SAVLOC, COMPUTER PROGRAM FOR AUTOMATIC CONTROL AND ANALYSIS OF X-RAY FLUORESCENCE EXPERIMENTS

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A program for a PDP-15 computer is presented which provides for control and analysis of trace element determinations by using X-ray fluorescence. The program simultaneously handles data accumulation for one sample and analysis of data from previous samples. Data accumulation consists of sample changing, timing, and data storage. Analysis requires the locating of peaks in X-ray spectra, determination of intensities of peaks, identification of origins of peaks, and determination of areal density of the element responsible for each peak. The program may be run in either a manual (supervised) mode or an automatic (unsupervised) mode.
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SUMMARY

A program for a PDP-15 computer is presented which provides for control and analysis of trace element determinations by using X-ray fluorescence. The program simultaneously handles data accumulation for one sample and analysis of data from previous samples. Data accumulation consists of sample changing, timing, and data storage. Analysis requires the locating of peaks in X-ray spectra, determination of intensities of peaks, identification of origins of peaks, and determination of areal density of the element responsible for each peak. The program may be run in either a manual (supervised) mode or an automatic (unsupervised) mode.

INTRODUCTION

The recent development of high-resolution solid-state X-ray detectors has made possible the use of X-ray fluorescence as a tool for the detection of trace elements in a variety of applications. However, analysis of environmental samples by means of X-ray fluorescence generates energy spectra for which quantitative hand analysis is prohibitively tedious. In addition, the number of samples generated by any comprehensive monitoring program requires a speed of data acquisition and analysis which is possible only through the use of a computerized system. The present report describes the software designed for control and data analysis of such a system. This report should permit the reader to operate the system.

PRINCIPLES OF X-RAY FLUORESCENCE AND CHARACTER OF DATA

When properly stimulated, the atoms of any element emit X-rays whose energy (or wavelength) is strictly dependent upon the atomic number of the emitting atom. Since
these energies may be quickly and accurately measured, and since the X-ray energies of all elements are well known and tabulated, it is possible to identify, with little ambiguity, the element responsible for the emission. In addition, the number of X-rays emitted is proportional to the number of atoms stimulated, so that after a proper calibration, quantitative measurements of areal densities are possible.

The X-ray detectors commonly employed provide data in the form of analog electric pulses. Data acquisition consists of the digitizing and storing of these pulses, which arrive with random timing at the rate of several thousand per second. A schematic representation of the X-ray fluorescence facility is shown in figure 1. A typical X-ray spectrum is shown in figure 2. This particular spectrum resulted from excitation of a sample by using X-rays from a tungsten X-ray tube. It contains a peak (labelled Rh) which resulted from the presence in the primary X-ray beam of a small, known amount of rhodium, whose purpose was to provide a monitor of the number of photons incident on the sample.

Data analysis consists of determining from this spectrum the number of X-ray counts contained in each peak, identifying the origin of the peak, and converting the number to an areal density by using the expression

\[
N(E) = N_i \left( \frac{d\sigma}{d\Omega} \right)_E \rho_X \Omega \varepsilon(E)
\]

where

- \( N(E) \) number of X-ray photons of energy \( E \) detected
- \( N_i \) number of X-ray photons incident on target
- \( \left( \frac{d\sigma}{d\Omega} \right)_E \) cross section for production of X-rays of energy \( E \) by exciting X-rays
- \( \rho_X \) areal density of atoms producing X-rays of energy \( E \)
- \( \Omega \) solid angle subtended by X-ray detector
- \( \varepsilon(E) \) efficiency of detector for detection of X-rays of energy \( E \)

In practice, only the quantity \( N(E) \) is determined absolutely. The number \( N_i \) is assumed to have the form

\[
N_i = K_{\text{Rh}} N_{\text{Rh}}
\]

where \( N_{\text{Rh}} \) is the number of rhodium (monitor) X-rays detected, so that the areal density may be written
The overall efficiency function

\[ \rho_x = \frac{N(E)}{K_{Rh} N_{Rh} \frac{d\sigma}{d\Omega}_E \Omega \varepsilon(E)} \]  \hspace{1cm} (3)

The overall efficiency function

\[ F(E) = \frac{1}{K_{Rh} \frac{d\sigma}{d\Omega}_E \Omega \varepsilon(E)} \]  \hspace{1cm} (4)

is then determined experimentally by using samples of known areal density of a number of elements. For elements other than those for which \( F(E) \) is measured directly, an interpolation is carried out with the assumption that the function varies smoothly with energy. The areal density then, in terms of directly measurable quantities, becomes

\[ \rho_x = \frac{N(E) F(E)}{N_{Rh}} \]  \hspace{1cm} (5)

Analysis then requires only the determination of the intensity and energy of each line in the X-ray spectrum and the intensity of the line used for normalization \( N_{Rh} \).

DATA ACQUISITION AND ANALYSIS

The entire X-ray fluorescence operation (sample changing, data acquisition, and data analysis) is carried out under the control of a PDP-15 computer. Communication between the computer and the X-ray fluorescence hardware is by means of a CAMAC system (ref. 1). The programmable interface between the computer and the CAMAC system has been described in detail elsewhere (ref. 2). The control panel of the PDP-15 computer, shown in figure 3, allows the input of a number of parameters as well as the selection of a number of different modes of operation, so that a sufficient degree of flexibility is provided to make the system useful for a variety of applications.

