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AUTOMATION OF THE JARRELL-ASH MODEL 70-314 EMISSION SPECTROMETER

W. F. Morris
E. R. Fisher
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April 17, 1978

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Automation of the Jarrell-Ash Model 70-314 Emission Spectrometer

ABSTRACT

We describe automation of the Jarrell-Ash 3.4-Meter Ebert direct-reading emission spectrometer with digital scaler readout. The readout is interfaced to a Data General NOVA 840 minicomputer. The automation code consists of BASIC language programs for interactive routines, data processing, and report generation. Call statements within the BASIC programs invoke assembly language routines for real-time data acquisition and control. In addition, we present the automation objectives as well as the spectrometer-computer system functions, coding, and operating instructions.

INTRODUCTION

The Jarrell-Ash direct-reader emission spectrometer consists of an excitation light source, a 3.4-Meter Ebert optical grating spectrometer model 70-314, and a 22-channel photomultiplier detector-readout model 66-110. It is used to determine 20 elements in water samples. Table 1 shows two alternative element lists of which the element channels "In" and "Y" are for background monitoring and internal standardization, respectively; the remaining element channels monitor the 20 elements determined in the spectrometric analysis. A high-voltage ac spark source excites the sample that is introduced into the spark gap by a rotating disk electrode. Prior to excitation, most samples are concentrated by evaporating enough of the sample to yield a dissolved solids content of 100 mg per 5 ml.

The method applies to a wide range of water samples.^{1,2}

Table 1. Elements determined by the Jarrell-Ash emission spectrometer.

Element list 1						Element list 2					
1. In	9. Ag	16. Mo	1. In	9. Ag	16. Mo	1. In	9. Ag	16. Mo	1. In	9. Ag	16. Mo
2. Y	10. Ni	17. B	2. Y	10. Ni	17. Sb	2. Y	10. Ni	17. Sb	2. Y	10. Ni	17. Sb
3. Fe	11. Co	18. Li	3. Fe	11. Co	18. Sn	3. Fe	11. Co	18. Sn	3. Fe	11. Co	18. Sn
4. Zn	12. Pb	19. Be	4. Zn	12. Pb	19. Be	4. Zn	12. Pb	19. Be	4. Zn	12. Pb	19. Be
5. Cd	13. Cr	20. Ti	5. Cd	13. Cr	20. Ti	5. Cd	13. Cr	20. Ti	5. Cd	13. Cr	20. Ti
6. As	14. V	21. Al	6. As	14. V	21. Al	6. As	14. V	21. Al	6. As	14. V	21. Al
7. Mn	15. Tl	22. Ba	7. Mn	15. Tl	22. Ba	7. Mn	15. Tl	22. Ba	7. Mn	15. Tl	22. Ba
8. Cu			8. Cu			8. Cu			8. Cu		

MANUAL OPERATION

After preparing the water sample, the operator places a small volume of sample into a porcelain boat, sets the pre-exposure and exposure timers, and visually checks the Hg monitor for spectrum alignment. He then positions a motor-mounted graphite disk in the solution, moves the counter electrode to within 3 mm of the top of the disk, and depresses the excitation START button. The disk rotates in the solution and feeds sample into the high-voltage spark gap between the disk and the counter electrode where elements in the sample are excited.

During the excitation, each of the detector-capacitor channels detects and stores light from each of the 22 element lines. When excitation is completed, a Nixie tube display generates a test count signal and the operator determines if the value is within a predetermined level (to check electronic stability). The operator

then depresses a sequencer button to read each of the 22 element channels. He reads and records the value from the Nixie tube display for each of the 22 steps of the sequencer.

The spectrometer is operated in either the calibration or analysis mode. In the calibration mode, the analyst runs a range of standards containing the elements of interest. He then reads and records corresponding count values, averages these values, and performs a least squares fit of the data, thus producing a calibration curve that relates known concentration with counts. In the analysis mode, the analyst checks the averaged count values of an unknown sample against the calibration curve to determine the concentrations of the elements of interest. In addition, he makes background corrections on all channels in both the calibration and analysis modes by running a "blank" at the beginning

of a series of calibrations or analyses, or at intervals during the series of runs, at his discretion. A "blank" is a water matrix typical of the waters being run and free of the trace elements of interest. The operator re-

cords the values of the blank for each channel and then subtracts them from the standards or samples after they have been run.

AUTOMATION GOALS

The principal objectives in automating the emission spectrometer, stated in Ref. 3, are to increase throughput and decrease errors, and at the same time preserve interaction between the operator, the instrument, and the data being generated. The following specific operations have been designated for automation: (1) sequential readout of the element channels; (2)

data logging for standards and samples; (3) calculations of standards data and fitting of the standard reference curves; (4) storage and retrieval of standards data; (5) calculation of sample data and results; (6) generation of detailed data sheets of standards and samples; and (7) generation of analysis reports.

PROPOSED AUTOMATION

Automation of the emission spectrometer is provided by interfacing the spectrometer readout to a Data General NOVA 840 computer system. The operator communicates with the automation computer by means of a video terminal with a teletype keyboard.

The automation designed for the emission spectrometer provides the operator with several options, including direct-count and count-ratio methods for line-intensity measurement, static and dynamic background correction, and two procedures for the calculation of detection limits. The system may be operated in either calibration or analysis modes and a variety of prompts allow the operator to interact with the program.

Calibration and Analysis Modes

In both the calibration and analysis modes, the system automatically reads the outputs of a test channel and the 22 element channels. The readings are displayed automatically on a terminal immediately after the sample or standard is run. The operator views the results, determines their acceptability, and elects to continue replicate (four or less) excitations. When the replicate excitations are completed, the operator examines the results and designates the two most acceptable runs. A sequence of dynamic retrieval, calculation, and display operations are then performed as follows: the data for the two acceptable runs are retrieved and displayed sequentially as they are retrieved; the values are averaged, corrected for background, ratioed to the internal standard (if that option is being used), and displayed.

At this point, if standards are being run (calibration mode), the mean counts or count ratios for all replicates of each standard run are calculated, displayed, and stored. If samples are being run (analysis mode), the concentrations in the processed and original samples are calculated and displayed. When all the data for

all 22 elements have been retrieved, calculated, and displayed, the operator essentially views the detailed summary data for the current sample or standard being run. By a keyboard command, he can obtain a printout of the detailed summary data sheet followed, in the case of samples, by a more concise report containing only the sample identification and the concentration values.

The calibration mode of operation is used to acquire data from known standards to establish standard working curves. Data for each concentration of each element in a number of standards will be acquired over an extended period of time, e.g., one run of each standard per day over several days. Standards and samples are run in the same way. The interactive instrument-operator sequence is the same for the calculation of the background corrected count or count ratio values. For standards, running mean values of the counts or count ratios for each element are calculated using values from the current standard and running mean values based on all standard runs up to the current run. All the data are dynamically displayed at the spectrometer terminal. A summary data sheet can be requested after each run of each standard. In practice, five runs of each standard are made—one run per standard per day. The final mean values, calculated from the accumulated data of the five runs, are used in the calibration fit that relates either background-corrected counts or count ratios to known concentrations. The operator may choose a linear or polynomial fit of the data in a normal or logarithmic form of the equation.

The analysis mode of operation is used to acquire and process sample data. Concentrations of the 20 elements in a sample are determined using the average background-corrected counts or count ratios of the elements from two acceptable runs of the sample. The concentrations are calculated using an equation with the coefficients of the currently stored standard calibration.

Background Corrections and Calculation of Detection Limits

The automation program provides static and dynamic methods for background correction and two methods for calculating detection limits. In the static method the background values for each element channel are derived from a separate run (average of two excitations) of a blank standard or sample. The background values are stored for subsequent retrieval and subtracted from standards and samples when they are run. When the static method of background correction is used, the detection limits are calculated to be those concentrations equivalent to count values 10% above the background level.

The second method of background correction is termed "the dynamic background correction." In this method, background correction is made possible by assigning one channel of the array of 22 photomultiplier channels to monitor a location on the focal curve that is responsive to differing levels of background from one excitation to another. Of the 22 channels currently installed, the Indium channel (45.11.3 A) has been found to be the most appropriate background monitor. The actual background correction on each element channel is performed by the computer using the reading from the background channel and previously stored factors relating each element channel to the background channel. The latter factors are established in the initial standardization (calibration mode) procedure using data

from 10 replicate exposures of a standard solution blank free of the 20 elements of analytical interest. When the standard solution blank is run, the mean number of counts for each of the 22 channels is determined and the background factors are calculated by dividing the mean counts for each element channel by the mean counts for the background channel. Once established, the factors are stored in files for later retrieval.

When dynamic background correction is being used, the detection limits are determined while the automation program is run in the analysis mode. The limits for the 20 analysis elements are established by making multiple runs of a sample blank (10 are recommended). The mean count values and standard deviations for the 20 analysis elements are calculated and the detection limits are established as the concentration equivalent to the blank plus 2 times the standard deviation of the mean of the blank.

Operator Decisions

Certain operator decisions, e.g., selection of the most acceptable runs, are retained in the overall system operation. These are necessary because of the diversity of the water samples and the nature of the sample electrode and high-voltage spark discharge. In most instances, precision is $\pm 10\%$. The operator determines whether replicate excitations fall within the specified precision and makes allowances where matrix effect is an overriding factor.

SPECTROMETER-COMPUTER SYSTEM

Figure 1 is a schematic of the Jarrell-Ash spectrometer--NOVA 840 computer system. The system includes a Data General NOVA 840 minicomputer with disk storage and line printer, as well as Data General's real-time disk operating system (RDOS) and multiuser BASIC software. The latter software has been modified to provide CALLS to invoke assembly language subroutines for real-time data acquisition and other functions.

One of the key items in the system is the video display. It allows the operator to view the results almost immediately after they are returned from the computer. He can compare data from successive excitations and choose those data suitable for further processing. He can also compare current and stored data during a

calibration run as well as the parameters of the least squares fit.

The computer monitors the pre-exposure and exposure timer relays of the spectrometer source and controls the channel sequencer. It automatically "homes" the sequencer prior to an exposure and causes it to step through 22 channels immediately after an exposure has been completed. On each step through the 22 channels, the capacitor-stored photomultiplier output is read, stored, and displayed under control of the computer. For each excitation, a single column of 22 values is displayed. Up to four columns of data representing four excitations can be displayed side by side for comparison.

SYSTEM FUNCTIONS

The term "system" includes the spectrometer, excitation light source, computer, operator, and interactive processes that produce reports.

Operator Functions

The operator is responsible for the following functions:

Fig. 1. Configuration of the spectrometer - computer system.

- Prepares samples and standards.
- Chooses the program mode.
- Selects the type of background correction (static or dynamic).
- Inputs identifications, descriptions of samples and number of replicates.
- Sets excitation source parameters.
- Sets pre-exposure and exposure timers.
- Checks the Hg monitor and adjusts the refractor plate as necessary to ensure alignment.
- Prepares the electrode system and initiates the excitation.
- Examines the data after each excitation and judges its quality.
- Determines the number of replicate excitations required to obtain two acceptable excitations.
- Selects the two acceptable excitations.
- Determines the number of replicate runs of each standard when carrying out a calibration.
- Chooses the order of the least squares calibration fit and if it is to be a normal or log equation.
- Chooses appropriate data and types of analysis reports.

Spectrometer and Source Functions

The high-voltage ac spark source excites the elements of interest in the sample. The spectrometer disperses the light from the source and detects the spectrum. The duration of exposure and integration of the 22 spectrum line signals are determined by the settings on the source timers. Each element channel signal is stored on an electronic capacitor; capacitor-stored signals are converted to pulsed signals by a circuit in the spectrometer readout.

Computer Functions

The computer issues prompts relative to each required input, e.g. *operation mode and sample number*. It also issues prompts relative to the next step in the procedure, e.g., *select excitation runs*. It senses the start of the excitation as well as the start and completion of the integration interval. It cycles the channel sequencer to the test position, reads the value, and evaluates whether it is within tolerance; it then cycles the channel sequencer to each of 22 channels, reads the integrated counts on each channel, displays the value on the video screen, and stores the value in a disk file. The channel sequencer is then cycled back to the initial readout position (HOME) after all 22 channel values have been read, displayed and stored. The above sequence of

functions is repeated for each excitation. When the 22 values for each succeeding excitation are displayed, the preceding excitation values are also displayed to a maximum of four excitations. Thus a maximum of four columns of data each containing 22 values can be displayed. The computer processes the data from two of a maximum of four excitations. The two columns of data to be processed are chosen by the operator and the choices entered via the keyboard. The data are processed in any of several ways depending on whether an analysis or calibration is being carried out, whether direct counts or count ratios vs concentration are being used, or whether static or dynamic background corrections are being applied.

In the data processing procedure, values for the 22 elements in each of the two selected excitation runs are retrieved, one element at a time. The two values for each element are averaged and corrected for background by means of the static or dynamic method. If internal standardization is used, the intensity ratios of the analysis elements to the internal standard are calculated. Subsequent steps will depend on whether calibrations or analyses are being performed.

If a calibration is being carried out, the background-corrected counts or count ratios are stored in a disk file. As replicates of each standard are run (usually five replicates of each standard), the computer calculates and stores a running mean value of the counts or count ratios for each element in each standard.

When the operator has established that enough standards and replicates have been run, he requests a least squares fit of the data. The computer then requests the degree of fit and the selection of a log or normal form of the equation. The computer performs the least squares fit and outputs both the coefficients of the fit as well as the coefficient of determination for each element. It also outputs a line printer report of the least squares data.

In the analysis mode, after the background corrected counts or count ratios are calculated, the computer calculates the concentration of each element in the sample by an iterative procedure using the coefficients of the least squares fit.

When data processing is completed, the computer outputs appropriate printed reports in response to operator input. The reports contain header information such as date, sample number, standard number, description, etc. Reports can be obtained for individual standard runs, least squares fit parameters, laboratory data records, and customer sample analysis report.

SPECTROMETER-COMPUTER INTERFACING

The emission spectrometer interfacing links the Jarrell-Ash model 66-110 scaler readout to the compu-

ter system. The interfacing monitors completion of the test signal counting and provides control signals to se-

quentially step the element channel selector to read the accumulated counts as well as to step the channel selector switch back to the starting test position (HOME). The control signals actuate solid-state relays in the scaler readout.

Some modifications of the scaler readout were required to implement the interfacing. We modified the 12AU7 analog-to-digital converter circuit by adding solid-state FETRONS for better reliability. These were mounted under the 12AU7 circuit box and were connected to the interfacing by a twisted-pair cable. The

data signal was routed from the box to the interface mounted in the scaler chassis and in turn through a plug and cable to the digital interface at the computer. Figure 2 shows a simplified schematic of the interfacing. More detailed schematics are included in Appendix A*

*The automation software and hardware will be described in more detail in a later section of the text. Note that the description pertains to the original automation software developed by LLL for the EPA. Subsequent changes in both hardware and software have been made by EMSL to accommodate modifications to the Jarrell-Ash scaler readout system. Requests for information regarding any changes should be directed to EMSL in Cincinnati, Ohio.

Fig. 2. Simplified schematic of system interfacing.

COMPUTER AUTOMATION CODES

The automation code for operating the emission spectrometer is composed of BASIC and Assembly language programs. Four programs ES1, ES2, ES3, and ES4, written in high-level BASIC (Data General extended BASIC language), are linked to one another by a chaining technique described on pages 5 through 16 of Ref. 4. The ES1 program makes BASIC language CALLS invoking assembly language programs that read the spectrometer element channel signals, control the channel sequencer, and sense the timer relays. The calls are summarized in Table 2 and are described later.

Table 2. Summary of assembly language calls.

Call	Function
12	Resets channel cycle-sense switch and data counter
2	Resets channel cycle switch to home position
3	Reads data counts

Flow charts of the BASIC program functions and operator interactions are shown in Appendix B. Functions controlled by the computer are designated by a "C" in the flow chart symbols. Listings of the BASIC language programs are given in Appendix C; tables and descriptions of the variables, arrays, and files used in the programs are shown in Appendix D.

The division of the BASIC coding into four programs is for the most part according to inputs, calculations, and outputs.

ES1 contains the statements and routines to:

- Issue prompts either requesting input information or indicating the next step to be carried out.
- Acquire initial excitation data from the spectrometer.
- Store instrument data or descriptive information keyed in by the operator.

ES2 contains the statements and routines to:

- Retrieve initial data from two designated acceptable excitations.
- Calculate the average counts for each of 22 elements.

● Calculate background factors for use in dynamic background correction.

- Calculate static background corrections.
- Calculate density ratios.
- Calculate detection limits.
- Calculate concentrations in the processed sample and original samples.

● Store the calculated data in appropriate files for further processing or report generations.

ES3 contains the statements and routines to:

- Retrieve standard data from the files.

- Conduct the least squares fit of the standard data.
- Store the least squares fit coefficients.
- Print the reports of the standard concentrations, the corresponding counts or count ratios, the least squares fit coefficients, and the coefficients of determination.

ES4 contains the statements and routines to:

- Retrieve standard and sample data from the files.
- Print reports of the initial standard data, working data relative to samples, and customer reports of sample analysis.

Note that ES4 does most of the hard-copy output report generation. The latter part of ES3 does the hard-copy output report of the least squares fit coefficients. The dynamic outputs to the visual display (ADM-1) are generated throughout all four programs as evidenced in the program listings by the numerous PRINT statements that display the data as it is being acquired, retrieved, or calculated.

Calibration Mode

Initial excitation data are acquired in ES1 by means of the assembly call, CALL 3,X. The data are placed in the array C(I,J) for printing on the ADM-1 display as well as into the array E(I) for transfer into the initial data file INDAT. Data from 22 channels for a maximum of four excitations are stored both in the array C(I,J) and in the INDAT file and are displayed on the ADM-1.

When the program asks the operator "GIVE RUN SELECTIONS" and he responds with two numbers that represent his two selected excitations (e.g., 2,3), certain variables will be stored in the SPECVAR file (e.g., operation mode, sample number, etc.). The ES1 program will be cleared from core and ES2 will be loaded from the disk by means of the statement CHAIN ES2. The variables saved in the SPECVAR file allow contiguous operation with the newly loaded program.

ES2 conducts the calculations needed to convert the raw data from the two selected runs into averaged, background-corrected values for the standards. As stated earlier, the program provides for both static and dynamic background corrections. In the static method the background values are derived from the blank standard. The average count values of the element channels for the two designated excitations of the blank are stored in files BCOUNTSAB or BCOUNTSCD for programs A,B,C, or D. The background values are retrieved from these files when the background corrections are made. When dynamic background corrections are used, background factors for each channel must first be established from multiple runs of a standard blank, each run consisting of two to four excitations of

the blank standard. When data from two selected excitations of the blank standard are retrieved, the ratio of the count level for each element channel to that of the background channel is calculated and the resultant factors are stored in file BFAB or BFCD, depending on whether program A,B,C, or D is being run. As succeeding runs of the blank standards are made, a running mean-background factor is calculated for each element using the stored background factors and the current factors. As many as ten runs are made to establish the mean background factors to be used in subsequent calibration (and analysis) runs. When standards containing known levels of the elements of interest are run, the ES2 program calculates the background corrections by multiplying the stored background factors for each element channel times the background channel reading of the current excitation and then dynamically subtracting the background corrections from each channel reading. The background-corrected values are stored in the files SCNTSA or SCNTSC for programs A or C. If the count ratio method is used, the ratio of the background-corrected counts for each element relative to the internal standard is calculated and stored in the files STARB or STARD for programs B or D. The successive retrieved and calculated values are stored in the array L(I,J) as follows:

- L(1,1): first selected value for element channel 1.
- L(1,2): second selected value for element channel 1.
- L(1,4): average value for 1 and 2 for element channel 1.
- L(1,7): average value minus background for 1.
- L(1,8): count ratio, i.e. ratio of average value for element 1, relative to the average value for the internal standard.

When the operator determines that enough standards and replicates have been run for a calibration, ES3 performs a least squares fit of the standard data. The least squares fit program is invoked by the statement "CHAIN ES3," and will handle up to seven standards each with one internal standard and 20 analysis elements in the concentration scheme shown in Table 3.

