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L. H. Christensen and A. C. Thompson

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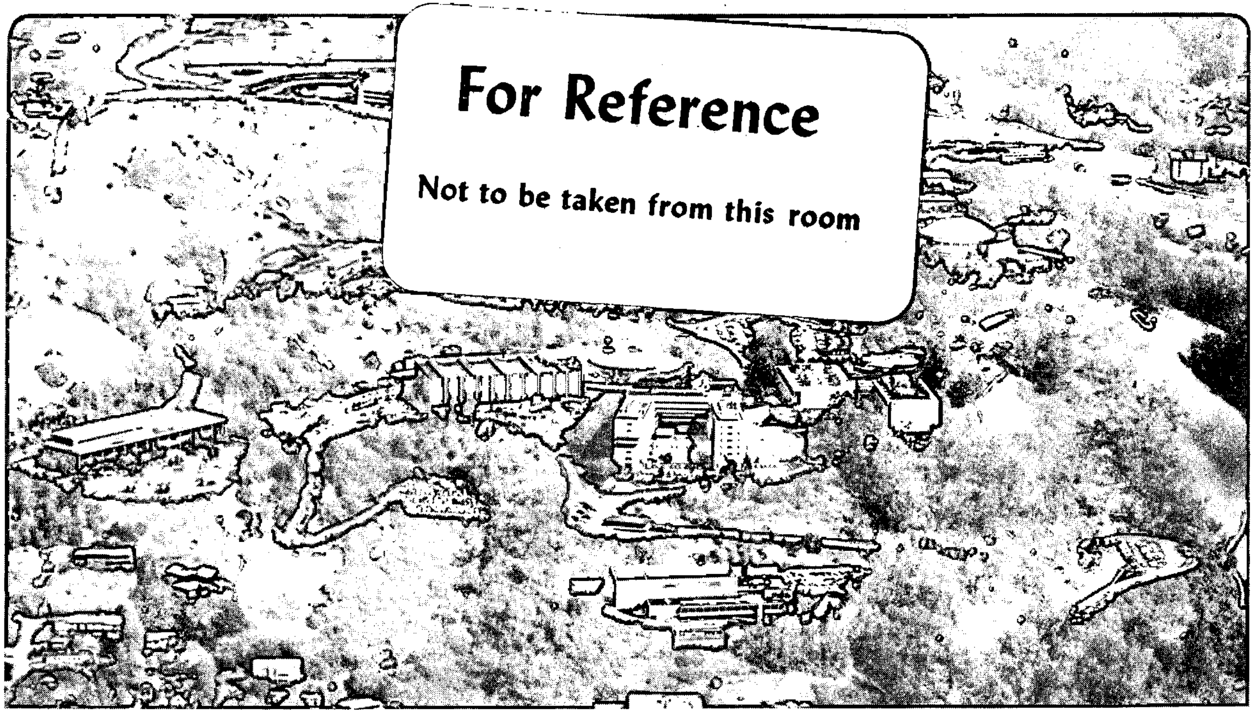

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SOFTWARE MANUAL

SCANNING X-RAY FLUORESCENCE HAIR ANALYZER

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Software Manual for the
Scanning X-ray Fluorescence Hair Analyzer

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I. INTRODUCTION

This manual will describe the software developed for the Lawrence Berkeley Laboratory Automated Hair Analyzer. The system measures hair samples using a special high-voltage Mo x-ray tube together with a high-resolution Si(Li) detector. Hair samples are mounted in plastic frames which can then be moved into position for analysis. The system is completely automated so that once the hair frames are placed in one of the 16 sample trays they will be sequentially moved into position, scanned down the hair and the results for 19 elements in ppm/mm and the mass in μgm/mm will be written on a 3M cassette tape. This tape can then be used to produce plots or printed output of the concentration of any element or mass versus sample position.

The first part of this manual will give a user oriented description and the second part a programmer oriented description. Reading the first part should make it possible for a relative inexperienced user to run the spectrometer and to obtain useful results. Part two demands that the programmer is familiar with the Basic Language and understands the general idea behind the spectrometer hardware and hardware functions.

The computer part of the hair analyzer consists of a Textronix 4051 computer with 32 K words and a Texas Instrument 9900 microprocessor with 16 K of 24-bit memory. The 4051 is programmed in Basic and the TI 9900 in assembler language. The Basic Language used is described in the 4051 manuals.[1] The TI 9900 software will be described elsewhere.[2]

Figure 1 shows an overall diagram for the hair analyzer. The central computer, which is operated from the keyboard, is connected to the microprocessor via the interface bus. This interface is an integral part of the 4051 and as such described in the manuals.[3] Some of the program works in an interactive way and the Graphic Display is used by the programs to question the user. The display can also be used to plot an acquired spectrum or the concentration versus hair length for a given element. All the programs and the data results are stored on 3M magnetic cassette tapes. The use of the Magnetic Tape Deck and the Graphic Display is described in the 4051 manuals.[1]

The collimator choice, sample changer, x-ray controller and the analog-to-digital converter (ADC) are all program controlled. Except for the ADC all these control functions can be operated via front panel push-button switches in what is called the 'manual' mode. The front panel of the hair analyzer is shown in Fig. 2.

The software for the hair analyzer consists of five main programs:

1) The Running Program
2) The Setup Program
3) The Data Tape Marking Program
4) The Data Presentation Program
5) The Hardware Test Program

These programs use various subroutines, which are divided into three groups:

1) Control Subroutines
2) Service Subroutines
3) Data Analysis Subroutine

The purpose of the Control Subroutines is to take care of sample handling and to select the experimental conditions (collimator, HV, etc.). The Service Subroutines takes care of all the necessary data manipulation (input/output, plot, etc.). The Data Analysis Subroutine is designed to facilitate automatic elemental analysis (area, concentrations, etc.).

II. USER ORIENTED DESCRIPTION OF SOFTWARE

All programs are stored on the Program Tape. By pressing the AUTO LOAD key on the 4051 a small program will be loaded which will load any of the five Basic programs.

The program asks which program you wish to run in the form

```
HAIR ANALYZER PROGRAM TAPE
WHICH PROGRAM DO YOU WANT TO LOAD
  R - Running Program
  P - Ploting + Printing Program
  S - Setup Program
  M - Tape Marking Program
  T - Hardware Test Program
```

Answer the question by typing the appropriate character. The designated program is then loaded from the tape.

1. Running Program

The general scheme for using the Running Program is shown in Fig. 3. Two modes of operation are possible: AUTO and SEMI AUTO. The only differences between these two modes are the input to and output from the program. In the AUTO mode all the necessary information about the sample and the running conditions for the spectrometer is stored on the Data Tape (see II. 3) and the final results will automatically be stored on the tape. In the SEMI AUTO mode the information has to be supplied on-line before the analysis, and the final results will only be displayed on the 4051 screen. The SEMI AUTO mode is useful if the user only wants to run one sample at a time and does not want to permanently record the data on magnetic tape.

When the Running Program has been loaded, the first question asked by the program is:

```
HAVE YOU LOADED ALL YOUR SAMPLES, AND PLACED
THE SPECTROMETER IN AUTO MODE  (Y  OR  N)?
```

If the answer is Y the program will ask:

```
HAVE YOU REFILLED THE LIQUID NITROGEN DEWAR RECENTLY?
```

This question is asked to remind the operator to refill the dewar. The dewar should be refilled at least once every four days. After refilling wait at least one hour before using the system to enable the system to stabilize properly. The next question is:

```
DO YOU WANT TO USE DATA TAPE OR
SCREEN INPUT  (T  OR  S)?
```

In the AUTO mode the Data Tape contains the necessary information and the program will ask:

```
INSERT DATA TAPE - WHICH TAPE FILE FOR FIRST SAMPLE?
```

The program refers to the Data Tape previously marked and the answer should be obvious (see II. 3). The last question in this mode is:

```
HOW MANY SAMPLES DO YOU WANT TO ANALYZE IN ONE RUN?
```

Again the answer should be obvious.

In the SEMI AUTO mode the following seven questions will be asked:

```
TYPE DATE (DDDDDD)?
WHICH KV SETTING DO YOU WANT (1, 2, 3)?
WHICH COLLIMATOR DO YOU WANT (1, 2, 3, 4)?
TYPE MM ADVANCE/STEP AND TOTAL NO. OF STEPS?
TYPE MM TO ADVANCE BEFORE ANALYSIS?
TYPE COUNTING TIME?
SAMPLE POSITION IN TRAY?
```

The user is referred to II. 3 for explanation.

All the necessary information is now in the computer and the system will start.

For each hair segment analyzed the output from the program will display the mass/mm and the elemental concentrations in ppm/mm. Figures 4 and 5 give an example of the output.

In the AUTO mode the elemental concentrations, an error estimate on these and the mass for each segment are all stored on the Data Tape. The Data Presentation Programs allows the user to print or plot the concentration versus length (see II. 4) at a later time.

If an unusual combination of collimator and high voltage have been selected then the program will ask:

```
SPECIAL SENSITIVITY FACTOR REQUIRED--
TYPE IN DESIRED FACTOR
```

The user should respond with either 1, 2, 3 or 4. Special care should be used in answering this question as the calibration factor presently stored in the system may not be the appropriate one for the particular HV-current and collimator chosen. Results may be in error by a constant factor if an error is made at this point.

2. Setup Program

The purpose of the Set-Up Program is to perform the necessary calibration of the spectrometer. The calibration is related to the quantitative data analysis (see II. 5) and this analysis is based on:

1) A stored background spectrum
2) Stored shape standard spectra
3) A calibration table
4) An attribution table (Part of 3)

Besides measuring the different spectra and creating the tables the program makes it possible to display previously stored spectra and to display and edit the Calibration Table.

Other options are: energy calibration, transfer of calibration information stored in the TI 9900 memory to a backup tape and vice versa. Figure 6 shows a list of the different options or menu items.

The TI 9900 16 K memory is organized as follows:

Buffer	1,2	:	Data acquisition
	3	:	Calibration table
	4	:	Background spectrum
	5-8	:	Shape standard spectra
	9-16	:	Temporary data storage

The Setup Program uses buffer 1 and buffer 3 to 8.

The following will explain how to run the program and give a stepwise description of the calibration procedure.

2.1 ELEMENTAL CALIBRATION

The Setup Program is stored as a binary file on the Calibration Tape (see II. 3). Pressing the AUTO LOAD key will load the program into the computer and execute it. The screen will display the MENU as shown in Fig. 6. The program is also stored on the Program Tape and can be loaded from it also.

The program works in an interactive way and questions will be displayed on the screen.

STEP #1: EXPERIMENTAL CONDIIONS

The calibration standard must be placed in one of the sample trays and the tray lowered so that it will enter the spectrometer (with the HAIR analyzer controller in the MANUAL mode). The spectrometer should then be placed in the AUTO mode and the program will ask how many steps you wish to insert the sample, what voltage (1, 2 or 3) to use and which collimator to use.

STEP #2: ENERGY CALIBRATION ITEM 11

The energy calibration is based on a knowledge of the energies and centroids for two well defined peaks. The energies (keV) and limits (channel numbers) for the two peaks are given as input. The centroids (i_o) are calculated according to

$$i_o = \frac{\sum_i i \cdot I_i}{\sum_i I_i}$$

where I_i is the intensity in channel i.

To perform the calibration place a sample in the spectrometer, choose ITEM 11 and input the counting time (sec) when the program asks for it. The spectrometer will then acquire a calibration spectrum and display it on the screen as shown in Fig. 7.

The next step is to supply the program with the energies and limits for two peaks. The program will then calculate the centroids and the number of electron volts per channel. Figure 8 shows an example of the energy calibration.

The calibration should not change very much from time to time. If the location of the centroid of the Mo coherent peak shifts more than one channel from its typical channel positin of 531.25, minor adjustments of the amplifier gain or zero controls may be necessary.

STEP #3: BACKGROUND MEASUREMENT ITEM 6 and 7

Place an appropriate background sample in the spectrometer, choose MENU ITEM 6 and input the counting time (sec). The acquisition time should be chosen in such a way that the spectrum has good statistics.

The program will display the background spectrum as shown in Fig. 9 and asks for the limits for Mo scattered peaks. The scatter peak region is shown in Fig. 10.

The limits for the coherent and incoherent peaks are determined as well as the integrated peak intensities. The intensity for the incoherent peak is used to normalize the background spectrum before subtracting it from the shape standard spectrum or from an unknown spectrum. The coherent peak centroid is also calculated and used as a fixed point for shifting an unknown spectrum (see II. 5).

Figure 11 shows the coherent peak and Fig. 12 shows the incoherent peak. The limits for these peaks can be changed until the user is satisfied with the two regions. The following parameters are used in Step #4 and should be noted:

		Typical Values
Mo coherent:	Limits	524 - 538
	Centroid	531.25
Mo incoherent:	Limits	490 - 519
	Integral/sec	224.51

It is possible to change the background spectrum without changing the rest of the calibration by measuring the background from an appropriate sample.

Use of MENU ITEM 7 will display the background spectrum currently in the calculator (see Fig. 13).

STEP #4: CALIBRATION TABLE FOR MS ITEM 2

MENU ITEM 2 is used in this case because it is the easiest way to store the calibration parameters for one element. The Ms information is part of the Calibration Table and this table will be described in greater detail under STEP #8.

The program will ask the user:

WHICH ELEMENT DO YOU WANT TO EDIT (2 CHAR.)?

and the answer should be Ms (Mass). The program will ask for which parameter you wish to change. After the user answers with the number of the parameter (1-32) the program types the current value of this parameter and asks for the new value. When you have finished editing parameters, type "-1" for the parameter number and the program will return to the initial MENU.

The mass calibration parameters are defined as:

Parameter 1 : Group number (=0)
2 : Z-value (=100)
3 : Peak centroid coherent peak
4 : Left limit for coherent peak
5 : Right limit for coherent peak
6 : Left limit for incoherent peak
7 : Right limit for incoherent peak
8 : Normalizing factor
9 : Intercept mass calibration for sensitivity 1

10 : Slope mass calibration for sensitivity 1
11 : Intercept mass calibration for sensitivity 2
12 : Slope mass calibration for sensitvity 2
13 : Intercept mass calibration for sensitvity 3
14 : Slope mass calibration for sensitvity 3
15 : Intercept mass calibration for sensitvity 4
16 : Slope mass calibration for sensitvity 4
17 : Counting time
18 : Background integral for incoherent peak (counts/sec)
19 : Start of Background Region 1
20 : Start of Background Region 2
21 : Start of Background Region 3
22 : End of Background Region 3
23 : Start of normalizing region for Background Region 1
24 : End of normalizing region for Background Region 1
25 : Integral normalizing region for Background Region 1 (c/s)
26 : Start of normalizing region for Background Region 2
27 : End of normalizing region for Background Region 2
28 : Integral normalizing region for Background Region 2 (c/s)
29 : Start of normalizing region for Background Region 3
30 : End of normalizing region for Background region 3
31 : Integral normalizing region for Background region 3 (c/s)
32 : Unassigned

It is possible at this time that not all the parameters have been determined, and the user can then set these parameters to 1. In order to measure the shape standard spectra the parameters 3 to 7, 17 and 18 must be given the right values.

STEP #5: ENERGY CALIBRATION ITEM 11

This step may not be necessary, but the user has to make sure that energy calibration is the same before and after measuring the shape standard spectra. Otherwise this measurement will be wrong. Anyway, STEP #5 is like STEP #2.

STEP #6: MEASUREMENT OF SHAPE STANDARD SPECTRA ITEM 5

As explained in II. 5 the Data Analysis Subroutine is a straight forward spectrum stripping routine in which the contribution due to scattered background and individual fluorescence peaks are sequentially subtracted from the spectrum to be analyzed. STEP #6 measures these standard fluorescence spectra for individual elements sequentially.

In order to store all the necessary spectral data in the TI 9900 memory it is necessary to compress the shape spectra using the limits on the important regions entered by the user. The spectral data for a particular element will typically consist of two regions (see Fig. 14) and in some cases of a third region. Region 1 covers the Kα line, region 2 the Kβ line and region 3 for example an escape line of a L line. The user also has to specify a fourth region: the fit region. This region is a part of region 1. The three regions will be stored in the TI 9900 memory buffer 5 to 8.

Before measuring the shape spectra be sure that the right background is in buffer 4, the Mo calibration information is stored properly and that all 19 samples are available:

Element List:

K _ Ca Ti V _ Cr Mn Fe Co Ni Cu Zn As Se Br Rb SR HG Pb

After the user has answered the questions:

DO YOU WANT TO ADVANCE SAMPLE?
WHAT HV DO YOU WANT?
INPUT COUNTING TIME?

and

HAVE YOU LOADED THE SAMPLE FOR *** K _ *** (Y OR N)?

the program will acquire the first spectrum and when finished display it as shown in Fig. 15. The program will then ask for the limits for each region, subtract the background and then display that particular region. The limits can be changed until the user is satisfied. For most elements it is not necessary to define a third region and the limits should be set to zero. It is suggested that region 1 and 2 are adjacent and if possible also region 3. The limits of region 1-3 should typically be chosen to include the peak until it is near the background. The limits of region 4 should normally be selected to include the peak from 3/4 down on the lower side to 3/4 down on the upper side.

When all the limits have been determined the program will store the three spectral regions and then print and copy the final results as shown in Fig. 16. The same procedure should be done for all the elements. Some elements can be omitted if no analysis will be done for them.