Data Acquisition

The two principal control tasks which the PDP-15 must perform are the changing of targets and the control (stop, start, and data transfer) of the 1024-channel analog-to-digital converter (ADC), through which all pulse-height data pass.
A typical data-taking cycle is initiated upon input of the last piece of sample identification data by means of the computer teletype unit. The ADC is turned on, and data transfers from the ADC to the computer memory take place autonomously by way of the CAMAC interface. During data acquisition the pulse-height spectrum is displayed on a video unit, which assures the user that all systems are functioning properly.

By means of push buttons on the computer control panel, data acquisition may be terminated at any time, either by pressing B4, which causes data to be recorded on magnetic tape, or by pushing B2, which ends the run without recording of the data. Data acquisition also terminates, with all accumulated data being recorded on tape, when the elapsed time reaches the preset value as entered (in tenths of seconds) on control panel thumb switch TH2.

Following termination and depending on the mode of operation selected, either another run is started automatically (T15 up) or a halt occurs (T15 down) until the operator chooses to continue by pressing B2. In either case sample changing may or may not be done, depending on the setting of rotary switch R1 on the control panel (sample is changed when R1=2).

The data recorded upon completion of a run include the run identification (a five-character file name and a three-digit file number), the time elapsed during data acquisition, and, of course, the pulse-height spectrum itself.

Because analog-to-digital conversion and data transfers take place at data-channel level, they proceed autonomously once initiated, so that the computer central processing unit is free at main-stream level to proceed with analysis of a previous data set if so instructed.

Data Analysis

Analysis of previous data sets may either be initiated by the operator (press B1) or take place automatically when the computer is operating in an automatic mode (T15 up). Analysis begins with the recalling of two previous runs from tape: one with the data of interest and one that is a background or blank run, which is subtracted to remove events resulting from scattering or impurities in the system or sample-supporting matrix.

When analysis is initiated by an operator, the program requests a file name and file number for each of these data sets. In the automatic mode the program searches for a data set with the same name as that previously analyzed, increases the file number to obtain the next data set, and uses the same background data set. Hence, it is always necessary that at least the first set be analyzed manually.

The first step in the analysis is the determination of the number of events $N_{Rh}$ contained in the monitor (rhodium) peak for both the sample data and background data.
This is accomplished by locating the rhodium peak and then fitting that portion of the spectrum within 20 channels of it with a Gaussian peak plus linear background. The number of events within the Gaussian peak is then the $N_{Rh}$ of equation (5). The amount of background in this region provides the normalization for subtraction of the blank spectrum.

It is assumed that since the blank spectrum results from an unloaded sample of the supporting matrix, it is identical in shape to that encountered in the loaded sample. Consequently, after normalization and smoothing over three channel segments, the two spectra are subtracted channel by channel to arrive at the spectrum to be analyzed.

The recalled spectrum (with background subtracted) then replaces the live display of data currently being accumulated on the video unit. Figure 4 shows the recalled spectrum derived from the data of figure 2. The number of events under each peak, that is, the number of detected X-ray photons of each energy, is determined by a least-squares fitting to each peak of a Gaussian distribution of adjustable height, width, and location. Initial estimates of peak locations may be supplied by the researcher by means of the light pen and video display (T11 down), or they may be located automatically by the program (T11 up). The automatic location procedure is described in appendix A.

Depending on the setting of toggle switches, an energy calibration may be supplied at this time (T16 down). The user may supply through the teletype console the energies of the first two peaks selected with the light pen. For operation in the automatic mode (T16 and T15 up) the program retains the energy calibration from the previous run. Hence, again at least one run must be done manually. The researcher is also asked to supply through the teletype console (unless the computer is operating in the automatic mode) an estimate of the full width at one-half of the maximum (FWHM) of a typical peak.

The fitting routine does each peak in turn from the lowest to the highest energy. When two peaks are found to lie within four times the estimated FWHM, they are fitted simultaneously. Up to five peaks may be treated as a multiplet and done simultaneously. A more detailed description of the fitting procedure is given in appendix B.

Following analysis of each line for energy and intensity, an identification is made by comparing the measured energy with a table of energies and atomic symbols. The elements which are included in this table are listed in table I. If a peak is identified as a $K_{\alpha}$ line, a check is made to determine whether the $K_{\beta}$ line can also be observed. If a line of the proper energy is located, the expected intensity of the $K_{\beta}$ line (determined from the intensity of the $K_{\alpha}$ line) is subtracted from the $K_{\beta}$ candidate. The remainder of the peak is tested for other identification. No peak may be identified as an $L$ series X-ray unless both the $L_{\alpha}$ and $L_{\beta}$ lines are observed.

The experimental intensity is converted to an areal density by using the stored efficiency function $F(E)$. This function is assumed (for $K$ series X-rays) to have the form
The parameters $P(i)$ are determined by measuring the X-ray yield for a number of samples (approximately 10 to 15) of known areal density and performing a least-squares fit of the function given in equation (6) to that data. The parameters $P(i)$ vary with any change in detector or source geometry and must be redetermined each time such a change occurs. A typical set of parameters $P(i)$ is listed in table II. For heavier elements, which are measured by means of D series X-rays, tabulated efficiencies are used for those elements which the program can identify.

The estimates of errors in the computed areal density are based on the number of counts in each peak, given by

$$N(E) = I(E)\sigma(E)\sqrt{\pi}$$

where $I$ and $\sigma$ (as defined in appendix B) are the height and width, respectively, of the Gaussian distribution derived from the data. The areal density, given by equation (5), then becomes

$$\rho_X = \frac{I(E)\sigma(E)\sqrt{\pi} F(E)}{N_{Rh}}$$

Therefore, assuming the error in $N_{Rh}$ to be small gives

$$\frac{\delta \rho_X}{\rho_X} = \frac{\delta I(E)}{I(E)} + \frac{\delta \sigma(E)}{\sigma(E)} + \frac{\delta F(E)}{F(E)}$$

or

$$\frac{\delta \rho_X}{\rho_X} = \left| \frac{\delta I(E)}{I(E)} \right| + \left| \frac{\delta \sigma(E)}{\sigma(E)} \right| + \left| \frac{1}{F(E)} \frac{dF(E)}{dE} \delta E \right|$$

The errors in each of the quantities $I(E)$, $\sigma(E)$, and $E$ are derived in the usual way from the residuals of the least-squares fitting process.