The options available in the program are: first-through third-order least squares fit of the standard data using a normal or log form of the linear-through third-order polynomial equations. Prior to conducting the least squares fit, the operator may examine the standard data in the SCNTS or STAR files. When the fit is being carried out, pertinent information is displayed on ADM-1. Examples are shown in a later section. A hard-copy report of the least squares fit may be obtained with a "Y" response to a computer prompt indicating its availability. The report lists the degree of fit, the pertinent equations, the concentration and corres-

ponding mean counts (or count ratios of the standards for each element, the coefficients of the fit, and the coefficients of determination. The least squares coefficients, the degree of fit, and an indication that a log or normal equation was used are stored in the files SLINTA, SLINTB, SLINTC, or SLINTD, depending on the spectrographic program being run.

After completing the least squares fit, appropriate prompts will indicate the next options available to the operator. Operation can either be terminated or the program will chain back to ES1 where the operator can choose to conduct analyses or run new standards.

Analysis Mode

When the operator chooses to carry out a sample analysis, the operation of the computer program is virtually the same as in the calibration mode including initial data acquisition, storage, selection of excitation data, and calculations of the background corrections. At this point, the background-corrected counts or count ratios are used to calculate concentration. The computer program calculates concentration in the processed sample by an iterative procedure with the number of iterations being a function of the degree of fit of the current calibration.

Just as in calibration mode, background corrections are made on the average counts of all samples that are run. If the static background correction is used, the background is derived from a BLANK sample that is usually run at the beginning of a series of sample runs or at the operators discretion. The average counts derived from two designated excitations of the BLANK are stored in files BCOUNTSAB and BCOUNTSCD and are retrieved when the background correction is made. If dynamic background correction is used, the background is calculated as described earlier for the calibration mode.

In the analysis mode, as in calibration, the successive retrieved and calculated values are placed in array L(I,J). In turn, the values are stored in files SAMFILE and SAMREP and are later retrieved when line printer reports are generated. SAMFILE contains all of the values required for the laboratory data report, while SAMREP contains only the concentration values reported to the customer. Examples of both of these reports are shown in Appendix E.

Detection Limits

The sample blank is used to determine detection limits. However, they are calculated differently depending on whether static or dynamic background correction is used. With the static method the detection limit is defined as the concentration that corresponds to an average count value that is 10% above background. Every time a blank sample is run, the detection limits

for the 20 analysis elements are calculated by the iterative concentration calculation procedure referred to earlier. They are stored in files DLIMITA or DLIMITB for the elements in lists 1 and 2 respectively (see Table 1).

When the dynamic background correction method is used, the detection limit is defined as the concentration equivalent to the mean value of the sample blank plus two times the standard deviation of the mean of the blank. Ten replicate runs of the sample blank are recommended to establish the mean value. The equivalent concentration is calculated in the program by the iterative procedure described in a later section. The detection limit concentrations are stored in files DLA, DLB, DLC, and DLD for programs A,B,C, and D respectively.

Table 3. Makeup of standards.

	1	2	3	4	5	6	7
In	BKG	BKG	BKG	BKG	BKG	BKG	BKG
Y	IS	IS	IS	IS	IS	IS	IS
Fe	1	2	4	10	20	40	100
Zn	1	2	4	10	20	40	100
Cd	1	2	4	10	20	40	100
As	1	2	4	10	20	40	100
Mn	1	2	4	10	20	40	100
Cu	1	2	4	10	20	40	100
Ag	0.01	0.02	0.04	0.1	0.2	0.4	1
Ni	1	2	4	10	20	40	100
Co	1	2	4	10	20	40	100
Pb	1	2	4	10	20	40	100
Cr	1	2	4	10	20	40	100
V	1	2	4	10	20	40	100
Ti	1	2	4	10	20	40	100
Mo	1	2	4	10	20	40	100
B	1	2	4	10	20	40	100
Li	1	2	4	10	20	40	100
Be	0.004	0.008	0.016	0.04	0.08	0.16	0.40
Tl	1	2	4	10	20	40	100
Al	1	2	4	10	20	40	100
Ba	0.1	0.2	0.4	1.0	2.0	4.0	10

BKG = Background (i.e., dynamic background correction).

IS = Internal standard.

Numbers = $\mu\text{g/liter}$.

Assembly Language Calls

The Assembly language subroutines for acquiring data and controlling the emission spectrometer are called into operation by the BASIC language programs through the BASIC statements CALL2, CALL3, and CALL12. The assembly language subroutine assigns a special user table, transfers control to an interrupt service routine, and then performs the requested function. When the function is completed the interrupt service routine passes control back to the assembly lan-

guage subroutine which transfers the data and control to the BASIC program. The following are brief descriptions of the three calls:

- CALL2—Sets to the "home" position the stepper relay that selects the photomultiplier channel of the emission spectrometer. This call does not have arguments and executes in approximately two seconds.

- CALL3—Acquires data sequentially from each photomultiplier. The call checks a sense flag to confirm completion of stepping to each photomultiplier position. When the flag is set (at each photomultiplier position), readings are taken until stability is achieved (a minimum of six identical readings). The reading is passed back to the BASIC program and the stepper

relay is activated to step to the next photomultiplier position. This call has one argument, the data reading, and executes in a minimum time of approximately three seconds.

- CALL12—Delays data acquisition until the sample excitation has been completed. Completion is determined by checking a hard-wired on-off condition in the spectrometer source. There are no arguments associated with CALL12.

Flowcharts of the assembly language calls and descriptions of other subroutines and conventions used by the assembly language programs are given in Appendix F. Listings of the assembly language programs are included in Appendix G.

CALCULATIONS AND THEIR CODING

The various calculations described in the preceding sections are represented by algebraic equations. In this section we present some of the principal equations, their corresponding representations in BASIC language code, and the statement numbers where the equations appear in the automation code.

Standard Calibration Calculations by Least Squares

The least squares method is used to calibrate the spectrometric analysis using known standards. The method provides a logical procedure for fitting a line through a set of data points that possess the coordinates x and y . This method minimizes the sum of the squares of the point deviations from the "best fitting" line. The least squares fit of data assumes that errors in the measurement of the independent variable are insignificant compared with those of the dependent variable.

In standardizing a spectrometric analysis, it would seem logical to assign the independent variable (X) to the concentration because it is accurately known. In a physical sense, the magnitude of the measured signal depends on the concentration. Also, the systematic and random errors in measurement of the signal are greater than the uncertainty in the concentrations of the standards. Therefore, it follows that the dependent variable (Y) should be assigned to the measured signal.

It has been found that a polynomial equation produces the best fit to analytical calibration data. The normal or logarithmic form of the polynomial may be used. The equations are:

$$Y = a_1 + a_2X + a_3X^2 + \dots + a_{N-1}X^{(N-1)}$$

and

$$\text{Log } Y = a_1 + a_2 \text{ Log } X + a_3 \text{ Log } X^2 + \dots + a_{N-1} \text{ Log } X^{(N-1)}$$

where Y is the element line intensity or intensity ratio measured in counts or count ratio, and X is the concentration.

A polynomial of X_1 terms (degree $X_1 - 1$) may be fitted to an array of X_2 data points by solving the following matrix equations:

$$[F] = \begin{bmatrix} X_2 & \Sigma X & \Sigma X^2 & \dots \\ \Sigma X & \Sigma X^2 & \Sigma X^3 & \dots \\ \vdots & \vdots & \vdots & \ddots \\ \Sigma X^{(X_1-1)} & \dots & \Sigma X^{2(X_1-1)} & \dots \end{bmatrix}$$

and

$$[M] = \begin{bmatrix} \Sigma Y \\ \Sigma X \cdot Y \\ \Sigma X^2 \cdot Y \\ \vdots \\ \Sigma X^{X_1-1} \cdot Y \end{bmatrix} \quad \text{and} \quad [A] = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a^{X_1} \end{bmatrix}$$

$$\text{Then } [F] \times [A] = [M]$$

$$[G] = [F]^{-1}$$

$$\text{and } [A] = [G] \times [M]$$

The coefficients of the desired polynomial are calculated by inputting the degree of fit desired and generating the $[F]$ and $[M]$ matrices from the concentration and counts or count ratios of the calibration set, $X(i)$ and $Y(i)$.

The coefficient of determination, $A(0)$ is defined as:

$$A(0) = (\text{Regression sum of squares}) / (\text{total sum of squares})$$

$$= (\Sigma Y_{\text{calc}} - \bar{Y}^2) / (\Sigma Y_{\text{meas}} - \bar{Y})^2, \text{ and may be written as:}$$

$$A(0) = \left[\frac{\sum Y_{\text{rate}}^2 - (\sum Y_{\text{meas}})^2}{\sum Y_{\text{meas}}^2 / X_s} \right] X_2 / \sum Y_{\text{meas}}^2 -$$

or in matrix notation

$$A(0) = \begin{bmatrix} A'FA & - \\ & \end{bmatrix} \begin{bmatrix} M(1) \\ \end{bmatrix} / X_2 \\ / [Y'Y - M(1)]^2 / X_2.$$

The BASIC language statements corresponding to the above matrix algebraic functions are found in program ES3 between statements 210 and 1300.

Sample Concentration Calculations

Concentrations in unknown samples are calculated by substituting the experimentally measured intensity counts or count ratios of the samples into the polynomial equation along with the coefficients derived from the standard calibration fit. Concentrations are calculated by an iterative approximation procedure, the number of iterations being a function of the degree of fit of the current calibration. For example, if the current calibration is a third-order polynomial that relates concentration (X) to counts or count ratios (Y), then the concentration in the sample will be calculated in three steps. The first approximation of concentration is:

$$X' = \frac{Y - a_1}{a_2};$$

the second approximation is

$$X'' = \frac{(Y - a_1) - a_3 (X')^2}{a_2};$$

and the final concentration is

$$X = \frac{(Y - a_1) - a_3 (X'')^2 - a_4 (X'')^3}{a_2}.$$

The BASIC language statements corresponding to the above equations are found in program ES2, statements 1730, 1810 and 1870 for the normal versions of the equations, and statements 1710, 1790 and 1890 for the logarithmic versions.

The first approximation (statement 1730) is

$$\text{LET } L(1,9) = [L(1,8) - Y(k,1)]/Y(k,2);$$

the second approximation (statement 1810) is

$$\text{LET } L(1,9) = [L(1,8) - Y(k,1) - (k,3)*D1\uparrow 2] \\ / (k,2);$$

and the final concentration (statement 1870) is

$$\text{LET } L(1,9) = [L(1,8) - Y(k,1) - (k,3)*D2\uparrow 2 \\ - Y(k,4)*D2\uparrow 3] / Y(k,2).$$

D1 and D2 are variables assigned to the first and second approximations of concentration. Y(k,1), Y(k,2), Y(k,3), and Y(k,4) are the calibration coefficients. L(1,8) is the element of array L containing the background-corrected count or count ratio, and L(1,9) is the element of array L where the concentration value of the processed sample (Cp) is placed. The program then calculates the concentration in the original sample (Co) by multiplying Cp by the concentration factor. The value Co is placed in the element L(1,10) of array L.

Dynamic Background and Detection Limit Calculations

The equations included in this section are used in the dynamic background correction method to calculate background corrected counts, count ratios, and detection limits. For each calculation, the algebraic expression is presented followed by the corresponding BASIC language coded statement.

Calculation of Background Factor — Algebraic Equation

$$BF_c = \frac{AC_c}{AB},$$

where

BF_c = background factor, current channel,
current run,

AC_c = average counts, current channel,

AB = average counts, background channel.

Calculation of Background Factor — BASIC Coded Statement

Statement 7350, ES2:

$$\text{LET } B(1,1) = L(1,4)/L(1,3),$$

where

$$B(1,1) = BF_c,$$

$$L(1,4) = AC_c,$$

$$L(1,3) = AB.$$

Calculation of Running Mean Background Factor — Algebraic Equation

$$MBF = \frac{MBF_n(n-1)}{n} + \frac{BF_c}{n},$$

where

MBF = running mean background factor,
MBF_p = running mean background factor, previous,
n = run number,
BF_c = background factor, current channel, current run.

Calculation of Running Mean Background Factor — BASIC Coded Statement

Statement 7470, ES2:

LET B(I,1) = (B(I,3)*(W(3) - 1))/W(3) + Y1/W(3),

where

B(I,1) = MBF,
B(I,3) = MBF_p,
W(3) = n,
Y1 = BF_c.

Calculation of Running Mean Standard Deviation of the Background Factor — Algebraic Equation

$$MSDBF = \left[(MSDBF_p)^2 + \frac{n(MBF - BF_c)^2}{(n - 1)^2} \right]^{1/2}$$

where

MSDBF = running mean standard deviation of background factor,
MSDBF_p = previous running mean standard deviation of background factor,
MBF = running mean background factor,
BF_c = background factor, current channel, current run,
n = run number.

Calculation of Running Mean Standard Deviation of the Background Factor — BASIC Coded Statement

Statement 7480, ES2:

LET B(I,2) = ((B(I,4))/A2
+ ((W(3)*(B(I,1) - Y1)/A2/W(3) - 1)/A2))/A.5,

where

B(I,2) = MSDBF,
B(I,4) = MSDBF_p,
B(I,1) = MBF,
Y1 = BF_c,
W(3) = n,
B_c = BF_c (AB).

Calculation of Background for Current Channel, Current Run — Algebraic Equation

$$B_c = BF_c (AB),$$

where

B_c = background, current channel, current run,
BF_c = background factor, current channel,
AB = average counts, background channel, current run.

Calculation of Background for Current Channel, Current Run — BASIC Coded Statement

Statement 6000, ES2:

LET L(I,6) = L(I,5)*L(I,3),

where

L(I,6) = B_c,
L(I,5) = BF_c,
L(I,3) = AB.

Calculation of Background-Corrected Counts, Current Channel, Current Run — Algebraic Equation

$$ACBC_c = AC_c - B_c,$$

where

ACBC_c = average counts, background-corrected, current channel, current run,
AC_c = average counts, current channel, current run,
B_c = background, current channel, current run.

Calculation of Background-Corrected Counts, Current Channel, Current Run — BASIC Coded Statement

Statement 6010, ES2:

LET L(I,7) = L(I,4) - L(I,6),

where

L(I,7) = ACBC_c,
L(I,4) = AC_c,
L(I,6) = B_c.

Calculation of Running Mean Background-Corrected Counts — Algebraic Equation

$$MC = \frac{MC_p(n-1)}{n} + \frac{ACBC_c}{n}$$

where

MC = running mean counts, background-corrected,
 MC_p = previous running mean counts, background-corrected,
 ACBC_c = average counts, background-corrected, current channel, current run,
 n = run number.

Calculation of Running Mean Background Corrected Counts — BASIC Coded Statement

Statement 6180, ES2:

$$\text{LET } D(I,1) = (Q*(B9-1)/B9) + L(I,7)/B9$$

where

D(I,1) = MC,
 Q = MC_p,
 L(I,7) = ACBC_c,
 B9 = n.

Calculation of Running Mean Standard Deviation of the Background-Corrected Counts — Algebraic Equation

$$MSDC = \left[(MSDC_p)^2 + \frac{n(MC - ACBC_c)^2}{(n-1)^2} \right]^{1/2}$$

where

MSDC = running mean standard deviation of the background-corrected counts,
 MSDC_p = previous running mean standard deviation of the background-corrected counts,
 MC = running mean counts, background-corrected,
 ACBC_c = average counts, background-corrected, current channel, current run,
 n = run number.

Calculation of Running Mean Standard Deviation of the Background-Corrected Counts — BASIC Coded Statement

Statement 6190, ES2:

$$\text{LET } D(I,3) = RA2 + ((B9*(D(I,1) - L(I,7)/A2)/(B9 - 1)/A2))A.5.$$

where

D(I,3) = MSDC,
 R = MSPDC_p,
 D(I,1) = MC,
 L(I,7) = ACBC_c,
 B9 = n.

Calculation of the Detection Limit in Count Units — Algebraic Equation

$$D.L. = 2(MSDC).$$

Calculation of the Detection Limit in Count Units — BASIC Coded Statement

Statement 6200, ES2:

$$\text{LET } D(I,2) = 2*D(I,3),$$

where

D(I,2) = D.L.,
 D(I,3) = MSDC.

Calculation of the Detection Limit in Concentration Units — BASIC Coded Statements

Refer to the ES2 program statements 1640, 1700, and the BASIC language statements for calculating concentrations referred to earlier in section entitled *Analysis Mode*.

Calculation of Background-Corrected Count Ratio, Current Channel, Current Run — Algebraic Equation

$$CR_c = \frac{ACBC_c}{ACBC_{is}}$$

where

CR_c = count ratio, background-corrected, current channel, current run,
 ACBC_c = average counts, background-corrected, current channel, current run,
 ACBC_{is} = Average counts, background-corrected, internal standard channel, current run.

Calculation of Background-Corrected Count Ratio, Current Channel Current Run — BASIC Coded Statement

Statement 6610, ES2:

LET L(I,8) = L(I,7)/X3,

where

$$\begin{aligned} L(I,8) &= CR_c, \\ L(I,7) &= ACBC_c, \\ X3 &= ACBC_{IS}. \end{aligned}$$

Note that X3 is calculated by a series of statements including 6010, 6060, and 7020.

Calculation of Running Mean Background-Corrected Count Ratio — Algebraic Equation

$$MCR = \frac{MCR_p (n - 1)}{n} + \frac{CR_c}{n},$$

where

$$\begin{aligned} MCR &= \text{running mean count ratio,} \\ MCR_p &= \text{previous running mean count ratio,} \\ CR_c &= \text{count ratio, background-corrected,} \\ &\quad \text{current channel, current run,} \\ n &= \text{run number.} \end{aligned}$$

Calculation of Running Mean Background-Corrected Count Ratio — BASIC Coded Statement

Statement 6380, ES2:

LET D(I,1) = (Q*(B9-1)/B9) + L(I,8)/B9,

where

$$\begin{aligned} D(I,1) &= MCR, \\ Q &= MCR_p, \\ L(I,8) &= CR_c, \\ B9 &= n. \end{aligned}$$

Calculation of Running Mean Standard Deviation of the Background-Corrected Count Ratio — Algebraic Equation

$$MSDCR = \left[(MSDCR_p)^2 + \frac{n(MCR - CR_c)^2}{(n-1)^2} \right]^{1/2},$$

where

$$\begin{aligned} MSDCR &= \text{running mean standard deviation of} \\ &\quad \text{background-corrected count ratio,} \\ MSDCR_p &= \text{previous running mean standard} \\ &\quad \text{deviation of background-corrected} \\ &\quad \text{count ratio,} \\ MCR &= \text{running mean count ratio, back-} \\ &\quad \text{ground-corrected,} \\ CR_c &= \text{count ratio, background-corrected,} \\ &\quad \text{current channel, current run,} \\ n &= \text{run number.} \end{aligned}$$

Calculation of Running Mean Standard Deviation of the Background-Corrected Count Ratio — BASIC Coded Statement

Statement 6390, ES2:

LET D(I,3) = (RA2 + ((B9*(D(I,1) - L(I,8))/ (B9-1))^2))/A.5,

where

$$\begin{aligned} D(I,3) &= MSDCR, \\ R &= MSDCR_p, \\ D(I,1) &= MCR, \\ L(I,8) &= CR_c, \\ B9 &= n. \end{aligned}$$

Calculation of the Detection Limit in Count Ratio Units — Algebraic Equation

$$D.L. = 2(MSDCR).$$

Calculation of the Detection Limit in Count Ratio Units — BASIC Coded Statement

Statement 6200 (via statement 6400), ES2:

LET D(I,2) = 2 * D(I,3)

where

$$\begin{aligned} D(I,2) &= D.L., \\ D(I,3) &= MSDCR. \end{aligned}$$

Calculation of the Detection Limit in Concentration Units — Algebraic Equations

Refer to the equations in section entitled *Sample Concentration Calculations*.

Calculation of the Detection Limit in Concentration Units — BASIC Coded Statements

Refer to the ES2 program statements 1640, 1700, and the BASIC language statements for calculating concentrations referred to earlier in section entitled *Sample Concentration Calculations*.