STEP #7: ENERGY CALIBRATION ITEM 11

The energy calibration should be checked after all the shape spectra have been measured. The calibration should not have changed compared with the calibration in STEP #5. If the calibration has changed it is probably necessary to remeasure the shape spectra in order to get the best data analysis results.

STEP #8: CREATE A CALIBRATION TABLE FOR 19 ELEMENTS ITEM 1

The Calibration Table contains all the information which is necessary to perform the data analysis. The table is stored in buffer 3 in the TI 9900.

For each element the following information is stored:

Parameter 1 : Group number
2 : Z-value
3 : Peak centroid
4 : Left limit region 1
5 : Right limit region 1
6 : Left limit region 2
7 : Right limit region 2
8 : Left limit region 3
9 : Right limit region 3
10 : Left limit fit region
11 : Right limit fit region
12 : First address buffer 5
13 : Last address buffer 5
14 : Number of data points
15 : Not used (=0)
16 : Not used (=0)
17 : Counting time
18 : Integral region 1 counts/sec
19 : Integral region 4 counts/sec
20 : Sensitivity 1
21 : Sensitivity 2
22 : Sensitivity 3
23 : Sensitivity 4
24 : Z-value for interference 1
25 : A_{ij} correction
26 : Z-value for interference 2
27 : A_{ij} correction
28-32 : Not used

The 19 elements can be divided into four groups numbered 1 to 4. Parameter 1 is the group number. If this parameter is not determined yet then set it to 1. The Z-value is found in the periodic table.

Parameters 3 to 19 are determined when the shape standard spectra are measured and the user should refer to the output from ITEM 5.

Parameters 20 to 23 are the sensitivity factors for example expressed as counts per sec per ng. These numbers will be determined in STEP #13.

As explained in II. 5 overlapping lines in a spectrum cause problems. Interference between two lines will result in erroneous intensities if no correction is applied. The correction α_{ij} has to be determined experimentally. It is assumed that at most only two elements interfere with the element of interest. Parmeter 24 to 27 contains the Z-values and correction factors.

It is possible that not all the parameters have been determined at this moment. The parameter is then set to 1 and can then be changed later on using MENU ITEM 2.

At any time it is possible to look at the Calibration Table using MENU ITEM 3. Up to five elements can be displayed at the same time.

STEP #9: CREATE AN ATTRIBUTION TABLE ITEM 4

To ensure that interference effects between elements are minimal it is necessary to carefully choose the order in which elements are stripped from the spectrum (see II. 5). In the Data Analysis Subroutine the sequence of removal of elements is specified by including each element in one of four groups. These groups are analyzed in order, but the elements within a group are removed from the spectrum in order of decreasing intensity. Some knowledge of possible interferences for a given sample type is necessary in order to create the table.

The group table is part of the Calibration Table stored in buffer 3. The 32 parameters are used as follows:

Parameter	1	9	17	25	:	Group number
	2	8	10	26	:	Number of elements in group
	3	11	19	27	:	Peak centroid. Position in element list for peak 1
	4	12	20	28	:	Same but for peak 2
	5	13	21	29	:	Same but for peak 3
	6	14	22	30	:	Same but for peak 4
	7	15	23	31	:	Same but for peak 5
	8	16	24	32	:	Same but for peak 6

Each group may contain up to six elements. The position in the element list is calculated automatically when the program is given the chemical symbol.

The program asks the user three questions:

1) HOW MANY ELEMENTS DO YOU WANT TO PLACE IN THIS GROUP (1 - 6)?
2) INPUT APPROXIMATE PEAK CENTROID
3) INPUT ELEMENT (2 CHAR.)

and the answers should be obvious. The last two questions will be asked for each element and the first question for each group. It is possible to place zero elements in a group.

When the program has stored the table it will display the whole table on the screen as shown in Fig. 17. At any time the user can look at the table using MENU ITEM 3 and the element symbol 'MC'.

2.2 TRANSFER TI MEMORY CONTENT ONTO TAPE

In case of a power failure all the calibration information will be lost. It is therefore necessary to store the information on a Calibration Tape every time this information is changed. MENU ITEM 9 gives that option.

Figure 18 is a listing of the files on the Calibration Tape. File 1 is a load program which loads the Set-Up Program, file 2, into the 4051 memory when the AUTO LOAD key is activated. Each Calibration Tape may contain up to four different calibrations (1, 2, 3, 4). In this example only calibration 1 is used.

Executing the program (MENU ITEM 9) will be followed by these two questions:

HAVE YOU LOADED THE SET-UP TAPE (Y OR N)?

and

TYPE OUTPUT TAPE FILE #(1-4)

When the tape has been inserted, the first answer is of course Y and the second answer should be 1, 2, 3 or 4 corresponding to calibration 1, 2, 3 or 4. Then the program will transfer the content of buffers 3 to 8 onto the tape automatically.

MENU ITEM 10 transfers calibration information previously stored on the Calibration Tape from the tape into the TI 9900 memory in the appropriate buffers. Two similar questions are asked as in MENU ITEM 9.

To create a new Calibration Tape it should first be marked in the same way as Fig. 18 shows and then the Load Program and the Set-Up Program should be stored in file 1 and 2, respectively.

2.3 MASS CALIBRATION

In order to transform absolute concentrations to relative concentrations (e.g. ng to ppm) it is necessary to determine the mass of the analyzed hair segment. It is assumed that the mass M (μg/mm) is linearly correlated to the intensity of the Mo incoherent scatter peak, I_{MI} (counts/sec).

$$M\ (\mu g/mm) = CM1 + I_{MI}/CM2$$

Before the mass can be calculated, CM1 and CM2 have to be determined. CM1 and CM2 are determined by measuring I_{MI} for different known masses, M. Again MENU ITEM 6 is used. CM1 and CM2 must be measured for each sensitivity (i.e. operational values of HV and collimator settings).

CM1 and CM2 are then stored in the Calibration Table for element MS as parameters 9 and 10 for sensitivity 1, 11 and 12 for sensitivity 2, 13 and 14 for sensitivity 3 and 15 and 16 for sensitivity 4. ITEM 2 is used to put the values in the calibration table.

2.4 BACKGROUND SPECTRUM

The background from different sample types will most likely be different. It is therefore necessary to measure the background and store it every time the sample type is changed using MENU ITEM 6. It is important to use a blank sample with very low elemental concentrations from Ca to Pb and of similar composition to the material being analyzed because a normalized background spectrum is subtracted before the elemental concentrations are calculated and a poor choice of background can give wrong concentrations.

Before the elemental concentrations are calculated, the background is subtracted from the raw spectrum using three different normalizing regions. This procedure reduces the dependence of the background subtraction on sample composition since the normalizing factor is determined for each element using a few channels which are close to the peak.

At the start of each background region are parameters 19, 20 and 21 in the mass calibration table (each region is assumed to continue to one channel before the start of the next). Parameter 22 is the end of the third background region. Parameters 22-23, 26-27 and 29-30 are the first and last channels of the window in each background region which are used to normalize the background. Parameters 25, 28 and 31 are the integral in (counts/sec) in each of the three window regions. The region integrals can be determined using MENU ITEM 6 and the parameters can be entered in the table using MENU ITEM 2.

2.5 DETERMINATION OF THE SENSITIVITY FACTORS

The sensitivity factors can be determined by using appropriate samples and running them using the Running Program in the SEMI AUTO mode. The user then has to correlate measured intensities with the known concentrations of the individual elements (e.g. ng/mm).

The sensitivity factors are stored as parameters 20 to 23 for each element using MENU ITEM 2.

3. Data Tape Marking Program

As mentioned in Section II. 1, the Master Program can be used in two modes: an AUTO and a SEMI AUTO mode. The AUTO mode assumes that a Data Tape has been marked before the analysis. The Data Tape Marking Program fulfills this requirement. It is loaded from the Program Tape by typing "M" following the first MENU.

The purpose of the program is:

1) to preset the experimental conditions (e.g. HV, collimator, step, etc.) under which each sample will be analyzed and,

2) to create element data files on a magnetic tape, where the acquired data can be stored. Each sample has to be marked individually, but the job is simplified if the samples are grouped together in such a way that the experimental conditions are the same for that particular group.

The program has the option to mark a new tape or to extend the marking on old partly used tape. The latter allows the user to add new and maybe completely different samples to an existing tape.

The space required on the tape for a given sample depends on the number of steps to advance and the number of elements analyzed. Given all the input information the program automatically computes the space requirements, marks the appropriate number of files and tells the user when the tape is filled.

The Data Tape is organized as follows:

File	1	:	A Directory (overall sample heading)
	2	:	Sample header for sample 1
	3	:	Data file element number 2
	4	:	Data file element number 3
		:	
		:	
		:	Sample header for sample 2

The Directory contains:

1) Number of bytes still available on the tape.
2) Number of samples on the tape.
3) Last file used.
4) List of element symbols.
5) Sample codes one for each sample.

The Directory will be updated automatically each time a new sample is added to the tape.

Each sample header code consists of a 72 characters word, which contains:

1) Date (dddddd 6 characters).
2) Instrument setting. Parameter P1 to P8 (4 characters each).
3) First file for that element; e.g. sample header file. Parameter P9 (4 characters).
4) Element list code (20 characters).
5) Sample label (8 characters).

Numbers 1) through 5) are all given as input to the program.

The instrument setting parameters are defined as:

P1	KV + current setting (1, 2, 3)
P2	Collimator setting (1, 2, 3)
P3	MM to advance/step (1, 2 ..., 10 mm)
P4	Total number of steps (1-200)
P5	MM to advance before analysis
P6, P7	Counting time = P6 * P7
P8	Horizontal/vertical position code

The sample position code is defined by the sum of the 10 * tray number plus the horizontal position (1, 2, 3 or 4). The horizontal position is defined as:

1 if the sample is a 12" frame
2 if the sample is a 9" frame
3 if the sample is a 6" frame
4 if the sample is a 3" frame

The vertial position or tray number is labelled on the trays and ranges from 1 to 16. Several examples of this code are:

Tray Number	Frame Size	Position Code
1	12"	11
8	6"	83
12	3"	124

The eight parameters contain all the information which is necessary for the Running Program to run a sample. When the Running Program is used in the SEMI AUTO mode the same input is used, but the output from the analysis will not be stored on a tape.

The element files will contain concentration/uncertainty in concentration as a function of hair length after an analysis. The files are empty when they are marked.

Figure 19 shows an example of how the Data Tape Marking Program works. The user's answers are marked with a *.

The 'preset values' for the instrument setting are the initial values. If the user changes one or more of the parameters the 'preset values' will change.

It is possible to analyze for 19 elements, but it will save time and space on the tape if a smaller number of elements are analyzed.

Figure 20 shows the Data Tape Marking Program output when all the information is supplied and all the files created. In fact the output is the content of the Directory. Figure 21 shows a TLIST of the Data Tape after the program has been used.

4. Data Presentation Program

The Data Presentation Program gives different presentations of data previously stored on a Data Tape (see II. 3). The MENU item list for the program is shown in Fig. 22. The overall sample head is the Directory mentioned in Section II. 3. The program is loaded from the Program Tape by typing 'P' after the MENU.

An example of item #1 is shown in Fig. 23. The parameter list is defined in II. 3. Twenty samples have been marked on the Data Tape using the Data Tape Marking Program. In this case the parameter list is the same for all these samples. Only the sample identification is different.

Figure 24 shows the output when menu item #2 is used. The user has to specify the file number for the sample header file. This number is given as parameter P9 in the sample code.

Menu item #3 and #4 plots the concentration (ppm) versus length of hair (mm) for a given sample and a given element. The program allows the user to plot the same list of elements (maximum 5) from all the samples stored on the tape. The starting and ending addresses (step) has to be the same for all the samples. If not all the elements in the specified list have been analyzed in all the samples, the program will automatically skip that element for that particular sample. Given all the necessary information, the program needs no further attention. Use of item #4 will give a hard copy of the results. The automatic scaling of the data can be suppressed. If the maximum step is greater than the value on this tape then the program plots from 0 rather than the minimum data point.

Figure 25 shows the questions asked by the program and Fig. 26 an example of the output from the program.

Menu item #5 and #6 print the concentration versus length for a given sample and a given list of elements. The printing options works in the same way as the plotting options.

Figure 27 shows the questions asked by the program and Fig. 28 an example of the output from the program. In this example no analysis has been made for K, Ti and Cr (zeroes in the columns).

5. Data Analysis Subroutine

The Data Analysis Subroutine, which is included in the Running Program, performs the spectrum analysis of an acquired pulse-height spectrum. The approach used in the analysis is basically the same as the one used in other LBL x-ray fluorescence spectrometers.

Crucial to the problem of converting a measured counting rate into an elemental concentration is the extraction of an accurate peak area from the spectrum. Since the energy resolution capabilities of the Si(Li) detector does not prohibit some interference of peaks from neighbouring elements in the periodic table, it is necessary to accurately subtract out the lines produced by each element so that the value for an adjacent element is not affected. This problem has received considerable attention in the literature and general formalisms exist for extracting peak areas from complex pulse-height spectra. Limitations in the computer core size necessitates certain, and in a lot of cases, reasonable assumptions to be made, which also can simplify the problem. Specifically, the number of possible lines in a spectrum is limited and the energies or channel positions and relative intensities of the lines from any one element are known beforehand. Thus, to a good approximation the only free parameters in the problem are the magnitude and shape of the background under the peaks and the relative intensity for each of the constituent elements.

When analyzing a series of alike samples, the continuous background due to scattering from the matrix is similar from sample to sample. Furthermore, the variation in background due to varying matrix contributions is mainly one of relative magnitude, rather than shape, provided the average Z at the matrix remains unchanged.

In the analysis of air filters used for particulate collection this fact has been used to advantage by using for a background shape a spectrum acquired by analyzing a blank filter. It may be more difficult to find a blank hair, but it could be useful to analyze synthetic fiber threads and use these as backgrounds. It is important to find a sample where the background resembles the background from hair samples since a normalized background is subtracted before peak areas are determined.

Calculation of the areas of the x-ray peaks is potentially a more difficult problem due to the variation in relative intensities of the elements and the possibility of interferences from spectral lines. The usual approach to this problem is to mathematically generate a function which simulates the response of the system to a particular photon energy. The shape is then fitted to the experimental data, usually by a least square fitting, and peak location and area determined. As noted earlier the peak location for a line is fixed; furthermore, the complexity of the x-ray lines, both in terms of $K\alpha/K\beta$ ratios and with regard to partially resolved $K\alpha_1$, $K\alpha_2$ lines makes the synthesis of such line shapes difficult. Fortunately, the profile of the instrumental response to the x-rays of an element can be established by running a spectrum from a pure sample of the element. This approach takes advantage of this by using a stored spectrum of the instrumental response to the x-rays of an element as a shape standard for that element. Thus the problem of determining the area of a given peak reduces to that of comparing the intensity of the unknown peak to that of a stored shape standard spectrum. Once this intensity ratio has been established, the total contribution of that element to the spectrum, including all x-ray lines, can be subtracted from the spectrum.

Figure 29 illustrates the operation of the subroutine on a schematic spectrum as shown in the upper left hand portion of the figure. The blank sample spectrum is first compared to the unknown sample over the specified shaded region, normalized, and then subtracted point by point to give the #2 spectrum. The lines due to elements #1, #2, etc. are then sequentially stripped out after first comparing intensities over the shaded regions to derive normalizing factors. Any selected portion of a spectrum can be specified for comparison. This is necessary when considering complex spectra where regions with overlapping lines must be avoided in making the comparison. After subtraction of the last element, the residual counts in the spectrum should be zero within statistics.

In practice, the problem is slightly more complicated. Samples used for generating shape standards must be made of material sufficiently thin to prevent changes in $K\alpha/K\beta$ ratios due to self-absorption. Also, to ensure that interference effects between elements are minimal, it is necessasry to carefully choose the order in which elements are removed from the spectrum (for example Pb before As, Fe before Co, etc.). In the present program, the sequence of removal of elements is specified by including each element in one of four groups. These four groups are analyzed in order, but the elements within a group are removed from the spectrum in order of decreasing intensity. In the above case, Pb and Fe might be in group 1 while As and Co could be in groups 2, 3 or 4. This pre-supposes some knowledge of possible interferences on the part of the person specifying the order. The order may be different from one sample type to another.

Other features of the subroutine include a peak-shifting routine to correct for any small shifts in peak location which might have occurred between the time that the shape standards were stored and that when the unknown spectrum was run. Experience with other systems indicates that the stability of the system when running continuously is adequate so that the same shape standards can be used for many weeks of running. Small shifts in the energy calibration can be corrected by adjustment of the amplifier gain.

The next step in the data analysis is to convert elemental peak intensities to absolute concentratons. The sensitivity of the instrument when running under certain experimental conditions has to be determined for each element. In order to transform absolute concentrations to relative concentrations (e. g. ng to ppm) it is necessary to determine the mass. For hair analysis it is assumed that the mass is linearly correlated to the intensity of the Mo incoherent scatter peak. Equipped with the mass calibration constants the subroutine calculates the ppm concentration for all the elements.

To summarize, the data analysis is based on:

1) A stored background spectrum
2) Stored shape standard spectra for each element
3) A calibration table
4) An attribution table (part of 3).

The Calibration Table contains limits for the comparison regions, sensitivity factors, etc., and the attribution table for the grouping of the elements. Measurements of the background spectrum, shape standard spectra and how to create the tables are more fully explained in II. 2.

The actual calculations of the areas and concentrations are given in Appendix 1.

