASIC Language of Interest to
Other Spectrochemistry Laboratories

Appendix II contains summaries of the nature of the calculations and examples of input data and of output for several programs written in this laboratory which are deemed to be of interest to other spectroscopists. Listings of the programs and instructions for their use are available on request to the authors of this Report.

Statistical treatment of data are taken from NBS Handbook 91, "Experimental Statistics" (9).

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KAISER

KAISER is a program for calibration of photographic emulsions from the percent transmission readings on lines of known relative intensity, such as readings on lines photographed through a step sector or filter. More detailed information on the method of calculation is given in the text of this report.

Example

The first number in line 900 controls an option, setting the step factor equal to 2 and determining that lines from 0 to 100 percent transmission will be accepted. The second number is the wavelength of calibration. Alternatively, this line could have a format such as

```
900 DATA 0,3600,3,5,90.
```

In this case, the step factor would be 3 and the pairs of light-dark readings would be used only if the percent transmission for the dark line was larger than 5 and the percent transmission for the light line less than 90.

Lines 901 to 909 contain pairs of light step--dark step percent transmission readings. The final number, 0, indicates the end of the data set.

In the example, the output has been truncated to save space.

900 DATA 1,3600
 901 DATA 089.0,050.3,097.4,082.5,082.5,037.1,037.1,008.3,094.2,
 902 DATA 068.1,068.1,022.6,022.6,004.1,090.8,053.6,053.6,012.7,
 903 DATA 012.7,001.8,090.4,053.4,053.4,013.0,013.0,001.9,096.8,
 904 DATA 081.4,081.4,037.8,037.8,006.9,090.7,050.9,050.9,011.6,
 905 DATA 084.2,039.0,039.0,008.2,092.7,058.6,095.4,069.2,
 906 DATA 089.8,053.3,094.2,061.8,061.8,017.2,069.5,022.3,022.3,
 907 DATA 005.0,093.5,059.6,059.6,017.4,017.4,003.6,092.6,058.2,
 908 DATA 058.2,015.3,056.8,014.4,014.4,003.5,070.4,021.7,
 909 DATA 086.2,043.4,0

KAISER 16:18 04/12/67

PLATE CALIBRATION BY FIT TO KAISER TRANSFORM
 WAVELENGTH= 3600 ANGSTROMS
 PCT. T LIMITS: 0 TO 100
 NO. OF INPUT PAIRS= 36
 NO. OF LIMIT REJECTS= 0

AVE. A	STD. DEV.	S.D. [MEAN]	SETS USED	3S REJ.
.138146	.16976	1.72365 E-2	97	3

AVE. SLOPE	STD. DEV.	S.D. [MEAN]	FRS. USED	3S REJ.
.363719	1.98032 E-2	3.34736 E-3	35	1

DO YOU WANT SUMMARY OF SLOPE VS. FCT. T, YES[1] OR NO[0]? 1

RANGE OF LIGHT T VALUES

FROM	TO	NO. OF PRS.	AVE. SLOPE	PCT. DEV.
10	20	3	.36165	-.568989
20	30	2	.390938	7.48345
30	40	3	.360449	-.899247
50	60	6	.356427	-2.00493
60	70	3	.361437	-.627402
70	80	1	.343948	-5.43597
80	90	6	.369912	1.70249
90	100	11	.363247	-.129943

DO YOU WANT INDIVIDUAL SLOPES, YES[1] OR NO[0]? 1

LIGHT T	DARK T	LOW K	HIGH K	SLOPE
89	50.3	-.77557	3.67355 E-2	.370587
97.4	82.5	-1.35462	-.568845	.383099
82.5	37.1	-.568845	.257092	.364471
37.1	8.3	.257092	1.04849	.380378
94.2	68.1	-1.0398	-.260807	.386437
68.1	22.6	-.260807	.550002	.371271
22.6	4.1	.550002	1.37155	.36642
90.8	53.6	-.85115	-1.65777 E-2	.3607
53.6	12.7	-1.65777 E-2	.845359	.349248
12.7	1.8	.845359	1.73793	.337262
90.4	53.4	-.833302	-1.33442 E-2	.367129
53.4	13	-1.33442 E-2	.833931	.355292
13	1.9	.833931	1.71407	.342027
96.8	81.4	-1.27422	-.540198	.410111
81.4	37.8	-.540198	.244786	.383486
37.8	6.9	.244786	1.13439	.338386
90.7	50.9	-.846625	2.70395 E-2	.34456
50.9	11.6	2.70395 E-2	.889392	.34908
84.2	39	-.615953	.223921	.358423
39	8.2	.223921	1.05416	.362581

INTEN2

INTEN2 is a program for conversion of percent transmission values to relative intensities, with provision for correction for background and for step if needed. One to ten sets of emulsion calibration functions from the program KAISER may be entered, and either a standard (1:2) or non-standard step sector or filter may have been used. The program is written so that the machine will, by inspection of the data, decide which of the many alternative calculations are required. The processor time and console time are determined by the length of the data set.