PROGRAM OPERATING INSTRUCTIONS

The emission spectrometer program will acquire and process data from one test channel and 22 element detector channels positioned to detect either of the two lists of elements shown in Table 1. It will process the data based on direct counts from each channel or on count ratios of each of 20 analysis channels compared to the Yttrium internal standard channel. Background corrections are made on all channels by either the static or dynamic background-correction methods described earlier.

The program is replete with prompts that are displayed on the CRT display terminal to which the operator responds via the terminal keyboard. Instructions for operating the program are facilitated in the following text by using examples of actual input/output copy. In the examples, the underlined information is the input entered by the operator via the keyboard. Each input must be followed by a carriage return indicated by a $\rightarrow$.

Prior to running the program, the operator logs into the system, loads the ESI program, and types RUN, or more simply "Run ESI" as shown in the following example. After the RUN command, the system will begin displaying prompts requesting input or reminding the operator of the next step to be carried out. Questions requiring Y (Yes) or N (No) answers will be displayed. These are usually points in the program where optional modes of operation or output are chosen by the operator.

If the operator mistypes a response to a prompt and the error occurs before a carriage return, he simply strikes the RUB-OUT key for each erroneous character and types the correct response followed by a carriage return. If the error has been followed by a carriage return, the program in all likelihood will have proceeded

to a wrong branch of the program. To correct this problem, the operator can either start over by typing RUN, "ESI," or he can go back to the place in the program (statement number) where the last prompt occurred. The statement number of the prompt can be found quite easily in the program listing. After the number has been found, the operator types RUN followed by the statement number. The prompt where the input error occurred will again be displayed and the operator can now respond with the correct entry.

To illustrate the operation of the program, we present examples of a standard calibration followed by a sample analysis. We also illustrate the dynamic background correction along with the determination of detection limits.

Standard Calibration

The first of a series of inputs and responses (dialog) is shown in Fig. 3. The prompts are self explanatory and in virtually all cases single-character entries are all that are needed. Of the series of standards to be run in calibration mode, the first is a blank followed by succeeding replicates of the blank for establishing the background factors. The program automatically identifies the blank standard as standard zero. It also keeps track of the blank run number to properly calculate the mean background factors derived from replicate runs of the standard blanks. Operator response to the prompt, "GIVE PROGRAM A,B,C,D", directs the program to either the direct counts or count ratio method and element lists 1 or 2 (Table 1). The prompt also reminds the operator to check the setting of the ABCD program switch on the spectrometer read-out chassis. The

```
RUN "ESI"  
EMISSION SPECTROMETER PROGRAM  
ANALYSIS OR CALIBRATION MODE A OR C > C  
DO YOU WANT BKG CHANNEL CORRECTION Y OR N > Y  
IS THIS A BLANK MATRIX Y OR N > Y  
GIVE BLANK RUN > 1  
GIVE PROGRAM A,B,C,D > B  
CHECK THE HG MONITOR
```

Fig. 3. Initial interactive dialog.

prompt "CHECK THE HG MONITOR" reminds the operator to visually check the HG monitor on the spectrometer and take whatever action is necessary to ensure alignment.

Following the above I/O, the program prompts "LOAD ELECTRODES — EXCITE" immediately followed by "HIT START". These are illustrated in Fig. 4. In response, the operator loads the electrode into the excitation stand and initiates the start button on the sequential readout chassis. This starts the excitation, signal integration, and readout sequence. The excitation number is displayed on the terminal, and when the excitation ceases, the test count followed by the counts from each of the 22 element channels is displayed. For reasons of space, only 9 element channels are shown in these examples. Following the first excitation only, the prompt "IS DATA OK" will be displayed. This is a reminder for the operator to view the data from the first excitation conditioning run to determine if the data are correct to continue additional excitations. In the above example he has responded Y.

Alternatively, if he were to respond N, the program would prompt "PREP NEW SAMPLE-CHANGE ELECTRODES", "LOAD ELECTRODES-EXCITE". The Y response allows the operator to proceed to the next excitation. The display then shows two columns of data, namely the first and second excitation, so that the operator can compare the data. He usually proceeds to a third and sometimes a fourth excitation, depending on the quality of the data. If the response to the prompt "MORE EXCITATIONS" is N, the program displays the message "YOU HAVE COMPLETED EXCITATIONS" and requests that the operator designate two of the four (or less runs) as acceptable data via the prompt "GIVE RUN SELECTIONS". In the example the response is 1,2 for excitations 1 and 2.

Response to the prompt "GIVE RUN SELECTIONS" immediately initiates a series of storage, retrieval, data processing, and output operations. The complexity of these operations is a function of whether a blank, standard or sample is being run. In I/O example, (Fig. 5) certain identifying information is displayed in the header followed by the element symbols, two columns of selected data, their averaged values, calculated background factors, and the standard deviations of the factors. Each time a run is completed the program asks the operator if he wants a line-printer copy of the displayed data and if he wishes to continue to a next run. If he chooses to continue additional runs, the process is repeated for each run. In the next I/O example (Fig. 6) the data for a seventh (and final) standard of a series of standards are illustrated. Having run enough standards, the operator indicates that he is ready to fit the standard data. The computer then re-

LOAD ELECTRODES-EXCITE

HIT START > S

EXCITATION 1

3100 OK

IN	60
Y	136
FE	205
ZN	145
CD	135
AS	414
MN	165
CU	133
AG	492

IS DATA OK > Y

LOAD ELECTRODES-EXCITE

HIT START > S

EXCITATION 2

3100 OK

IN	60	63
Y	136	141
FE	205	211
ZN	145	148
CD	135	138
AS	414	417
MN	165	167
CU	133	132
AG	492	490

MORE EXCITATIONS — Y OR N > N

YOU HAVE COMPLETED EXCITATIONS

GIVE RUN SELECTIONS > 1,2

Fig. 4. Initial data output.

quests the form of the equation, the degree of fit, and the number of standards to be used in the fit. After the operator responds to the input requests, the program performs the fit and displays the known concentrations of the standards, the running mean counts (or count ratios), certain summations (e.g., ΣX , ΣX^2 , ΣX^3 , ΣY , ΣY^2 , etc.) pertinent to the calculation, and the coefficient of determination (refer to the section entitled *Method of Least Squares*). If the operator had indicated the log form of the polynomial, the log equivalent values of concentration and counts (or count ratios) would have been displayed. The above example shows the least squares calibration data for only the first of 20 analysis elements that are actually displayed.

A line-printer report of the calibration coefficients for all 20 elements from the least squares fit can be obtained with a Y response to the appropriate prompt displayed when the program has completed all of the calculations. If a third-order fit has been performed, the line-printer report will include the coefficients for the

DATE 3/12/1976
PROGRAM-B

	C1	C2	AC	BF	STDEV	STANDARD RUN 2
IN	60.	60.	60.0			
Y	136.	136.	136.0	2.26	0.0103	
FE	205.	205.	205.0	3.40	0.0244	
ZN	145.	146.	145.5	2.40	0.0303	
CD	135.	135.	135.0	2.23	0.0215	
AS	414.	424.	419.0	6.87	0.1607	
MN	165.	165.	165.0	2.72	0.0359	
CU	133.	133.	133.0	2.19	0.0440	
AG	492.	492.	492.0	8.09	0.1529	

DO YOU WANT A REPORT ON THE SLPT > Y

DO YOU WANT TO CONTINUE Y OR N > Y

ANALYSIS OR CALIBRATION MODE A OR C > C

Fig. 5. Data from selected excitations.

DATE 3/11/1976
PROGRAM-B

	C1	C2	AC	ACBC	CR	STANDARD RUN 1
IN	71.	73.	72.0			
Y	515.	560.	537.5	374.8		
FE	5277.	5751.	5514.0	5269.2	14.06	
ZN	413.	434.	423.5	250.4	0.67	
CD	747.	776.	761.5	600.6	1.60	
AS	1094.	1155.	1124.5	629.9	1.68	
MN	7089.	7824.	7456.5	7260.3	19.37	
CU	4088.	4464.	4276.0	4118.6	10.99	
AG	841.	908.	874.5	291.9	0.78	

STD DATA FILED

DO YOU WANT A REPORT ON THE SLPT > N

ARE YOU READY TO FIT STD DATA > Y

DO YOU WANT LOG EQUATION FOR FIT > N

DEGREE OF FIT- LINEAR = 1 > 1

NUMBER OF STDS > 7

1	9.2849819E-02
2	.27119507
4	.56953228
10	1.4584252
20	3.0089453
40	5.9007182
100	14.057809
7	177
177	12121

25.359475

1719.4861

5.6675245E-02

.14103247

COEF. OF DETERMINATION = .99942745

Fig. 6. Data output from final standard and least squares fit.

DO YOU WANT A REPORT ON THE SLPT > Y
DO YOU WANT TO CONTINUE > Y OR N > Y
ANALYSIS OR CALIBRATION MODE A OR C > A
DO YOU WANT BKG CHANNEL CORRECTION Y OR N > Y
SAMPLE NUMBER > BLANK
GIVE SAMPLE TYPE > DL
GIVE SAMPLE SOURCE > 2
GIVE VOL. (ML) OF ORIG SAMPLE ALIQUOT > 1
GIVE VOL. (ML) OF PROCESSED SAMPLE > 1
DO YOU WANT TO ESTABLISH NEW DETECTION LIMITS
RECOMMENDED OF BLANKS TO ESTABLISH D.L. IS 10
GIVE PROGRAM A,B,C,D > B
CHECK THE HG MONITOR
LOAD ELECTRODES-EXCITE
HIT START > S
EXCITATION 1
3100 OK
IN 61
Y 151
FE 215
ZN 158
CD 156
AS 457
MN 164
CU 149
AG 571
IS DATA OK > Y
LOAD ELECTRODES-EXCITE
HIT START > S
EXCITATION 2
3100 OK
IN 61 59
Y 151 150
FE 215 217
ZN 158 161
CD 156 150
AS 457 457
MN 164 169
CU 149 151
AG 571 576
MORE EXCITATIONS - Y OR N > N
YOU HAVE COMPLETED EXCITATIONS
GIVE RUN SELECTIONS > 1,2

	DATE 3/12/1976 TYPE DL				SAMPLE BLANK SOURCE 2		
	01	02	AC	ACBC	CR (RM)	SD	DLIM
IN	61.	59.	60.0				
Y	151.	150.	150.5	14.9			
FE	215.	217.	216.0	12.0	0.85	0.0604	6.4714
ZN	158.	151.	159.5	15.3	1.03	0.0049	15.4903
CD	156.	150.	153.0	18.9	1.26	0.0157	7.4033
AS	457.	457.	457.0	44.8	3.06	0.0913	19.5493
MN	164.	169.	166.5	3.0	0.25	0.0642	1.5989
CU	149.	151.	150.0	18.9	1.25	0.0177	9.2962
AG	571.	576.	573.5	88.0	5.88	0.0142	7.5512

DO YOU WANT A REPORT ON THE SLPT > Y
DO YOU WANT TO CONTINUE Y OR N > Y
ANALYSIS OR CALIBRATION MODE A OR C > A

Fig. 7. Interactive dialog and data output for deflection limits.

20 elements for the three orders of the fit. An example of a report of the least squares data is shown in Appendix H. Again, for the sake of brevity, only a limited number of channels are shown in the example.

Sample Analysis

After having completed the standard calibration and printing the least squares data, the program issues a series of prompts to provide the operator with the option to discontinue or continue operations and to input additional information. Figure 7 illustrates some I/O for the sample analysis mode of operation and specifically for the determination of detection limits by means of sample blanks described earlier. Operator-program interactions are virtually identical to those described for the running of calibration standards except for the ob-

vious prompts that apply to the analysis mode and detection limit calculations. In the example given here, after the operator selects the two most acceptable excitations, the program prints the columns of data containing the counts for the two excitations, their averages, the background-corrected averages, the count ratios, the running mean-standard deviations of the count ratios, the running mean standard deviations of the count ratios up to the current run, and the corresponding detection limits.

Figure 8 shows the output generated for a typical sample after the operator has selected the two most acceptable excitation runs. When a sample analysis has been completed, the operator can choose a line printer report of the detailed analytical data. In addition, the program provides a separate, more concise report of the sample identity, the elements sought, the concentrations found and the detection limits of the elements not detected. Examples are given in Appendix E.

DATE 3/12/1976 TYPE WATER					SAMPLE 1200 SOURCE RIVER				
	C1	C2	AC	ACBC	CR	CP	CO		
IN	62.	66.	64.0						
Y	573.	598.	585.5	440.9					
FE	912.	944.	928.0	710.4					
ZN	247.	257.	252.0	98.2	1.61	11.023	11023.4		
CD	322.	329.	325.5	182.5	0.22	ND-	15.490	ND-	15490.3
AS	539.	566.	552.5	112.8	0.41	ND-	7.403	ND-	7403.3
MN	835.	877.	856.0	681.6	0.26	ND-	19.549	ND-	19549.3
CU	744.	777.	760.5	620.6	1.55		7.627		7627.2
AG	592.	591.	591.5	73.6	1.41	ND-	10.405	ND-	10405.3
					0.17	ND-	7.551	ND-	7551.2

DO YOU WANT A REPORT ON THE SLPT >

Fig. 8. Data output from sample analysis.

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- 3) J.W. Frazer, Lawrence Livermore Laboratory, Internal Document JWF: 73-2222 (1974). Readers outside the Laboratory who desire further information on LLL internal documents should address their inquiries to the Technical Information Department, Lawrence Livermore Laboratory, Livermore, California 94550.
- 4) *Extended Basic Users Manual*, Data General Corporation 093-000065-05, (1974).

APPENDIX A

COMPUTER INTERFACE SCHEMATICS

Fig. A-1. Block diagram of the spectrometer interface.

Note:

Wiring to be done inside analog to digital

1. Pin 6 - +200V
2. Pin 7 - signal side of 100PF cap.
3. Pin 8 - GND

Fig. A-3. Spectrometer interface.

Fig. A-1. Computer interface.

APPENDIX B **FLOWCHARTS OF THE BASIC LANGUAGE PROGRAMS** **FOR THE EMISSION SPECTROMETER**

Fig. B-1. ES-1.

Fig. B-2. ES-2.

Fig. B-3. ES-3.

Fig. B-4. ES-4.

Fig. B-5. ES-5.

Fig. B-6. ES-6.

Fig. B-7. ES-7.

APPENDIX C

LISTINGS OF THE BASIC LANGUAGE PROGRAMS

```

0010 REM      **** FMISSION SPECTROMETER PROGRAM ****
0020 REM
0030 REM ***** ES1 *****
0040 REM THE OVERALL PROGRAM IS A COMPOSITE OF 4 PROGRAMS
0050 REM THE PROGRAMS ARE "ES1", "ES2", "ES3", "ES4"
0060 REM THE FILE NAMES AND ASSOCIATED CHANNELS TO BE ESTABLISHED
0070 REM IN THE FOUR PROGRAMS ARE AS FOLLOWS:
0080 REM CHANNEL 1 - "INRDT", INITIAL DATA (EXCITATIONS)
0090 REM CHANNEL 1 - "DI IMITA", DETECTION LIMITS, PROG A
0100 REM CHANNEL 1 - "DI IMTB", DETECTION LIMITS, PROG B
0110 REM CHANNEL 1 - "DI A", DETECTION LIMITS, PROG A, DYNAM BKG
0120 REM CHANNEL 1 - "DLB", DETECTION LIMITS, PROG B, DYNAM BKG
0130 REM CHANNEL 1 - "DI C", DETECTION LIMITS, PROG C, DYNAM BKG
0140 REM CHANNEL 1 - "DI D", DETECTION LIMITS, PROG D, DYNAM BKG
0150 REM CHANNEL 1 - "STINFO", STANDARDS INFO
0160 REM CHANNEL 3 - "BLFILEAR", BLANK STD DATA FOR $LPT REPORT, PROG A,B
0170 REM CHANNEL 3 - "BI FILECD", BLANK STD DATA FOR $LPT REPORT, PROG C,D
0180 REM CHANNEL 3 - "STFILEAC", STD DATA FOR $LPT REPORT
0190 REM CHANNEL 3 - "STAFILED", STD DATA FOR $LPT REPORT
0200 REM CHANNEL 3 - "SAMFILE", SAMPLE DATA FOR $LPT REPORT
0210 REM CHANNEL 4 - "SAMRFP", SAMPLE CONC. DATA FOR CUSTOMER $LPT REPORT
0220 REM CHANNEL 5 - "SPECVAR", FILE OF PROGRAM VARIABLES
0230 REM CHANNEL 5 - "BCDINTSAB", FILE OF BKG COUNTS, 22 EL, PROG A,B
0240 REM CHANNEL 5 - "BCDINTSCN", FILE OF BKG COUNTS, 22EL, PROG C,D
0250 REM CHANNEL 5 - "RFB", FILE OF BKG FACTORS, PROGS A,B, DYNAM BKG
0260 REM CHANNEL 5 - "BFCB", FILE OF BKG FACTORS, PROGS C,D, DYNAM BKG
0270 REM CHANNEL 6 - "STARB", STD RATIOS, PROG B
0280 REM CHANNEL 6 - "STAR", STD RATIOS, PROG D
0290 REM CHANNEL 6 - "SCNTSA", STD COUNTS, PROG A
0300 REM CHANNEL 6 - "SCNTSC", STD COUNTS, PROG C
0310 REM CHANNEL 7 - "SLINTA", STD COEFFICIENTS, PROG A
0320 REM CHANNEL 7 - "SLINTB", STD COEFFICIENTS, PROG B
0330 REM CHANNEL 7 - "SLINTC", STD COEFFICIENTS, PROG C
0340 REM CHANNEL 7 - "SLIND", STD COEFFICIENTS, PROG D
0350 PRINT "FMISSION SPECTROMETER PROGRAM"
0360 REM CLOSE ALL FILES AT START OF PROGRAM
0370 CLOSE
0380 DIM B(30), C(12,4), E(40)
0390 DIM W(24)
0400 DIM M(3), N(5)
0410 LET W(4)=0
0420 LET W(14)=20
0430 LET B=1
0440 GOSUB 1960
0450 DIM X(47)
0460 DIM Z(17), Z0(17), Z4(12), Z5(16)
0470 DIM Z4(15), Z7(15), Z11(8)
0480 DIM A(130), A1(50), A2(50), A3(60), A4(60), A5(70)
0490 DIM A6(34), A7(40), A8(20)
0500 DIM B7(50)
0510 DIM D(22,2)
0520 DIM L(22,10)
0530 DIM D4(3), X8(5), Z9(5)
0540 DIM W(24)
0550 INPUT "ANALYSIS OR CALIBRATION MODE A OR C?", Z4#
0560 LET Z6=0
0570 LET Z=1
0580 LET Z1=1
0590 LET X8="N"
0600 LET Z9="N"
0610 LET Z8="NO"
0620 LET Z5="NO"
0630 INPUT "DO YOU WANT BKG CHANNEL CORRECTION Y OR N?", Z9#
0640 IF Z4#="A" THEN GOTO 0790
0650 INPUT "SAMPLE NUMBER > ", Z5#
0660 INPUT "GIVE SAMPLE TYPE > ", Z6#
0670 INPUT "GIVE SAMPLE SOURCE > ", Z7#
0680 INPUT "GIVE VOL (ML) OF ORIG SAMPLE ALIQUOT > ", Z
0690 INPUT "GIVE VOL (ML) OF PROCESSED SAMPLE > ", Z1
0700 REM CALCULATE CONC FACTOR
0710 LET W(1)=(1000*Z1)/Z
0720 IF Z5#="BLANK" THEN GOTO 0780
0730 IF Z6#="Y" THEN GOTO 0760
0740 INPUT "DO YOU WANT TO ESTABLISH NEW DETECTION LIMITS", X8#
0750 IF X8#="Y" THEN GOTO 0760
0760 PRINT "RECOMMENDED # OF BLANKS TO ESTABLISH D.L. IS 10"

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```

0760 LET W(1)=1
0770 GOSUB 0940
0780 GOTO 0980
0790 INPUT "IS THIS A BLANK MATRIX Y OR N > ",Z$
0800 LET B9=0
0810 IF Z$="Y" THEN GOTO 0860
0820 INPUT "GIVE BLANK RUN # > ",W(2)
0830 LET Z8=0
0840 LET W(3)=W(2)
0850 GOTO 0980
0860 INPUT "GIVE STANDARD # > ",Z8
0870 INPUT "GIVE STANDARD RUN # > ",W(3)
0880 IF Z8<1 THEN GOSUB 0940
0890 GOTO 0980
0900 IF W(3)<1 THEN GOSUB 0940
0910 GOTO 0980
0920 LET W(4)=0
0930 GOTO 0980
0940 OPEN FILE(5,3), "SPECVAR"
0950 READ FILE(5),W(4),B9
0960 CLOSE FILE(5)
0970 RETURN
0980 INPUT "GIVE PROGRAM A,B,C,D > ",Z0$
0990 LET A$="INY FEZNCDSMNCUAGNICOPBCRV TLMOB LIRETIALRA"
1000 LET R2$="INY FEZNCDSMNCUAGNICOPBCRV TLMOSBRNBETIALRA"
1010 IF Z0$="A" THEN GOTO 1070
1020 IF Z0$="B" THEN GOTO 1060
1030 IF Z0$="C" THEN GOTO 1070
1040 IF Z0$="D" THEN GOTO 1050
1050 LET B2$=A$
1060 PRINT
1070 PRINT "CHECK THE HG MONITOR"
1080 LET W(5)=1
1090 PRINT "LOAD ELE-TR0DES-EXCITE"
1100 PRINT "HIT START"
1110 PRINT "EXCITATION # ",W(5)
1120 CALL 2
1130 CALL 12
1140 GOTO 1380
1150 INPUT "IS DATA OK > ",X1$
1160 IF X1$="N" THEN GOTO 1190
1170 LET W(5)=W(5)+1
1180 GOTO 1090
1190 PRINT "PAFF NEW SAMPLE CHANGE ELECTRODES"
1200 GOTO 1090
1210 PRINT
1220 PRINT " YOU HAVE COMPLETED EXCITATIONS"
1230 CLOSE FILE(1)
1240 LET W(5)=W(5)-1
1250 INPUT "GIVE RUN SELECTIONS > ",W(6),W(7)
1260 IF Z8="Y" THEN GOTO 1280
1270 LET B9=1
1280 OPEN FILE(5,1), "SPECVAR"
1290 WRITE FILE(5),W(4),B9
1300 WRITE FILE(5),Z$,Z0$,Z1$,Z4$,Z5$,Z6$,Z7$
1310 WRITE FILE(5),W(1),W(2),W(3),Z8,A2$
1320 WRITE FILE(5),W(5),W(6),W(7)
1330 WRITE FILE(5),Z8,Z9$
1340 CLOSE FILE(5)
1350 PRINT
1360 PRINT
1370 CHAIN "E52"
1380 IF W(5)=4 THEN GOTO 1740
1390 IF W(5)=3 THEN GOTO 1720
1400 IF W(5)=2 THEN GOTO 1700
1410 LET J=1
1420 LET X=0
1430 IF Z4$="C" THEN GOTO 1460
1440 PRINT "THIS IS A CALIB RUN, STD ",Z8
1450 PRINT " " RUN # ",W(3)
1460 FOR I=1 TO 23
1470 CALL 3,X
1480 IF I<1 THEN GOTO 1510
1490 GOSUB 1570
1500 GOTO 1540
1510 LET C(I-1,J)=X
1520 GOSUB 1760
1530 LET E(I-1)=X
1540 NEXT I
1550 CALL 2
1560 IF J>1 THEN GOTO 1580
1570 OPEN FILE(1,1), "IN DAT"
1580 FOR I=1 TO 22
1590 WRITE FILE(1),E(I)
1600 NEXT I