III. PROGRAMMER ORIENTED DESCRIPTION OF SOFTWARE

1. Input/Output

Figure 1 shows the communication diagram for the Hair Analyzer. The Input/Output operations between the 4051 computer and the spectrometer or more precisely the TI 9900 microprocessor has to go through the 4051 Interface. A detailed description of this interface and how it operates is given in the manuals[3] and the following will only give a brief discussion in relation to how it is used in the Hair Analyzer.

The Interface has a set of programmable parameters: data code and handshake (n1), interrupt mask setting (n2), number of data lines (n3), number of command lines (n4), data and command logic (n5) and transfer logic (n6), which can be programmed using one of the Environmental Statements: PRINT at 61, 6: "n1 n2 n3 n4 n5 n6". Table 1 shows the chosen Interface programming for the input operation and Table 2 the same for the output operation.

TABLE 1: Interface Programming for the Input Operation

Parameter	Value	Statement
Data code and handshake	Signed Magnitude and two-wire	PRI @ 61,6: "0....."
Interrupt mask setting	Off	PRI @ 61,6: ".0...."
Number of data lines	32	PRI @ 61,6: "..8..."
Number of command lines	8	PRI @ 61,6: "...2.."
Data and command ligic	High, High	PRI @ 61,6: "....3."
Transfer logic	High, High, High, High	PRI @ 61,6: ".....F"

TABLE 2: Interface Programming for the Output Operation

Parameter	Value	Statement
Data code and handshake	Signed Magnitude and two-wire	PRI @ 71,6: "5....."
Interrupt mask setting	Off	PRI @ 71,6: ".0...."
Number of data lines	32	PRI @ 71,6: "..8..."
Number of command lines	8	PRI @ 71,6: "...2.."
Data and command ligic	High, Low	PRI @ 71,6: "....1."
Transfer logic	High, Low, Low, Low	PRI @ 71,6: ".....8"

PRI @ 71,6: "508218"

The General Interface Bus is organized with 1 to d data lines, d + 1 to d + c command lines, d + c + 1 to 40 unused lines, 41 to 44 transfer lines, 45 trigger line, 46 to 49 ground lines and 50 to 52 unused lines. Both the Input and Output use 32 data lines and 8 command lines. The 32 lines are used to transfer a signed datum and the 8 lines are used to transfer the command.

The handshake in the system has caused problems. So far only a two-wire handshake has been used, and every Output operation must be followed by "nonsense" Input operation in order to avoid a hang-up.

Three Input/Output statements are used in the programs:

PRINT @ p,26: n	Programs the command as the value n
PRINT @ p,12: e	Outputs the value of the data parameter e
PRINT @ p,13: t	Inputs datum and assigns it to the target value t

The primary address p selects the peripheral, and the secondary address (26, 12, 13) selects the operation to be performed. In fact, each peripheral device has two primary addresses: one for the Output and one for the Input (e.g. p = 61,71). According to the syntax for the last two statements it should be possible to Output or Input an array, but at the moment only one parameter can be sent at a time. This fact slows the Input/Output operation down.

The control and Service subroutines described in the next two sections (III. 2 and III. 3) make use of various 8-bit ASCII Command Codes and a 32-bit Status Word. The Codes and Status Word are defined in Tables 4 and 5, respectively, and Table 3 gives two examples to illustrate their use.

TABLE 3: Examples of the Use of Command Codes and Status

Ex. 1: Read Status of a sample	Ex. 2: Lower Stack
$S2 = 83$	$S2 = 76$
$S1 = 2^{29}$	$S1 = 0$ (arbitrary)

PRI @ 61,26: S2	Ex. 1 and Ex. 2
PRI @ 61,12: S1	
INP @ 71,13: S4	Ex. 1 only
INP @ 71,13: S3	

The first input (S4) is a nonsense input and the second input (S3) returns the status of instrument, (i.e. the status of the sample). In order to get the status of, for example, the collimator at the same time it is necessary to set $S1 = 2^{29} + 2^9 + 2^8$. The TI 9900 Microprocessor will then return the summed value of bit 30, 10 and 9. The program will have to decode the message. In Ex. 2, S1 can arbitrarily be set to zero, only the Lower Stack action will be performed.

TABLE 4: Command Codes

Comand Character		BITS								DESCRIPTION
		8	7	6	5	4	3	2	1	
L	76	0	1	0	0	1	1	0	0	LOWER STACK
U	85	0	1	0	1	0	1	0	1	RAISE STACK
I	73	0	1	0	0	1	0	0	1	INSERT SAMPLE
P	80	0	1	0	1	0	0	0	0	WITHDRAW SAMPLE
C	67	0	1	0	0	0	0	1	1	ADC ON
S	83	0	1	0	1	0	0	1	1	READ STATUS
T	84	0	1	0	1	0	1	0	0	TIME
A	65	0	1	0	0	0	0	0	1	ADVANCE SAMPLE
X	88	0	1	0	1	1	0	0	0	ROTATE COLLIMATOR
D	68	0	1	0	0	0	1	0	0	CLEAR BUFFER
E	69	0	1	0	0	0	1	0	1	CLEAR TIMER
	64	0	1	0	0	0	0	0	0	SELECT ADC BUFFER
B	66	0	1	0	0	0	0	1	0	SELECT BUFFER
R(A1,A2)*	82	0	1	0	1	0	0	1	0	READ BUFFER
W(A1,A2)*	87	0	1	0	1	0	1	1	1	WRITE BUFFER
F	70	0	1	0	0	0	1	1	0	ADC OFF
V	86	0	1	0	1	0	1	1	0	INITIATE HV CONTROLLER
y	89	0	1	0	1	1	0	0	1	HV TO STANDBY
1	49	0	0	1	1	0	0	0	1	SELECT HV1
2	50	0	0	1	1	0	0	1	0	SELECT HV2
3	51	0	0	1	1	0	0	1	1	Select HV3
Z	90	0	1	0	1	1	0	1	0	ADVANCE TO CALIB. POS.
M	77	0	1	0	0	1	1	0	1	X-RAYS OFF
O	79	0	1	0	0	1	1	1	1	X-RAYS ON

TRIGGER OUTPUT	PRINT @ 71,2:
TRIGGER INPUT	PRINT @ 61,2:

*Where A1 = FIRST ADDRESS

*Where A2 = LAST ADDRESS

TABLE 5: Status Word

BIT	DESCRIPTION	$2^n + 1$
32		
31		
30	SAMPLE LOCATED	5.36870912E8
29	CALIBRATE POSITION	
28	BETWEEN SAMPLES	1.34217728E8
27	FULL INSERTED	6.7108864E7
26	FULL WITHDRAWN	3.3554432E7
25	STACK LOADER FULL UP	16777216
24	STACK LOADER FULL DOWN	8388608
23	STACK LOADER LOCATED	4194304
22	ADC ON	2097152
21	HV BUSY	1048576
20	HV STANDBY	524288
19	X-RAY ON	262144
18	HV ON	131072
17		
16	HV AUTO	32768
15	HV 1	16384
14	HV 2	8192
13	HV 3	4096
12	HV TROUBLE	2048
11	HV DOOR OPEN	1024
10	COLLIMATOR POSITION	512
09	COLLIMATOR POSITION	256
08	COLLIMATOR LOCATED	128
07	AUTO/MANUAL	64
06		
05		
04		
03		
02		
01		

2. Control Subroutines

The purpose of the Control Subroutines is to set up the experimental conditions (HV, collimator, X-rays on/off, ADC on/off) for the spectrometer and to perform the necessary sample manipulation (Stack Loader up/down, Insert/Withdraw, Advance Sample). Table 6 is a list of the different subroutines, and the following will give a short description of each of them:

TABLE 6: CONTROL SUBROUTINES

SUBCON 1:	Stack loader up and down
SUBCON 2:	Select collimator
SUBCON 3:	X-rays on/off
SUBCON 4:	High voltage setting
SUBCON 5:	Initiate ADC (count)
SUBCON 6:	HV control to standby
SUBCON 7:	Insert/Withdraw
SUBCON 8:	Advance Sample

Description of SUBCON 1:

Purpose: This subroutine moves the Stack loader L steps down or U steps up

Input:

L	Number of steps down
U	Number of steps up

If L is greater than 0 then U = 0
If U is greater than 0 then L = 0

L = -1 if want full down
U = -1 if want full raise

Commands: Lower Stack
S2 = 76

Raise Stack
S2 = 85

Status Bits:

S24	Stack loader full down
S25	Stack loader full up
S23	Stack loader located

Subroutines:

1	SUBSER	1 + 2	Status/Command
2	SUBSER	12	Error
3	SUBSER	13	Time Delay

Errors: Error 1: Stack failure
Error 2: Stack position not found

Comment: Error 1 occurs when the Stack loader initially is not located. Check the hardware.

Error 2 occurs when the Stack loader is not located after a move. Check the hardware.

Description of SUBCON 2:

Purpose: This subroutine changes or rotates the collimator.

Input: X Collimator position
X = 1, 2, 3 or 4

Commands: Change collimator to next position
S2 = 88

Status Bits:
S8 Collimator located
S9 Collimator position (LSB)
S10 Collimator position (MSB)
S3 Collimator position value

for
X = 1 : S3 = 0
X = 2 : S3 = 512
X = 3 : S3 = 256
X = 4 : S3 = 768

Subroutines:

1	SUBSER 1 + 2	Status/Command
2	SUBSER 12	Error
3	SUBSER 13	Time Delay

Errors:
Error 3: Motors or timer is not in AUTO MODE
Error 4: Collimator not in position

Comment: Error 3 occurs when either the timer or motor control is not in the AUTO mode.

Error 4 occurs when the wanted collimator did not show up after a change command.

Description of SUBCON 3:

Purpose: This subroutine turns the X-rays on or off.

Input:
M = 1 X-rays off
O = 1 X-rays on

Commands:
X-rays off
S2 = 77

X-rays on
S2 = 87

Status Bits:

S21	HV busy
S19	X-ray on
S20	X-ray off

Subroutines:

1	SUBSER 1 + 2	Status/Command
2	SUBSER 12	Error message
3	SUBSER 13	Time delay

Errors:

Error 6: HV not on - cannot turn on X-rays
Error 7: Final status check of X-rays not OK

Comments:

Error 6 occurs when the high voltage has not been successfully turned on. Check X-ray controller.

Error 7 occurs when the wanted status of the X-rays is not OK. Check the X-ray controller.

Description of SUBCON 4:

Purpose:

This subroutine selects the HV voltage setting and initiates it.

Input:

V High voltage setting
V = 1, 2 or 3

Commands:

Initiate HV controller
S2 = 86
Select HV1
S2 = 49
Select HV2
S2 = 50
Select HV3
S2 = 51

Status Bits: S11 HV door open
S12 HV trouble
S13 HV 3
S14 HV 2
S15 HV 1
S16 HV auto
S18 HV on
S20 HV standby

Subroutines: SUBSER 1 + 2 Status/Command
SUBSER 12 Error message
SUBSER 13 Time delay

Errors: Error: 8 HV door open
Error: 9 HV trouble
Error: 10 HV not in AUTO mode
Error: 11 Final HV status not OK
Error: 11a Unexplained error in HV controller

Comments: The first four errors explain themselves. Error 11a indicates there is a major problem in the HV controller.

Description of SUBCON 5:

Purpose: This subroutine initiates the ADC for a certain time period and places the accumulated data in buffer 1 or 2.

Input: B Buffer number B = 1 or 2
T Time (sec.)

Commands: Select ADC buffer B
S2 = 64

Set Timer Interval
S2 = 84

Status Bits: S22 ADC on S22 = 1
ADC off S22 = 0

Subroutines: 1 SUBSER 1 + 2 Status/Command

Errors: Hardware error: No HV, fully inserted or not in AUTO

Commands: Error message occurs when high voltage is not on, the sample has gone in too far and activated the fully inserted microswitch, or the controller is not in the AUTO mode.

Description of SUBCON 6:

Purpose: This subroutine sets HV control to standby

Input: None

Commands: HV to standby
S2 = 89

Status Bits: S20 HV to standby S20 = 1

Errors: Error: unable to put HV to standby

Comments: Error indicates that the X-ray controller is either already in standby or there is a hardware problem and it cannot be put in standby.

Description of SUBCON 7:

Purpose: This subroutine inserts or withdraws a sample in the sample tray.

Input:
I = 1 Insert
P = 1 Withdraw
If I = 1 then P = 0
If P = 1 then I = 0

Commands:
Insert
S2 = 73

Withdraw
S2 = 80

Status Bits:
S27 Full inserted
S26 Full withdraw
S28 Between samples
S30 Sample located

Subroutines:

1	SUBSER 1 + 2	Status/Command
2	SUBSER 12	Error message
3	SUBSER 13	Time delay

Errors:
Error 12: Insert failure - may have no sample in tray
Error 13: Withdraw failure

Comments: Error 12 usually occurs when the routine tries to insert a sample and there is no sample in the tray. Check the location of the tray.

Error 13 occurs when the routine tries to withdraw a sample and there is no sample located. Check hardware.

Description of SUBCON 8:

Purpose: This subroutine advances a sample a certain number of steps.

Input: A Number of steps

Commands: Advance sample one step
S2 = 65

Subroutines:

1	SUBSER 1 + 2	Status/Command
2	SUBSER 12	Error message
3	SUBSER 13	Time delay

Errors: Error 14: Sample is fully inserted

3. Service Subroutines

The purpose of the Service Subroutines is to send status or command to the microprocessor, program interface and perform the necessary data manipulation (e.g. input/output, data storage, plot, etc.). Table 7 is a list of the different subroutines and the following will give a short description of each of them:

TABLE 7: Service Subroutines

SUBSER 1 + 2:	Status check and command
SUBSER 3	Program interface
SUBSER 4 + 5:	Read or write TI 9900 memory
SUBSER 6:	Read sample head on tape
SUBSER 7:	Read sample head from terminal
SUBSER 8:	Store data results temporarily in TI 9900 memory
SUBSER 9:	Store data results on tape
SUBSER 11:	Plot spectrum
SUBSER 14:	Data Analysis

Description of SUBSER 1 + 2:

Purpose: A to send and receive the status. 4051 ⇄ TI 9900 SPECTROMETER
B to send a command to the TI 9900

Input: S1 Mask
S2 Command
See the command codes and the status word.

Commands: See the command codes

Output: S3 return status

Description of SUBSER 3:

Purpose: This subroutine programs and initiates the interface.

Input: None

Commands: None

Output: None

Comments: See Input/Output manuals for the interface

Description of SUBSER 4 + 5:

Purpose: This subroutine reads/writes an array U0 from the TI 9900/4051 memory into the 4051/TI 9900 memory.

Input:
B Buffer number in TI 9900 memory
A1, A2 First and last address
S2 Command:
S2 = 82 Read U0 (A2 - A1 + 1) Output
S2 = 87 Write U0 (A2 - A1 + 1) Input

Output: If S2 = 82 then array U0 (A2 - A1 + 1)

Subroutines: SUBSER 1 + 2

Comments: If S2 = 87 then the U0 has to be dimensioned outside the subroutine. If S2 = 82 then U0 is dimensioned within the subroutine.

Description of SUBSER 6:

Purpose: This subroutine reads the sample header on a previously marked Data Tape (see II. 3).

Input: F1 File number for sample head file on Data Tape

Output: A$ Sample code
D1(9) Experimental parameters
P2(20) Element list

Comments: A$, P1(9) and P2(20) are defined and described in detail in Section II. 3.

Description of SUBSER 7:

Purpose: This subroutine reads the sample header information from the keyboard (SEMI-AUTO mode).

Input: A$ Sample code
P1(9) Experimental parameters

Output: None

Description of SUBSER 8:

Purpose: This subroutine stores concentration information temporarily in the TI 9900 memory buffer 9-12.

Input: E2 Number of time subroutine is called (e.g. steps)
Q0(19,5) Elemental data results array (19 elements)
P2(20) Element list code

Output: Q1(F5) Elemental concentration array
F5 is the number of elements analyzed

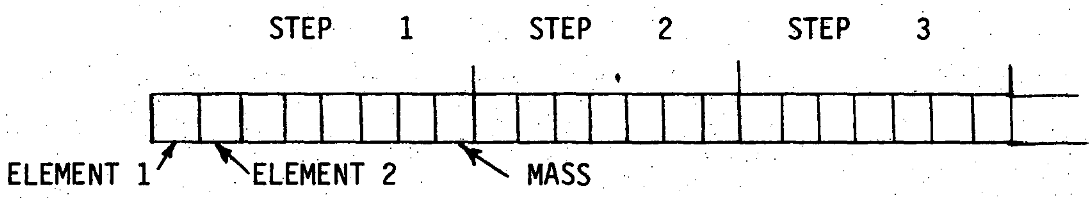
Subroutines: SUBSER 4 + 5 write TI 9900 memory

Comments: Q0(19,5) is defined in III. 6 and P2(20) in II. 3.

Comments: (continued)

The subroutine uses buffer 9 as a base buffer and depending on the number of elements analyzed and the number of steps some of the buffers 10 to 12 are used.

The data results are stored in TI 9900 memory as shown below.



Description of SUBSER 9:

Purpose: This subroutine rearranges the data results temporarily stored in the TI 9900 memory and stores the rearranged results on a previously marked Data Tape (see II. 3) and prints the output on the external printer if it is connected.

Input:
P1(9) Experimental parameters (see II. 3)
P2(20) Element list code (see II. 3)

Output: None

Subroutines: SUBSER 4 + 5 Read TI 9900 memory

Comments: The way the final results are stored on the Data Tape is explained in II. 3.

Description of SUBSER 11:

Purpose: This subroutine plots a spectrum.