Example

The first line of input data shown is the emulsion calibration data for two wavelength ranges (for each, the lower and upper wavelength, and the values of A and the slope from KAISER). The number 0 indicates the end of the list of calibration data. The first number in line 901 is the wavelength at which the microphotometer reading was made. The next number, 5, shows the number of readings at that wavelength. The program counts the number of data points until it reaches the next number larger than 1000 (the next wavelength). Since there are five points for the five readings, the program recognized that these must be sets of percent transmission readings for the line. In line 902, there are eight data points for four readings, and line 903 also has twice as many data points as readings. In line 902, the second data point is larger than 6, and the program uses this information to determine that the data points in line 902 represent sets of readings on line and background. Similarly, the program determines that the data points in line 903 represent line percent transmission readings followed by step numbers. Line 904 contains sixteen data points for four readings, and the program recognizes that there are

four data points per reading so this must be a list of line and background percent transmission readings, each followed by a step number. The final data entry, 0, indicates the end of the data block and stops processing.

900 DATA 3000, 3590, .8, .7, 3590, 4000, .9, .8, 0
 901 DATA 3400, 5, 15, 55, 60, 65, 70
 902 DATA 3500, 4, 55, 90, 60, 91, 65, 92, 15, 90
 903 DATA 3700, 5, 10, 6, 20, 6, 10, 5, 10, 4, 10, 2
 904 DATA 3800, 4, 10, 6, 90, 6, 10, 3, 90, 6, 20, 2, 80, 3, 10, 2, 80, 5, 0

INTEN2 14:59 04/14/67

RELATIVE INTENSITIES OF SPECTRAL LINES

WAVELENGTH= 3400 ANGSTROMS

PERCENT T REL. INT.

15	3.68854
55	1.35893
60	1.25772
65	1.16716
70	1.0845

WAVELENGTH= 3500 ANGSTROMS

LINE PCT. T	BKGD. PCT. T	LINE INT.	BKGD. INT.	CORR. INT.
55	90	1.35893	.779884	.579042
60	91	1.25772	.762544	.495172
65	92	1.16716	.744357	.422803
15	90	3.68854	.779884.	2.90866

WAVELENGTH= 3700 ANGSTROMS

PERCENT T	STEP	REL. INT.
10	6	6.25661
20	6	3.55978
10	5	12.5132
10	4	25.0265
10	2	100.106

WAVELENGTH= 3800 ANGSTROMS

LINE PCT. T	STEP	LINE INT.	BKGD. INT.	CORR. INT.
10	6	6.25661	.904911	5.3517
10	3	50.0529	.904911	49.148
20	2	56.9565	8.40815	48.5483
10	2	100.106	2.10204	98.0038

TIME: 5 SECS.

CODEBC and CFIT2

CODEBC and CFIT2 are programs for converting intensity ratios or other instrument readings to concentrations. The programs fit least-square polynomial equations to data for standards, starting with the first degree and continuing as high as the eleventh degree if there are enough standards. Two statistical parameters, the index of determination and the standard error of Y, are given for each degree of polynomial, and the operator selects the polynomial to be used on the basis of this information. The equation is then applied to the data on the standards to provide a comparison between given and found concentrations. Finally, the equation is applied to the data for the samples to convert the instrument readings to concentrations.

Both programs provide for fitting either concentration vs. instrument reading or log concentration vs. log instrument reading. CODEBC also provides for the use of the concentration ratio (variable internal standard) method. CFIT2 gives a briefer output than CODEBC, and this output is often suitable as an analysis report.

Examples

CODEBC: The first number on line 900 is the number of standards. The second number, 1, controls an option, giving a log-log fit. If this number were 0, the fit would be concentration vs. instrument reading. Data on the standards are given on lines 901 and 902. For each standard, the average instrument reading and the percent concentration are given, in that order. Lines 903 and 904 contain data on two samples. The information given for each is the sample number, the number of runs, the percent content of the internal standard element, and the individual readings. The final number, 0, marks the end of the data block.

On the first run, the index of determination was lower and the standard error of Y higher than expected. The operator chose a first-degree polynomial (straight line) and to take complete output. He stopped the processing after output of the data on the standards by pressing the "BREAK" key. Comparison of the given and found concentrations shows that the second standard has a large positive percentage difference, while for the other standards the percentage differences are smaller and mostly negative. The operator then changed lines 900 and 901 to delete the data for the second standard, and ran the program a second time, giving more satisfactory values for the index of determination and the standard error of Y. Neither of these factors improved after the first degree, so a straight-line fit was selected. The fit to the standards was judged to be satisfactory, and the computer then processed the data for the samples.

CFIT2: The initial data, for the standards, is arranged in the same way as for CODEBC. The number 3, at the end of line 902, is the number of runs per sample. The data on lines 903-912 give, for each sample, the sample number and three readings.

When the program was run, the operator noted that the two statistical parameters improved considerably going from the first to the second degree, but showed little change for higher degrees. Accordingly, he selected the second degree. Inspection of the data for the standards shows that the absolute difference between given and found concentrations is small in all cases. The data for the samples were then processed, giving the output shown.

Selection of Polynomial and Rejection of Standards

The selection of the polynomial is guided by the operator's judgement, and only some general rules can be given. In most cases, it is preferable that the number of standards be large compared to the number of coefficients in the equation - normally, at least two standards per coefficient. When a satisfactory fit is obtained, the index of determination will approach a value near 1, and the standard error of Y will approach a fixed number. (The standard error of Y will always be 0 when the number of coefficients equals the number of standards.) If neither statistical factor shows a large improvement after the first degree, the first degree polynomial should be selected. In some cases, the two statistical parameters will show a sudden improvement in going from degree N to degree N + 1 and only a small change for higher degrees. The degree to be chosen is then N + 1.