```

```

1610 IF 74#C="C" THEN GOTO 1640
1620 IF 74#="Y" THEN GOTO 1640
1630 LET W(4)=1
1640 IF W(5)=1 THEN GOTO 1150
1650 LET W(5)=W(5)+1
1660 INPUT "MORE EXCITATIONS - Y OR N >",X1$
1670 IF X1$="N" THEN GOTO 1210
1680 PRINT "NEXT"
1690 GOTO 1090
1700 LET J=2
1710 GOTO 1430
1720 LET J=3
1730 GOTO 1430
1740 LET J=4
1750 GOTO 1430
1760 PRINT TAB(4);A2#[I+1-3,I+1-2]; TAB(4);
1770 IF W(5)=1 THEN GOTO 1850
1780 IF W(5)=2 THEN GOTO 1840
1790 IF W(5)=3 THEN GOTO 1820
1800 PRINT C[I-1,J-3]; TAB(11);C[I-1,J-2]; TAB(18);C[I-1,J-1]; TAB(25);
1810 GOTO 1850
1820 PRINT C[I-1,J-2]; TAB(11);C[I-1,J-1]; TAB(18);
1830 GOTO 1850
1840 PRINT C[I-1,J-1]; TAB(11);
1850 PRINT C[I-1,J]
1860 RETURN
1870 RFN ROUTINE TO CHECK TEST COUNTS
1871 RFN ***** 1872 IS A TEMPORARY CHANGE UNTIL TEST COUNTER IS FIXED *****
1872 LET X=3000
1880 PRINT X;
1890 IF X<200 THEN GOTO 1930
1900 IF X<2800 THEN GOTO 1930
1910 PRINT "OK"
1920 GOTO 1950
1930 PRINT "TEST CNT OUTSIDE 3000<200> LIMIT"
1940 GOTO 1090
1950 RETURN
1960 OPEN FILE$(5,1,"SPECVAR"
1970 WRITE FILE$(5),W(4),B9
1980 CLOSE FILE$(5)
1990 RETURN
2000 FND

```

```

0010 RFN **** E82 ****
0020 DIM C(22,4),E(40),LC(22,10),N(22)
0030 DIM V(2,4);W(24)
0040 DIM A$(50),A1$(50),A2$(50),A3$(60),A4$(60)
0050 DIM A5$(70),A6$(34),A7$(40),A8$(20),B2$(50)
0060 DIM R$(5),X1$(2),Z$(2),Z0$(2),Z1$(2),Z4$(2)
0070 DIM Z5$(3),Z6$(15),Z7$(15)
0080 DIM F$(3),X8$(5),Z9$(5)
0090 OPEN FILE$(5,1,"SPECVAR"
0100 READ FILE$(5),W(4),B9
0110 READ FILE$(5),Z$,Z0$,Z1$,Z4$,Z5$,Z6$,Z7$
0120 READ FILE$(5),W(1),W(2),W(3),Z8$,A2$
0130 READ FILE$(5),W(5),W(6),W(7)
0140 READ FILE$(5),X8$,Z9$
0150 CLOSE FILE$(5)
0160 IF Z0$="Y" THEN GOTO 0190
0170 DIM D(22,4),D(22,4)
0180 GOTO 0200
0190 DIM D(30),D(22,2)
0200 IF Z4$="C" THEN GOTO 0500
0210 IF Z5$="BLANK" THEN GOTO 0400
0220 IF Z6$="Y" THEN GOTO 0390
0230 IF Z0$="B" THEN GOTO 0320
0240 OPEN FILE$(1,3,"DLIMITA"
0250 FOR I=3 TO 32
0260 READ FILE$(1),L(1,7),L(1,9)
0270 LET D(1,1)=L(1,7)
0280 LET D(1,2)=L(1,9)
0290 NEXT I
0300 CLOSE FILE$(1)
0310 GOTO 0390
0320 OPEN FILE$(1,3,"DLIMITB"
0330 FOR I=3 TO 22
0340 READ FILE$(1),L(1,7),L(1,9)
0350 LET D(1,1)=L(1,7)
0360 LET D(1,2)=L(1,9)
0370 NEXT I
0380 CLOSE FILE$(1)
0390 IF Z4$="C" THEN GOTO 0500
0400 GOSUB 4040

```

```

0410 GOSUB 0510
0420 IF Z54="Y" THEN GOTO 0460
0430 GOSUB 7230
0440 IF Z54="BLANK" THEN GOTO 0460
0450 IF B51 THEN GOSUB 7070
0460 PRINT A$(1:21:25)
0470 PRINT A$
0480 PRINT B$
0490 GOTO 0700
0500 GOSUB 4360
0510 GOSUB 0510
0520 IF Z54="Y" THEN GOTO 0560
0530 IF Z54="Y" THEN GOTO 0550
0540 IF W51:2 THEN GOTO 0560
0550 GOSUB 7230
0560 PRINT Z$
0570 PRINT A$
0580 PRINT W$
0590 PRINT B$
0600 GOTO 0700
0610 PRINT A$
0620 PRINT SYS(21):"/":SYS(1):"/":SYS(3):
0630 IF Z54="C" THEN GOTO 0660
0640 PRINT A$(1:10):A19(6:11):
0650 RETURN
0660 PRINT A$(1:11):A19(6:14):
0670 RETURN
0680 REM ROUTINE FOR READING INITIAL COUNT DATA
0690 REM FROM A FILE INTO AN ARRAY C(1,J)
0700 OPEN FILE(1:31,"INDAT")
0710 IF W51:4 THEN GOTO 0730
0720 GOTO 0770
0730 IF W51:2 THEN GOTO 0760
0740 DIM C(22:3)
0750 GOTO 0770
0760 DIM C(22:3)
0770 FOR J=1 TO W51
0780 FOR I=1 TO 22
0790 READ FILE(1:31,C(1,J))
0800 NEXT I
0810 NEXT J
0820 CLOSE FILE(1)
0830 REM START CALCULATIONS ON DATA FROM 2 SELECTED RIMS
0840 IF Z54="C" THEN GOTO 0860
0850 IF Z54="Y" THEN GOTO 0860
0860 LET I=0
0870 LET J=W$
0880 LET I=I+1
0890 PRINT A$(I+1-1:1+1):
0900 PRINT TAB(4):
0910 PRINT USING "#### ".C(1,J):
0920 LET C(1,J)=C(1,J)
0930 LET J=W$
0940 PRINT TAB(10):
0950 PRINT USING "#### ".C(1,J):
0960 LET C(1,J)=C(1,J)
0970 LET LFI.41=(LFI.13+LFI.21)/2
0980 PRINT TAB(16):
0990 PRINT USING "#### #".LFI.41:
1000 IF Z54="Y" THEN GOTO 2460
1010 IF Z54="BLANK" THEN GOTO 2730
1020 IF Z54="Y" THEN GOTO 5930
1030 IF I:1 THEN GOTO 1130
1040 IF Z54="C" THEN GOTO 1080
1050 IF Z54="D" THEN GOTO 1080
1060 OPEN FILE(5:31,"BCOUNTSAB")
1070 GOTO 1090
1080 OPEN FILE(5:31,"BCOUNTSCD")
1090 FOR I=1 TO 22
1100 READ FILE(53,BK)
1110 NEXT I
1120 CLOSE FILE(5)
1130 LET I=1
1140 IF I:2 THEN GOTO 1170
1150 LET LFI.71-LFI.41
1160 GOTO 1180
1170 LET LFI.71-LFI.41-BK
1180 IF Z54="E" THEN GOTO 1370
1190 IF Z54="D" THEN GOTO 1370
1200 LET NC(1)=I:71
1210 IF I:3 THEN GOTO 1240
1220 PRINT TAB(24):
1230 PRINT USING "#### #".NC(1):
1240 IF Z54="C" THEN GOTO 1310
1250 IF Z54="E" THEN GOTO 1300

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```

1260 IF Z01="D" THEN GOTO 1300
1270 IF I=23 THEN GOTO 2340
1280 LET X1=1
1290 LET L11,83=L11,73
1300 GOTO 1660
1310 FF1N1
1320 GOSUB 4620
1330 IF I=23 THEN GOTO 1350
1340 GOTO 9370
1350 CLOSE FILE(F3)
1360 GOTO 3420
1370 IF I=23 THEN GOTO 1400
1380 PRINT TAB(24);
1390 PRINT USING "#### N",L11,73;
1400 IF I=23 THEN GOTO 1510
1410 LET L11,83=L11,73/X3
1420 IF Z44="C" THEN GOTO 1610
1430 LET N11=L11,83
1440 PRINT TAB(35);
1450 PRINT USING "#### N",N11;
1460 GOSUB 4620
1470 IF I=23 THEN GOTO 1490
1480 GOTO 9370
1490 CLOSE FILE(F3)
1500 GOTO 3290
1510 PRINT
1520 IF I=23 THEN GOTO 1570
1530 GOTO 1590
1540 PRINT
1550 GOSUB 4620
1560 IF I=23 THEN GOTO 1600
1570 GOSUB 4620
1580 GOTO 9370
1590 LET Y3=L11,73
1600 GOTO 1570
1610 PRINT TAB(35);
1620 PRINT USING "#### N",L11,83;
1630 IF Y3<="Y" THEN GOTO 1650
1640 LET L11,83=DCI,13+DCI,23
1650 LET X1=1
1660 LET F3="N"
1670 GOSUB 2960
1680 LET F=I-2
1690 IF F<="Y" THEN GOTO 1730
1700 DEF FNI(A)=LOG(A)/LOG(10)
1710 LET L11,93=EXP(((FNI(L11,83)-YEK,13)/YEK,21)*2.303)
1720 GOTO 1740
1730 LET L11,93=(L11,83-YEK,13)/YEK,21
1740 IF Y0=2 THEN GOTO 1900
1750 LET D1=L11,93
1760 GOSUB 2960
1770 LET F=I-2
1780 IF F<="Y" THEN GOTO 1810
1790 LET L11,93=EXP(((FNI(L11,83)-YEK,13)-YEK,31*D1^2)/YEK,21)*2.303)
1800 GOTO 1820
1810 LET L11,93=((L11,83-YEK,13)-YEK,31*D1^2)/YEK,21
1820 IF Y0=2 THEN GOTO 1900
1830 LET D3=L11,93
1840 GOSUB 2960
1850 LET F=I-2
1860 IF F<="Y" THEN GOTO 1890
1870 LET L11,93=((L11,83-YEK,13)-YEK,31*D2^2-YEK,41*D2^3)/YEK,21
1880 GOTO 1900
1890 LET L11,93=EXP(((FNI(L11,83)-YEK,13)-YEK,31*D2^2-YEK,41*D2^3)/YEK,21)*2.303)
1900 IF Z54="BIANK" THEN GOTO 1970
1910 IF Y3<="Y" THEN GOTO 1950
1920 PRINT TAB(45);
1930 PRINT USING "## ####",DCI,31;
1940 GOTO 1970
1950 PRINT TAB(45);
1960 PRINT USING "#### N",L11,93;
1970 IF Z04="B" THEN GOTO 2170
1980 IF Z04="N" THEN GOTO 2170
1990 IF Z54="BIANK" THEN GOTO 2010
2000 GOTO 2250
2010 IF L11,73<DCI,11 THEN GOTO 2050
2020 PRINT TAB(45);
2030 PRINT USING "#### N",L11,93;
2040 GOTO 2250
2050 LET N3="ND="
2060 PRINT TAB(43);N3;
2070 IF Z54="Y" THEN GOTO 2110
2080 PRINT USING "#### N",DCI,43;
2090 LET D0=DCI,41+NCI1
2100 GOTO 2130