Computed areal densities may be modified by an arbitrary multiplicative factor $G$, which may be entered by means of thumb wheel TH1. The value of $G$ may be between
0 and 9.9999, and its effect is included in all areal densities and errors listed as output. The principal purpose of this factor is to permit the user to convert to a convenient system of units if so desired. If \( G \) is set equal to 1, the results are in units of micrograms per square inch.

Output may consist of either one or two pages of teletype output as well as a record of the results on magnetic tape. These options are selected through the control panel toggle switches (p. 1, T14 up; p. 2, T12 up; and tape, T13 up). Samples of the two pages of teletype output are shown in figures 5 and 6. More detailed information on the results of the least-squares fitting process may be obtained by replying "T" (true) when the program inquires, through the teletype console, "Do you wish extra output? Output=." A sample of this augmented output is shown in figure 7. It includes the height, width, and location, as well as the standard deviation of each, for each line fitted by the program.

A flow chart for the entire program is shown in figure 8. A guide to the loading of the program into the PDP-15 is given in appendix C. Appendix D contains the details of the overlay structure necessary in order to fit the program into the available core. Appendix E contains a listing of the FORTRAN sections of the program.

CONCLUDING REMARKS

The program described in this report permits trace element analysis of environmental samples at a rate which would make meaningful monitoring surveys feasible. Specifically, data analysis requires between 3 and 12 minutes, depending on the complexity of the spectrum, while data acquisition requires 5 to 30 minutes, depending on the primary radiation source and associated hardware employed. The program works reliably in an automatic mode; it changes samples, takes data, locates peaks, measures intensities, and identifies elements. As a result samples may be processed without an operator in attendance, which makes around-the-clock analysis possible. In addition, when operated under the supervision of the user, the program is capable of treating a wide variety of nonroutine samples, such as those containing elements not automatically recognized and those containing a number of heavy elements and thus having extremely complex spectra. For these, the program permits the extraction of meaningful data with a minimum amount of effort on the part of the user.

Lewis Research Center,  
National Aeronautics and Space Administration,  
Cleveland, Ohio, December 2, 1976,  
506-25.
APPENDIX A

AUTOMATIC PEAK LOCATING PROCEDURE

If the operator so desires, initial estimates of peak locations are determined by the program, using a method described by Mariscotti (ref. 3). The method is based on the construction of smoothed second differences of the experimentally measured energy spectrum. The smoothed second difference is defined by

\[
S_i(z, m) = \sum_{j=1-m}^{i+m} \cdot \cdot \cdot \sum_{h=l-m}^{l+m} (N_{l+1} - 2N_l + N_{l-1})
\]

or equivalently

\[
S_i(z, m) = \sum_{\text{all } j} C_{ij}(z, m)N_j
\]

where the \( C_{ij} \) are weighting factors derived by Mariscotti, given by

\[
C_{ij}(z, m) = \sum_{l=i-m}^{i+m} C_{lj}(z-1, m)
\]

and

\[
C_{ij}(0, m) = \begin{cases} 
0 & \text{if } |j - i| \geq 2 \\
1 & \text{if } |j - i| = 1 \\
2 & \text{if } j = i 
\end{cases}
\]

The values of \( z \) and \( m \) used here are those found by Mariscotti to be most suitable, namely,

\[
z = 5
\]

\[
m = \frac{(0.6\Gamma - 1)}{2}
\]
The resulting function $S$ then vanishes for a linear spectrum and is similar to the second derivative of a Gaussian function if $N_j$ is a Gaussian function. The program assumes that a peak exists in channel $i$ if three conditions are present: First,

$$|S_i| > 1.6 |\delta S_i|$$  \hspace{1cm} (A5)

where $\delta S_i$ is the standard deviation in the function $S_i$, approximated by Mariscotti as

$$\delta S_i = \left( \sum C_{ij}^2 \right)^{1/2} \delta N_i$$

where $\delta N_i$ is the standard deviation in the data point $N_i$. The program assumes

$$\delta N_i = (N_i + B_i)^{1/2}$$

where $B_i$ is the amount of background previously subtracted from channel $i$ of the spectrum. Second,

$$S_i < 0$$  \hspace{1cm} (A6)

Third,

$$S_{i-1} < |S_i| > S_{i+1}$$  \hspace{1cm} (A7)

The code does not reject any peak on the basis of its width as suggested by Mariscotti.
APPENDIX B

LEAST-SQUARES FITTING

Once initial estimates of peak locations and widths have been obtained, a least-squares fitting is carried out by using the Gaussian function

\[ f(x) = I \exp \left( \frac{(x - x_0)^2}{\sigma^2} \right) \]  \hspace{1cm} (B1)

to represent that portion of the spectrum being treated. In the event that several peaks fall within 4FWHM of each other, they are fitted simultaneously as the sum of as many as five Gaussian distributions, each of which has independently variable width.

For initial estimates, \(x_0\) is taken to be the channel \(i\) either found by the automatic search routine described in appendix B or supplied through the light pen. The initial estimate of the intensity \(I\) is taken to be the number of counts in that \(i^{th}\) channel, and \(\sigma\) is calculated from the FWHM input (for a Gaussian distribution, \(\sigma = \text{FWHM}/1.665\)).