The output comparing the given and found concentrations for the standards provides information for rejection of standards which do not fit the curve properly. If standards are to be rejected, the operator can stop processing of the program by pressing the "BREAK" key on the teletypewriter. The decision to reject may be based on absolute or percentage differences. When concentration has been fitted vs. instrument reading, the absolute difference has been minimized, in the least-squares fitting, and this is the criterion for rejection. When a log-log fit has been made, the percentage difference has been minimized, and it is the basis for judgement. The level of difference requiring rejection of a standard depends on the precision expected in the analysis.

900 DATA 6,1
 901 DATA 409.5,1.11, 633,.634, 254.5,.387
 902 DATA 154,.178, 134.5,.14, 923.5,4.59
 903 DATA 9182,5,75.3,147,143,146,149,148
 904 DATA 9183,4,76.8,785,782,778,784
 905 DATA 0

CODEBC 13:57 10/30/67

DEGREE	INDEX OF DETN	STD ERROR OF Y
1	.85819	.234579
2	.817817	.265882
3	.825702	.260065
4	.897868	.199074
5	.897868	0

WHAT DEGREE DO YOU WANT TO USE? 1
 DO YOU WANT COEFFICIENTS [1] OR FULL LIST[2]? 2

TERM	COEFFICIENT
0	-4.13739
1	1.54412

INTEN RATIO	CONC GIVEN	CONC FOUND	DIFF	PCT DIFF
409.5	1.11	.787496	-.322504	-29.0544
633.	.634	1.54283	.908831	143.349
254.5	.387	.37782	-9.17962 E-3	-2.372
154.	.178	.173944	-4.05611 E-3	-2.27871
134.5	.14	.141129	1.12935 E-3	.806675
923.5	4.59	2.76443	-1.82557	-39.7728

STOP.
 READY.

900 DATA 5,1
 901 DATA 409.5,1.11, 254.5,.387
 RUN
 WAIT.

CODEBC 14:01 CEIR 10/30/67

DEGREE	INDEX OF DETN	STD ERROR OF Y
1	.997377	3.53085 E-2
2	.996328	4.17762 E-2
3	.998115	2.99274 E-2
4	.998115	0

WHAT DEGREE DO YOU WANT TO USE? 1
 DO YOU WANT COEFFICIENTS [1] OR FULL LIST[2]? 2

TERM	COEFFICIENT
0	-4.75698
1	1.8274

INTEN RATIO	CONC GIVEN	CONC FOUND	DIFF	PCT DIFF
409.5	1.11	1.03907	-7.09288 E-2	-6.38998
254.5	.387	.43568	4.86797 E-2	12.5787
154.	.178	.173976	-4.02379 E-3	-2.26055
134.5	.14	.135844	-4.15555 E-3	-2.96825
923.5	4.59	4.59251	2.51167 E-3	5.47204 E-2

RESULTS FOR SAMPLES

SAMPLE NO.	INTEN RATIO	CONCEN RATIO	CONCENTRATION
9182	147.	.159798	.120328
9182	143.	.151941	.114412
9182	146.	.157817	.118836
9182	149	.163793	.123336
9182	148	.16179	.121828
9182	AVERAGE=	.159028	.119748
9182	STD. DEV.=	4.54458 E-3	3.42207 E-3
9183	785.	3.41268	2.62094
9183	782.	3.38889	2.60267
9183	778.	3.35728	2.57839
9183	784.	3.40474	2.61484
9183	AVERAGE=	3.3909	2.60421
9183	STD. DEV.=	2.44994 E-2	1.88155 E-2

TIME: 9 SECS.

900 DATA 5.0
 901 DATA 1075.0, 1654.5, 3764.2.5
 902 DATA 5940.5, 9602.10, 3
 903 DATA 221, 1620, 1620, 1641
 904 DATA 222, 1660, 1664, 1664
 905 DATA 223, 1714, 1704, 1689
 906 DATA 224, 1723, 1723, 1711
 907 DATA 225, 1645, 1647, 1656
 908 DATA 226, 2250, 2265, 2184
 909 DATA 227, 2290, 2294, 2290
 910 DATA 228, 2759, 2759, 2765
 911 DATA 229, 5766, 5714, 5792
 912 DATA 231, 1598, 1596, 1610
 913 DATA 0

CFIT2 14:24 10/30/67

DEGREE	INDEX OF DETN	STD ERROR OF Y
1	.995102	.401285
2	.999991	1.75589 E-2
3	.999992	1.60697 E-2
4	.999992	0

WHAT DEGREE DO YOU WANT TO USE? 2

TERM	COEFFICIENT
0	-.842798
1	7.40564 E-4
2	4.05085 E-8

INTEN.	CONC. GIVEN	CONC. FOUND	DIFF.	PCT. DIFF.
1075	0	1.21821 E-4	1.21821 E-4	INFINITE
1654	.5	.492916	-7.08427 E-3	-1.41685
3764	2.5	2.5186	1.85991 E-2	.743964
5940	5	4.98544	-1.45589 E-2	-.291178
9602	10	10.0029	2.92218 E-3	2.92218 E-2

ANALYSES FOR UTECH AND EARLY -- ELEMENT: BI

RESULTS FOR SAMPLES

SAMPLE NO.	AVE. INTEN.	AVE. CONC.	STD. DEV. CONC.	NO. OF RUNS
221	1627	.469336	1.05805 E-2	3
222	1662.67	.500498	2.02139 E-3	3
223	1702.33	.535285	1.10527 E-2	3
224	1719	.549935	6.09456 E-3	3
225	1649.33	.488836	5.12302 E-3	3
226	2233	1.01292	3.96715 E-2	3
227	2291.33	1.06676	2.13884 E-3	3
228	2761	1.5107	3.34006 E-3	3
229	5757.33	4.76365	4.79171 E-2	3
231	1601.33	.446969	6.59104 E-3	3

TIME: 7 SECS.