```

```

2110 PRINT USING "####.###",DEI,21;
2120 LET DO=DEI,21*WEI;
2130 PRINT TAB(54);N3;
2140 PRINT USING "####.###",DO
2150 GOSUB 4620
2160 GOTO 2350
2170 IF Z5="BLANK" THEN GOTO 2190
2180 GOTO 2250
2190 IF Z9="Y" THEN GOTO 2220
2200 IF ICI,81>DEI,11 THEN GOTO 2050
2210 GOTO 2230
2220 IF ICI,71>DEI,11 THEN GOTO 2050
2230 PRINT TAB(45);
2240 PRINT USING "####.###",LCI,9;
2250 IF X9="Y" THEN GOTO 2290
2260 PRINT TAB(56);
2270 PRINT USING "###.###",LCI,9;
2280 GOTO 2320
2290 LET LFI,101=LFI,91*WEI;
2300 PRINT TAB(56);
2310 PRINT USING "#####.###",LCI,101;
2320 IF Z5="BLANK" THEN GOTO 2340
2330 IF Z9="Y" THEN GOTO 2500
2340 GOSUB 4620
2350 IF I=22 THEN GOTO 2370
2360 GOTO 0870
2370 CLOSE FILE(3)
2380 CLOSE FILE(4)
2390 IF Z5="BLANK" THEN GOSUB 5640
2400 GOTO 2650
2410 PRINT TAB(24);
2420 PRINT USING "####.###",ICI,71;
2430 PRINT
2440 GOSUB 4620
2450 GOTO 0870
2460 REM ROUTINE FOR STORING BKG COUNTS IN FILE BCOUNTS
2470 IF Z5="Y" THEN GOTO 5930
2480 LET BCI1=LCI,41
2490 GOSUB 4620
2500 IF I=22 THEN GOTO 2530
2510 PRINT
2520 GOTO 0870
2530 CLOSE FILE(3)
2540 PRINT
2550 IF Z0="C" THEN GOTO 2590
2560 IF Z0="D" THEN GOTO 2590
2570 OPEN FILE(5),1,"BCOUNTSAB"
2580 GOTO 2600
2590 OPEN FILE(5),1,"BCOUNTSCD"
2600 FOR J=1 TO 22
2610 WRITE FILE(5),BCI1
2620 NEXT J
2630 CLOSE FILE(5)
2640 IF Z5="BLANK" THEN GOTO 5790
2650 PRINT
2660 INPUT "DO YOU WANT A REPORT ON THE ALPT > ",X1$
2670 IF X1$="Y" THEN GOTO 3760
2680 PRINT
2690 DIM X1$(2)
2700 INPUT "DO YOU WANT TO CONTINUE Y OR N > ",X1$
2710 IF X1$="N" THEN GOTO 2660
2720 CHAIN "F$1" THEN GOTO 0450
2730 REM SAMPLE BLANK FOR BKG CORRECTION
2740 IF Z9="Y" THEN GOTO 5930
2750 LET BCI2=LCI,41
2760 IF I=22 THEN GOTO 2790
2770 LET LFI,71=BCI1
2780 GOTO 2820
2790 LET LCI,71=1*BCI1
2800 PRINT TAB(24);
2810 PRINT USING "####.###",LCI,71;
2820 LET NCI1=ICI,71
2830 IF I=22 THEN GOTO 2930
2840 IF Z0="D" THEN GOTO 2890
2850 IF Z0="D" THEN GOTO 2890
2860 GOSUB 4620
2870 PRINT
2880 GOTO 0870
2890 IF I=2 THEN GOTO 2910
2900 GOTO 2860
2910 LET X9=BCI1
2920 GOTO 2860
2930 IF Z0="D" THEN GOTO 1410
2940 IF Z0="D" THEN GOTO 1410
2950 GOTO 1280

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3260 IF Z0$="B" THEN GOTO 3280
3270 IF Z0$="D" THEN GOTO 3250
3280 RPN ROUTINE FOR READING STD COEFF, PROG A & C
3290 RPN FOR USE IN CALCULATING CONCENTRATIONS, DIR COUNTS METHOD
3300 IF Z0$="A" THEN GOTO 3040
3310 OPEN FILE(7,0), "SLINTC"
3320 READ FILE(7,0), F$
3330 GOTO 3060
3340 OPEN FILE(7,0), "SLINTA"
3350 READ FILE(7,0), F$
3360 LET Y1=X1+1
3370 GOTO 3310
3380 LET W(12)=X1
3390 IF Y1<2 THEN GOTO 3140
3400 LET W(12)=1
3410 LET X=W(12)
3420 READ FILE(7,X), X0
3430 LET W(12)=W(12)+1
3440 FOR I=1 TO 20
3450 FOR L=1 TO W(12)
3460 LET X=W(12)
3470 READ FILE(7,X), Y(K,L)
3480 LET W(12)=W(12)+1
3490 NEXT L
3500 NEXT K
3510 CLOSE FILE(7)
3520 RETURN
3530 RPN ROUTINE FOR READING STD COEFF, PROG B & D
3540 IF Z0$="B" THEN GOTO 3280
3550 OPEN FILE(7,0), "SLINTD"
3560 READ FILE(7,0), F$
3570 GOTO 3300
3580 OPEN FILE(7,0), "SLINTB"
3590 READ FILE(7,0), F$
3600 LET X1=X1+1
3610 IF X1<4 THEN GOTO 3340
3620 DIM Y(22,4)
3630 GOTO 3080
3640 IF Y1<3 THEN GOTO 3370
3650 DIM Y(22,3)
3660 GOTO 3080
3670 DIM Y(22,2)
3680 GOTO 3080
3690 RPN
3700 RPN ROUTINE TO WRITE STD COUNTS INTO A FILE CALLED SCNTS
3710 RPN ROUTINE TO WRITE STD COUNT RATIOS INTO A FILE CALLED STAR
3720 IF W(3)<1 THEN GOTO 3770
3730 IF Z0$="A" THEN GOTO 3670
3740 IF Z0$="C" THEN GOTO 3600
3750 IF Z0$="D" THEN GOTO 3480
3760 OPEN FILE(6,0), "STARB"
3770 GOTO 3490
3780 OPEN FILE(6,0), "STARD"
3790 LET W(14)=20
3800 IF Z0$="A" THEN GOTO 3530
3810 LET W(15)=1
3820 GOTO 3540
3830 LET W(15)=(W(14)*(Z0-1)+1)
3840 FOR I=1 TO W(14)
3850 LET X=W(15)
3860 WRITE FILE(6,X), N(I)+2)
3870 LET W(15)=W(15)+1
3880 NEXT I
3890 GOTO 3440
3900 OPEN FILE(6,0), "SCNTSC"
3910 GOTO 3630
3920 OPEN FILE(6,0), "SCNTSA"
3930 LET W(14)=20
3940 GOTO 3500
3950 GOTO 3570
3960 CLOSE FILE(6)
3970 PRINT "STD DATA FILED"
3980 INPUT "DO YOU WANT A REPORT ON THE $IPT > ", X1$
3990 IF X1$="Y" THEN GOTO 3760
4000 PRINT
4010 DIM Y1$C(2)
4020 INPUT "ARE YOU READY TO FIT STD DATA > ", X1$
4030 IF X1$="Y" THEN GOTO 3750
4040 GOTO 3630
4050 CHAIN "ES2"
4060 CHAIN "ES4"
4070 RPN ROUTINE FOR CALCULATING RUNNING MEAN COUNTS OR COUNT RATIOS
4080 IF Z0$="A" THEN GOTO 3960
4090 IF Z0$="C" THEN GOTO 3960
4100 IF Z0$="D" THEN GOTO 3830

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3810 OPEN FILE(6,01,"STARR"
3820 GOTO 3840
3830 OPEN FILE(6,01,"STARD"
3840 LET W(14)=20
3850 IF Z8="I" THEN GOTO 3880
3860 LET W(15)=1
3870 GOTO 3890
3880 LET W(15)=(W(14)*(Z8-1)+1)
3890 FOR I=1 TO W(14)
3900 LET X=W(15)
3910 READ FILE(6,X),E(1)
3920 LET N(1+2)=(N(1+2)+(E(1)*(W(3)-1)))/W(3)
3930 LET W(15)=W(15)+1
3940 NEXT I
3950 GOTO 4020
3960 IF Z0="A" THEN GOTO 3990
3970 OPEN FILE(6,01,"SCNTSC"
3980 GOTO 4000
3990 OPEN FILE(6,01,"SCNTSA"
4000 LET W(14)=20
4010 GOTO 3950
4020 CLOSE FILE(6)
4030 GOTO 3430
4040 RHM ROUTINE TO STORE SPEC ANAL DATA & HEADER
4050 LET A$=""
4060 LET A1$="DATE SAMPLE TYPE SOURCE"
4070 LET B=LEN(Z1$)
4080 LET A3$=A$[1,4],A1$[1,4],A$[1,2]
4090 LET B1=LEN(Z6$)
4100 LET A4$=A$[1,4],A1$[13,16], " ",Z6$,A$[1,25-B1],A1$[18,23], " ",Z7$
4110 LET A6$="SPECTROGRAPHIC ANALYSIS REPORT"
4120 LET A7$=A$[1,8], "ELEMENT CONCENTRATION"
4130 LET A8$="MICROGRAMS/LITER"
4140 IF Z0$="B" THEN GOTO 4250
4150 IF Z0$="D" THEN GOTO 4250
4160 IF Z5$="BLANK" THEN GOTO 4230
4170 IF Z5$="Y" THEN GOTO 4230
4180 IF Z5$="Y" THEN GOTO 4210
4190 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,4], "ACBC(RM)", A$[1,4], "STDEV", A$[1,8], "DLIM"
4200 RETURN
4210 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,16], "DLIM"
4220 RETURN
4230 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,18], "CP", A$[1,8], "CO"
4240 RETURN
4250 IF Z5$="BLANK" THEN GOTO 4300
4260 IF Z9$="Y" THEN GOTO 4340
4270 IF Z5$="Y" THEN GOTO 4320
4280 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,6], "CR(RM)", A$[1,6], "SD", A$[1,7], "DLIM"
4290 RETURN
4300 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,8], "CR", A$[1,11], "CP", A$[1,7], "CO"
4310 RETURN
4320 LET A5$=A$[1,6], "C1 C2 AC ACBC", A$[1,8], "CR", A$[1,8], "DLIM"
4330 RETURN
4340 LET A5$=A$[1,6], "C1 C2 AC 10X(AC)", A$[1,7], "CR", A$[1,11], "CP", A$[1,7], "CO"
4350 RETURN
4360 RHM HEADER FOR STD REPORT
4370 LET A$=""
4380 LET A1$="DATE STANDARD RHM PROGRAM"
4390 LET B=LEN(Z1$)
4400 LET A3$=A$[1,4],A1$[1,4],A$[1,2]
4410 IF Z0$="A" THEN GOTO 4440
4420 LET A4$=A$[1,4],A1$[21,27], "-A", A$[1,23], A1$[16,19]
4430 GOTO 4520
4440 IF Z0$="B" THEN GOTO 4470
4450 IF Z0$="C" THEN GOTO 4490
4460 IF Z0$="D" THEN GOTO 4510
4470 LET A4$=A$[1,4],A1$[21,27], "-B", A$[1,23], A1$[16,19]
4480 GOTO 4520
4490 LET A4$=A$[1,4],A1$[21,27], "-C", A$[1,23], A1$[16,19]
4500 GOTO 4520
4510 LET A4$=A$[1,4],A1$[21,27], "-D", A$[1,23], A1$[16,19]
4520 IF Z6$="Y" THEN GOTO 4570
4530 LET A5$=A$[1,6], "C1 C2 AC ACBC"
4540 IF Z0$="A" THEN GOTO 4560
4550 LET A5$=A$[1,8], "CR"
4560 GOTO 4610
4570 IF Z9$="Y" THEN GOTO 4600
4580 LET A5$=A$[1,6], "C1 C2 AC BF", A$[1,8], "STDEV"
4590 RETURN
4600 LET A5$=A$[1,6], "C1 C2 AC"
4610 RETURN
4620 RHM ROUTINE TO STORE FILS FOR DATA TO BE USED IN REPORTS
4630 IF Z4$="C" THEN GOTO 5010
4640 RHM DATA FOR STD REPORTS
4650 IF Z6$="Y" THEN GOTO 4820

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4660 IF Z0#="C" THEN GOTO 4710
4670 IF Z0#="D" THEN GOTO 4710
4680 IF I>1 THEN GOTO 4770
4690 OPEN FILE(3,1),"BLFILEAB"
4700 GOTO 4730
4710 IF I=1 THEN GOTO 4770
4720 OPEN FILE(3,1),"BLFILEBD"
4730 WRITE FILE(3),A$,Z$,A$,W(3),A$
4740 IF Z$="Y" THEN GOTO 4800
4750 WRITE FILE(3),L(1,1),L(1,2),L(1,3)
4760 RETURN
4770 IF Z$="Y" THEN GOTO 4800
4780 WRITE FILE(3),L(1,1),L(1,2),L(1,4),B(1,3),B(1,4)
4790 RETURN
4800 WRITE FILE(3),L(1,1),L(1,2),B(1)
4810 RETURN
4820 IF Z0#="B" THEN GOTO 4930
4830 IF Z0#="D" THEN GOTO 4930
4840 IF I>1 THEN GOTO 4870
4850 OPEN FILE(3,1),"STAFLEAB"
4860 WRITE FILE(3),A$,Z$,A$,W(3),A$
4870 IF Z$="Y" THEN GOTO 4910
4880 IF I=1 THEN GOTO 4910
4890 WRITE FILE(3),L(1,1),L(1,2),L(1,3)
4900 RETURN
4910 WRITE FILE(3),L(1,1),L(1,2),L(1,4),N(1)
4920 RETURN
4930 IF I=1 THEN GOTO 4960
4940 OPEN FILE(3,1),"STAFLEBD"
4950 WRITE FILE(3),A$,Z$,A$,W(3),A$
4960 IF I=2 THEN GOTO 4990
4970 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7)
4980 RETURN
4990 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7),N(1)
5000 RETURN
5010 REM DATA FOR SAMPLE REPORTS
5020 IF I=1 THEN GOTO 5080
5030 OPEN FILE(3,1),"SAMPLE"
5040 OPEN FILE(4,1),"SAMPLE"
5050 LET N$="ND-"
5060 WRITE FILE(3),A$,A$,A$
5070 WRITE FILE(4),A$,A$,A$,A$,A$,A$
5080 IF Z0#="B" THEN GOTO 5380
5090 IF Z0#="D" THEN GOTO 5380
5100 IF I=3 THEN GOTO 5140
5110 IF Z$="BLANK" THEN GOTO 5220
5120 IF L(1,7)<D(1,1) THEN GOTO 5290
5130 GOTO 5260
5140 IF Z$="Y" THEN GOTO 5180
5150 IF I=1 THEN GOTO 5180
5160 WRITE FILE(3),L(1,1),L(1,2),L(1,4)
5170 RETURN
5180 WRITE FILE(3),L(1,1),L(1,2),L(1,4),N(1)
5190 IF Z$="BLANK" THEN GOTO 5210
5200 PRINT
5210 RETURN
5220 IF Z$="Y" THEN GOTO 5260
5230 WRITE FILE(3),L(1,1),L(1,2),L(1,4),D(1,1),D(1,3),D(1,4)
5240 WRITE FILE(4),D(1,4)
5250 RETURN
5260 WRITE FILE(3),L(1,1),L(1,2),L(1,4),N(1),L(1,9),L(1,10)
5270 WRITE FILE(4),L(1,10)
5280 RETURN
5290 IF Z$="Y" THEN GOTO 5330
5300 WRITE FILE(3),L(1,1),L(1,2),L(1,4),N(1),N$,D(1,4)
5310 LET D=D(1,4)+N(1)
5320 GOTO 5350
5330 WRITE FILE(3),L(1,1),L(1,2),L(1,4),N(1),N$,D(1,2)
5340 LET D=D(1,2)+N(1)
5350 WRITE FILE(3),N$,D
5360 WRITE FILE(4),N$,D
5370 RETURN
5380 IF I=1 THEN GOTO 5420
5390 IF Z$="Y" THEN GOTO 5430
5400 WRITE FILE(3),L(1,1),L(1,2),L(1,4)
5410 RETURN
5420 IF I=2 THEN GOTO 5450
5430 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7)
5440 RETURN
5450 IF Z$="BLANK" THEN GOTO 5510
5460 IF Z$="Y" THEN GOTO 5490
5470 IF L(1,8)<D(1,1) THEN GOTO 5580
5480 GOTO 5550
5490 IF L(1,7)<D(1,1) THEN GOTO 5610
5500 GOTO 5530

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5510 IF X8<>"Y" THEN GOTO 5550
5520 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7),D(1,1),D(1,3),D(1,4)
5530 WRITE FILE(4),D(1,4)
5540 RETURN
5550 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7),L(1,8),L(1,9),L(1,10)
5560 WRITE FILE(4),L(1,10)
5570 RETURN
5580 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7),L(1,8),N8,D(1,4)
5590 LET D=D(1,4)*W(1)
5600 GOTO 5350
5610 WRITE FILE(3),L(1,1),L(1,2),L(1,4),L(1,7),L(1,8),N8,D(1,2)
5620 LET D=D(1,2)*W(1)
5630 GOTO 5350
5640 IF Z04="B" THEN GOTO 5720
5650 IF Z04="D" THEN GOTO 5720
5660 FOR I=3 TO 22
5670 IF I>3 THEN GOTO 5690
5680 OPEN FILE(1,1),"DLIMITA"
5690 WRITE FILE(1),L(1,7),L(1,9)
5700 NEXT I
5710 GOTO 5770
5720 FOR I=3 TO 22
5730 IF I>3 THEN GOTO 5750
5740 OPEN FILE(1,1),"DLIMITB"
5750 WRITE FILE(1),L(1,7),L(1,9)
5760 NEXT I
5770 CLOSE FILE(1)
5780 GOTO 5550
5790 RETURN
5800 PRINT TAB(45);
5810 PRINT USING "#### ###",L(1,9);
5820 PRINT TAB(56);
5830 PRINT USING "#### #",L(1,10)
5840 RETURN
5850 OPEN FILE(5,1),"SPECVAR"
5860 WRITE FILE(5),W(4),B9
5870 WRITE FILE(5),Z0,Z04,Z1,Z4,Z5,Z6,Z7
5880 WRITE FILE(5),W(1),W(2),W(3),Z8,A2
5890 WRITE FILE(5),W(5),W(6),W(7)
5900 WRITE FILE(5),X8,Z9
5910 CLOSE FILE(5)
5920 RETURN
5930 REM
5940 IF I>1 THEN GOTO 5990
5950 LET L(1,3)=L(1,4)
5960 GOSUB 6420
5970 PRINT
5980 GOTO 6870
5990 IF Z4<>"Y" THEN GOTO 7340
6000 LET L(1,6)=L(1,5)+L(1,3)
6010 LET L(1,7)=L(1,4)+L(1,6)
6020 PRINT TAB(24);
6030 PRINT USING "#### #",L(1,7);
6040 LET N(1)=L(1,7)
6050 IF X8<>"Y" THEN GOTO 6640
6060 IF I=2 THEN GOTO 7020
6070 IF Z04="B" THEN GOTO 6290
6080 IF Z04="D" THEN GOTO 6410
6090 IF Z04="C" THEN GOTO 6250
6100 IF I>3 THEN GOTO 6120
6110 OPEN FILE(1,1),"DLA"
6120 IF B9=1 THEN GOTO 6160
6130 LET D(1,1)=L(1,7)
6140 LET D(1,3)=0
6150 GOTO 6200
6160 LET D=D(1,1)
6170 LET R=D(1,3)
6180 LET D(1,1)=(R*(B9-1)/B9)+L(1,7)/B9
6190 LET D(1,3)=(R^2+((B9*(D(1,1)-L(1,7))^2)/(B9-1)^2))^ .5
6200 LET D(1,2)=2*D(1,3)
6210 IF L4<>"Y" THEN GOTO 6240
6220 LET L(1,8)=D(1,1)
6230 GOTO 1410
6240 GOTO 6420
6250 GOTO 6420
6260 IF I=3 THEN GOTO 6270
6270 OPEN FILE(1,1),"D(C)"
6280 IF B9=1 THEN GOTO 6160
6290 GOTO 6420
6300 GOSUB 6420
6310 IF I=3 THEN GOTO 6320
6320 OPEN FILE(1,1),"DLB"
6330 IF B9=1 THEN GOTO 6360
6340 LET D(1,1)=L(1,8)
6350 LET D(1,3)=0
6360 GOTO 6200

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6360 LET Q=DEI.13
6370 LET R=DEI.33
6380 LET D(1,13)=(Q*(B9-1)/B9)+L(1,83)/B9
6390 LET D(1,33)=(R^2+((B9*(DEI.13-L(1,83)^2)/(B9-1)^2))^ 5
6400 GOTO 6200
6410 GOSUB 6610
6420 IF I=3 THEN GOTO 6440
6430 OPEN FILE(1,13,"DLB")
6440 IF B%1 THEN GOTO 6360
6450 GOTO 6390
6460 IF Z0%="B" THEN GOTO 1610
6470 IF Z0%="D" THEN GOTO 1610
6480 LET I(1,83)=L(1,73)
6490 GOTO 1610
6500 LET D(1,43)=L(1,93)
6510 WRITE FILE(13,DEI.13,D(1,23),D(1,33),D(1,43)
6520 GOSUB 6620
6530 IF I=22 THEN GOTO 6550
6540 GOTO 0870
6550 CLOSE FILE(13)
6560 CLOSE FILE(14)
6570 CLOSE FILE(33)
6580 LET B=B+1
6590 GOSUB 5550
6600 GOTO 7660
6610 LET L(1,83)=L(1,73)/X3
6620 RETURN
6630 GOTO 2660
6640 IF Z0%="B" THEN GOTO 6870
6650 IF Z0%="D" THEN GOTO 6870
6660 IF Z4%="C" THEN GOTO 6690
6670 LET N(13)=L(1,73)
6680 GOTO 1240
6690 GOSUB 7070
6700 IF Z5%="BLANK" THEN GOTO 6730
6710 LET K=1
6720 GOTO 1240
6730 LET N(13)=L(1,73)
6740 LET D3=ABS(L(1,73)-D(1,13))
6750 IF D3>D(1,33) THEN GOTO 6830
6760 IF I=2 THEN GOTO 6800
6770 LET L(1,93)=D(1,43)
6780 LET L(1,103)=L(1,93)+N(13)
6790 GOSUB 5500
6800 GOSUB 4620
6810 IF I=32 THEN GOTO 6850
6820 GOTO 0870
6830 PRINT "QSD"
6840 GOTO 6760
6850 CLOSE FILE(33)
6860 GOTO 2660
6870 IF I=2 THEN GOTO 7020
6880 LET I(1,83)=L(1,73)/X3
6890 IF Z4%="C" THEN GOTO 6910
6900 GOTO 1420
6910 GOSUB 7070
6920 IF Z5%="BLANK" THEN GOTO 6950
6930 LET K=1
6940 GOTO 1420
6950 PRINT TAB(35);
6960 PRINT USING "####.###",L(1,83);
6970 LET D3=ABS(L(1,83)-D(1,13))
6980 IF D3>D(1,33) THEN GOTO 7000
6990 GOTO 6770
7000 PRINT "QSD"
7010 GOTO 6900
7020 LET X3=L(1,73)
7030 LET N(13)=L(1,73)
7040 GOSUB 4620
7050 PRINT
7060 GOTO 0870
7070 IF Z0%="B" THEN GOTO 7180
7080 IF Z0%="C" THEN GOTO 7160
7090 IF Z0%="D" THEN GOTO 7200
7100 OPEN FILE(1,33,"DLA")
7110 FOR I1=3 TO 22
7120 READ FILE(13,D(1,13),D(1,23),D(1,33),D(1,43)
7130 NEXT I1
7140 CLOSE FILE(13)
7150 RETURN
7160 OPEN FILE(1,33,"DLB")
7170 GOTO 7110
7180 OPEN FILE(1,33,"DLB")
7190 GOTO 7110
7200 OPEN FILE(1,33,"DLB")

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7210 GOTO 7110
7220 RETURN
7230 IF Z0#="C" THEN GOTO 7320
7240 IF Z0#="D" THEN GOTO 7320
7250 OPEN FILE(5,3), "BFAB"
7260 FOR I1=3 TO 22
7270   READ FILE(5), B(1,3), B(1,4)
7280   LET L(1,3)=B(1,3)
7290 NEXT I1
7300 CLOSE FILE(5)
7310 RETURN
7320 OPEN FILE(5,3), "BFCD"
7330 GOTO 7380
7340 REM
7350 LET B(1,1)=L(1,4)/L(1,3)
7360 LET Y1=B(1,1)
7370 IF W(3)=1 THEN GOTO 7470
7380 LET B(1,2)=0
7390 GOSUB 7510
7400 GOSUB 4620
7410 IF I=22 THEN GOTO 7440
7420 PRINT
7430 GOTO 0870
7440 CLOSE FILE(5)
7450 CLOSE FILE(3)
7460 GOTO 2640
7470 LET B(1,1)+((B(1,3)+(W(3)-1))/W(3))+Y1/W(3)
7480 LET B(1,2)+((B(1,4))^2+((W(3)+(B(1,1)-Y1)^2)/(W(3)-1)^2))^.5
7490 GOSUB 7510
7500 GOTO 7400
7510 LET B(1,3)=B(1,1)
7520 LET B(1,4)=B(1,2)
7530 PRINT TAB(24)
7540 PRINT USING "##.##", B(1,3)
7550 PRINT TAB(35)
7560 PRINT USING "#####", B(1,4)
7570 IF Z0#="C" THEN GOTO 7630
7580 IF Z0#="D" THEN GOTO 7630
7590 IF I=2 THEN GOTO 7610
7600 OPEN FILE(5,1), "BFAB"
7610 WRITE FILE(5), B(1,3), B(1,4)
7620 RETURN
7630 IF I=2 THEN GOTO 7610
7640 OPEN FILE(5,1), "BFCD"
7650 GOTO 7610
7660 END

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0010 REM **** ERS ****
0020 DIM B(30), D(22,2), F(40), L(22,10), N(22)
0030 DIM A%(50)
0040 DIM D(22,7), Y(22,7), W(24)
0050 DIM C(2,4), H(22,3), F(4)
0060 DIM B%(45), B1%(25), B2%(50), B3%(30)
0070 DIM B4%(30), B5%(45), B6%(30), B7%(30)
0080 DIM B9%(45), B9%(40)
0090 DIM X1(2), Z(2), Z0(2), Z1(8), Z4(2), Z5(6)
0100 DIM Z6(15), Z7(15)
0110 DIM X8(5), Z8(5)
0120 OPEN FILE(5,3), "SPECVAR"
0130 READ FILE(5), W(4), B9
0140 READ FILE(5), Z6, Z0, Z1, Z4, Z5, Z6, Z7
0150 READ FILE(5), W(1), W(2), W(3), Z8, A%
0160 READ FILE(5), W(5), W(6), W(7)
0170 READ FILE(5), X8, Z8
0180 CLOSE FILE(5)
0190 INPUT "WHICH PROGRAM A,B,C,D ? ", Z0
0200 GOSUB 1970
0210 REM LEAST SQUARES FIT ROUTINE
0220 MAT F=ZFR(4,4)
0230 MAT N=ZER(4)
0240 MAT A=ZER(4)
0250 MAT G=ZER(4,4)
0260 MAT U=ZER(4)
0270 INPUT "DO YOU WANT LOG EQUATION FOR FIT > ", F%
0280 INPUT "DPOREE OF FIT- LINEAR = 1 > ", X0
0290 INPUT "NUMBER OF STDS > ", X2
0300 LET X1=1
0310 LET X1=X1+1
0320 LET W(24)=1
0330 FOR I=1 TO W(14)
0340   MAT D=ZER(X2)
0350   MAT R=ZER(X2)
0360   MAT F=ZFR(X1, X1)

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0370 MAT M=ZEREX(1)
0380 MAT A=ZEREX(1)
0390 FOR J=1 TO X2
0400 IF Z0<="B" THEN GOTO 0480
0410 IF Z0<="D" THEN GOTO 0480
0420 IF F<C>"Y" THEN GOTO 0460
0430 IF Y(I,J)<0 THEN GOTO 0530
0440 LET R(I,J)=OG(Y(I,J))/LOG(10)
0450 GOTO 0530
0460 LET R(I,J)=Y(I,J)
0470 GOTO 0530
0480 IF F<C>"Y" THEN GOTO 0520
0490 IF O(I,J)<0 THEN GOTO 0530
0500 LET R(I,J)=OG(O(I,J))/LOG(10)
0510 GOTO 0530
0520 LET R(I,J)=O(I,J)
0530 IF J>1 THEN GOTO 0790
0540 IF F<C>"Y" THEN GOTO 0670
0550 IF I=7 THEN GOTO 0610
0560 IF I=17 THEN GOTO 0630
0570 IF I=18 THEN GOTO 0650
0580 IF I=20 THEN GOTO 0650
0590 LET O(I,J)=LOG(1)/LOG(10)
0600 GOTO 0910
0610 IFT O(I,J)=LOG(.01)/LOG(10)
0620 GOTO 0910
0630 LET O(I,J)=LOG(.004)/LOG(10)
0640 GOTO 0910
0650 LET O(I,J)=LOG(.1)/LOG(10)
0660 GOTO 0910
0670 IF I=7 THEN GOTO 0730
0680 IF I=17 THEN GOTO 0750
0690 IF I=18 THEN GOTO 0770
0700 IF I=20 THEN GOTO 0770
0710 LET O(I,J)=1
0720 GOTO 0910
0730 LET O(I,J)=.01
0740 GOTO 0910
0750 LET O(I,J)=.004
0760 GOTO 0910
0770 LET O(I,J)=1
0780 GOTO 0910
0790 IF F<C>"Y" THEN GOTO 0860
0800 IF J=4 THEN GOTO 0840
0810 IF J=7 THEN GOTO 0840
0820 LET O(I,J)=O(I,J-1,1)*(LOG(2)/LOG(10))
0830 GOTO 0910
0840 LET R(I,J)=R(I,J-1,1)*(LOG(2.5)/LOG(10))
0850 GOTO 0910
0860 IF J=4 THEN GOTO 0900
0870 IF J=7 THEN GOTO 0900
0880 LET O(I,J)=O(I,J-1,1)*2
0890 GOTO 0910
0900 LET R(I,J)=O(I,J-1,1)*2.5
0910 NEXT J
0920 RM STORE CNTS,CR OR LOGCNTS,LOGCR IN STINFO FILE
0930 GOSUB 3360
0940 FOR J=1 TO X2
0950 LET W(18)=R(I,J)
0960 LET W(19)=O(I,J)
0970 LET W(20)=1
0980 FOR L=1 TO 2*X1-1
0990 IF L>X1 THEN GOTO 1030
1000 LET F(1,L)=F(1,L)+W(20)
1010 LET M(L,1)=M(L,1)+W(18)
1020 GOTO 1040
1030 LET F(L-X1+1,X1)=F(L-X1+1,X1)+W(20)
1040 LET W(20)=W(19)+W(20)
1050 LET W(18)=W(18)+W(19)
1060 NEXT L
1070 NEXT J
1080 FOR J=2 TO X1
1090 FOR L=1 TO X1-1
1100 LET F(L,L)=F(L,J-1,L+1)
1110 NEXT L
1120 NEXT J
1130 MAT G=ZEREX(1,X1)
1140 MAT G=INV(F)
1150 MAT A=G*M
1160 MAT Z=TRN(R)
1170 MAT I=Z*A
1180 LET C=-DC(1,1)
1190 LET C3=M(1,1)*M(1,1)/X2
1200 MAT Z=F*A
1210 MAT U=TRN(A)

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```

1220 MAT DIM=2
1230 LET CA=DEL(1,1)
1240 LET AC03=(C04-C05)/(C02-C03)
1250 FOR J=1 TO X2
1260 PRINT OF(J,1),RE(J,1)
1270 NEXT J
1280 MAT PRINT F
1290 MAT PRINT M
1300 MAT PRINT A
1310 PRINT " COEF OF DETERMINATION = ",AC03
1320 PRINT
1330 PRINT
1340 IF X1=2 THEN GOTO 1370
1350 LET WC133=1
1360 GOTO 1470
1370 IF X1=3 THEN GOTO 1400
1380 LET WC133=2
1390 GOTO 1460
1400 IF X1=4 THEN GOTO 1430
1410 LET WC133=4
1420 GOTO 1450
1430 PRINT "100 HIGH - MAX DEGREE OF FIT = 3"
1440 GOTO 0080
1450 LET CCI,43=AC4,13
1460 LET CCI,33=AC3,13
1470 LET CCI,23=AC2,13
1480 LET CCI,13=AC1,13
1490 IF WC133=2 THEN GOTO 1560
1500 IF WC133=3 THEN GOTO 1540
1510 IF WC133=4 THEN GOTO 1520
1520 LET HCI,33=AC03
1530 GOTO 1570
1540 LET HCI,23=AC03
1550 GOTO 1570
1560 LET HCI,13=AC03
1570 NEXT I
1580 IF Z04="B" THEN GOTO 1750
1590 IF Z04="D" THEN GOTO 1720
1600 IF Z04="A" THEN GOTO 1640
1610 OPEN FILE(7,01,"SLINTC"
1620 WRITE F(1),F(7,03),F#
1630 GOTO 1660
1640 OPEN FILE(7,01,"SLINTA"
1650 WRITE FILE(7,03),F#
1660 IF X1=2 THEN GOTO 1820
1670 LET WC123=1
1680 LET X=WC123
1690 WRITE FILE(7,X),X0
1700 LET WC123=WC123+1
1710 GOTO 1820
1720 OPEN FILE(7,01,"SLIND"
1730 WRITE FILE(7,03),F#
1740 GOTO 1770
1750 OPEN FILE(7,01,"SLINTB"
1760 WRITE F(1),F(7,03),F#
1770 IF X1=2 THEN GOTO 1820
1780 LET WC123=1
1790 LET X=WC123
1800 WRITE FILE(7,X),X0
1810 LET WC123=WC123+1
1820 FOR I=1 TO 20
1830 FOR J=1 TO WC133
1840 LET X=WC123
1850 WRITE FILE(7,X),CCI,J3
1860 LET WC123=WC123+1
1870 NEXT J
1880 NEXT I
1890 CLOSE FILE(7)
1900 IF X1=X0+1 THEN GOTO 1920
1910 GOTO 0310
1920 INPUT "DO YOU WANT A REPORT ON THE %LPT >",X14
1930 IF X14="Y" THEN GOTO 2440
1940 INPUT "DO YOU WANT TO CONTINUE >",X14
1950 IF X14="N" THEN GOTO 4060
1960 CHAIN "ESI" THEN GOTO 0420
1970 IF Z04="B" THEN GOTO 2060
1980 IF Z04="D" THEN GOTO 2080
1990 IF Z04="C" THEN GOTO 2020
2000 OPEN FILE(6,03,"SCNTSA"
2010 GOTO 2030
2020 OPEN F(1),F(6,03,"SCNTSC"
2030 LET WC143=20
2040 GOTO 2100
2050 REM EXAMINATION OF STAR FILE OF STD COUNT RATIOS
2060 OPEN FILE(6,01,"STARB"

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2070 GOTO 2090
2080 OPEN FILE(6,01,"STARD"
2090 LET W(141)=20
2100 DIM C(20,41),H(20,31)
2110 REM 7 STDs
2120 FOR J=1 TO 7
2130 LET Z6=J
2140 IF Z6>1 THEN GOTO 2170
2150 LET W(15)=1
2160 GOTO 2190
2170 LET W(15)=(W(143)*(Z6-1)+1)
2180 REM 20 CHANNELS FE TO RA
2190 FOR I=1 TO W(141)
2200 IF Z6="B" THEN GOTO 2250
2210 IF Z6="D" THEN GOTO 2250
2220 LET X=W(15)
2230 READ FILE(6,X),Y(I,J)
2240 GOTO 2270
2250 LET Y=W(15)
2260 READ FILE(6,X),O(I,J)
2270 LET W(15)=W(15)+1
2280 NEXT I
2290 NEXT J
2300 IF Z6="B" THEN GOTO 2340
2310 IF Z6="D" THEN GOTO 2340
2320 INPUT "DO YOU WANT TO OUTPUT COUNTS FROM SCNTS > ",X1$
2330 GOTO 2350
2340 INPUT "DO YOU WANT TO OUTPUT RATIOS FROM STAR > ",X1$
2350 IF X1$="Y" THEN GOTO 2370
2360 GOTO 2420
2370 IF Z6="B" THEN GOTO 2410
2380 IF Z6="D" THEN GOTO 2410
2390 MAT PRINT Y
2400 GOTO 2420
2410 MAT PRINT O
2420 CLOSE FILE(6)
2430 RETURN
2440 REM REPORT OF LEAST SQUARES FIT DATA AND COEFFICIENTS
2450 LET B$="STANDARD DATA AND CALIBRATION COEFFICIENTS"
2460 LET B1$="ELEMENT=DEGREE OF FIT ="
2470 LET B2$="EQUATION FOR DEGREE OF FIT ="
2480 LET B4$="Y = A1 + A2X + A3X^2 + A4X^3"
2490 LET B5$="LOG Y = A1 + (2LOGX + A3LOGX^2 + A4LOGX^3"
2500 LET B6$="COEFFICIENT OF DETERMINATION ="
2510 LET B7$="STD CONC (X) STD COUNTS (Y)"
2520 LET B8$="LOG STD CONC (LOGX) LOG STD COUNTS (LOGY)"
2530 LET B9$="STD RATIOS (Y) LOG STD RATIOS (LOGY)"
2540 LET X1=1
2550 GOSUB 3630
2560 GOSUB 3470
2570 OPEN FILE(7,1),"$LPT"
2580 PRINT FILE(7,1),"<11>"
2590 PRINT FILE(7,1),TAB(10);B$
2600 PRINT FILE(7,1),TAB(6);B1$(1,13)
2610 PRINT FILE(7,1),TAB(6);B2$(9,23);X0
2620 LET X=1
2630 IF F$="Y" THEN GOTO 2750
2640 PRINT FILE(7,1),TAB(6);B3$;X;TAB(3);
2650 IF X=3 THEN GOTO 2710
2660 IF X=2 THEN GOTO 2690
2670 PRINT FILE(7,1);B4$(1,12)
2680 GOTO 2720
2690 PRINT FILE(7,1);B4$(1,20)
2700 GOTO 2720
2710 PRINT FILE(7,1);B4$
2720 LET X=X+1
2730 IF X=4 THEN GOTO 2860
2740 GOTO 2640
2750 PRINT FILE(7,1),TAB(6);B5$;X;TAB(3);
2760 IF X=3 THEN GOTO 2820
2770 IF X=2 THEN GOTO 2800
2780 PRINT FILE(7,1);B5$(1,19)
2790 GOTO 2830
2800 PRINT FILE(7,1);B5$(1,30)
2810 GOTO 2830
2820 PRINT FILE(7,1);B5$
2830 LET X=X+1
2840 IF X=4 THEN GOTO 2860
2850 GOTO 2750
2860 PRINT FILE(7,1)
2870 FOR K=1 TO 20
2880 LET K=K+2
2890 PRINT FILE(7,1),TAB(6);B1$(1,6);A2$(K+1,K+K)
2900 IF F$="Y" THEN GOTO 2990
2910 IF Z6="B" THEN GOTO 2960

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2920 IF Z0$="D" THEN GOTO 2970
2930 PRINT FILE(7), TAB(6);B9#[1,12]; TAB(24);B9#[21,34]
2940 PRINT FILE(7), TAB(6);B9#[14,19]; TAB(24);B9#[36,41]
2950 GOTO 3040
2960 PRINT FILE(7), TAB(6);B9#[1,12]; TAB(24);B9#[16,29]
2970 PRINT FILE(7), TAB(6);B9#[14,19]; TAB(24);B9#[31,36]
2980 GOTO 3040
2990 IF Z0$="B" THEN GOTO 3030
3000 IF Z0$="D" THEN GOTO 3030
3010 PRINT FILE(7), TAB(6);B7#[1,12]; TAB(24);B7#[14,27]
3020 GOTO 3040
3030 PRINT FILE(7), TAB(6);B7#[1,12]; TAB(24);B9#[1,14]
3040 LET K=K-2
3050 FOR J=1 TO X2
3060 PRINT FILE(7), TAB(6);C(K,J); TAB(24);Y(K,J)
3070 NEXT J
3080 PRINT FILE(7), TAB(6);"A1=";C(K,1); TAB(21);"A2=";C(K,2);
3090 IF X12 THEN GOTO 3190
3100 PRINT FILE(7)
3110 PRINT FILE(7), TAB(6);B6#;H(K,1)
3120 PRINT FILE(7)
3130 NEXT K
3140 IF X0=1 THEN GOTO 3340
3150 CLOSE FILE(7)
3160 GOSUB 3630
3170 OPEN FILE(7,1);"%LPT"
3180 GOTO 2870
3190 PRINT FILE(7), TAB(15);"A3=";C(K,3);
3200 IF X103 THEN GOTO 3300
3210 PRINT FILE(7)
3220 PRINT FILE(7),B6#;H(K,2)
3230 PRINT FILE(7)
3240 NEXT K
3250 IF X0=2 THEN GOTO 3340
3260 CLOSE FILE(7)
3270 GOSUB 3630
3280 OPEN FILE(7,1);"%LPT"
3290 GOTO 2870
3300 PRINT FILE(7), TAB(15);"A4=";C(K,4)
3310 PRINT FILE(7),B6#;H(K,3)
3320 PRINT FILE(7)
3330 NEXT K
3340 CLOSE FILE(7)
3350 GOTO 1940
3360 OPEN FILE(1,0);"STINFO"
3370 LET X=WC(24)
3380 FOR J=1 TO 7
3390 WRITE FILE(1,X),R(J,1)
3400 LET X=X+1
3410 WRITE FILE(1,X),Q(J,1)
3420 LET X=X+1
3430 NEXT J
3440 LET W(24)=X
3450 CLOSE FILE(1)
3460 RETURN
3470 LET W(24)=1
3480 OPEN FILE(1,0);"STINFO"
3490 FOR I=1 TO 20
3500 LET X=WC(24)
3510 FOR J=1 TO 7
3520 READ FILE(1,X),R(J,1)
3530 LET X=X+1
3540 READ FILE(1,X),Q(J,1)
3550 LET X=X+1
3560 LET Y(I,J)=R(J,1)
3570 LET Q(I,J)=Q(J,1)
3580 NEXT J
3590 LET W(24)=X
3600 NEXT I
3610 CLOSE FILE(1)
3620 RETURN
3630 IF Z0$="B" THEN GOTO 3970
3640 IF Z0$="D" THEN GOTO 3940
3650 REM
3660 REM
3670 IF Z0$="A" THEN GOTO 3710
3680 OPEN FILE(7,0);"SLINTC"
3690 READ FILE(7,0),F#
3700 GOTO 3730
3710 OPEN FILE(7,0);"SLINTA"
3720 READ FILE(7,0),F#
3730 LET X1=X1+1
3740 GOTO 4000
3750 LET W(19)=X1

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3760 IF X102 THEN GOTO 3830
3770 LET W123=1
3780 GOTO 3800
3790 LET W123=W123+1
3800 LET X=W123
3810 READ FILE(7,X),X0
3820 LET W123=W123+1
3830 FOR K=1 TO 20
3840   FOR L=1 TO W123
3850     LET Y=W123
3860     READ FILE(7,X),CFK,L3
3870     LET W123=W123+1
3880   NEXT L
3890 NEXT K
3900 CLOSE FILE(7)
3910 RETURN
3920 REM
3930 REM
3940 OPEN FILE(7,0), "SLINTD"
3950 READ FILE(7,0),F#
3960 GOTO 3730
3970 OPEN FILE(7,0), "SLINTB"
3980 READ FILE(7,0),F#
3990 GOTO 3730
4000 IF X14 THEN GOTO 4030
4010 DIM C22,41
4020 GOTO 3750
4030 IF X14 THEN GOTO 4060
4040 DIM C22,31
4050 GOTO 3750
4060 DIM C22,21
4070 GOTO 3750
4080 END