Fitting is carried out by standard methods. In the event a satisfactory fit cannot be obtained within a specified number of iterations, the peak of highest energy is dropped from the multiplet, and the fitting process is restarted for the remainder of the peaks. In the event that a single peak cannot be satisfactorily fitted, a message to that effect is included on output page 1, and the peak is assigned intensity zero and a location equal to the starting channel number.
APPENDIX C

LOADING THE PROGRAM

As presented in this report the program (entitled SAVLOC) is too large to be loaded directly into a 16K PDP-15 computer. As a result it can only be used as a series of overlays, constructed by using the routine CHAIN (ref. 4). A listing of the execute file, titled SAVLOC, is given in appendix D; the listing includes the resident code as well as the structure of each of the links and a machine constructed map of the file.

At execution time the user must assign handlers to three slots in the device assignment table (dat): dat slot 1, for writing of raw data; dat slot 2, for reading of raw data; and dat slot 3, for writing of results of analysis (fig. 6). Dat slots 1 and 2 are normally assigned the same magnetic tape (dectape) unit, and dat slot 3 is assigned a second dectape unit.

An example of the entire loading sequence is as follows:

```
KMS15 V5C
$A DTE6 1,2/DTE7 3
$E SAVLOC

EXECUTE V4A
FNAME(A) =
```

where the underlined expressions are output from the computer.
APPENDIX D
OVERLAY STRUCTURE AND MEMORY MAP FOR EXECUTE FILE SAVLOC

\CHAIN

CHAIN V5B

NAME XCT FILE
>SAVLOC
LIST OPTIONS & PARAMETERS
>PGR, 16K, SZ
DEFINE RESIDENT CODE
>SIMUL2, CAMADC, IPK3, PICKER
DESCRIPTION LINKS & STRUCTURE
>LKI=PEDE, RITE
>LK2=FITALL, FITALL, GAUS
>LK3=ECAL1, ECAL2
>LK4=PGEOUT, XXYN
>LK5=LABEL, SOFT
>LK6=S, SCALI, LOCUM
-MULT:SIT2:EPPO:ENERG:IDENT

LINK TABLE
37825-37836 00412

RESIDENT CODE
SIMUL2 36527-37224 00476
CAMADC 35731-36526 00576
IPK3 34742-35732 00771
PICKER 34305-34737 00433
SEARCH 34226-34304 00257
PTIME 34146-34225 00269
REC16 34126-34145 00022
SEND16 34113-34125 00013
CAMAC 33631-34112 00262
PANEL 33477-33630 00139
CPASS 33347-33476 00139
HIST01 33226-33346 00121
PENSW 33200-33225 00226
UPVECT 33014-33177 00164
VIDEO 32515-33013 00277
TIMAGE 32470-32514 00025
CLOCK 32372-32467 00076
RITEST 32350-32371 00022
GETALK 32267-32347 00261
IPPOOL 32224-32266 00243
TPED 32000-32223 00224
*S 31150-32177 00056
FLOAT 32117-32127 00011
FLOAT? 32071-32116 00026
.BR 32024-32073 00045
FIOPS 31302-32023 00052
INTEAE 31171-31301 02111
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.CB 22760-22776 00017

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SOPT 24621-24756 02136
ABS 24602-24620 00017

LINK -- LK6
S 27117-27344 00226
SCALI 24651-27116 00246
LOCUM 24730-26650 01721
IFIX 24712-24727 00016
ARS 24673-24711 00017
LIMIT 24650-24672 00023
.RC 24554-24647 00074
SOQT 24441-24553 00113
DIFF 24220-24440 00221

LINK -- REED
PEED 26775-27344 00350
BCDEXT 26726-26774 00947
INPUT1 26637-26725 00667
XPEAD 26323-26636 00314
PACKEP 24222-26322 00101
MOD 26201-26221 00021
BCDIO 23544-26220 02435
BINIO 23317-23543 00225
FILE 23040-23316 00257
.CB 23021-23037 00017

LINK -- MAXER
MAXER 27275-27344 00050

LINK -- SETI
SETI 27003-27344 00342

LINK -- SUBTP
SUBTP 26527-27344 06616
INPUT1 26440-26526 02967
XPEAD 26124-26437 00314
PACKER 26023-26123 00101
BCDIO 23366-26022 02435
.CB 23347-23365 00017

LINK -- OUTER
OUTER 27041-27344 00304
BCDIO 24404-27040 02435
.CB 24365-24403 00017

LINK -- MULT
MULT 26665-27344 00460
IFIX 26647-26664 00016

LINK -- SIT2
SIT2 26032-27344 01313
BCDIO 23375-26031 02435
.CB 23356-23374 00017

14
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ERRO  27033-27344 00312  
BCDIO  24376-27032 02435  
.CB  24357-24375 00017  

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RCDEXT  26017-26069 00047  
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BCDIO  23221-25655 22435  
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BLANK COMMON  
XX  12723-22722 10000  