Input:
U0 (A2 - A1 + 1) Data array
A1, A2 First and last channel

Output: Plot on screen

Comments: The plot subroutine is a modified version of the Tektronix plot subroutine.

Description of SUBSER 14:

Purpose: This subroutine performs the data analysis. The analysis is based on a stored background spectrum and shape standard spectra (see II. 5).

Input:
1 19 shape standards stored in buffer 5-8.
2 1 background sectrum stored in buffer 4.
3 A calibration table stored in buffer 3.
4 An unknown spectrum stored in either buffer 1 or 2.
5 T Time in seconds.
6 Q2(2) Calibration option.
  (1) Buffer number for unknown spectrum (1 or 2).
  (2) Sensitivity factor used (1 to 4).

Data Arrays:
U0(A2 - A1 + 1) General data array
Z1 (A2 - A1 + 1) Data array unknown spectrum
I0(32) } Calibration information (see III. 2)
I1(32) }

Subroutines: SUBSER 4 + 5 Read/Write

Output:
Q0(19,5) Data analysis results
  (i,1) Area of peak
  (i,2) Delta area
  (i,3) Background in fit region
  (i,4) Concentration
  (i,5) Delta concentration

MS 1. Error message: shift exceeds more than one channel
2. Warning counting rate greater than 10K
3. Anal error: zero counts in spectrum

Comments: First error message indicates the amplifier gain has drifted. The second message indicates that the sample is too concentrated to give good results under this HV-current setting. Message 3 usually indicates the x-ray tube has tripped off.

4. The Running Program

Purpose: This program is designed to perform a complete analysis of one or more samples automatically after some preliminary information has been given.

Input:

A$	Sample code (see II. 3)
P1(9)	Experimental parameters given as tape or screen input (see II. 3 and II. 1)
Q2(2)	Calibration option (see II. 2)
F1	File for first sample head on the Data Tape (see II. 3)
F2	Number of samples to analyze in one run
F3	Tape (F3 = 1) or screen (F3 = 2) input

Output: Q0(19, 5) Data Analysis results (see III. 3)

Subroutines: All control and service subroutines

Parameters:

D1	Horizontal position
D2	Vertical position
F4	Stack Position
E1	Sample Loop Counter
E2	Step Loop Counter

Command Codes (see II. 3)

Comments: A central part in the program is the Data Analysis Subroutine

5. The Setup Program

Purpose: This program sets up the spectrometer for quantitative analysis; creates a calibration table, measures background spectrum and shapes standard spectra; performs energy calibration and transfers the stored information from the TI 9900 memory to a tape and vice versa.

Input:

Parameter	Description
M	Menu item
IO(32)	Calibration information
B$	Chemical symbol
C$(1)	Yes/No answer
I$(16)	Part of element list
A1, A2	Limits (channels)
T	Counting time
I9	First calibration on tape
E1, E2	Energies
A3, A4	Limits (channels)

Output:

Spectrum	Background, shape calibration
IO	Calibration information
B$	Chemical symbol
A1, A2	Limits (channels)
Q(4,2)	Limits
Integral	
Centroid	

Subroutines: SUBSER 1 + 2, 3, 4 + 5, 11, 13
SUBCON 3, 4, 5, 8

Parameters:	General	
	I1(32)	
	U0, U1	Arrays (general)
	E$	Element list
	L	Number of elements
	B1	Element position in element list
	P1(5)	Array. Element positions in element list
	S1	Status
	S2	Command

Comments: The program is described in great detail in Sec. II.

Because of the size of the program and especially the size of some of the arrays it is in some cases necessary to delete parts of the program and then reload it. This is done automatically when the program is stored on a Calibration Tape file 2 (Binary version).

6. The Data Tape Marking Program

Purpose: This program is used to set up the experimental conditions when the user wants to run a lot of samples automatically. The Data Tape is used to store the information.

Input:
Q$(1): New or add to old tape answer (N or A)
K: Number of parameter to change
E: Number of elements analyzed
N: Number of samples

P$(6) Bit 1-6: Date (dddddd)
P(9) Experimental conditions where:
  P(1) Bit 7-10: KV + Current setting (1,2,3)
  P(2) Bit 11-14: Collimator setting (1,2,3,4)
  P(3) Bit 15-18: MM to advance/step (1,2,...10 mm)
  P(4) Bit 19-22: Total number of steps (1 to 200)

P(5)	Bit 23-26:	MM to advance before analysis
P(6)	Bit 27-30:	
P(7)	Bit 31-34:	Counting time (=P(6) * P(7))
P(8)	Bit 35-38:	Sample head file
P(9)	Bit 39-42:	Horizontal/vertical position
P1(20)	Bit 44-63:	Element list code. One bit per element. (Bit = 0 if ot analyzed; bit = 1 if analyzed)
Z$(8)	Bit 65-72:	Additional remarks or sample I.D.

Output:

Y	Number of bytes still available
S	Number of samples on tape
T	Last file used
E$	List of element symbols
D$	Date
P(9)	Experimental conditions
P1(20)	
Z$	Sample I.D.

Error message: parameter outside preset range

Parameters: A$(72) Sample code

Comments: The program is described in great detail in Sec. II. 3.

7. The Data Presentation Program

Purpose: This program presents data stored on the Data Tape during the analysis of one or more hair samples.

Input:

Menu Item	Input Parameters	
1	None	
2	T	File number for sample heading
3,4,5,6	S1	Number of samples to plot or print
	F1(S1)	Array for sample head files
	Y1(S1)	Array for starting addresses (steps)
	Y2(S1)	Array for ending addresses (steps)
	I$(10)	Contains the chemical symbols (2 characters) for a given list of elements (max 5)

Output:	M = 1:	Y	Number of bytes available
		S	Number of samples on tape
		T	Last used file on tape
		E$	List of element symbols
		A$	Sample Code (see III. 6)
	M = 2:	D$	Date (dddddd)
		P(9)	Array for experimental parameters
		Z$(20)	Element list code (equivalent to P1(20) in Sec. III. 6)
		S$(10)	Additonal remarks or sample I.D.
	M = 3,4:	A$	Sample code
		Plot	Concentration or mass versus hair length
	M = 5,6:	A$	Sample code
		Print	Concentration or mass versus hair length for a given list of elements

Parameters:	General	
	P1(5)	Array. Positions in element list
	P2(20)	Array. Element list code
	C1(P4)	Array. Contains concentration. Delta concentration versus length as stored on the Data Tape
	C2(Y2-Y1+1,L)	Array. Contains concentration versus length for L elements
	L	Number of elements to be plotted or printed

Comments: See II. 3 and II. 4

The plot routine is a modified version of the Textronix routine.

APPENDIX I

FORMULA USED

Symbols Used:

F	$\sum$ fit region
P	$\sum$ primary region
N_R	channel counts in raw spectrum
N_B	channel counts in background spectrum
N_S	channel counts in shape standard spectrum
Δ	uncertainty
N	normalizing factor
S	sensitivity factor
COR_i	correction to the concentration of element i
α_{ij}	interelement coefficient
CONC	concentration
EI_i	interelement error
E	total error on $CONC_i$
N_P	$= N_R - N_B$
i	i'th element

FORMULA:

Area/Concentration

$$*\mathrm{AREA} = \frac{N_P{}^F}{N_S{}^F} \times N_S{}^P$$

$$*\Delta\mathrm{AREA} = \left(\left(\frac{\Delta N_P{}^F}{N_P{}^F}\right)^2 + \left(\frac{\Delta N_S{}^F}{N_S{}^F}\right)^2 + \left(\frac{\Delta N_S{}^P}{N_S{}^P}\right)^2\right)^{1/2} \times \mathrm{AREA}$$

$$\left(\frac{\Delta N_P{}^F}{N_P{}^F}\right)^2 = \frac{2 * N_B{}^F + N_P{}^F}{\left(N_P{}^F\right)^2}$$

$$\left(\frac{\Delta N_S{}^F}{N_S{}^F}\right)^2 = \frac{1}{N_S{}^F}$$

$$\left(\frac{\Delta N_S{}^P}{N_S{}^P}\right)^2 = \frac{1}{N_S{}^P}$$

If $N_p < 0$ THEN AREA $\leq 3\sqrt{N_S{}^F}$

If $\left(\frac{\Delta N_p{}^F}{N_p{}^F}\right)^2 \geq 1$ then $\Delta\mathrm{AREA} \leq 3\sqrt{N_S{}^F}$

$$*\mathrm{CONC}_i = \frac{N \times \mathrm{AREA}_i}{S_i}$$

$$\Delta\mathrm{CONC}_i = \frac{N \times \Delta\mathrm{AREA}_i}{S_i}$$

APPENDIX II

CONTROL ERROR MESSAGES:

ERROR	1:	Stack failure	SUBCON 1
	2:	Stack position not found	SUBCON 1
	3:	Motors or timer is not in AUTO MODE	SUBCON 2
	4:	Collimator not in position	SUBCON 2
	5:	Hardware error - no HV, fully inserted or not in AUTO MODE	SUBCON 5
	6:	HV not on - cannot turn on x-rays	SUBCON 3
	7:	Final status check of X-ray not OK	SUBCON 3
	8:	HV door open	SUBCON 4
	9:	HV trouble error	SUBCON 4
	10:	HV not in AUTO mode	SUBCON 4
	11:	Final HV status not OK	SUBCON 4
	11a:	Unexplained error in HV controller	SUBCON 4
	12:	Insert failure - may have no sample in tray	SUBCON 7
	13:	Withdraw failure	SUBCON 7
	14:	Sample is fully inserted	SUBCON 8
	15:	Unable to put HV to standby	SUBCON 6
	16:	Warning - Counting rate greater than 10K	SUBCON 14
	17:	Anal error - zero counts in spectrum	SUBCON 14
	18:	Shift exceeds one channel	SUBCON 14
	19:	Unable to shift spectrum correctly	SUBCON 14

REFERENCES

1. Tektronix 4051 Manuals.
2. Texas Instruments 9900 Software Documentation.
3. Tektronix General Purpose Input/Output Manuals for 4051.

FIGURES

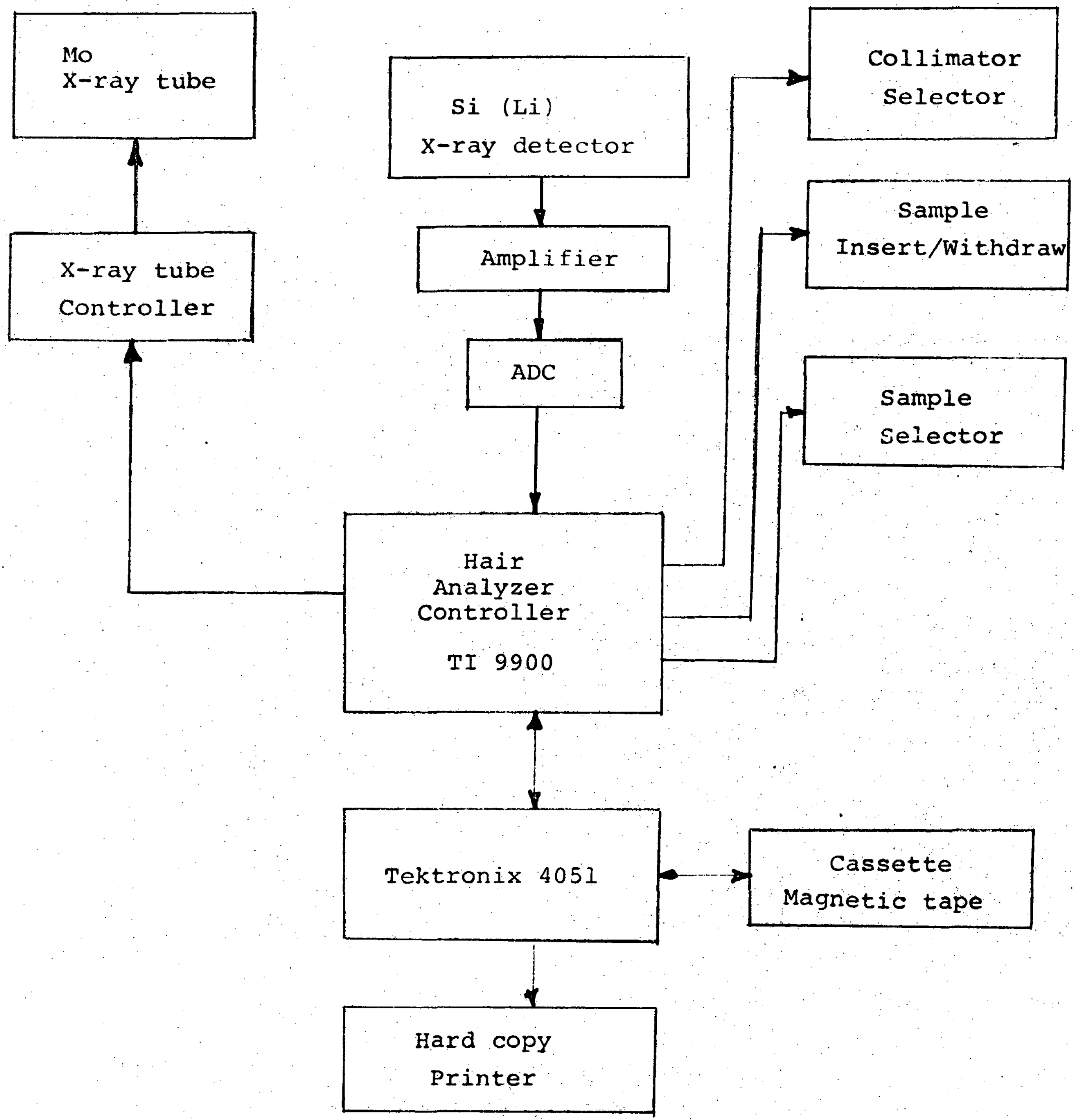
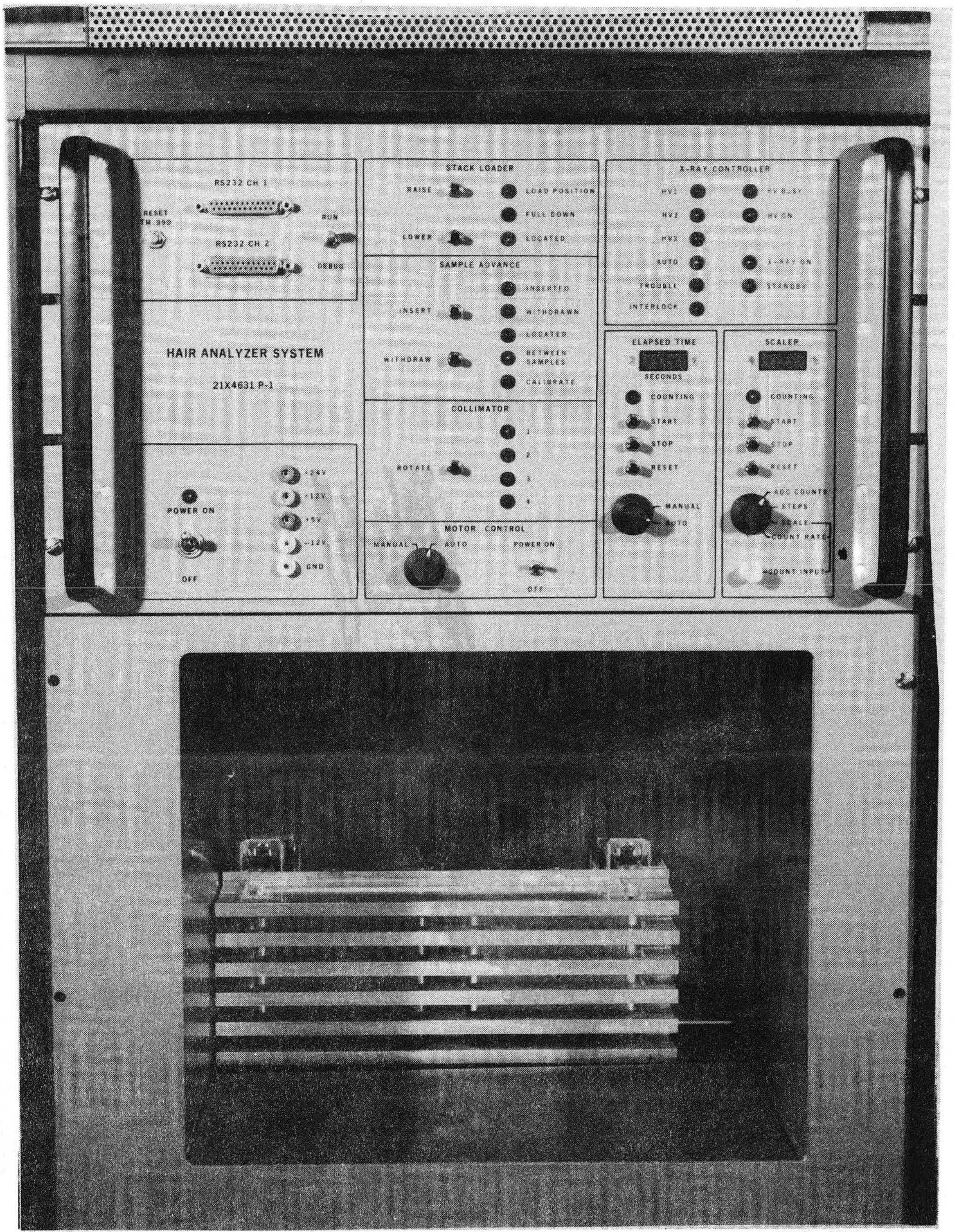