```

```

0010 REM **** ESA ****
0020 DIM C(22,43),E(403),L(22,101),N(221)
0030 DIM D(70,73),Y(22,73),W(243)
0040 DIM A$(301),A1$(501),A2$(501),A3$(601),A4$(601)
0050 DIM A5$(801),A6$(343),A7$(401),A8$(201),B2$(501)
0060 DIM N$(51),X1$(23),Z1$(23),Z0$(23),Z1$(81),Z4$(12)
0070 DIM Z5$(16),Z6$(153),Z7$(151)
0080 DIM X8$(53),Z9$(53)
0090 OPEN FILE(5,3), "SPECVAR"
0100 READ FILE(5),W(43),B9
0110 READ FILE(5),Z5,Z0,Z1,Z4,Z5,Z6,Z7
0120 READ FILE(5),W(13),W(23),W(33),Z8,A2$
0130 READ FILE(5),W(53),W(63),W(73)
0140 READ FILE(5),X8,Z9
0150 CLOSE FILE(5)
0160 IF Z9<0 THEN GOTO 0190
0170 DIM B(22,43),D(22,41)
0180 GOTO 0200
0190 DIM B(301),D(22,41)
0200 LET A$=""
0210 IF Z4$="C" THEN GOTO 0400
0220 IF Z5$="BLANK" THEN GOTO 0400
0230 IF Z0$="Y" THEN GOTO 0400
0240 IF Z0$="B" THEN GOTO 0330
0250 OPEN FILE(1,3), "DLIMITA"
0260 FOR I=3 TO 22
0270   READ FILE(1),L(1,73),L(1,93)
0280   LET D(1,13)=L(1,73)
0290   LET D(1,23)=L(1,93)
0300 NEXT I
0310 CLOSE FILE(1)
0320 GOTO 0400
0330 OPEN FILE(1,3), "DLIMITB"
0340 FOR I=3 TO 22
0350   READ FILE(1),L(1,73),L(1,93)
0360   LET D(1,13)=L(1,73)
0370   LET D(1,23)=L(1,93)
0380 NEXT I
0390 CLOSE FILE(1)
0400 REM
0410 REM RTN TO RETRIEVE HEADERS (SAMPLES) FOR PRINTING ON LPT
0420 REM RTN TO RETRIEVE HEADER (STDs) FOR LPT
0430 REM ROUTINE TO RETRIEVE DATA AND PRINT REPORTS ON $LPT
0440 IF Z4$="C" THEN GOTO 1640
0450 REM DATA FOR STD REPORTS
0460 LET A1$="DATE STANDARD# RUN# PROGRAM"
0470 IF Z0$="Y" THEN GOTO 0930
0480 IF Z0$="C" THEN GOTO 0530
0490 IF Z0$="D" THEN GOTO 0930

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0500 RPN BLANK STD REPORT
0510 OPEN FILE(3,3), "BLFILEAB"
0520 GOTO 0540
0530 OPEN FILE(3,3), "BLFILECD"
0540 FOR I=1 TO 22
0550 IF I>1 THEN GOTO 0570
0560 READ FILE(3,3), A$, Z$, A4$, W(3), A5$
0570 IF Z$="Y" THEN GOTO 0600
0580 READ FILE(3,1), C1, I1, L(1,2), B(1,3)
0590 GOTO 0640
0600 IF I=1 THEN GOTO 0630
0610 READ FILE(3,1), L(1,1), L(1,2), L(1,3)
0620 GOTO 0640
0630 READ FILE(3,1), L(1,1), L(1,2), L(1,3), L(1,4), B(1,3), B(1,4)
0640 NEXT I
0650 CLOSE FILE(3)
0660 OPEN FILE(3,1), "%LPT"
0670 PRINT FILE(3), "<11>"
0680 IF Z$="Y" THEN GOTO 0710
0690 LET A5$=A$(1,12), "C1 C2 AC BF", A$(1,8), "STDEV"
0700 GOTO 0720
0710 LET A5$=A$(1,12), "C1 C2 AC"
0720 FOR I=1 TO 22
0730 IF I>1 THEN GOTO 0800
0740 GOSUB 2310
0750 PRINT FILE(3), Z$
0760 PRINT FILE(3), A4$, W(3)
0770 PRINT FILE(3)
0780 PRINT FILE(3), A5$
0790 PRINT FILE(3)
0800 IF Z$="Y" THEN GOTO 0890
0810 IF I>1 THEN GOTO 0840
0820 PRINT FILE(3), TAB(6), A2$(I+I-1, I+I); TAB(10); L(1,1); TAB(16); L(1,2); TAB(22); L(1,3)
0830 GOTO 0900
0840 PRINT FILE(3), TAB(6), A2$(I+I-1, I+I); TAB(10); L(1,1); TAB(16); L(1,2); TAB(22); L(1,4); TAB(29);
0850 PRINT FILE(3), USING "### ##", B(1,3);
0860 PRINT FILE(3), TAB(8);
0870 PRINT FILE(3), USING "#####", B(1,4)
0880 GOTO 0900
0890 PRINT FILE(3), TAB(6), A2$(I+I-1, I+I); TAB(10); L(1,1); TAB(16); L(1,2); TAB(22); B(1)
0900 NEXT I
0910 CLOSE FILE(3)
0920 CHAIN "ES2" THEN GOTO 2680
0930 IF Z$="B" THEN GOTO 1260
0940 IF Z$="D" THEN GOTO 1260
0950 REM STD REPORT PROGRAMS A & C
0960 OPEN FILE(3,3), "STAFLEAC"
0970 FOR I=1 TO 22
0980 IF I>1 THEN GOTO 1030
0990 READ FILE(3,3), A$, Z$, A4$, W(3), A5$
1000 IF Z$="Y" THEN GOTO 1030
1010 READ FILE(3,1), L(1,1), L(1,2), L(1,3)
1020 GOTO 1040
1030 READ FILE(3,1), L(1,1), L(1,2), L(1,3), N(1)
1040 NEXT I
1050 CLOSE FILE(3)
1060 OPEN FILE(3,1), "%LPT"
1070 PRINT FILE(3), "<11>"
1080 LET A5$=A$(1,12), "C1 C2 AC ACBC"
1090 FOR I=1 TO 22
1100 IF I>1 THEN GOTO 1190
1110 GOSUB 2310
1120 PRINT FILE(3), Z$
1130 PRINT FILE(3), A4$, W(3)
1140 PRINT FILE(3)
1150 PRINT FILE(3), A5$
1160 PRINT FILE(3)
1170 PRINT FILE(3), TAB(6), A2$(I+I-1, I+I); TAB(10); L(1,1); TAB(16); L(1,2); TAB(22); L(1,4)
1180 GOTO 1230
1190 IF Z$="Y" THEN GOTO 1210
1200 IF I=2 THEN GOTO 1170
1210 PRINT FILE(3), TAB(6), A2$(I+I-1, I+I); TAB(10); L(1,1); TAB(16); L(1,2); TAB(22); L(1,4); TAB(32);
1220 PRINT FILE(3), USING "#####", N(1)
1230 NEXT I
1240 GOTO 1580
1250 RPN STD REPORT PROGRAMS B & D
1260 OPEN FILE(3,3), "STAFLEBD"
1270 FOR I=1 TO 22
1280 IF I>1 THEN GOTO 1300
1290 READ FILE(3,3), A$, Z$, A4$, W(3), A5$
1300 IF I=2 THEN GOTO 1330
1310 READ FILE(3,1), L(1,1), L(1,2), L(1,3), L(1,4), L(1,7)
1320 GOTO 1340
1330 READ FILE(3,1), L(1,1), L(1,2), L(1,3), L(1,4), L(1,7), N(1)
1340 NEXT I

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1350 CLOSE FILE(3)
1360 OPEN FILE(3,1), "%LPT"
1370 PRINT FILE(3), "<11>"
1380 LET A$=A$(1,12), "C1 C2 AC ACBC", A$(1,9), "CR"
1390 FOR I=1 TO 22
1400 IF I=1 THEN GOTO 1490
1410 GOSUB 2310
1420 PRINT FILE(3), Z$
1430 PRINT FILE(3), A$:WC(3)
1440 PRINT FILE(3)
1450 PRINT FILE(3), A$
1460 PRINT FILE(3)
1470 PRINT FILE(3), TAB(6), A$(I+1-1, I+1), TAB(10), L(I,1), TAB(16), L(I,2), TAB(22), L(I,4)
1480 GOTO 1570
1490 IF I=2 THEN GOTO 1530
1500 PRINT FILE(3), TAB(6), A$(I+1-1, I+1), TAB(10), L(I,1), TAB(16), L(I,2), TAB(22), L(I,4), TAB(30),
1510 PRINT FILE(3), USING "####.###", L(I,7)
1520 GOTO 1570
1530 PRINT FILE(3), TAB(6), A$(I+1-1, I+1), TAB(10), L(I,1), TAB(16), L(I,2), TAB(22), L(I,4), TAB(30),
1540 PRINT FILE(3), USING "####.###", L(I,7)
1550 PRINT FILE(3), TAB(4),
1560 PRINT FILE(3), USING "####.###", N(I)
1570 NEXT I
1580 CLOSE FILE(3)
1590 INPUT "ARE YOU READY TO FIT STD DATA > ", X1$
1600 IF X1$="Y" THEN GOTO 1620
1610 GOTO 1630
1620 CHAIN "ES3"
1630 CHAIN "ES2" THEN GOTO 2680
1640 REM ROUTINE TO PRINT SAMPLE REPORTS ON %LPT
1650 LET A1$="DATE SAMPLE TYPE SOURCE"
1660 LET N$="ND-"
1670 GOSUB 4000
1680 IF Z$="E" THEN GOTO 2390
1690 IF Z$="D" THEN GOTO 2390
1700 REM SAMPLE REPORT PROGRAMS A & C
1710 OPEN FILE(3,1), "SAMPLE"
1720 FOR I=1 TO 22
1730 IF I=1 THEN GOTO 1780
1740 READ FILE(3), A$, A$, A$
1750 IF Z$="Y" THEN GOTO 1780
1760 READ FILE(3), L(I,1), L(I,2), L(I,4)
1770 GOTO 1860
1780 READ FILE(3), L(I,1), L(I,2), L(I,4), N(I)
1790 IF I=2 THEN GOTO 1810
1800 GOTO 1860
1810 IF Z$="BLANK" THEN GOTO 1830
1820 IF N(I)<D(I,1) THEN GOTO 1850
1830 READ FILE(3), L(I,9), L(I,10)
1840 GOTO 1860
1850 READ FILE(3), N$, L(I,9), N$, L(I,10)
1860 NEXT I
1870 CLOSE FILE(3)
1880 OPEN FILE(3,1), "%LPT"
1890 PRINT FILE(3), "<11>"
1900 IF Z$="BLANK" THEN GOTO 1930
1910 LET A$=A$(1,6), "C1 C2 AC ACBC", A$(1,21), "CP", A$(1,14), "CO"
1920 GOTO 2000
1930 IF Z$="Y" THEN GOTO 1990
1940 IF Z$="Y" THEN GOTO 1970
1950 LET A$=A$(1,6), "C1 C2 AC ACBC(RM)", A$(1,19), "STDEV", A$(1,11), "DLIM"
1960 GOTO 2000
1970 LET A$=A$(1,6), "C1 C2 AC ACBC", A$(1,21), "DLIM"
1980 GOTO 2000
1990 LET A$=A$(1,6), "C1 C2 AC 10X(AC)", A$(1,21), "CP", A$(1,14), "CO"
2000 FOR I=1 TO 22
2010 IF I=1 THEN GOTO 2060
2020 GOSUB 2310
2030 PRINT FILE(3), A$(1,2), Z$
2040 PRINT FILE(3), A$
2050 PRINT FILE(3)
2060 PRINT FILE(3), A$
2070 PRINT FILE(3)
2080 PRINT FILE(3), A$(I+1-1, I+1), TAB(4), L(I,1), TAB(10), L(I,2), TAB(16), L(I,4), TAB(25),
2090 IF I=1 THEN GOTO 2110
2100 GOTO 2140
2110 PRINT FILE(3), USING "####.###", N(I)
2120 PRINT FILE(3), TAB(14),
2130 IF I=2 THEN GOTO 2160
2140 PRINT FILE(3)
2150 GOTO 2260
2160 IF Z$="BLANK" THEN GOTO 2180
2170 IF N(I)<D(I,1) THEN GOTO 2230
2180 PRINT FILE(3), TAB(5),
2190 PRINT FILE(3), USING "####.###", L(I,9),

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2200 PRINT FILE(3), TAB(9);
2210 PRINT FILE(3), USING "#### #", L(I, 10)
2220 GOTO 2280
2230 PRINT FILE(3), TAB(2); N%;
2240 PRINT FILE(3), USING "###.###", L(I, 9);
2250 PRINT FILE(3), TAB(6); N%;
2260 PRINT FILE(3), USING "#### #", L(I, 10)
2270 GOTO 2280
2280 NEXT I
2290 CLOSE FILE(3)
2300 GOTO 3210
2310 PRINT FILE(3), A%;
2320 PRINT FILE(3), SYS(2); "/"; SYS(1); "/"; SYS(3);
2330 IF Z4="C" THEN GOTO 2360
2340 PRINT FILE(3), A%(1, 10); A%(6, 11);
2350 RETURN
2360 PRINT FILE(3), A%(1, 11); A%(6, 14);
2370 RETURN
2380 REM SAMPLE REPORT PROGRAMS B & D
2390 OPEN FILE(3), "SAMPLE"
2400 FOR I=1 TO 22
2410 IF I>1 THEN GOTO 2460
2420 READ FILE(3), A%, A%, A%
2430 IF Z9="Y" THEN GOTO 2460
2440 READ FILE(3), L(I, 1), L(I, 2), L(I, 4)
2450 GOTO 2410
2460 READ FILE(3), L(I, 1), L(I, 2), L(I, 4), L(I, 7)
2470 IF I=2 THEN GOTO 2490
2480 GOTO 2610
2490 IF Z5="BLANK" THEN GOTO 2560
2500 IF Z9="Y" THEN GOTO 2550
2510 READ FILE(3), L(I, 8)
2520 IF L(I, 8)<D(I, 1) THEN GOTO 2580
2530 READ FILE(3), L(I, 9), L(I, 10)
2540 GOTO 2610
2550 IF L(I, 7)<D(I, 1) THEN GOTO 2600
2560 READ FILE(3), L(I, 8), L(I, 9), L(I, 10)
2570 GOTO 2610
2580 READ FILE(3), N%, L(I, 9), N%, L(I, 10)
2590 GOTO 2610
2600 READ FILE(3), L(I, 8), N%, L(I, 9), N%, L(I, 10)
2610 NEXT I
2620 CLOSE FILE(3)
2630 OPEN FILE(3, 1), "SLPT"
2640 PRINT FILE(3), "<I>"
2650 IF Z5="BLANK" THEN GOTO 2680
2660 LET A5=A%(1, 6), "C1 C2 AC ACBC", A%(1, 9), "CR", A%(1, 12), "CP", A%(1, 14), "CO"
2670 GOTO 2750
2680 IF Z9="Y" THEN GOTO 2740
2690 IF Z8="Y" THEN GOTO 2720
2700 LET A5=A%(1, 6), "C1 C2 AC ACBC", A%(1, 8), "CR(RN)", A%(1, 11), "SD", A%(1, 11), "DLIM"
2710 GOTO 2750
2720 LET A5=A%(1, 6), "C1 C2 AC ACBC", A%(1, 10), "CR", A%(1, 11), "DLIM"
2730 GOTO 2750
2740 LET A5=A%(1, 6), "C1 C2 AC 10X(AC)", A%(1, 9), "CR", A%(1, 12), "CP", A%(1, 14), "CO"
2750 FOR I=1 TO 22
2760 IF I=1 THEN GOTO 2830
2770 GOSUB 2810
2780 PRINT FILE(3), A%(1, 2); Z5%
2790 PRINT FILE(3), A%
2800 PRINT FILE(3)
2810 PRINT FILE(3), A%
2820 PRINT FILE(3)
2830 PRINT FILE(3), A2%(I+1-I, I+1); TAB(4); L(I, 1); TAB(10); L(I, 2); TAB(16); L(I, 4); TAB(24);
2840 IF I=1 THEN GOTO 2860
2850 GOTO 2880
2860 PRINT FILE(3), USING "-#### #", L(I, 7);
2870 IF I=2 THEN GOTO 2900
2880 PRINT FILE(3)
2890 GOTO 3190
2900 PRINT FILE(3), TAB(4);
2910 PRINT FILE(3), USING "-#### #", L(I, 8);
2920 PRINT FILE(3), TAB(4);
2930 IF Z5="BLANK" THEN GOTO 2960
2940 IF Z9="Y" THEN GOTO 2970
2950 IF L(I, 8)<D(I, 1) THEN GOTO 3070
2960 GOTO 2980
2970 IF L(I, 7)<D(I, 1) THEN GOTO 3070
2980 PRINT FILE(3), TAB(5);
2990 IF Z9="Y" THEN GOTO 3050
3000 IF Z8="Y" THEN GOTO 3030
3010 PRINT FILE(3), USING "##.###", L(I, 9);
3020 GOTO 3130
3030 PRINT FILE(3), USING "###.###", L(I, 9);