CORE REQ'D  
12723-37636 24714  

KMS15 V5C  
$
APPENDIX E

SOURCE LISTING

C......PROGRAM TO SIMULTANEOUSLY TAKE AND ANALYZE DATA
INTEGER DATAD(4096), GATEX(64, 7), ORGN(8), DATUM(1024)
REAL FNAME(2), LT, LTI
LOGICAL ON, EXIST, BUTNS, RITEST
EXTERNAL ADCON
COMMON DATAD
EQUIVALENCE (GATEX(I, J), DATAD(3573)), (DATAD(I), DATUM(I))
DATA ND, NLAST/I024, I/
1 FNAME(1), FNAME(2)/5HSPECT, 1H /
CALL CLKON
CALL PSTART
CALL REDE(FNAME, NEXT, NLAST)
I4= IROTOR(4)
I3= IROTOR(3)
I2= IROTOR(2)
EXIST=.TRUE.
NY= IROTOR(4)+6
NF= 256*I2-255
NX= I3+7
CALL ZERO(DATUM)
CALL CLKON
CALL VSTOP
CALL HISTO1(DATUM, NF, NX, NY, NSAW, I)
CALL VPSTRT
CALL ECAMCK
CALL RTCOFF
IF(ON) CALL ADCOFF
MODE= 0
IPT= ITHUMB(2)
ILT= 0
IF(NEXT, GT, NLAST) GO TO 122
CALL ADCSTR(DATAD, GATEX, ORGN, ILT, ON, MODE)
CALL RTCOSTR(IRT, ADCOFF)
CALL RTIME(IS)
CALL LAMPON(1)
CALL BUTNS(1B)
IF(IB, EQ, 1) GO TO 101
IF(IB, EQ, 2) GO TO 501
IF(.NOT. ON) GO TO 96
122 IF(IB, EQ, 4) GO TO 98
CALL TOGLS(1T)
IF(RITEST(I, 15) .AND. EXIST) GO TO 101
GO TO 120
101 CALL VSTOP
CALL IPK2(EXIST)
CALL VSTOP
CALL HISTO1(DATUM, NF, NX, NY, NSAW, 1)
CALL VPSTRT
IF(ON) GO TO 122
96 IF(NEXT, GT, NLAST) GO TO 122
93 CALL RTCOFF
CALL ADCOFF
CALL LAMP0F(1)
CALL TOGGLS(IT)
IF(CIPTOR(1),EQ,2) CALL PELAON(3)
CALL RITE(FNAME, NEXT, TS, IRT, ILT, ND)
NEXT=NEXT+1
CALL TOGGLS(IT)
IF(BITEST(IT,15)) G0 TO 3
CALL LAMPON(2)

500 CALL BUITNS(1B)
IF(IB.NE.2) G0 TO 500

522 CALL LAMPOF(2)
501 CALL TOGGLS(IT)
IF(BITEST(IT,17)) G0 TO 2
G0 TO 3
END

SUBROUTINE IPK2(EXIST)
C......SUBROUTINE TO DO PEAK ANALYSIS AFTER LIGHT PEN SELECTION,
C......FOR USE WITH SIMUL2, TO TAKE DATA SIMULTANEOUSLY.
C......USED TO BUILD XCT FILE

INTEGER LIST(520), DATA(1024), RKGND(1024), GATE(5,30), CH0(30),
1, CHMAX, DATAD(4096), REXT, IR(5)
REAL FNAME(2), PARAM(15), DP(15), POINT(100), BNAME(2), XCH(2),
1, ELE(30), ENORM(30), BNGMX(30), DRC(30)
LOGICAL EXIST, DOUBLE, UNDOUR, TRIPLE, UNTRIP, QUAD, UNQUAD, GUIN,
1, UNQUIN, BUITNS, PENSW, OUTPT, BITEST
EXTERNAL GAUSS
COMMON/DISPL/NF, NX, NY
COMMON/ERR/PHI2, IMIN, ITELL
COMMON/STUFF/GATE
COMMON/MUP/DOLL, UNDOUR, TRIPLE, UNTRIP, QUAD, UNQUAD, GUIN, UNGUIN,
1, JPEAK, GAM, IDUB, ITRIP, IQUAD, IGUIN
COMMON/FINOUT/ELE, A1, A2
COMMON/DATAD
EQUIVALENCE (DATA(1), DATAD(525)), (RKGND(1), DATAD(1024)),
1, LIST(1), DATAD(3073)), (CH0(1), DATAD(4021)),
2, (POINT(1), DATAD(3593)), (ENORM(1), DATAD(3800)),
3, (BNGMX(1), DATAD(3861)), (DRC(1), DATAD(3821)),
4, (IR(1), DATAD(4051)), (PARAM(1), DATAD(4056))
CALL LAMPON(3)
CALL REED(1, FNAME, NEXT, EXIST)
IF(EXIST) 30 TO 3
CALL LAMPOF(3)
RETURN
3
NEXT=NEXT+1
2
CALL MAXER(DATA, CHMAX)
CALL SETI(CHMAX, DATA, POINT)
ITELL=1
CALL FITALL(GAUSS, POINT, PARAM, DP, 0, LIST)
CALL OUTER(PARAM, LIST, ANORM, APNORM, CHMAX)
CALL REED(2, RNAME, NEXT, EXIST)
CALL MAXER(RKGND, CHMAX)
CALL SETI(CHMAX, RKGND, POINT)
CALL FITALL(GAUSS, POINT, PARAM, DP, 0, LIST)
ITELL=0
CALL SURTR(ANORM, APNORM, CHMAX, OUTPT, GAM)
CALL PICKER
CALL TOGGLS(IT)
IF(BITEST(IT,10)) CALL USTOP
IF(BITEST(IT,11)) CALL LOCUM
CALL LAMPOF(7)
IF(BITEST(IT,16)) GO TO 87
DO RR J=1,2
CALL ECALI(J)
CALL FITALL(GAUSS,POINT,PARAM,DP,Q,LIST)
XCH(J)=FLOAT(CH(J)+PARAM(2)-4.
CONTINUE
88 CALL ECAL2(XCH,A1,A2)
87 CALL LAMPOF(7)
C.....BEGIN FITTING PEAKS
88 DO R9 J=3,JPEAK
89 CALL MULT(IMAX,IMIN,J)
CALL SIT2(IMAX,IMIN,J,ANORM)
CALL FITALL(GAUSS,POINT,PARAM,DP,Q,LIST)
NPARAM=LIST(6)
DO 85 I=1,NPARAM,3
IF(PARAM(I+1).GT.FLOAT(IMAX-IMIN+5)) LIST(4)=7
IF(PARAM(I+1).LT.-.5.) LIST(4)=8
CONTINUE
IF(LIST(4).EQ.0) GO TO 86
CALL ERROC(J,IMIN,DP)
IF(.NOT.DOUBLE) GO TO 86
GO TO 81
86 CALL ENERG(IMIN,A1,A2,J,DP)
CALL LABEL(J,JPEAK)
CALL REGOUT(OUTPT,ANORM,IMIN,DP,Q,J)
CONTINUE
CALL IDENT(ELE,ENORM,BNORMX,DP,JPEAK,FNAME,NEXT)
CALL LAMPOF(3)
CALL VPSTRT
RETURN
END