XRAY1

XRAY1 is a program for data analysis in testing proposed analytical methods, where all the data are from standard specimens and the calibration is presumed to be linear. (The assumption of linearity may be under test.) A calibration slope, the ratio of percent concentration to intensity, must be input and the average percent concentration for each specimen is known a priori, the derived range of percent concentration values being centered on this value.

A program option allows for a found concentration to be printed for each measured intensity or for suppressing this print out.

The statistical methods used in this program are outlined in NBS Handbook 91. The program consists of 70 active statements. Each set of data requires approximately 3 sec processor time and 1 min console time.

Example

The data entry begins in line 801 with the following parameters being input in the order given: print out option (1 for percentage print out for each intensity, 0 for no print out); number of measurements per standard; four slopes; specimen number; four known concentrations; a table, four columns wide by as many rows as there are measurements, which contains the measured intensities.

The data are in columns with each column being related to an element. If fewer than four elements are being studied the extra columns must be filled with zeros. In addition to numerical input, column headings may be changed by adjusting line 30.

If the labels are constant, several sets of data can be entered at one time by adding additional sets of data to the input. Line 450 must be adjusted to return control to the

proper read line (line 20 or 21) depending on whether the print out option, the number of measurements per standard, and the slopes change between data sets.

801 DATA 0, 4, .0091, .0012, .0016, .00017
 802 DATA 14, 74.50, 0.001, 0.10, 0.10
 901 DATA 3366, 2781, 0143, 0467
 902 DATA 3395, 2785, 0108, 0429
 903 DATA 3519, 2855, 0072, 409
 904 DATA 3569, 2869, 0074, 0497
 906 DATA 14, 74.50, 0.001, 0.10, 0.10
 907 DATA 3366, 2781, 0143, 0467
 908 DATA 3395, 2785, 0108, 0429
 909 DATA 3519, 2855, 0072, 409
 910 DATA 3569, 2869, 0074, 0497

XRAY1 15:09 04/14/67

ANALYSIS FOR 4 ELEMENTS FOR 4 RUNS ON SPECIMEN 14

ITEM	AGKA	CUSC	ZNKA	ZNKA
STATISTICAL ANALYSIS				
AVE PCT	74.5	.001	.1	.1
STD DEV PCT	.885442	5.51957 E-2	5.36318 E-2	6.67056 E-3
AVE INTEN	3462.25	2822.5	99.25	450.5
STD DEV INTEN	97.3015	45.9964	33.5199	39.2386
PCT COEF VAR	1.18851	5519.57	53.6318	6.67056
MAX PCT	75.4714	.0568	.17	.107905
MIN PCT	73.6241	-.0488	.0564	.092945
RANGE PCT	1.8473	.1056	.1136	.01496

ANALYSIS FOR 4 ELEMENTS FOR 4 RUNS ON SPECIMEN 14

ITEM	AGKA	CUSC	ZNKA	ZNKA
STATISTICAL ANALYSIS				
AVE PCT	74.5	.001	.1	.1
STD DEV PCT	.885442	5.51957 E-2	5.36318 E-2	6.67056 E-3
AVE INTEN	3462.25	2822.5	99.25	450.5
STD DEV INTEN	97.3015	45.9964	33.5199	39.2386
PCT COEF VAR	1.18851	5519.57	53.6318	6.67056
MAX PCT	75.4714	.0568	.17	.107905
MIN PCT	73.6241	-.0488	.0564	.092945
RANGE PCT	1.8473	.1056	.1136	.01496

OUT OF DATA IN 21

TIME: 5 SECS.

XRAY2

XRAY2 is similar in structure to XRAY1, but it has a different purpose. XRAY2 computes statistics for intensities measured on unknown specimens. A calibration slope, which is the ratio of percent concentration to intensity, is input so that the standard deviation may be computed in terms of percent concentration.

The statistical methods used in this program are outlined in NBS Handbook 91. The program consists of 54 active statements. Each set of data requires approximately 2 sec processor time and 1 min console time.

Example

The data entry begins in line 899 with the following parameters being input in the order given; four slopes; specimen number; number of measurements per unknown; a table, four columns wide by as many rows as there are measurements, which contains the measured intensities.

The data are in columns with each column related to an element. If fewer than four elements are being studied the extra columns must be filled with zeros. In addition to numerical input, column headings may be changed by adjusting line 130.

If the labels are constant, several sets of data can be entered at one time by adding additional sets of data to the input. Line 310 must be adjusted to return control to the proper line (12, 14, or 15) depending on what data are common to all sets.