Mo
X-ray tube
Si (Li)
X-ray detector
Collimator
Selector
X-ray tube
Controller
Amplifier
Sample
Insert/Withdraw
ADC
Sample
Selector
Hair
Analyzer
Controller
TI 9900
Tektronix 4051
Cassette
Magnetic tape
Hard copy
Printer

Figure 1



CBB 793-3550

Figure 2

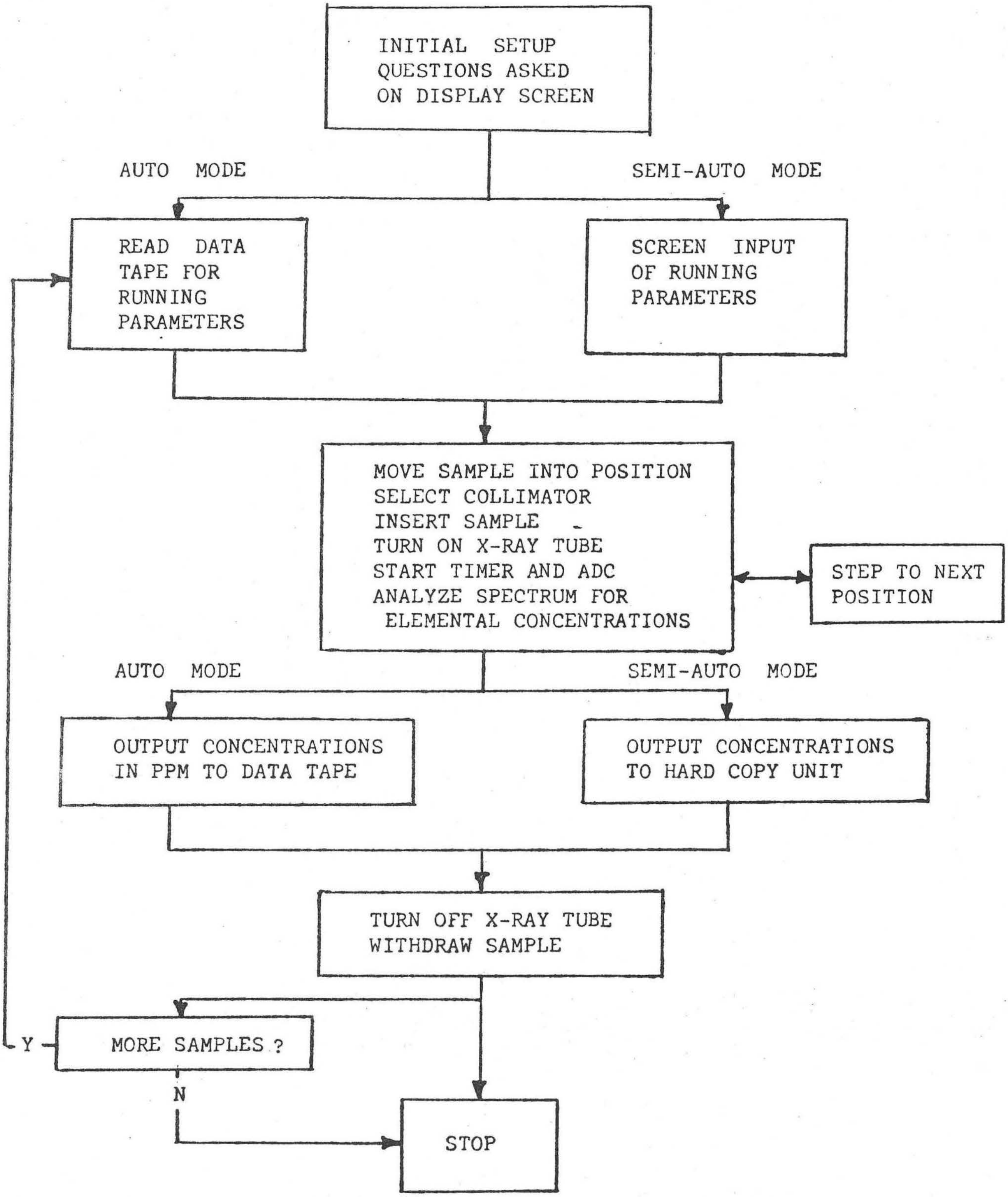
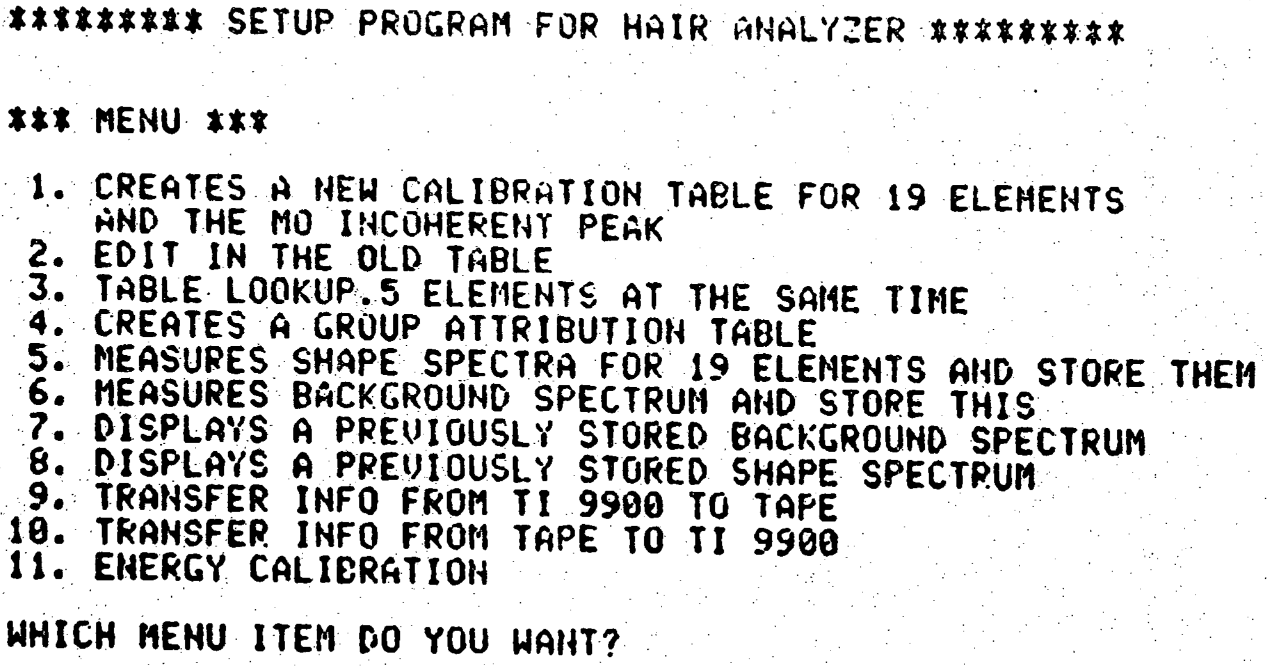

INITIAL SETUP
QUESTIONS ASKED
ON DISPLAY SCREEN
AUTO MODE
SEMI-AUTO MODE
READ DATA
TAPE FOR
RUNNING
PARAMETERS
SCREEN INPUT
OF RUNNING
PARAMETERS
MOVE SAMPLE INTO POSITION
SELECT COLLIMATOR
INSERT SAMPLE
TURN ON X-RAY TUBE
START TIMER AND ADC
ANALYZE SPECTRUM FOR
ELEMENTAL CONCENTRATIONS
STEP TO NEXT
POSITION
AUTO MODE
SEMI-AUTO MODE
OUTPUT CONCENTRATIONS
IN PPM TO DATA TAPE
OUTPUT CONCENTRATIONS
TO HARD COPY UNIT
TURN OFF X-RAY TUBE
WITHDRAW SAMPLE
Y
MORE SAMPLES ?
N
STOP

Figure 3

```
 SHOULD BE DOING DATA ANALYSIS ON POS 60
080779    3    2    2  60    5 100    6  63   86 11111111111111111111 A.OTTER
SPEC SHIFT=-0.096376327223
SPEC SHIFT=4.019417502E-4
MASS=                 6.63438999214
ZN CONC=     1008.44 PG/MM   +-     20.6
FE CONC=      273.46 PG/MM   +-     18.7
CU CONC=       88.13 PG/MM   +-     10.1
MN CONC=       66.32 PG/MM   +-     19.4
K  CONC=     3807.42 PG/MM   +-    248.9
CA CONC=     2730.96 PG/MM   +-    133.5
HG CONC=      385.18 PG/MM   +-     32.4
PB CONC=        0.00 PG/MM   +-    123.9
BR CONC=       48.76 PG/MM   +-     17.5
RB CONC=        0.00 PG/MM   +-     38.9
AS CONC=        0.35 PG/MM   +-     30.6
SR CONC=        0.00 PG/MM   +-     40.5
SE CONC=        0.00 PG/MM   +-     33.1
NI CONC=        0.00 PG/MM   +-     19.0
TI CONC=        0.00 PG/MM   +-     83.5
V  CONC=        0.00 PG/MM   +-     62.3
CR CONC=        0.00 PG/MM   +-     46.8
```

Figure 4

```
 090779    3    2    2   11   17 100    6   14    2 1111111111111111111 WT-H-1
K  CONC=
   827.034   900.036  1044.039   806.037   859.038   966.039  1062.042   981.041
  1113.042   903.037   888.032
CA CONC=
   286.016   323.017   345.018   313.017   339.018   353.018   417.020   377.019
   374.019   332.017   340.015
TI CONC=
     2.010    10.011     2.011     8.011    13.006    18.006    12.007     1.012
    21.007    16.006     8.009
V  CONC=
     0.008     2.008     0.008     0.008     2.009     3.009     5.009     0.009
     6.009     3.008     2.007
CR CONC=
     1.006     2.006     0.006     1.006     2.006     3.007     4.007     0.007
     9.004     0.006     1.005
MN CONC=
     0.004     2.004     0.005     0.005     0.005     0.005     0.005     0.005
     0.005     0.005     0.004
FE CONC=
    94.003    46.003    47.003    50.003    44.003    46.003    42.003    45.003
    44.003    51.003    67.003
CO CONC=
     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000
     0.000     0.000     0.000
NI CONC=
     9.001    15.001    16.002    15.002    20.002    17.002    12.002    20.002
    17.002    28.002    24.001
CU CONC=
    15.001    25.002    21.002    23.002    43.002    25.002    26.002    28.002
    23.002    26.002    33.001
ZN CONC=
    47.002    57.002    60.002    53.002    72.002    62.002    62.002    72.002
    71.002    68.002    67.002
GA CONC=
     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000
     0.000     0.000     0.000
AS CONC=
     0.004     3.004    10.002     0.004     0.004     0.004     6.002     0.004
     5.002     6.002     2.003
SE CONC=
     2.004     0.004     0.004     2.004     3.005     4.005     0.005     0.005
     1.005     1.004     0.004
BR CONC=
     7.002     6.002     7.002     8.002    14.002    12.002     4.005    10.003
     4.005     9.002     3.004
RB CONC=
     2.005     0.005     0.005     3.005     7.003     3.005     0.006     0.006
     2.006     0.005     0.004
SR CONC=
     0.005     0.005     0.005     0.005     1.006     4.006     0.006     0.006
     0.006     3.005     0.005
HG CONC=
     2.008     0.008     0.008     5.008     4.006     8.004     0.009     0.009
     0.009     0.008     0.007
PB CONC=
   133.009   112.009   125.009   150.010   161.010   158.010   134.010   162.010
   129.010   132.009   104.008
MS CONC=
     8.740     8.172     7.753     7.753     7.563     7.350     6.818     6.912
     6.940     7.981    10.005
```



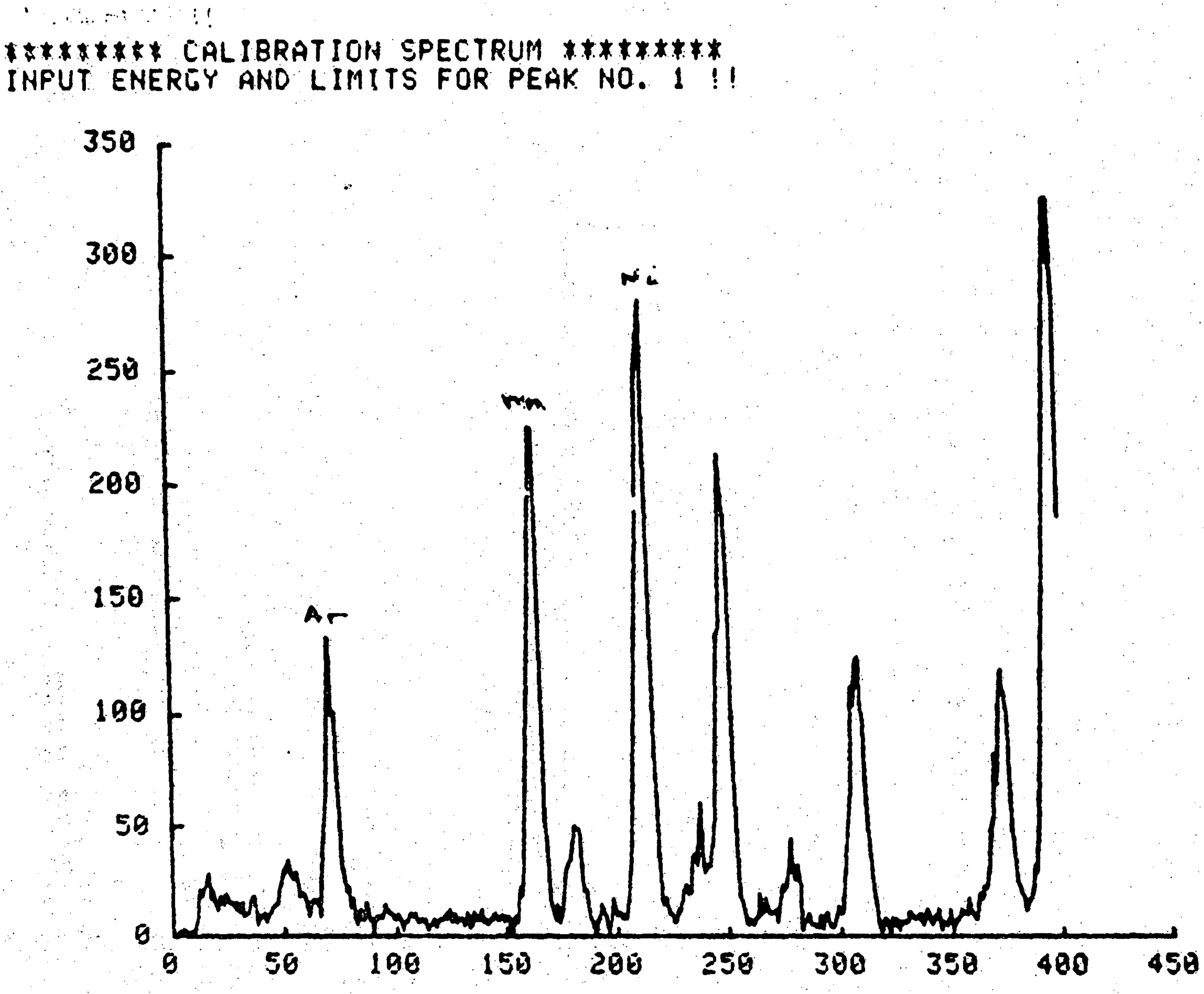
```
********* SETUP PROGRAM FOR HAIR ANALYZER *********

*** MENU ***

 1. CREATES A NEW CALIBRATION TABLE FOR 19 ELEMENTS
    AND THE MO INCOHERENT PEAK
 2. EDIT IN THE OLD TABLE
 3. TABLE LOOKUP.5 ELEMENTS AT THE SAME TIME
 4. CREATES A GROUP ATTRIBUTION TABLE
 5. MEASURES SHAPE SPECTRA FOR 19 ELEMENTS AND STORE THEM
 6. MEASURES BACKGROUND SPECTRUM AND STORE THIS
 7. DISPLAYS A PREVIOUSLY STORED BACKGROUND SPECTRUM
 8. DISPLAYS A PREVIOUSLY STORED SHAPE SPECTRUM
 9. TRANSFER INFO FROM TI 9900 TO TAPE
10. TRANSFER INFO FROM TAPE TO TI 9900
11. ENERGY CALIBRATION

WHICH MENU ITEM DO YOU WANT?
```

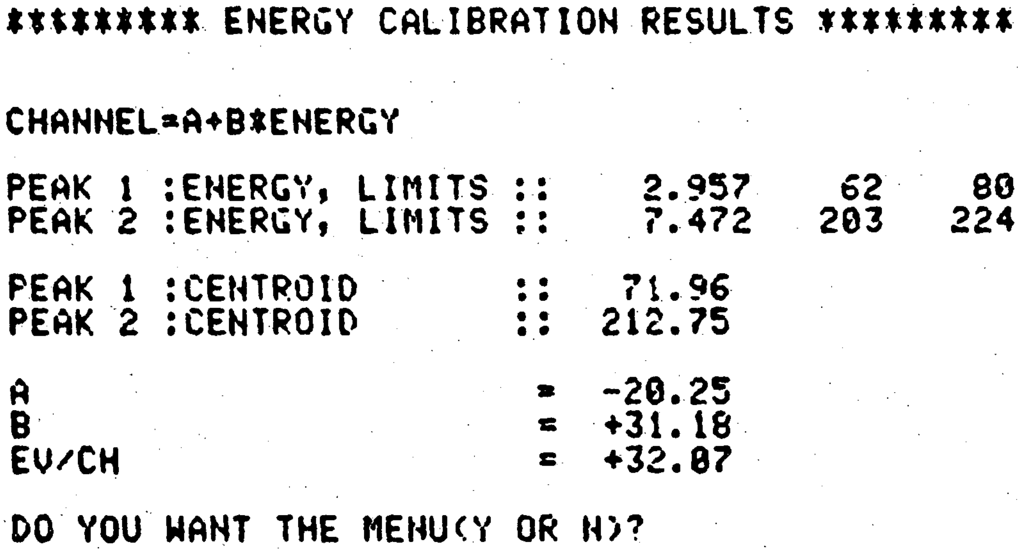
Figure 6



```
********* CALIBRATION SPECTRUM *********
INPUT ENERGY AND LIMITS FOR PEAK NO. 1 !!
```