SUBROUTINE PICKER
INTEGER GATE(5,30),CHO(30),DATA(1024),DATAD(4096),OFF,X,Y,
I,CHMAX
LOGICAL DOUBLE,UNDOUB,TRIPLE,UNTRIP,QUAD,UNQUAD,QUIN,UNQUIN,
I,BUTTONS,PENSW,BITEST
COMMON/STUFF/GATE
COMMON/MUP/DOURLE,UNDOUB,TRIPLE,UNTRIP,QUAD,UNQUAD,QUIN,
I,UNQUIN,JPEAK,GAM,IDUB,ITRIP,QUAD,QUIN
COMMON/DISPL/NF,NX,NY
COMMON DATAD
EQUIVALENCE (DATA(I),DATAD(I025),(CH0(I),DATAD(4021))
DATA OFF/-1/
100 FORMAT(1X,2H0)
ICHK=0
6 ISI=NX
IS2=NY
IS3=NF
CALL SCALI(NX,NY,NF)
CALL TOGGLS(II)
IF(ICHK.NE.1) GO TO 66
IF(ISI.NE.NX).OR.(IS2.NE.NY).OR.(IS3.NE.NF)) GO TO 66
GO TO 65
66 CALL VPSTOP
CALL HISTOJ(DATA,NF,NX,NY,NHIT,1)
CALL VPVECT(GATE,30,IHIT,2)
CALL VPSTRT
65 IF(BITEST(I,T,16)) RETURN
IF(ICHK.EQ.1) GO TO 12
IF(ICHK.EQ.-1) GO TO 13
CALL ZERO(GATE)
CALL ZERO(CH0)
JPEAK=0
CALL CROSS(X,Y,OFF,3)
JPEAK=JPEAK+1
8 IF(PENSW(.TRUE.)) GO TO 9
ICHK=1
GO TO 6
9 GATE(1,JPEAK)=NHIT
CH0(JPEAK)=NHIT
GATE(2,JPEAK)=DATA(NHIT)
GATE(3,JPEAK)=0
GATE(4,JPEAK)=128
GATE(5,JPEAK)=-10
ICHK=-1
GO TO 6
12 CALL LAMPON(7)
10 CALL RUNNS(IB)
IF(IR.EQ.128) GO TO 11
IF(IB.EQ.32) GO TO 14
IF(IR.EQ.64) RETURN
GO TO 10
14 JPEAK=JPEAK-1
11 CALL LAMPONF(7)
GO TO 8
END

SURROUNLE REDE(FNAME,NEXT,NLAST)
REAL FNAME(2)
CALL INPUT1 (FNAME(1),5HFNAME,6)
CALL INPUT1 (NEXT,4HNEXT,1)
CALL INPUT1 (NLAST,5HNLAST,1)
RETURN
END

FUNCTION S(ICHNL)
INTEGER DATA(1024),DATAD(4096)
REAL C(36),B(36)
COMMON/DIFF/C,B,M
COMMON DATAD
EQUIVALENCE (DATA(1),DATAD(1:25))
MI=5*M+2
X=C(1)*FLOAT(DATA(ICHNL))
DO 41 J=1,MI
I1=ICHNL+J
I2=ICHNL-J
JI=J+1
IF(I1.GT.1024) GO TO 42
IF(I2.LT.0) GO TO 42
X=X+C(JI)*FLOAT(DATA(I1))+C(JI)*FLOAT(DATA(I2))
GO TO 41
X=0
CONTINUE
S=X
RETURN

SUBROUTINE RITE(FNAME,NEXT,TS,IRT,ILT,ND)
REAL FNAME(2)
INTEGER DATAD(4096)
COMMON DATAD
CALL BCDEXT(FNAME,NEXT)
CALL ENTER(2,FNAME)
WRITE(2) TS,IRT,ILT,ND,(DATAD(I),I=1,ND)
CALL RELAOF(3)
WRITE(6,106) FNAME,TS,IRT,ILT
106 FORMAT(1X,2A5,5X,F12.5,16,3X,16)
CALL CLOSE(2)
RETURN
END