899 DATA .5, .5, .5, .5
 900 DATA 76, 5
 901 DATA 9, 7, 22, 7.6
 902 DATA 10, 9, 22, 7.7
 903 DATA 9, 8, 21, 7.8
 904 DATA 11, 9, 23, 6.9
 905 DATA 11, 7, 22, 6.7
 906 DATA 12, 9, 22, 6.9
 907 DATA 11, 8, 22, 7.1
 908 DATA 11, 9, 22, 6.9
 909 DATA 13, 7, 22, 7.7
 910 DATA 13, 7, 22, 7.5

XRAY2 15:17 04/14/67

AVERAGES OF 5 INTENSITIES FOR 4 ELEMENTS FROM SPECIMEN 76
 -- WITH STATISTICAL ANALYSIS. TEST SAMPLE 1

ITEM	AGKA	SN/AG	CUSC	ZNKA
AVERAGE	10.	.804242	22.	7.34
MAXIMUM	11	.9	23	7.8
MINIMUM	9	.636364	21	6.7
RANGE	2	.263636	2	1.1
STD. DEV.	1	.106551	.707107	.502991
STD. DEV. OF PCT	.5	5.32755 E-2	.353553	.251496
PCT. COF. VAR.	10.	13.2486	3.21412	6.85274

AVERAGES OF 5 INTENSITIES FOR 4 ELEMENTS FROM SPECIMEN 76
 -- WITH STATISTICAL ANALYSIS. TEST SAMPLE 1

ITEM	AGKA	SN/AG	CUSC	ZNKA
AVERAGE	12.	.674476	22.	7.22
MAXIMUM	13	.818182	22	7.7
MINIMUM	11	.538462	22	6.9
RANGE	2	.27972	0	.8
STD. DEV.	1	.128591	0	.363318
STD. DEV. OF PCT	.5	6.42955 E-2	0	.181659
PCT. COF. VAR.	8.33333	19.0653	0	5.0321

OUT OF DATA IN 110

TIME: 3 SECS.

PLATE1

PLATE1 is a program for calibrating plating thickness as a function of attenuation of x-ray fluorescent intensity. Intensities are measured as a function of the time required to reach a preset count, and are background corrected. The program makes a linear least squares regression of plating thickness as a function of the natural logarithm of the corrected fluorescent intensity of the substrate material.

The statistical methods used in this program are outlined in NBS Handbook 91. The program consists of 94 active statements. Each set of data requires approximately 5 sec processor time and 2 min console time.

Example

The data input begins in line 900 where the first number is the mass absorption coefficient in the plating material for the radiation of the substrate which is measured, followed by the density of the plating material in g/cm^3 , the preset x-ray count, the counting time for an infinitely thick plating, the counting time for the substrate with no plating, and the number of time measurements per standard. In line 901 and the following lines the thickness of a standard and the measured times for that standard are input.

900 DATA 90.0, 8.90, 256000, 191.2, 10.94, 4
 901 DATA 0, 10.87, 10.86, 10.88, 10.88, 0, 10.97, 11.00, 11.05, 11.01
 902 DATA .12, 20.78, 20.85, 20.77, 20.77, .12, 20.98, 21.00, 21.08, 20.8
 903 DATA .26, 41.04, 41.16, 41.25, 41.19
 904 DATA .26, 41.11, 40.86, 41.04, 40.98
 905 DATA .37, 61.56, 61.64, 61.28, 61.26
 906 DATA .37, 62.24, 62.35, 62.11, 62.38
 907 DATA .56, 109.61, 109.36, 109.63, 109.89
 908 DATA .56, 111.50, 111.38, 111.41, 111.34
 909 DATA .76, 149.97, 149.62, 149.69, 148.89
 910 DATA .76, 150.43, 149.69, 150.39, 150.37
 911 DATA .85, 159.19, 158.89, 158.81, 158.41
 912 DATA .85, 159.84, 159.72, 160.04, 159.82

PLATE1 16:05 04/22/67

COMPUTATIONS FOR PLATING THICKNESS CALIBRATION.

GIVEN THICKNESS	CORR. I	LN CORR I	LN(COR I/IO)	MU FOR AVE 0
0	22206.7	10.008	.007	-63871.3
0	21918.1	9.995	-.007	63426.5
.12	10973.3	9.303	-.698	.17
.12	10854.6	9.292	-.709	.179
.26	4880.74	8.493	-1.509	.169
.26	4905.4	8.498	-1.503	.167
.37	2828.13	7.947	-2.054	.144
.37	2772.23	7.927	-2.074	.15
.56	996.382	6.904	-3.097	.142
.56	958.959	6.866	-3.136	.149
.76	372.988	5.922	-4.08	.126
.76	365.262	5.901	-4.101	.129
.85	272.93	5.609	-4.392	.107
.85	262.54	5.57	-4.431	.111

LEAST SQUARES FIT OF DATA .

REGRESSION WITH THICKNESS AS THE INDEPENDENT VARIABLE .

$$\text{LN INTENSITY} = -5.23 [\text{THICKNESS}] + 9.913$$

$$\text{STANDARD ERROR OF LN INTENSITY} = .081$$

REGRESSION WITH LN INTENSITY AS THE INDEPENDENT VARIABLE .

$$\text{THICKNESS} = -.191 [\text{LN INTENSITY}] + 1.892$$

$$\text{STANDARD ERROR OF THICKNESS} = .016$$

TIME: 5 SECS.

PLATE2

PLATE2 is a program for computing plating thickness for measurements on unknown specimens, given a calibration equation as found in PLATE1. As in PLATE1, attenuation of characteristic x-rays originating in the substrate is the basis for measurement. Time to reach a preset count level is the quantity input; several such measurements for each unknown thickness are input. These quantities are converted to counts per second, background corrected, and averaged. The averaged value is substituted into the calibration equation found in PLATE1, and the determined thickness is printed out.