```

```

3040 GOTO 3130
3050 PRINT FILE(3), USING "#### #", LCI, 91;
3060 GOTO 3130
3070 PRINT FILE(3), TAB(3); N#;
3080 PRINT FILE(3), USING "###.###", LCI, 91;
3090 PRINT FILE(3), TAB(6);
3100 PRINT FILE(3); N#;
3110 PRINT FILE(3), USING "#### #", LCI, 101;
3120 GOTO 3190
3130 PRINT FILE(3), TAB(9);
3140 IF Z#<"Y" THEN GOTO 3130
3150 IF X#<"Y" THEN GOTO 3180
3160 PRINT FILE(3), USING "###.###", LCI, 101;
3170 GOTO 3190
3180 PRINT FILE(3), USING "#### #", LCI, 101;
3190 NEXT I
3200 CLOSE FILE(3)
3210 IF Z#="BLANK" THEN GOTO 3770
3220 OPEN FILE(4, 3), "SAMREP"
3230 READ FILE(4), A6#, A3#, A4#, A7#, A8#
3240 IF Z#="B" THEN GOTO 3330
3250 IF Z#="D" THEN GOTO 3330
3260 FOR I=3 TO 22
3270 IF N(I)<D(I, 1) THEN GOTO 3300
3280 READ FILE(4), LCI, 101;
3290 GOTO 3310
3300 READ FILE(4), N#, LCI, 101;
3310 NEXT I
3320 GOTO 3420
3330 FOR I=3 TO 22
3340 IF Z#<"Y" THEN GOTO 3370
3350 IF LCI, 81<D(I, 1) THEN GOTO 3400
3360 GOTO 3380
3370 IF LCI, 71<D(I, 1) THEN GOTO 3400
3380 READ FILE(4), LCI, 101;
3390 GOTO 3410
3400 READ FILE(4), N#, LCI, 101;
3410 NEXT I
3420 CLOSE FILE(4)
3430 OPEN FILE(4, 1), "SLPT"
3440 PRINT FILE(4), "<1>"
3450 REM CUSTOMER REPORT
3460 IF Z#="B" THEN GOTO 3610
3470 IF Z#="D" THEN GOTO 3610
3480 FOR I=3 TO 22
3490 IF I>2 THEN GOTO 3510
3500 GOSUB 3780
3510 PRINT FILE(4), TAB(16);
3520 PRINT FILE(4), A2#(I+1-1, 1+1);
3530 IF N(I)<D(I, 1) THEN GOTO 3570
3540 PRINT FILE(4), TAB(15);
3550 PRINT FILE(4), USING "#### #", LCI, 101;
3560 GOTO 3590
3570 PRINT FILE(4), TAB(12); N#;
3580 PRINT FILE(4), USING "#### #", LCI, 101;
3590 NEXT I
3600 GOTO 3760
3610 FOR I=3 TO 22
3620 IF I>2 THEN GOTO 3640
3630 GOSUB 3780
3640 PRINT FILE(4), TAB(16);
3650 PRINT FILE(4), A2#(I+1-1, 1+1);
3660 IF Z#<"Y" THEN GOTO 3690
3670 IF LCI, 81<D(I, 1) THEN GOTO 3730
3680 GOTO 3700
3690 IF LCI, 71<D(I, 1) THEN GOTO 3730
3700 PRINT FILE(4), TAB(15);
3710 PRINT FILE(4), USING "#### #", LCI, 101;
3720 GOTO 3750
3730 PRINT FILE(4), TAB(12); N#;
3740 PRINT FILE(4), USING "#### #", LCI, 101;
3750 NEXT I
3760 CLOSE FILE(4)
3770 CHAIN "ES2" THEN GOTO 2690
3780 PRINT FILE(4), TAB(20); A6#
3790 PRINT FILE(4);
3800 PRINT FILE(4), TAB(4); A3#;
3810 PRINT FILE(4), SYS(2); "/" ; SYS(1); "/" ; SYS(3);
3820 PRINT FILE(4), A#(1, 1); A1#(6, 1);
3830 PRINT FILE(4), A#(1, 2); Z#;
3840 PRINT FILE(4);
3850 PRINT FILE(4), TAB(4); A4#
3860 PRINT FILE(4);
3870 PRINT FILE(4), TAB(6); A7#
3880 PRINT FILE(4), TAB(30); A8#

```

```

3890 PRINT FILE(4)
3900 RETURN
3910 FOR I4=1 TO 6
3920 PRINT FILE(3)
3930 NEXT I4
3940 RETURN
3950 FOR I4=1 TO 6
3960 PRINT FILE(4)
3970 NEXT I4
3980 RETURN
3990 END
4000 IF Z04="B" THEN GOTO 4110
4010 IF Z04="C" THEN GOTO 4090
4020 IF Z04="D" THEN GOTO 4130
4030 OPEN FILE(1,3),"DLA"
4040 FOR I1=3 TO 22
4050 READ FILE(1,DCI1,13,DCI1,21,DCI1,33,DCI1,43
4060 NEXT I1
4070 CLOSE FILE(1)
4080 RETURN
4090 OPEN FILE(1,3),"DLC"
4100 GOTO 4040
4110 OPEN FILE(1,3),"DLB"
4120 GOTO 4040
4130 OPEN FILE(1,3),"DLD"
4140 GOTO 4040
4150 RETURN
4160 END

```

APPENDIX D

EMISSION SPECTROMETER PROGRAMS:

DESCRIPTIONS OF VARIABLES, ARRAYS, AND FILES

Variables (ES1)

<i>Variable</i>	<i>Description</i>
I	Control variable in a FOR loop
J	Control variable in a FOR loop
X	Location for data currently being acquired by CALL 3,X
Z	Milliliters of original sample
Z1	Milliliters of processed sample
Z8	Standard number
B9	Counter

String Variables (ES1)

<i>String Variable</i>	<i>Description</i>
A2\$	Element symbols, list 1
B2\$	Element symbols, list 2
X1\$	Y or N; "Is data OK"
Z\$	Y or N; "Is this a blank standard"
Z0\$	A, B, C
Z4\$	A or C, analysis or calibration mode
Z5\$	Sample number
Z6\$	Sample type
Z7\$	Sample source
Z8\$	Y or N; "Do you want to establish new detection limits"
Z9\$	Y or N; "Do you want BKG correction Y or N"

Arrays (ES1)

<i>Array</i>	<i>Dimension</i>	<i>Description</i>
C	22×4	Data array, initial excitation data
E	40×1	Data array, initial excitation data
W	24×1	Various information, e.g. W(2) = blank run No., W(3) = standard run No., W(4) = control variable, W(5) = excitation No., W(6) = run selection, W(7) = run selection.