Figure 7

MENU 11



```
********* ENERGY CALIBRATION RESULTS *********

CHANNEL=A+B*ENERGY

PEAK 1 :ENERGY, LIMITS ::    2.957    62    80
PEAK 2 :ENERGY, LIMITS ::    7.472   203   224

PEAK 1 :CENTROID       ::   71.96
PEAK 2 :CENTROID       ::  212.75

A                       =  -20.25
B                       =  +31.18
EV/CH                   =  +32.07

DO YOU WANT THE MENU(Y OR N)?
```

Figure 8

MENU 6

```
********* BACKGROUND SPECTRUM *********
LIMITS FOR THE MO SCATTERED PEAKS?
```

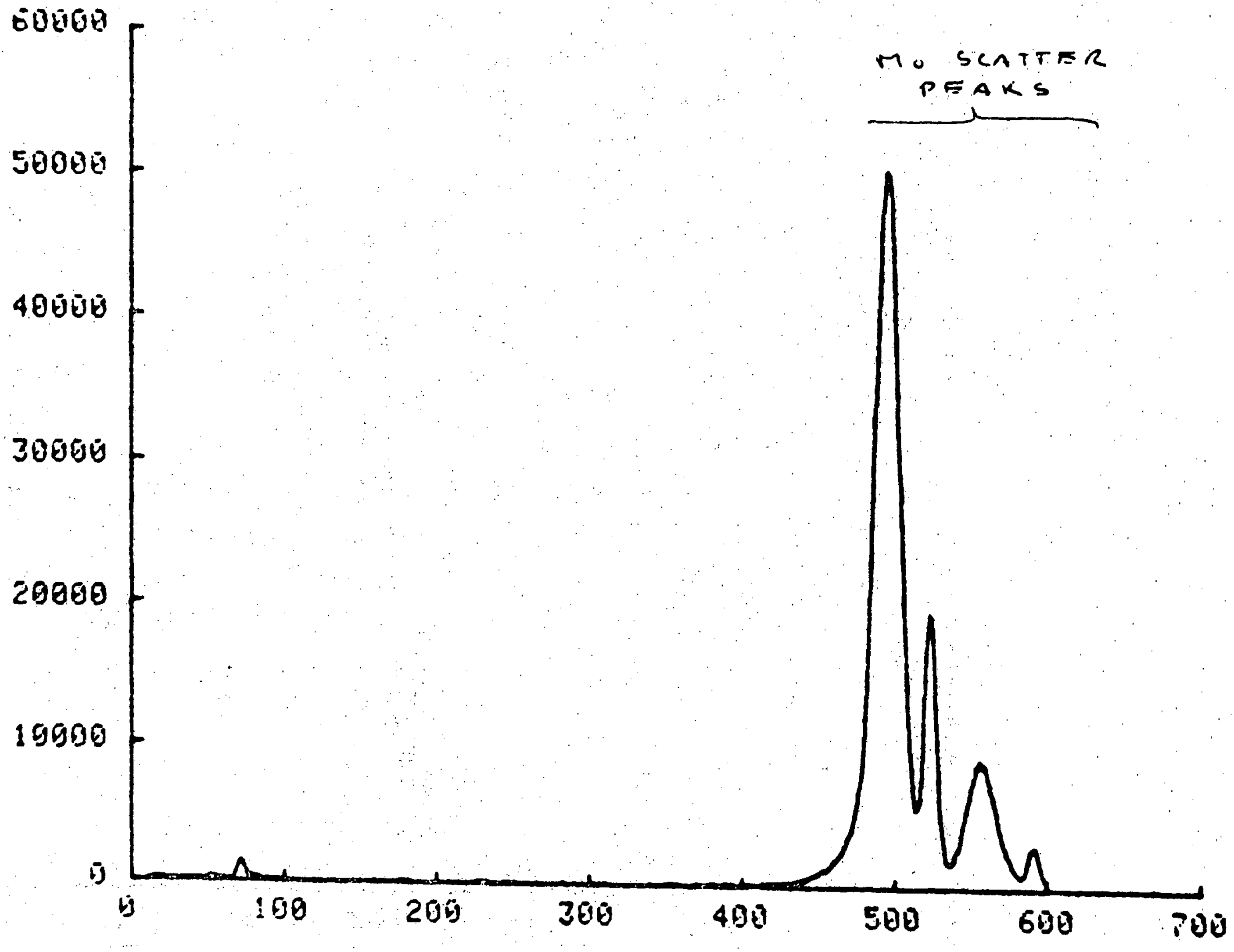


Figure 9

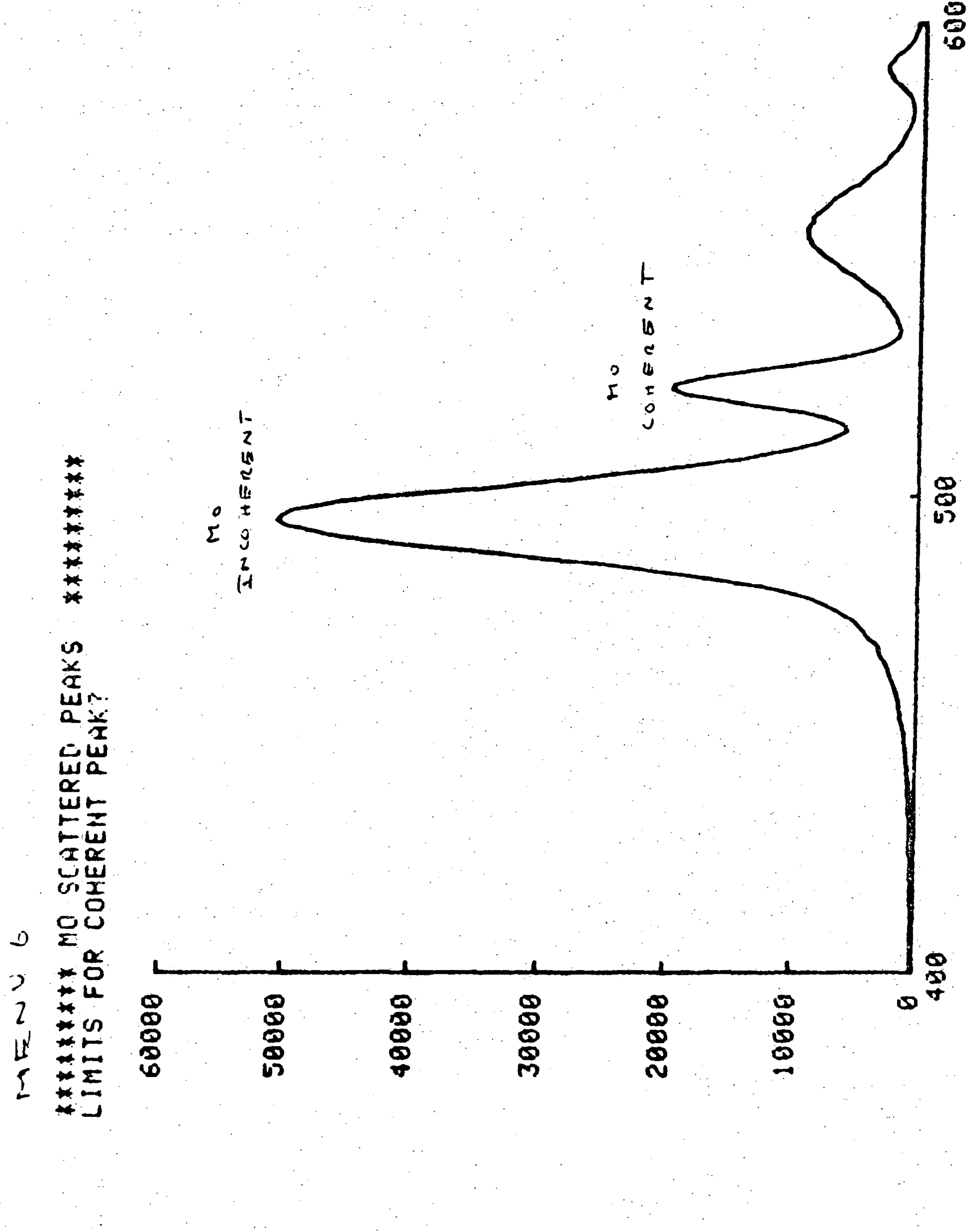

MENU 6
******** MO SCATTERED PEAKS *********
LIMITS FOR COHERENT PEAK?
60000
50000
40000
30000
20000
10000
0
400
500
600
Mo INCOHERENT
Mo COHERENT

Figure 10

```
MENV 6

MO COHERENT PEAK :LIMITS,CENTROID,INTEGRAL::: 512  532 522.16  227220
ARE THE LIMITS OK(Y OR N)?
```

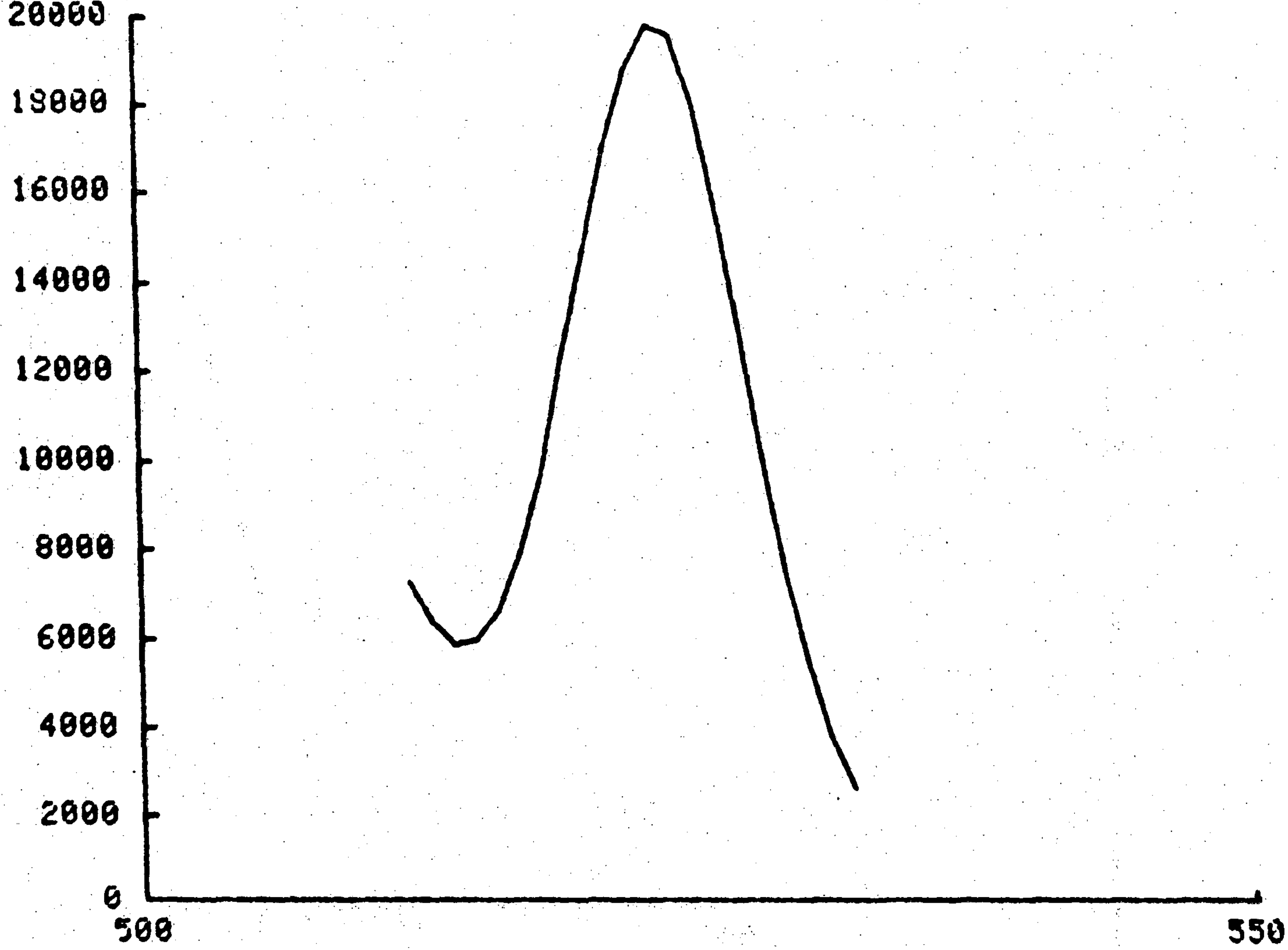
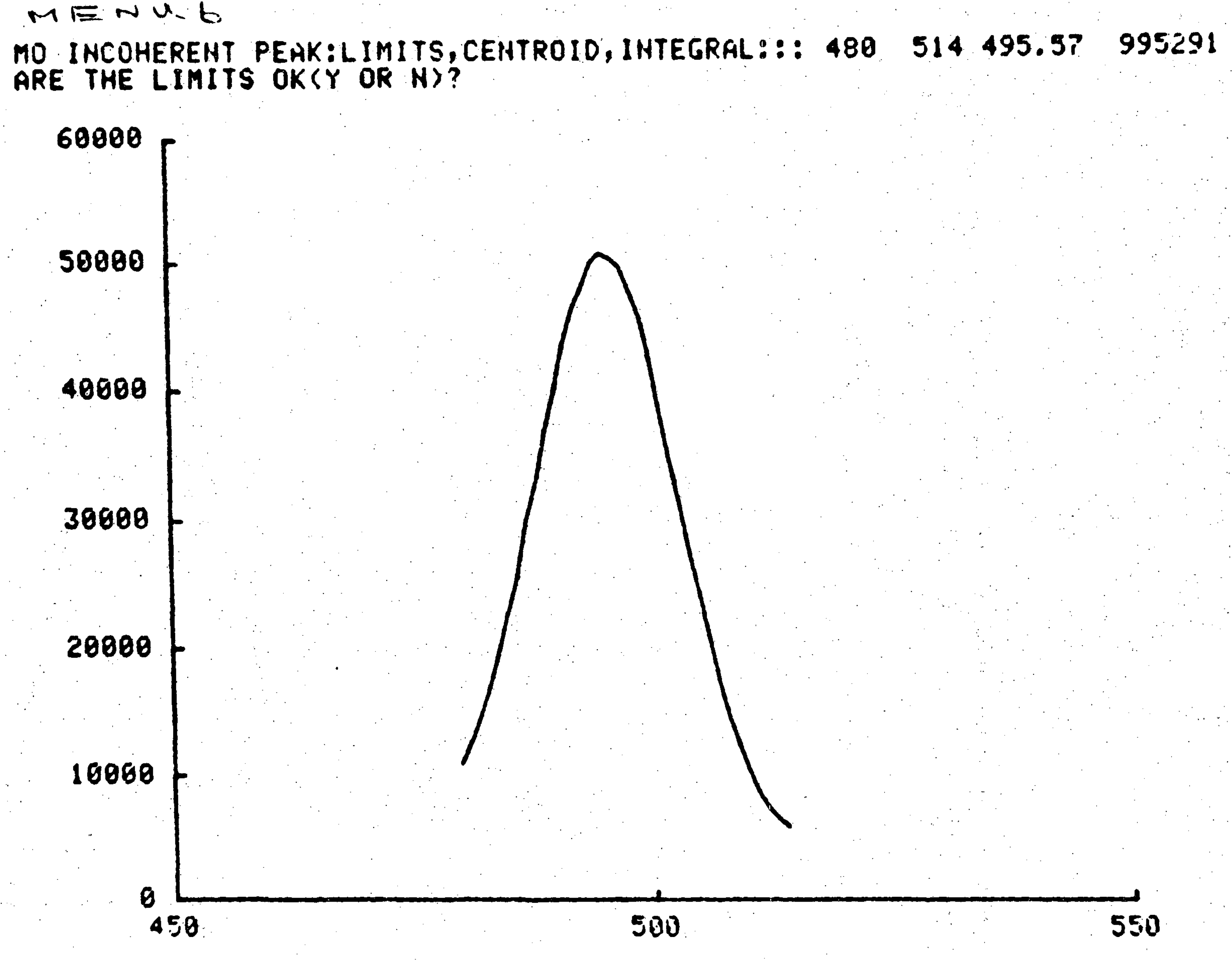