The statistical methods used in this program are outlined in NBS Handbook 91. The program consists of 33 active statements. Each set of data requires approximately 1 sec processor time and 1 min console time.

Example

The data entry begins in line 900 with the following parameters being input in the order given: test number, coefficient of the linear term, constant term, number of time measurements per unknown, test level for the coefficient of variation of found thickness, the background in cps, and the total number of counts taken in each measurement (preset count). In line 901 and the following lines the identification number of the unknown specimen is input, followed by the n time measurements for each.

900 DATA 75, -.192, 1.903, 4, .8, 1499, 256000
 901 DATA 2, 20.78, 21.00, 20.79, 20.80
 902 DATA 4, 62.00, 62.31, 62.13, 62.09
 903 DATA 6, 111.0, 111.2, 111.3, 111.3
 904 DATA 8, 89, 89, 89.4, 95

PLATE2 16:18 04/22/67

X-RAY THICKNESS DETERMINATIONS. 4 MEASUREMENTS PER UNKNOWN.

TEST NO.: 75

EQUATION : = -.192 [LN INTEN.] + 1.903

TEST LEVEL : COEFFICIENT OF VAR.= .8

UNKNOWN NO.	THICKNESS	PCT CV IF> .8	REMARKS
2	.1201	.92	
4	.3917	*	
6	.6188	*	
8	.5225	2.55	

TIME: 1 SECS.

STAT

STAT is a program which computes the following statistics for each of one to eight columns of numbers: average, maximum, minimum, range, standard deviation, 95% confidence limits for the standard deviation, percent coefficient of variation, and the 95% confidence limit for the lot mean. The columns of numbers need not be related, but must all have the same length.

An important feature of the program allows the operator to cause the data to be subgrouped by changing four parameters in one line of input. For example, a set of 80 data points may have been obtained at five different times. The computations can be made for the total set of 80 data points and for the original subsets of 16.

The statistical methods used in this program are outlined in NBS Handbook 91. The program consists of 119 statements. Running time for eight columns of 20 numbers is about 3 sec processor time and 2 min console time.

Example

The first number of the input, on line 899, controls an option. In this case, the program will read in N columns, each L long. Alternatively, if the first number was 1, the program would read $L \times N$ table. Line 900 contains the following data: number of columns, number of rows, number of rows to be computed each time, B upper, B lower, Student's T . B and T values may be found in NBS Handbook 91, pp. T34 and T5; if either of these computations is not desired, zeroes may be inserted. Lines 901 through 904 contain 4 columns of 8 numbers each. In the example given, the data have been subgrouped into groups of four. Calculations for the complete set, without subgrouping, could be obtained by changing the last four parameters on line 900.

899 DATA 2
 900 DATA 4, 8, 4, 3, 183, 5178, 3, 182
 901 DATA 631, 634, 645, 652, 614, 632, 643, 622
 902 DATA 555, 533, 544, 523, 533, 522, 541, 532
 903 DATA 211, 234, 231, 222, 234, 235, 253, 233
 904 DATA 123, 124, 122, 133, 133, 122, 123, 123

STAT 13:43 10/30/67

STATISTICAL ANALYSIS FOR 4 COLUMNS OF 4 NUMBERS

COL:	1	2	3	4
AVERAGE	640.5	538.75	224.5	125.5
MAXIMUM	652	555	234	133
MINIMUM	631	523	211	122
RANGE	21	32	23	11

ANALYSIS OF VARIANCE

STD. DEV.	9.74679	13.8173	10.3441	5.06623
95 CONF U LIM	31.024	43.9803	32.9252	16.1258
95 CONF L LIM	5.04689	7.15458	5.35616	2.62329
PCT COEF VAR	1.52175	2.56469	4.60761	4.03684

T TEST...95 PCT CONF INTERVAL FOR THE LOT MEAN.

UPPER LIMIT	658.406	564.134	243.503	134.807
LOWER LIMIT	622.594	513.366	205.497	116.193

STATISTICAL ANALYSIS FOR 4 COLUMNS OF 4 NUMBERS

COL:	1	2	3	4
AVERAGE	627.75	532	238.75	125.25
MAXIMUM	643	541	253	133
MINIMUM	614	522	233	122
RANGE	29	19	20	11

ANALYSIS OF VARIANCE

STD. DEV.	12.5532	7.78888	9.53502	5.18813
95 CONF U LIM	39.9569	24.792	30.35	16.5138
95 CONF L LIM	6.50006	4.03308	4.93724	2.68641
PCT COEF VAR	1.99972	1.46408	3.99373	4.14222

T TEST...95 PCT CONF INTERVAL FOR THE LOT MEAN.

UPPER LIMIT	650.812	546.309	256.267	134.781
LOWER LIMIT	604.688	517.691	221.233	115.719

TIME: 5 SECS.

TEMPER and PROFIL

Both of these programs calculate plasma temperatures from the relative intensities of spectral lines. They differ only in the form of output. The temperature and standard deviation of the **temperature** are found from the slope and standard deviation of the slope of a least-squares line fitted through $\log(I\lambda^3/gf)$ vs. E , where I is the relative intensity of a line, λ is its wavelength, g is the statistical weight of the line, f is the oscillator strength, and E is the excitation energy. The procedure for the least-squares fit is taken from NBS Handbook 91, Section 5-4.1.

For each value of E , a value of $\log(I\lambda^3/gf)$ is found from the curve, and from this is calculated the standard error of Y . Any point for which the difference between the input and calculated values of this log ratio is greater than twice the standard error of Y is rejected, and the line is refitted to the remaining points.