SUBROUTINE GAUSS(R,X,P,DP,V,KK,J)
C.....SUBROUTINE FOR US WITH FITALL TO FIT UP TO 4
C.....GAUSSIAN PACKS WITH OR WITHOUT BACKGROUND
REAL X(100),P(15),DP(15)
INTEGER BKGND(1024),DATA(1024),DATAD(4096)
COMMON/ERR/PHI2,ILOWER,ITELL
COMMON DATAD
EQUIVALENCE (DATA(1),DATAD(1225)),(BKGND(1),DATAD(2049))
NP=KK/3
IF(KK-NP.EQ.0) GO TO 1
R=X(J)*P(1)*FLOAT(J-P(2))
DP(1)=-P(1)
DP(2)=-1.
N=3
GO TO 3
1 N=1
P=X(J)
3 DO 2 I=N,KK,3
TP=P(I)*EXP(-(FLOAT(J)-P(I+1))**2/P(I+2)**2)
R=P-TP
DP(I)=TP/P(I)
DP(I+1)=-TP*2.*(FLOAT(J)-P(I+1))/P(I+2)**2
DP(I+2)=DP(I+1)*(FLOAT(J)-P(I+1))/P(I+2)
2 CONTINUE
IERR=ILOWER+J-3
IF(ITELL.EQ.0) V=(FLOAT(BKGND(IERR)+1))
IF(ITELL.EQ.1) V=1.
RETURN
END

SUBROUTINE ECALI(J)
C.....SUBROUTINE CALLED BY IPK2 TO DETERMINE ENERGY CALIBRATION.
INTEGER CH(30),LIST(520),DATAD(4096),DATA(1024)
LOGICAL BITEST
REAL PARAM(15),DP(15),POINT(100),X(2)
COMMON DATAD
COMMON/ERR/PHI2,IMIN,ITELL

20
EQUIVALENCE (DATA(1), DATA(1025)), (LIST(1), DATA(3073)),
1        (CH(1), DATA(4021)), (POINT(1), DATA(3593)), (PARAM(1)
1, DATA(4056))
CALL TOGGLS(IT)
IF(BITEST(IT, 16)) RETURN
LIST(1) = 7
LIST(2) = 3
LIST(3) = 15
LIST(4) = 2
LIST(5) = 3
LIST(6) = 3
IK = CH0(J)
PARAM(1) = FLOAT(DATA(IK))
PARAM(2) = 4.
PARAM(3) = 4.5/1.665
IMIN = CH0(J) - 3
DO 3 I = 1, 7
IC = CH0(J) - 4 + I
POINT(I) = FLOAT(DATA(IC))
3       CONTINUE
RETURN
END

SUBROUTINE ECAL2(X, A1, A2)
LOGICAL BITEST
CALL TOGGLS(IT)
IF(BITEST(IT, 16)) GO TO 99
WRITE(6, 100)
CALL INPUT1 (EI, 2HE1, 2)
CALL INPUT1 (E2, 2HE2, 2)
A1 = (EI - E2) / (X(1) - X(2))
A2 = EI - A1 * X(1)
99       G = FLOAT(ITHUMB(1)) / 10000.
WRITE(6, 103) G
103      FORMAT(1X, 2HG = , F6.4)
IF(BITEST(IT, 14)) WRITE(6, 101)
IF(BITEST(IT, 14)) WRITE(6, 102)
RETURN
101      FORMAT(1X, 6H PEAK, 9H CHANNEL, 12H STRENGTH,
1   10H ENERGY, 16H CONCENTRATION, 10H ERROR,
2   8H ELEM)
102      FORMAT(39X, 14H(UGRAMS/IN**2))
100      FORMAT(1X, 25H ENERGIES FOR CALIBRATION:)
END

SUBROUTINE REGOUT(OUTPT, ANORM, IMIN, DP, Q, J)
INTEGER LIST(520), DATA(4096)
REAL PARAM(15), ENORM(30), ELE(30), DP(15), BNORMX(30), DB(30)
LOGICAL OUTPT, BITEST
COMMON DATAD
COMMON/FIOUT/ELE, A1, A2
EQUIVALENCE (LIST(1), DATA(3073)), (ENORM(1), DATA(3600)),
1        (BNORMX(1), DATA(3861)), (DR(1), DATA(3921)),
2        (PARAM(1), DATA(4056))
NPARAM = LIST(6)

DO 92 I=1,NPARAM
DP(I)=SQRT(XQ)*DP(I))

92 CONTINUE
DO 91 I=1,NPARAM,3
IP2=I+1
ANORMX=PARAM(I)*PARAM(I+2)*1.7725/ANORM
BNORMX(J)=ANORM*XKYLDC ENORM(J)*FLOAT(IThumb(I))/1000.

91 CONTINUE
BNORMX(J),DB(J),ENORM(J)

BNORMX(J)=ANORMX*KYLDC ENORM(J)

CALL TOGGLST(1T)
IFBITEST(1T,14) WRITE(6,125) J,PARAM(IP2),ANORMX,ENORM(J),

IF(OUTPT) WRITE(6,l nj)
FORMAT(1X,F12.3,5X,F12.3)
RETURN

END

C.....FUNCTION XKYLD, TO TRANSFORM RATIO TO RHODIUM TO
1 NANOGRAMS/CMK**2
FUNCTION XKYLD(E)
REAL P(8)
DATA P(1),P(2),P(3),P(4),P(5),P(6),P(7)/
1 1.2347,30.8516,39.138,19.348,1677.202,
2 1661.891,7126.553/