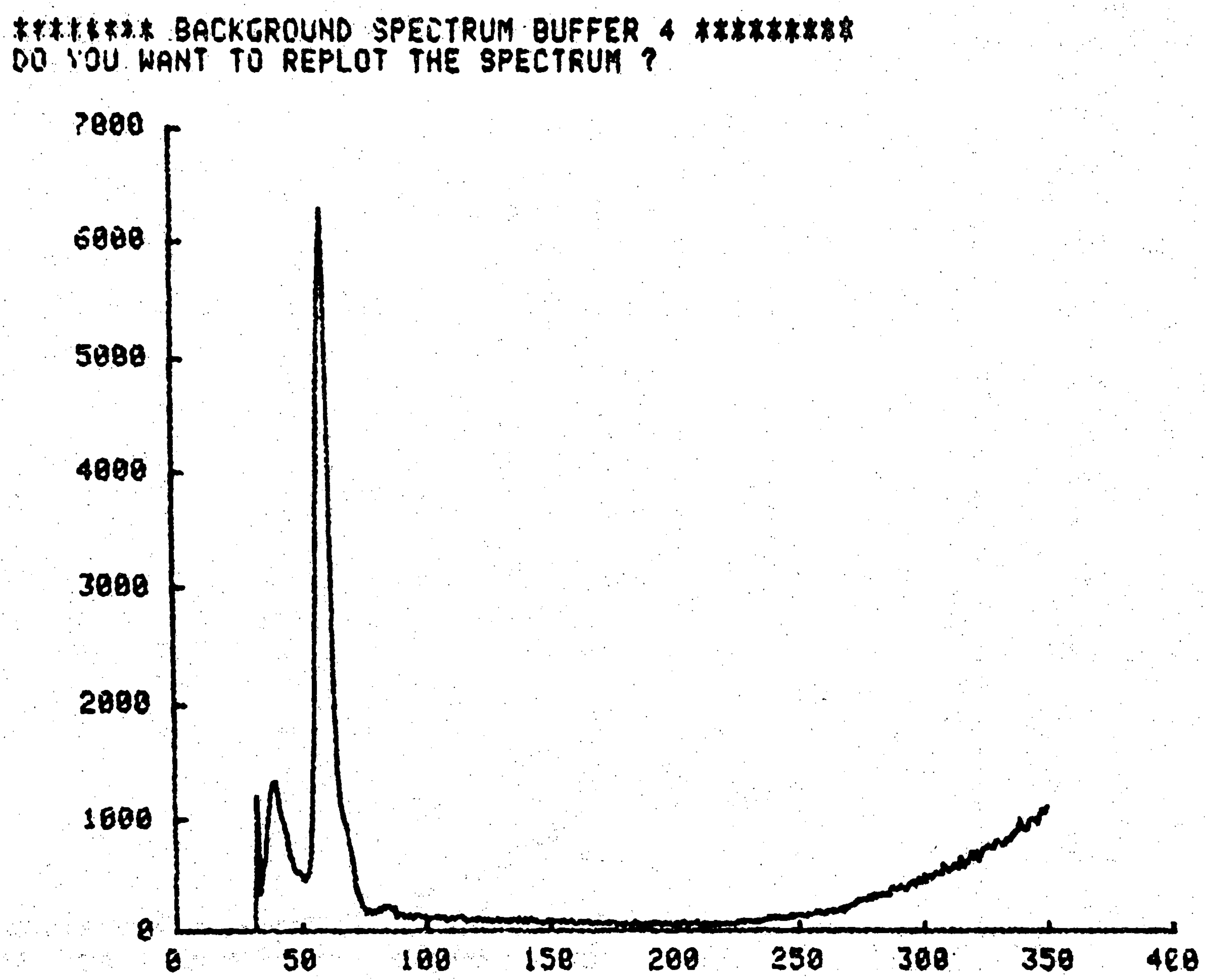
Figure 11

Figure 12



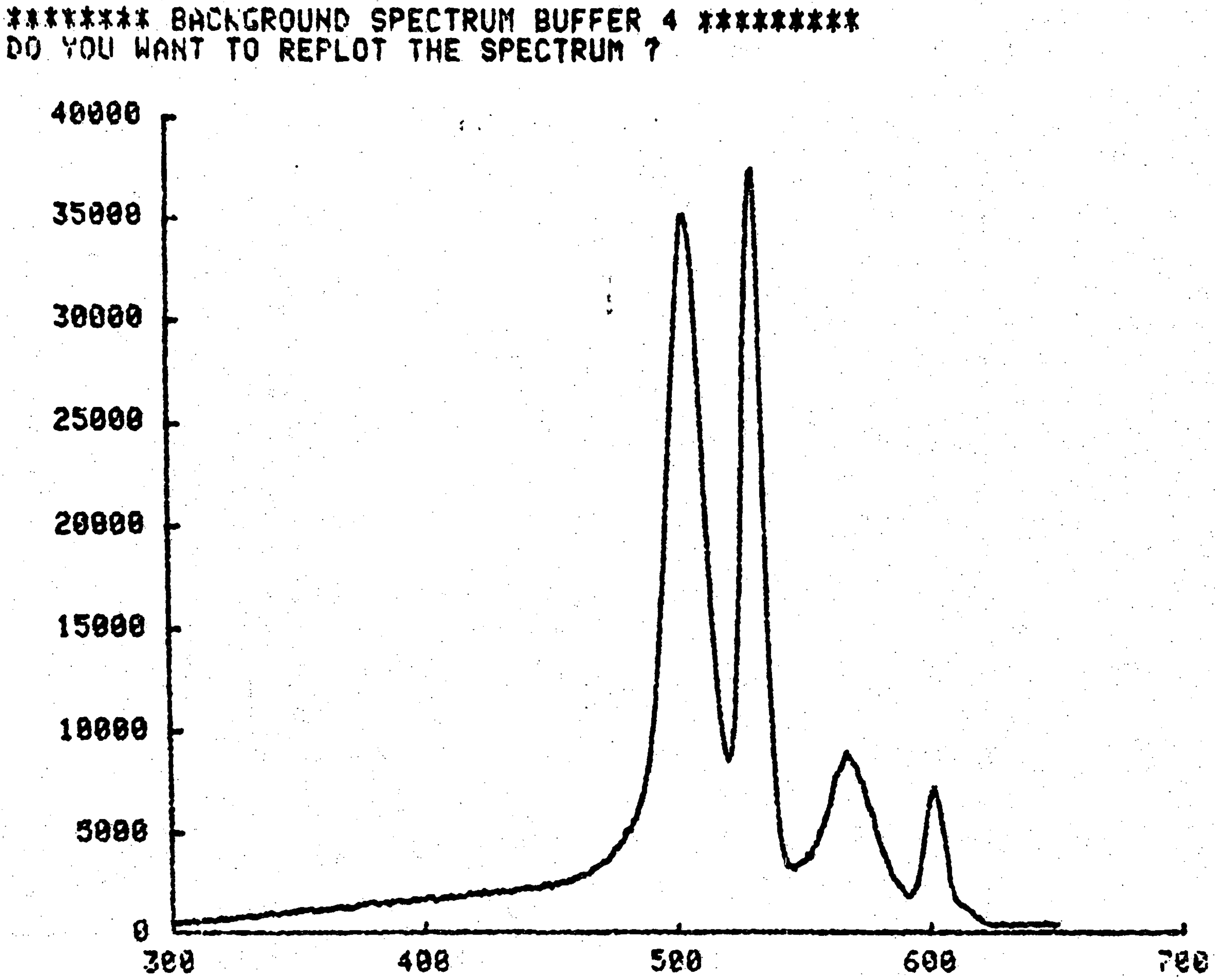
MENU 6

```
MO INCOHERENT PEAK:LIMITS,CENTROID,INTEGRAL::: 480  514 495.57  995291
ARE THE LIMITS OK(Y OR N)?
```



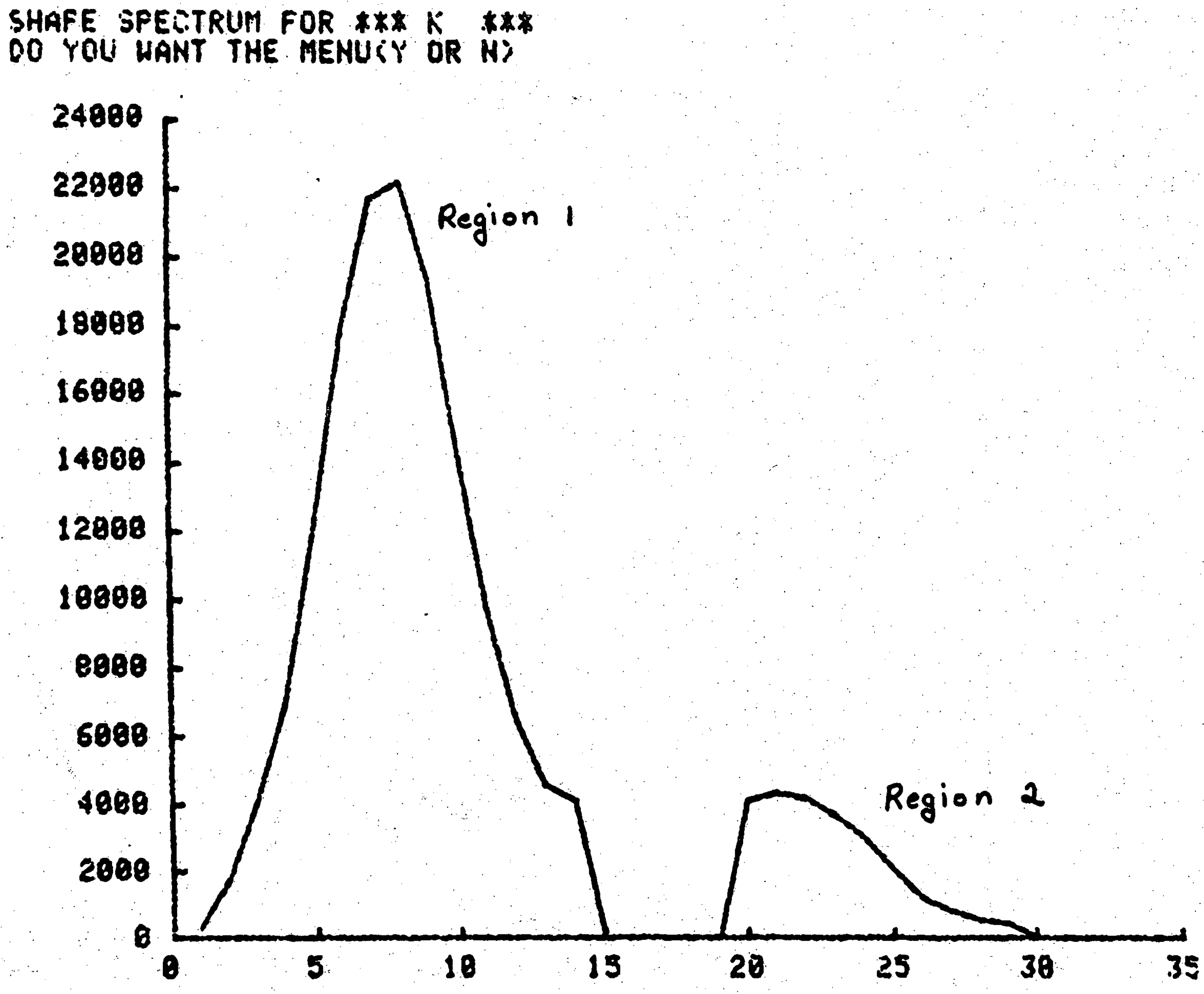
```
******** BACKGROUND SPECTRUM BUFFER 4 *********
DO YOU WANT TO REPLOT THE SPECTRUM ?
```

Figure 13 a



```
******** BACKGROUND SPECTRUM BUFFER 4 *********
DO YOU WANT TO REPLOT THE SPECTRUM ?
```

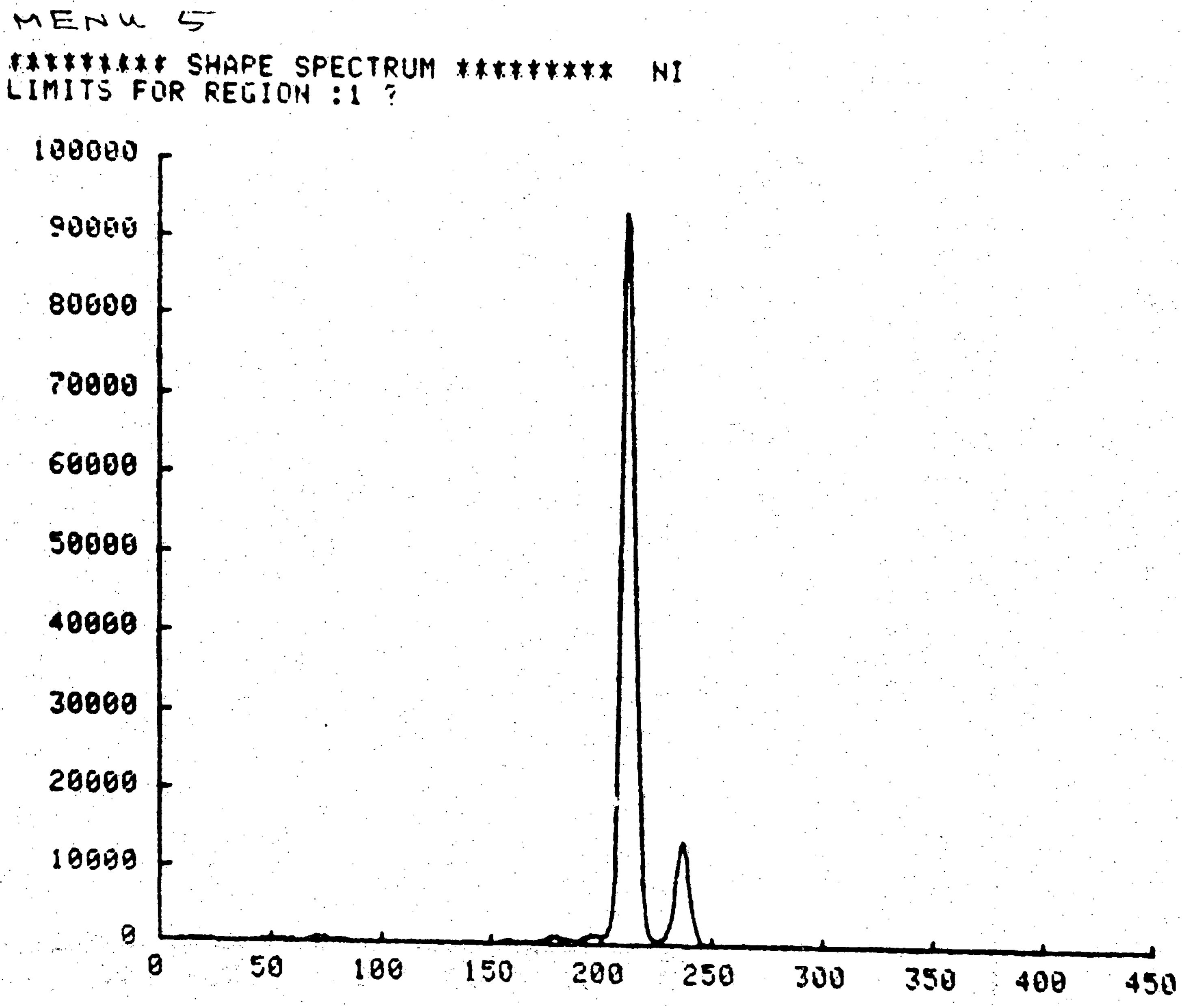
Figure 13 b



```
SHAPE SPECTRUM FOR *** K  ***
DO YOU WANT THE MENU(Y OR N)
```

Figure 14

Figure 15



MENU 5

```
********* SHAPE SPECTRUM *********  NI
LIMITS FOR REGION :1 ?
```

```
SHAPE STANDARD RESULTS FOR :HG

CENTROID                       :   288.57
LIMITS, INTEGRAL REGION 1 ::   278      299      1380.168
LIMITS REGION 2                :   300      434
LIMITS REGION 3                :   240      277
LIMITS, INTEGRAL REGION 4 ::   283      294      1257.992
FIRST ADDRESS                  :   722
LAST ADDRESS                   :   916
TIME (PAR 17)= 600
```

Figure 16

MENU 4

```
*** GROUP TABLE ***

GROUP 1 CONTAINS :

NUMBER OF ELEMENTS        :4
ELEMENT NUMBER            :3   CENTROID :124
ELEMENT NUMBER            :7   CENTROID :180
ELEMENT NUMBER            :9   CENTROID :202
ELEMENT NUMBER            :11   CENTROID :244

GROUP 2 CONTAINS :

NUMBER OF ELEMENTS        :0
ELEMENT NUMBER            :1   CENTROID :0

GROUP 3 CONTAINS :

NUMBER OF ELEMENTS        :0
ELEMENT NUMBER            :1   CENTROID :0

GROUP 4 CONTAINS :

NUMBER OF ELEMENTS        :0
ELEMENT NUMBER            :1   CENTROID :0

DO YOU WANT THE MENU(Y OR N)
```

Figure 17

CALIBRATION TAPE

```
1       ASCII   PROGRAM          768   — LOAD PROGRAM
2       BINARY  PROGRAM        30208  — SET UP PROGRAM
3       BINARY  DATA           10240  —
4       BINARY  DATA           10240
5       BINARY  DATA           10240
6       BINARY  DATA           10240      CALIBRATION 1
7       BINARY  DATA           10240
8       BINARY  DATA           10240  —
9       NEW                    10240
10      NEW                    10240
11      NEW                    10240
12      NEW                    10240      CALIBRATION 2
13      NEW                    10240
14      NEW                    10240  —
15      NEW                    10240
16      NEW                    10240
17      NEW                    10240
18      NEW                    10240      CALIBRATION 3
19      NEW                    10240
20      NEW                    10240  —
21      NEW                    10240
22      NEW                    10240
23      NEW                    10240
24      NEW                    10240
25      NEW                    10240      CALIBRATION 4
26      NEW                    10240  —
27      LAST                     768  —
```