Example of TEMPER

The first number in line 900 is the number of emission lines used. This is followed by the following data for each line: wavelength, excitation energy in Kaysers, and the gf -value. In the example there are two sets of relative intensities, listed in the same order as the emission lines. These two sets of emission intensities are identical except that in the second set two intensity values have been changed to demonstrate rejection of faulty data by the program.

Example of PROFIL

The first number in the data is the number of emission lines used. This is followed by the following data for each line: wavelength, excitation energy in Kaysers, and the gf -value. In the example there are three sets of

relative intensities, listed in the same order as the emission lines. In each case, the first number indicates the position in the arc at which the measurements were made. The first two sets are identical except that two intensities have been changed in the second set to demonstrate rejection of faulty data by the program.

900 DATA 10, 3278.3, 40426, .68, 3282.3, 40330, .59, 3308.8, 31301, .062
 901 DATA 3318.0, 31114, .072, 3329.5, 31114, .33, 3332.1, 40027, .91
 902 DATA 3335.2, 30959, .26, 3340.3, 30837, .19, 3343.8, 31114, .062
 903 DATA 3346.7, 30959, .072
 904 DATA 44.372, 33.716, 30.082, 40.456, 287.23, 70.666, 206.97
 905 DATA 149.90, 31.669, 43.529
 908 DATA 44.372, 33.716, 30.082, 40.456, 490
 909 DATA 70.666, 206.97, 149.9, 31.669, 23.529

TEMPER 16:33 04/12/67

WAVELENGTH	RATIO	ENERGY
3278.3	12.3615	40426
3282.3	12.3055	40330
3308.8	13.2449	31301
3318	13.3123	31114
3329.5	13.5069	31114
3332.1	12.4583	40027
3335.2	13.4703	30959
3340.3	13.4684	30837
3343.8	13.281	31114
3346.7	13.3553	30959

TEMP. IS 5731.39 +-342.694 DEGREES K.

WAVELENGTH	RATIO	ENERGY
3278.3	12.3615	40426
3282.3	12.3055	40330
3308.8	13.2449	31301
3318	13.3123	31114
3329.5	13.7388	31114
3332.1	12.4583	40027
3335.2	13.4703	30959
3340.3	13.4684	30837
3343.8	13.281	31114
3346.7	13.0881	30959

LINE AT 3329.5 A. OUT OF LIMITS.

LINE AT 3346.7 A. OUT OF LIMITS.

TEMP. IS 5846.26 +-351.037 DEGREES K.

OUT OF DATA IN 160

TIME: 3 SECS.

900 DATA 10, 3278.3, 40426.68, 3282.3, 40330.59, 3308.8, 31301.062
 901 DATA 3318.0, 31114.072, 3329.5, 31114.33, 3332.1, 40027.91
 902 DATA 3335.2, 30959.26, 3340.3, 30837.19, 3343.8, 31114.062
 903 DATA 3346.7, 30959.072
 904 DATA 1.23, 44.372, 33.716, 30.082, 40.456, 287.23
 905 DATA 70.666, 206.97, 149.90, 31.669, 43.529
 906 DATA 2.34, 44.372, 33.716, 30.082, 40.456, 490
 907 DATA 70.666, 206.97, 149.9, 31.669, 23.529
 908 DATA 3.45, 51.663, 38.962, 34.602, 46.774, 341.99
 909 DATA 83.86, 241.08, 186.27, 38.152, 49.375

PROFIL 16:42 04/12/67

SET NUMBER 12

POSN.-MM	TEMP.-DEG. K	T - 1S	T + 1S	STD. DEV.
1.23	5731.39	5388.7	6074.09	342.694
2.34	5846.26	5495.22	6197.3	351.037
LINE AT 3329.5	ANGSTROMS REJECTED			
LINE AT 3346.7	ANGSTROMS REJECTED			
3.45	5711.7	5348.26	6075.15	363.446

OUT OF DATA IN 160

TIME: 3 SECS.

COLS8

COLS8 is a subroutine which will print out 6 to 8 neat columns of tabular data. Exponential output is not allowed for and the columns are 6 digits wide. Thus, no entry in the table may be larger than 999999.

Example

In the example shown, the subroutine was appended to a program written to generate 8 columns of 10 numbers.

```
COLEX      16:29           04/22/67
20         40         60         80         100        120        140        160
40         80        120        160        200        240        280        320
60        120        180        240        300        360        420        480
80        160        240        320        400        480        560        640
100       200        300        400        500        600        700        800
120       240        360        480        600        720        840        960
140       280        420        560        700        840        980       1120
160       320        480        640        800        960       1120       1280
180       360        540        720        900       1080       1260       1440
200       400        600        800       1000       1200       1400       1600
```

TIME: 2 SECS.

WRITE1, WRITE2, and WRITE4

These subroutines are useful for having the results of one program punched onto a paper tape formatted for quick reentry as input data to another program.

Examples

In the example shown, the subroutines have been added to the program TEMPER. In each case, the normal output of TEMPER is followed by the output of the subroutine.

TEMPER 10:09 04/24/67

WAVELENGTH	RATIO	ENERGY
3278.3	12.3579	40426
3282.3	12.2962	40330
3308.8	13.2437	31301
3318	13.3074	31114
3329.5	13.5065	31114
3332.1	12.4542	40027
3335.2	13.4683	30959
3340.3	13.4687	30837
3343.8	13.2855	31114
3346.7	13.35	30959

TEMP. IS 5706.39 +-341.504 DEGREES K.