Variables (ES2)

<i>Variable</i>	<i>Description</i>
A	Dummy arithmetic variable in expression: LOG(A)/LOG(10)
B	Variable containing length of string variable
B1	Variable containing length of string variable
D1	First approximation of concentration
D2	Second approximation of concentration
I	Control variable in a FOR loop
J	Control variable in a FOR loop
K	Control variable in a FOR loop
L	Control variable in a FOR loop
X	File record number
X0	Degree of fit
X1	Control variable in a FOR loop
X3	Internal standard location
Z8	Standard number

String Variables (ES2)

<i>String Variable</i>	<i>Description</i>
AS	30 space characters
A1S	“DATE SAMPLE TYPE SOURCE”
A2S	Element symbols, list 1
A3S	Report header information, combination of strings and variables
A4S	Report header information combination of strings and variables
A5S	Report header information, combination of strings and variables
A6S	Report header information, combination of strings and variables
A7S	Report header information, combination of strings and variables
A8S	Report header information, combination of strings and variables
B2S	Element symbols, list 2
F5	Y or N, “Log or normal equation”
F5	Y or N, “Log or normal equation”
N5	“ND-”
X1S	Y or N
Z5	Y or N, blank standard
Z0S	A, B, C, or D, spectrometer program A, B, C, or D.
Z1S	Date
Z4S	A or C, analysis or calibration mode
Z5S	Sample No.
Z6S	Sample type
Z7S	Sample source

Arrays (ES2)

<i>Array</i>	<i>Dimension</i>	<i>Description</i>
B	30×1	Background counts from BLANK
C	22×4	Data array, data retrieved from INDAT file
D	22×2	Detection limits, equivalent counts or count ratios
E	40×1	Data array
L	22×10	Contains intermediate and final calculated data
N	22×1	Array for background corrected counts, programs A and C
W	24×1	Various information (see listing of ES1 arrays)
Y	22×4	Standard calibration coefficients

Variables (ES3)

<i>Variable</i>	<i>Description</i>
C2	Variable used to calculate coefficient of determination (see Appendix D, least squares)
C3	Variable used to calculate coefficient of determination (see Appendix D, least squares)
C4	Variable used to calculate coefficient of determination (see Appendix D, least squares)
I	Control variable in a FOR loop
J	Control variable in a FOR loop
K	Control variable in a FOR loop
X	File record number
X0	Degree of fit
X1	Control variable in a FOR loop
X2	Number of standards

String Variables (ES3)

<i>String Variable</i>	<i>Description</i>
BS	"STANDARD DATA AND CALIBRATION COEFFICIENTS"
B1S	"ELEMENT = DEGREE OF FIT ="
B3S	"EQUATION FOR DEGREE OF FIT ="
B4S	"Y = A1 + A2X + A3X ² + A4X ³ "
B5S	"LOGY = A1 + A2LOGX + A3LOGX ² + A4LOGX ³ "
B6S	"COEFFICIENT OF DETERMINATION"
B7S	"STD CONC (X) STD COUNTS (Y)"
B8S	"LOG STD CONC (LOGX) LOG STD COUNTS (LOG Y)"
B9S	"STD RATIOS (Y) LOG STD RATIOS (LOG Y)"

Arrays (ES3)

<i>Array</i>	<i>Dimension</i>	<i>Description</i>
C	22×4	Data array, data retrieved from standard coefficients file
H	22×3	Coefficients of determination
O	20×7	Standard count ratios, seven standards
W	24×1	Various information, refer to ES1 arrays
Y	20×7	Standard counts, seven standards

Variables (ES4)

<i>Variable</i>	<i>Description</i>
I	Control variable in a FOR loop
Z8	Standard number

String Variables (ES4)

<i>String Variable</i>	<i>Description</i>		
A\$	Same as ES2	Z1\$	Same as ES2
A1\$	Same as ES2	Z4\$	Same as ES2
A2\$	Same as ES2	Z5\$	Same as ES2
A3\$	Same as ES2	Z6\$	Same as ES2
A4\$	Same as ES2	Z7\$	Same as ES2
A4\$	Same as ES2		
A5\$	Same as ES2		
A6\$	Same as ES2		
A7\$	Same as ES2		
A8\$	Same as ES2		
B2\$	Same as ES2		
F\$	Same as ES2		
NS	Same as ES2		
X1\$	Same as ES2		
Z\$	Same as ES2		
Z0\$	Same as ES2		

Arrays (ES4)

<i>Array</i>	<i>Dimension</i>	<i>Description</i>
B	30×1	Same as ES2
C	22×4	Same as ES2
D	22×2	Same as ES2
E	40×1	Same as ES2
L	22×10	Same as ES2
N	22×1	Same as ES2
W	24×1	Same as ES2
Y	22×4	Same as ES2

Files Name of file	Description	Created (write file)	Used (read file)
INDAT	Contains initial excitation data for 22 elements for up to four replicate excitations.	ES1	ES2
SPECV.R	Contains spectrometer program variables that must be carried throughout the four programs.	ES1	ES1
DLIMITA DLIMITB	Contains detection limits, (A) for direct counts method, (B) for count ratio method.	ES2	ES2
BCOUNTSAB BCOUNTSCD	Contain background counts, (AB) for element list 1, (CD) for element list 2. The background counts are derived from runs of blank standards or samples.	ES2	ES2
BLFILEAB	Contain data for standard blanks, (AB) for element list 1, (CD) for element list 2. The data stored in these files are later retrieved for generation of a report of the standard blank.	ES2	ES4
STAFLEAC STAFLEBD	Contain data relative to standard runs, (AC) direct counts method, (BD) count ratio method. The data stored in these files are later retrieved to generate reports of standard runs.	ES2	ES4
SCNTSA SCNTSA	Contain standard counts data, (A) for element list 1, (C) for element list 2. These are random access files with the data filed in records corresponding to the standard No. The data stored in these files are later retrieved when the least squares fit of standard data is carried out.	ES2	ES3
STAR B STAR D	Contain standard ratio data, (B) for element list 1, (D) for element list 2. These are random access files, etc., see above.	ES2	ES3
SAMFILE	Contains sample data. These data are later retrieved to generate a laboratory sample data report.	ES2	ES4
SAMREP	Contains sample results. These data are later retrieved to generate a customer analysis report.	ES2	ES4
STINFO	Contains standards information, concentration, and corresponding count or count ratio for each element in each of seven standards. The data are retrieved to generate a report of the least squares fit parameters.	ES3	ES3

SLINTA SLINTB SLINTC SLINTD	Contain the least squares fit coefficients, the degree of the fit, and whether a log or normal equation was used. The data are retrieved for use in calculating concentrations in unknown samples.	ES3	ES2
BFAB BFCD	Contains background factors for use in dynamic background correction. BFAB - factors for list 1, programs A and B, BFCD - factors for element list 2, programs C and D.	ES2	ES2
DLA DLB DLL	Contains detection limits for elements determined by method using dynamic background correction.	ES2	ES2 ES4

APPENDIX E **EMISSION SPECTROMETER SAMPLE DATA REPORTS**

Detailed Analytical Data Report

	DATE TYPE	3/12/1976 WATER		SAMPLE 1200 SOURCE RIVER		
	C1	C2	AC	ACBC	CP	CO
In	62	66	64			
Y	573	598	585.5	585.50		
Fe	912	944	928	713.00	11.319	11318.6
Zn	247	257	252	93.50	20.240	20239.9
Cd	322	329	325.5	173.50	14.768	14768.2
As	539	566	552.5	96.50	5.455	5454.8
Mn	835	877	856	690.50	7.599	7598.7
Cu	744	777	760.5	611.50	10.484	10483.9
Ag	592	591	591.5	19.00	ND-0.046	ND-45.5

Spectrographic Analysis Report

DATE 3/12/76 SAMPLE 1200
 TYPE WATER SOURCE RIVER

Element	Concentration, μg/liter
Fe	11318.6
Zn	20239.9
Cd	14768.2
As	5454.8
Mn	7598.7
Cu	10483.9
Ag	ND- 45.5

FLOWCHARTS OF THE ASSEMBLY LANGUAGE CALLS AND DESCRIPTORS OF MISCELLANEOUS SUBROUTINES AND CONVENTIONS

Fig. F-1. Emission spectrometer calls.

The following are descriptions of miscellaneous subroutines and conventions used by the emission spectrometer assembly language programs.

Subroutines

- ES.W — This is a subroutine used throughout the emission spectrometer real-time code (E.S. RTC) for waiting a given period of time.
- FRRT — This is a subroutine used by the E.S. RTC. It is the final exit point from the real-time data acquisition routine.
- .RECS — This is a subroutine used in the emission spectrometer call routine. It suspends the BASIC user while data are being acquired.

Conventions

- C3 — This is a constant used to address in the emission spectrometer call routine.
- TR3 — This is a page-zero location (temporary register) that is saved and restored by BASIC. It is a linkage table address of the BASIC subroutine.

APPENDIX G. EMISSION SPECTROMETER ASSEMBLY LANGUAGE PROGRAMS.

E.S. RTC ROUTINE

ES.R:	JMP@	4,2	:	VECTOR TO ENTRY POINT
P1:	500		:	RELAY HOME TIME PERIOD
P2:	100		:	SENSE DONE WAIT LOOP
P3:	200		:	AFTER SENSE DONE BEFORE FIRST POINT
P4:	40		:	BETWEEN POINTS
P5:	20		:	CYCLE SET PERIOD
P6:	100			
.ESRW:	ES. MR			
.ESIW:	ES. W			
.ESRH:	ES. H			
.ESRS:	ES. S			
.ESRT:	ES. V			
ES. MR:	LDA	1, ESRT	:	WAIT ADDRESS
	STA	1,4,2	:	NEXT
	LDA	1,P6	:	5 SEC WAIT
	JSR@	ESIW	:	WAIT
	JMP	ESCCW		
ESRMW:	LDA	1,P2	:	WAIT
	JSR@	ESIW		
ESCCW:	SKPDN	DC. F	:	GET SENSE DONE
	JMP	ESRMW		
	ESCCO+DC.	A	:	COUNTER CLEAR
	ESCSS+DC.	F	:	CLEAR SENSE SET
	JMP@	PFRRT		
ES. H:	ESHMS+DC.	F	:	HOMESSET
	ESCSS+DC.	F	:	CLEAR SENSE SET
	ESCYC+DC.	F	:	CYCLE CLEAR
	ESCCO+DC.	A	:	COUNTER CLEAR
	LDA	1, ESRT	:	LOAD WAIT ADDRESS
	STA	1,4,2	:	NEXT ENTRY
	LDA	1,P1	:	5SECONDS
	JSR@	ESIW	:	WAIT
	ESHMC+DC.	F	:	HOME CLEAR
	JMP@	+1		
	FRRT			
ES.S:	LDA	1, ESRT	:	LOAD WAIT ADDRESS
	STA	1,4,2	:	NEXT ENTRY
	JMP	ES. CK	:	IS SENSE DONE
ES. SW:	LDA	1,P2	:	SENSE WAIT LOOP
	JSR@	ESIW	:	WAIT
ES. CK:	SKPDN	DC. F	:	SKIP SENSE DONE
	JMP	ES. SW	:	WAIT MORE
	LDA	1,P3	:	WAIT BEFORE THE FIRST POINT IS TAKEN
	JSR@	ESIW	:	WAIT
	SUB	0,1	:	ZERO
	STA	0,5,2	:	READING
	JMP	ES. D	:	SKIP WAIT LOOP FIRST TIME
ES. I:	SUBZL	0,0	:	ONE
	JMP	ES. M+1		


```

ES. M:  SUB      0,0           ; ZERO
        STA      0,11,2
        LDA      1,P4         ; WAIT BETWEEN READINGS
        JSR@     ESIW         ; WAIT
ES. D:  DIA      0,DC. G      ; GET DATA
        JMP      .+1
        JMP      .+1
        JMP      .+1
        DIA      1,DC. G
        SUB      0,1,SZR
        JMP      ES. M        ; COUNTER CHANGING NOW!
        LDA      1,5,2        ; LAST
        STA      0,5,2        ; THIS
        SUBZ     1,0,SZR      ; SKIP SAME
        JMP      ES. M        ; STILL CHANGING, WAIT
        DSZ      11,2
        JMP      ES. I
        ESCSS+DC. F          ; CLEAR SENSE TEST
        ESCCO+DC. A          ; COUNTER CLEAR
        ESCYS+DC. F          ; CYCLE SET
        LDA      1,P5         ; CYCLE SET WAIT
        JSR@     ESIW         ; WAIT
        ESCYC+DC. F          ; CYCLE CLEAR
        JMP@     PFRRT        ; RETURN TO CALL ROUTINE
PFRRT:  FRRT
; *****
; E. S.
CALL ROUTINE
ES. TP: ES. T
ESPSW:  LDA      1,.ESRW      ; PRE BURN SENSE ROUTINE
        SUB      0,0          ; ZERO ROUTINE I. D.
        JMP      ES. CR
ES. CH: LDA      1,.ESRS      ; ADDRESS OF ROUTINE
        SUB      0,0          ; ROUTINE IDENTIFIER
        JMP      ES. CR      ; USE COMMON ENTRY
ES. CS:  LDA      1,.ESRS      ; ADDRESS OF ROUTINE
        SUBZL    0,0          ; ONE
ES. CR:  STA      2,TR3        ; RETURN ADDRESS
        LDA      2,ES. TP     ; TABLE POINTER
        STA      0,6,2        ; STORE ROUTINE NUMBER FOR RETURN SEQUENCE
        STA      1,4,2        ; FIRST ADDRESS FOR RTC ROUTINE
        SUB      0,0          ; ZERO
        STA      0,3,2        ; X/R
        STA      0,0,2        ; FLAG
        LDA      0,C3         ; X?R DISPLACEMENT
        ADD      2,0          ; ADDRESS
        .RECS
        DSZ      6,2          ; RETURN A VALUE OR NOT
        JMP@     TR3          ; RETURN FROM RELAY HOME ROUTINE
        SUB      0,0          ; ZERO MOST SIG HALF
        LDA      1,5,2        ; VALUE FROM E.S.
        JSR@     .FLOT        ; FLOAT FOR BASIC
        JMP      .+1          ; ERROR?
        LDA      3,TR3        ; ADDRESS OF ADDRESS OF VARISABLE
        LDA      2,0,3        ; ADDRESS OF VARIABLE
        DOBS      2,FPU1      ; MOVE DATA

```

```

JMP      1,3      ; RETURN
, *****
; *****
; E.S. TABLE
ES.T:    1        ; FLAG
          ES. R    ; ENTRY
          STM. T    ; EXIT
          0        ; X/R LOC.
          0        ; 4 ENTRY ADDRESS AFTER RTC INTERRUPT
          0        ; 5 COUNT RETURNED
          0        ; 6 WHICH ROUTINE 0=>HOME RELAY 1=>STEP
                   & COUNT
          0        ; 7 ADDRESS AT END OF WAIT
          0        ; 10 TIME AT END OF WAIT
          0        ; 11 TEMP FOR DATA RELIABILITY COUNT
; *****

```

APPENDIX H

LINE PRINTER REPORT OF LEAST SQUARES DATA-EMISSION SPECTROMETER PROGRAM*

Standard Data and Calibration Coefficients

Standard data

Degree of fit = 1

Equation for degree of fit - 1 $Y = A1 + A2X$

Equation for degree of fit - 2 $Y = A1 + A2X$

+ $A3X^2$

Equation for degree of fit - 3 $Y = A1 + A2X$

+ $A3X^2$

+ $A4X^3$

Element = Fe

Std conc (X)

1

2

4

10

20

40

100

Std ratios (Y)

9.2849819E-02

0.27119507

0.56953228

1.4584252

3.9089453

5.9007182

14.057809

A1 = 5.6675245E-02

A2 = 0.14103247

Coefficient of determination = 0.99942745

Element = Zn

Std conc (X)

1

2

4

10

20

40

100

Std ratios (Y)

8.5432014E-03

3.9207078E-02

9.4328814E-02

0.11770476

0.25957838

0.32489145

0.66815895

A1 = 5.5979063E-02

A2 = 6.3308429E-03

Coefficient of determination = 0.96675173

Element = Cd

Std conc (X)

1

2

4

10

Std ratios (Y)

6.7105675E-02

0.10755033

0.17296798

0.34804067

20

40

100

0.58740583

0.90606364

1.6023334

A1 = 0.15531757

A2 = 1.5278218E-02

Coefficient of determination = 0.96623691

Element = As

Std Conc (X)

1

2

4

10

20

40

100

Std ratios (Y)

5.5455359E-02

4.8521984E-02

9.6239271E-02

0.13961266

0.32850595

0.64487926

1.6804573

A1 = 8.8064215H-03

A2 = 1.6565124E-02

Coefficient of determination = 0.99824962

Element = Mn

Std conc (X)

1

2

4

10

20

40

100

Std ratios (Y)

0.22266139

0.39935128

0.77194863

2.0077288

3.9405964

8.0979974

19.369823

A1 = 6.5826562E-02

A2 = 0.19406396

Coefficient of determination = 0.99967882

Element = Cu

Std conc (X)

1

2

4

10

20

40

100

Std ratios (Y)

0.11256518

0.27081529

0.56008902

1.4402457

2.706313

5.2279295

10.988112

A1 = 0.26356799

A2 = 0.10994968

Coefficient of determination = 0.99362354

*The example shows the least squares data for the first six of twenty elements printed.