Figure 18

```
  TAPE MARKING PROGRAM - PLEASE INSERT DATA TAPE

  ENTER DATE(DDDDDD) :
* 080879
  WHAT DATA TAPE NUMBER?
* 7
  DO YOU WANT TO MARK NEW TAPE OR ADD TO OLD TAPE(N or A)
* A


  THE PRESET  VALUES FOR INSTRUMENT SETTINGS ARE

  KV+CURRENT SETTING CODE     P1:3
  COLLIMATOR SETTING CODE     P2:2
  MM ADVANCE/STEP             P3:2
  TOTAL NO. OF STEPS          P4:10
  NM ADVANCE BEFORE ANALYSIS  P5:5
  TIME P(6)*P(7)             P6,P7:100 6
  SAMPLE POSITION IN TRAY     P8:11

  ELEMENT LIST :K CATIV CRMNFECONICUZNGAASSEBRRBSRHGPBMS

  TYPE IN ELEMENTS YOU WANT TO ANALYSE (2 CHAR/EL or ALL=-1)
* -1
  HOW MANY SAMPLES DO YOU WANT TO ANALYSE? :
* 1
  SAMPLE NUMBER :1
  HOW_MANY PARAMETERS DO YOU WANT TO CHANGE(MAX. 8)?
* ███3
  TYPE PARAMETER NUMBER,NEW VALUE!
*   (1)                 3,20
*   (2)                 4,4
*   (3)                 7,100
  ADDITIONAL REMARKS OR SAMPLE I.D.(MAX 8  CHARACTERS):
* 229E904
```

Figure 19

```
CONTENT OF OVERALL SAMPLE HEADING :   DATA TAPE  7

NUMBER OF BYTES STILL AVAIBLE          :368600
NUMBER OF SAMPLES ON TAPE              :5
LAST FILE ON TAPE USED                 :106
LIST OF ELEMENT SYMBOLS                :

K CATIV CRMNFECONICUZNGAASSEBRRBSRHGPBMS

SAMPLE CODES :

 DATE   P1  P2  P3  P4  P5  P6  P7  P8  P9   SAMPLE I.D.
        HV COL STEP  #  STRT  TIME  POS FILE

080779   3   2   2  11  17 100   6  14   2 11111111111111111111 WT-H-1

080779   3   2   2   8  24 100   6  24  23 11111111111111111111 WT-H-2

080779   3   2   2  23   5 100   6  44  44 11111111111111111111 WT-P-1

080779   3   2   2  10  20 100   6  54  65 11111111111111111111 WT-P-2

080779   3   2   2  60   5 100   6  63  86 11111111111111111111 A.OTTER

PROGRAM HAS ENDED
```

Figure 20

```
1       BINARY  DATA          10240   OVERALL HEAD
2       BINARY  DATA          768     SAMPLE HEAD      #1
3       NEW                   2048  } DATA RESULTS
4       NEW                   2048  }
5       NEW                   2048  } 5 ELEMENTS
6       NEW                   2048  }
7       NEW                   2048  }
8       BINARY  DATA          768     SAMPLE HEAD      #2
9       NEW                   2048
10      NEW                   2048
11      NEW                   2048
12      NEW                   2048
13      NEW                   2048
14      BINARY  DATA          768
15      NEW                   2048
16      NEW                   2048
17      NEW                   2048
18      NEW                   2048
19      NEW                   2048
20      BINARY  DATA          768
21      NEW                   2048
22      NEW                   2048
23      NEW                   2048
24      NEW                   2048
25      NEW                   2048
26      BINARY  DATA          768
27      NEW                   2048
28      NEW                   2048
29      NEW                   2048
30      NEW                   2048
31      NEW                   2048
32      BINARY  DATA          768
33      NEW                   2048
34      NEW                   2048
```

Figure 21

DATA PRESENTATION PROGRAM EX. 2

* USER ANSWERS

```
MENU FOR DATA PRESENTATION :

 1.:DISPLAY OF OVERALL SAMPLE HEADING(FILE 1)
 2.:DISPLAY OF A SPECIFIED SAMPLE HEADING
 3.:PLOT OF CONCENTRATION VERSUS LENGTH
 4.:NO.3 + HARD COPY OF THE RESULTS
 5.:PRINT OF CONCENTRATION VERSUS LENGTH
 6.:NO.5 + HARD COPY OF THE RESULTS
 7.:NEW MENU
 8.:STOP

WHICH MENU ITEM DO YOU WANT ?(TYPE NO.)
*-1
```

Figure 22

M = 1

```
CONTENT OF OVERALL SAMPLE HEADING :

NUMBER OF BYTES AVAIBLE                   :24000
NUMBER OF SAMPLES ON TAPE                 :20
LAST USED FILE ON TAPE                    :121
LIST OF ELEMENT SYMBOLS                   :

K CATIV CRMNFECONICUZNGAASSEBRRBSRHGPBMI

SAMPLE CODE  :

 DATE   P1  P2  P3  P4  P5  P6  P7  P8  P9       SAMPLE I.D.

012979   1   1   1 200   0 100  10  11   2 01010101010000000000 LHC 1

012979   1   1   1 200   0 100  10  11   8 01010101010000000000 LHC 2

012979   1   1   1 200   0 100  10  11  14 01010101010000000000 LHC 3

012979   1   1   1 200   0 100  10  11  20 01010101010000000000 LHC 4

012979   1   1   1 200   0 100  10  11  26 01010101010000000000 LHC 5

012979   1   1   1 200   0 100  10  11  32 01010101010000000000 LHC 6

012979   1   1   1 200   0 100  10  11  38 01010101010000000000 LHC 7

012979   1   1   1 200   0 100  10  11  44 01010101010000000000 LHC 8

012979   1   1   1 200   0 100  10  11  50 01010101010000000000 LHC 9

012979   1   1   1 200   0 100  10  11  56 01010101010000000000 LHC 10

012979   1   1   1 200   0 100  10  11  62 01010101010000000000 LHC 11
```

Figure 23

m = 2

```
INSERT DATA TAPE!!
FILE NUMBER FOR SAMPLE HEADING ?
2
INSTRUMENT SETTINGS AND SAMPLE I.D.:

DATE                                       :012979
SAMPLE HEAD FILE                         P9:2
KV+CURRENT SETTING                       P1:1
COLLIMATOR SETTING                       P2:1
MM ADVANCE/STEP                          P3:1
TOTAL NUMBER OF STEPS                    P4:200
MM TO ADVANCE BEFORE ANALYSIS            P5:0
TIME P6*P7                            P6,P7:100 10
SAMPLE POSITION IN TRAY                  P8:11
ELEMENT LIST CODE                          :01010101010000000000
SAMPLE I.D.                                : LHC 1


IF YOU WANT THE MENU PRINT 7 OR 8 IF STOP!
```

Figure 24

M = 3,4

```
  HOW MANY SAMPLES DO YOU WANT TO PLOT?
*-1
  INPUT HEAD FILE NUMBER FOR EACH FILE!
*-2
  INPUT STARTING AND ENDING ADDRESSES FOR EACH SAMPLE(STEPS)
*-     (1)              1,25
  WHICH ELEMENTS DO YOU WANT(MAX 5:2 CHAR EACH)?
*-████ CA
```

Figure 25

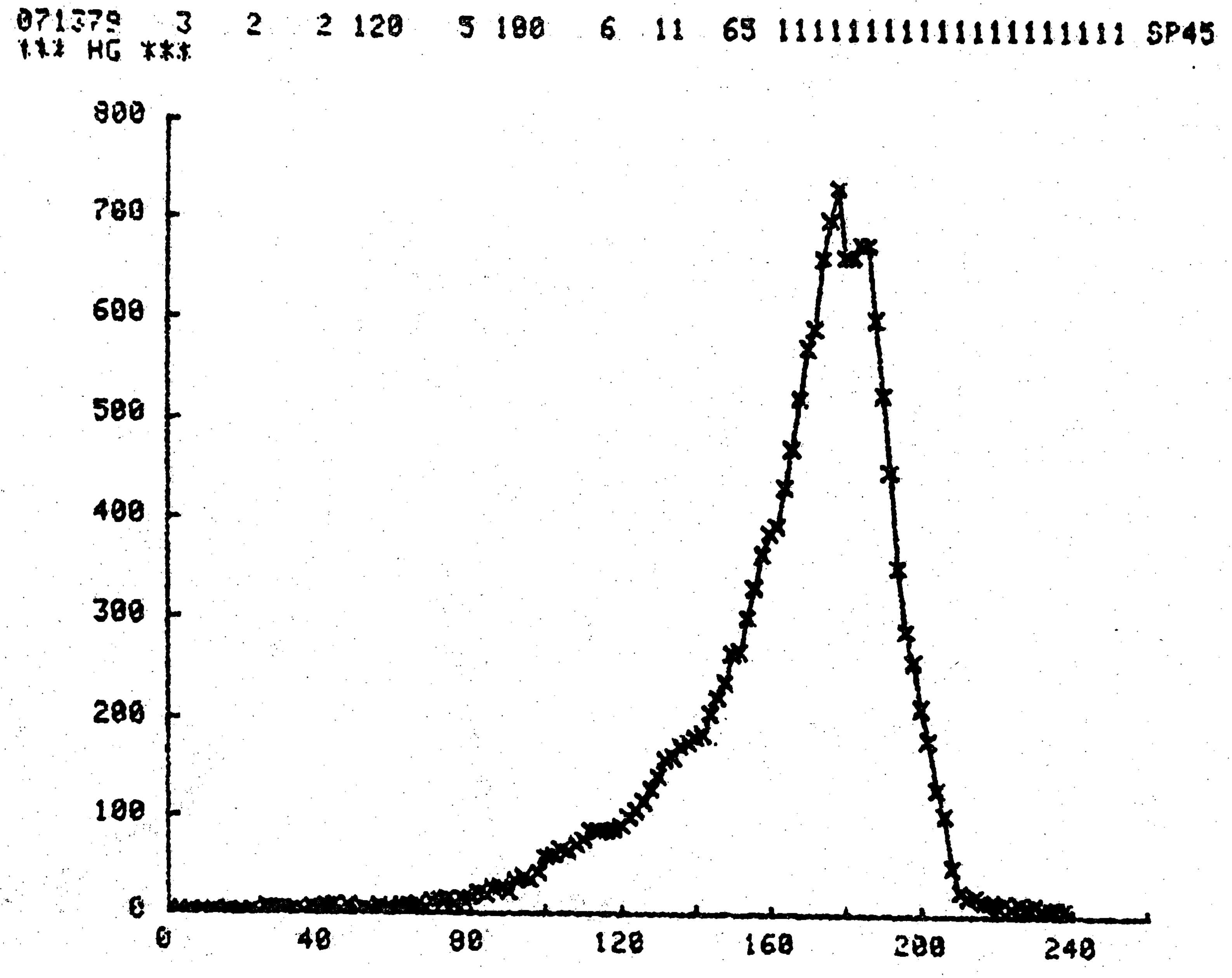

071379 3 2 2 120 5 100 6 11 65 11111111111111111111 SP45
*** HG ***
800
700
600
500
400
300
200
100
0
0
40
80
120
160
200
240

Figure 26

```
   PLEASE LOAD DATA TAPE
   HOW MANY SAMPLES DO YOU WANT TO PLOT?
*  1
   INPUT HEAD FILE NUMBER FOR EACH FILE!
*  65
   INPUT STARTING AND ENDING ADDRESSES FOR EACH SAMPLE(STEPS)
*      (1)            1,128
   WHICH ELEMENTS DO YOU WANT(MAX 5;2 CHAR EACH)?
*  HG
```

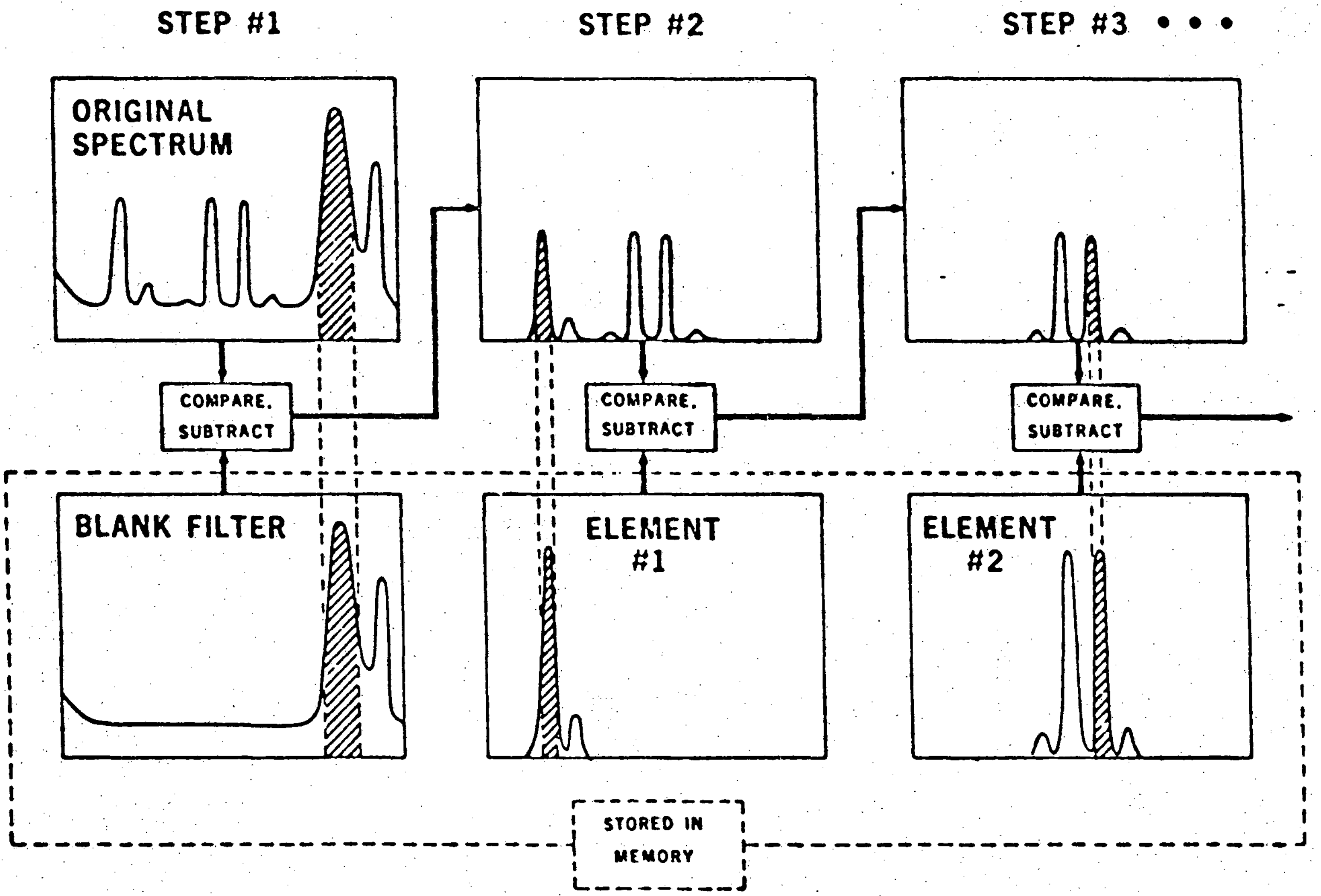
Figure 27

```
PAGE : 1
012979   1    1    1 200   0 100  10  11   2 01010101010000000000 LHC 1

 MM    K (PPM+-)      CA(PPM+-)      TI(PPM+-)      V (PPM+-)      CR(PPM+-;

  0        0     0      102   102       0     0      104   104       0     0
  1        0     0      102   102       0     0      104   104       0     0
  2        0     0      102   102       0     0      104   104       0     0
  3        0     0      102   102       0     0      104   104       0     0
  4        0     0      102   102       0     0      104   104       0     0
  5        0     0      102   102       0     0      104   104       0     0
  6        0     0      102   102       0     0      104   104       0     0
  7        0     0      102   102       0     0      104   104       0     0
  8        0     0      102   102       0     0      104   104       0     0
  9        0     0      102   102       0     0      104   104       0     0
 10        0     0      102   102       0     0      104   104       0     0
 11        0     0      102   102       0     0      104   104       0     0
 12        0     0      102   102       0     0      104   104       0     0
 13        0     0      102   102       0     0      104   104       0     0
 14        0     0      102   102       0     0      104   104       0     0
 15        0     0      102   102       0     0      104   104       0     0
 16        0     0      102   102       0     0      104   104       0     0
 17        0     0      102   102       0     0      104   104       0     0
 18        0     0      102   102       0     0      104   104       0     0
 19        0     0      102   102       0     0      104   104       0     0
 20        0     0      102   102       0     0      104   104       0     0
 21        0     0      102   102       0     0      104   104       0     0
 22        0     0      102   102       0     0      104   104       0     0
 23        0     0      102   102       0     0      104   104       0     0
 24        0     0      102   102       0     0      104   104       0     0
 25        0     0      102   102       0     0      104   104       0     0
 26        0     0      102   102       0     0      104   104       0     0
 27        0     0      102   102       0     0      104   104       0     0
 28        0     0      102   102       0     0      104   104       0     0
 29        0     0      102   102       0     0      104   104       0     0
```

Figure 28



XBL 731-86

Figure 29

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