DATA INPUT TAPE BEGINS, TYPE 1, TURN ON TAPE, HIT RETURN.
?1

900	DATA	40426	,	40330	,	31301	,	31114
901	DATA	31114	,	40027	,	30959	,	30837
902	DATA	31114	,	30959				

TIME: 4 SECS.

TEMPER 10:47 04/24/67

WAVELENGTH	RATIO	ENERGY
3278.3	12.3615	40426
3282.3	12.3055	40330
3308.8	13.2449	31301
3318	13.3123	31114
3329.5	13.5069	31114
3332.1	12.4583	40027
3335.2	13.4703	30959
3340.3	13.4684	30837
3343.8	13.281	31114
3346.7	13.3553	30959

TEMP. IS 5731.39 +-342.694 DEGREES K.

DATA TAPE BEGINS, TYPE 1, TURN ON TAPE, HIT RETURN.
?1

900	DATA	3278.3	,	12.3615	,	40426	,	40426
901	DATA	3282.3	,	12.3055	,	40330	,	40330
902	DATA	3308.8	,	13.2449	,	31301	,	31301
903	DATA	3318	,	13.3123	,	31114	,	31114
904	DATA	3329.5	,	13.5069	,	31114	,	31114
905	DATA	3332.1	,	12.4583	,	40027	,	40027
906	DATA	3335.2	,	13.4703	,	30959	,	30959
907	DATA	3340.3	,	13.4684	,	30837	,	30837
908	DATA	3343.8	,	13.281	,	31114	,	31114
909	DATA	3346.7	,	13.3553	,	30959	,	30959

TIME: 4 SECS.

TEMPER 10:34 04/24/67

WAVELENGTH	RATIO	ENERGY
3278.3	12.3615	40426
3282.3	12.3055	40330
3308.8	13.2449	31301
3318	13.3123	31114
3329.5	13.5069	31114
3332.1	12.4583	40027
3335.2	13.4703	30959
3340.3	13.4684	30837
3343.8	13.281	31114
3346.7	13.3553	30959

TEMP. IS 5731.39 +-342.694 DEGREES K.

DATA OUTPUT TAPE BEGINS, TYPE 1, TURN ON TAPE, HIT RETURN.
?1

900	DATA	12.3615	,	40426	,	12.3055	,	40330
901	DATA	13.2449	,	31301	,	13.3123	,	31114
902	DATA	13.5069	,	31114	,	12.4583	,	40027
903	DATA	13.4703	,	30959	,	13.4684	,	30837
904	DATA	13.281	,	31114	,	13.3553	,	30959

TIME: 4 SECS.

TIME

TIME is a program for computer terminal usage accounting and housekeeping. It functions by accumulating a block of usage data. The program accumulates the data automatically by instructing the operator how to load and save one line of data at the end of each use. Each operator should call TIME and type RUN before signing off the terminal. When a summary is desired type: "5 GO TO 130"; then type: RUN. At the beginning of each month the data of the previous month should be run and then unloaded by deleting all the data lines except 999.

Examples

Two examples are shown. The first shows entry of data by an operator at the end of a use. He calls up the program, types "RUN", and enters data according to the instructions given by the output of the program. In the second example, the operator types "5 GO TO 130" to skip over the first part of the program, and then types run. The program then summarizes the data that have been put in by individual operators to show the usage of the system from the first of the month.

OLD
OLD PROBLEM NAME--TIME

READY.

RUN

TIME 16:58 04/12/67

TYPE A LINE OF DATA NUMBERED: 959 USING THIS FORMAT:

959 DATA 959 , OPERATOR NO., TIME ON, TIME OFF, DAY OF MONTH

WHEN COMPLETE TYPE 'SAVE' AND SAY 'GOODBYE'.

**** ALWAYS USE PROPER FORMAT ****

\$\$\$\$ REMEMBER TO TYPE SAVE \$\$\$\$

TIME: 3 SECS.

959 DATA 959,7,1543,1658,12

SAVE

WAIT.

READY.

GOODEYE

*** OFF AT 16:58.

5 GO TO 130
 RUN
 WAIT.

TIME 15:46 04/12/67

SUMMARY OF COMPUTER USAGE TO THE 12 TH DAY OF THE MONTH

NO. CONTACTS	CONTACT HOURS	CONTACTS/WKDAY	AV.HRS/CONT.	PRED.HRS/MO
39	23.9333	3.9	.613675	50.26

USER NUMBER	NO. CONTACTS	CONTACT HOURS	PCT. ALL HRS	PRED.HRS/MO
6	6	6.06667	25.3482	12.74
7	4	1.5	6.26741	3.15
10	9	2.45	10.2368	5.145
11	4	4.06667	16.9916	8.54
15	2	1.11667	4.66574	2.345
16	2	1.86667	7.79944	3.92
19	1	.266667	1.11421	.56
27	8	5.75	24.0251	12.075
31	2	.683333	2.85515	1.435
32	1	.166667	.696379	.35

CHART OF DAILY USAGE

DAY	HOURS									
	0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	>
1	+	+	+	+	+	+	+	+	+	+
2	+	+	+	+	+	+	+	+	+	+
3	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
4	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
5	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
6	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
7	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
8	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
9	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
10	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
11	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
12	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
13	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
14	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

STOP.
 READY.

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