1 AMT=0.
DO 2 I=1,7
AMT=AMT+P(I)/(E)**(I-1)
2 CONTINUE
XKYLDC=10.**AMT
RETURN

END

SUBROUTINE LABEL(J,JPEAK)
REAL ENORM(30),ELE(30),KMN,CRMN,NI,NIBET,MO,BNORMX(30),DB(32)
INTEGER CH8(30),LIST(528),DATAD(4096)
LOGICAL CHECK
COMMON/F1NOUT/ELE,A1,A2
COMMON DATAD
EQUIVALENCE (CH8(1),DATAD(4211)),(LIST(1),DATAD(3073)),
1 (ENORM(1),DATAD(3002)),(BNORMX(1),DATAD(3861)),
2 (DB(1),DATAD(3921))
DATA CL,AP,K,SC,CA,TI/2HCL,2HAR,1HK,2HSC,2HCA,2HTL/, 
1 V,CR,MN,FE,Co,NI/IHV,2HCR,2HMN,0HFE,2HCO,2HNI/, 
2 CU,ZN,TL,L,SE,RR/2HCUS,2HZN,3HTLL,3HPP,2HSE,2HBP/, 
3 THL,RB,SR,ZR,MO/3HTHL,2HPP,2HSR,2HHR,2HM0/, 
4 CAS,SCI,TIV,VC,CRMN/5HCA-SC,5HSC-SC,5HSC-TI,4HTI-V, 
5 4HVC-5HCR-MN/, 
6 FEBET,NIBET,CUBET/5HFEBET,5HNI,5HSC/ 
7 ZNRET,PRRET,UNKWN/5HZNPET,5HRRRET,5H----/
NELE=(LIST(J))/3+J
DO 2 I=J,NELE
E=ENORM(I)
ELE(I)=UNKNOWN
IF(ABS(E-2.62) .LE. 0.06) ELE(I)=CL
IF(ABS(E-2.95) .LE. 0.06) ELE(I)=AR
IF(ABS(E-3.31) .LE. 0.06) ELE(I)=K
IF(ABS(E-3.69) .LE. 0.06) ELE(I)=CA
IF(ABS(E-4.09) .LE. 0.06) ELE(I)=S
IF(.NOT. CHECK .AND. (ABS(E-4.09) .LT. 0.06)) ELE(I)=SC
IF(ABS(E-4.95) .LE. 0.06) ELE(I)=T
IF(.NOT. CHECK .AND. (ABS(E-4.95) .LT. 0.06)) ELE(I)=V
IF(ABS(E-5.41) .LE. 0.06) ELE(I)=CR
IF(CHECK .AND. (ABS(E-5.41) .LT. 0.06)) ELE(I)=CR
IF(ABS(E-6.26) .LE. 0.06) ELE(I)=FE
IF(CHECK .AND. (ABS(E-6.26) .LT. 0.06)) ELE(I)=FE
IF(ABS(E-7.06) .LE. 0.06) ELE(I)=FERET
IF(CHECK .AND. (ABS(E-7.06) .LT. 0.06)) ELE(I)=FERET
IF(ABS(E-7.48) .LE. 0.06) ELE(I)=NI
IF(CHECK .AND. (ABS(E-7.48) .LT. 0.06)) ELE(I)=NI
IF(ABS(E-8.05) .LE. 0.06) ELE(I)=CU
IF(CHECK .AND. (ABS(E-8.05) .LT. 0.06)) ELE(I)=CU
IF(ABS(E-8.79) .LE. 0.06) ELE(I)=NI
IF(CHECK .AND. (ABS(E-8.79) .LT. 0.06)) ELE(I)=NI
IF(ABS(E-9.57) .LE. 0.06) ELE(I)=N
IF(CHECK .AND. (ABS(E-9.57) .LT. 0.06)) ELE(I)=N
IF(ABS(E-9.80) .LE. 0.06) ELE(I)=N
IF(CHECK .AND. (ABS(E-9.80) .LT. 0.06)) ELE(I)=N
IF(ABS(E-10.25) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-10.25) .LT. 0.06)) ELE(I)=T
IF(ABS(E-10.55) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-10.55) .LT. 0.06)) ELE(I)=T
IF(ABS(E-11.22) .LE. 0.06) ELE(I)=SE
IF(CHECK .AND. (ABS(E-11.22) .LT. 0.06)) ELE(I)=SE
IF(ABS(E-11.89) .LE. 0.06) ELE(I)=BR
IF(CHECK .AND. (ABS(E-11.89) .LT. 0.06)) ELE(I)=BR
IF(ABS(E-12.21) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-12.21) .LT. 0.06)) ELE(I)=T
IF(ABS(E-12.61) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-12.61) .LT. 0.06)) ELE(I)=T
IF(ABS(E-12.96) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-12.96) .LT. 0.06)) ELE(I)=T
IF(ABS(E-13.29) .LE. 0.06) ELE(I)=T
IF(CHECK .AND. (ABS(E-13.29) .LT. 0.06)) ELE(I)=T
SUBROUTINE SORT(CHECK,X,JPEAK)
INTEGER CHI(30),DATA(4096)
LOGICAL CHECK
REAL ELE(I),R(30),IPEAK
COMMON/INOUT/ELE,A1,A2
COMMON DATAD
EQUIVALENCE (CHI(1),DATA(4021)), (R,NORMX(1),DATA(3861)),
           (E,DATA(3921))
CHECK=.FALSE.
DO 2 I=1,JPEAK
     E=AI+FLOAT(CHI(I))A2
     IF(ABS(E-X),LE,0.13)GO TO 5
2 CONTINUE
      CHECK=.TRUE.
CONTINUE
RETURN
END

SUBROUTINE SCALI(NX,NY,NF)
C......SUBROUTINE TO CHANGE SCALES ON DISPLAY,
C........FOR USE WITH IPICK
INTEGER GATE(5,30),DATA(1024),CHI(30),DATAD(4096),CHMAX
COMMON/STUFF/GATE
COMMON DATAD
EQUIVALENCE (DATA(1),DATA(1025)), (CHI(1),DATA(4021))
I2=IROTOR(2)
NF=LIMIT(1256*I2-255,1024)
I3=IROTOR(3)
NX=LIMIT(8,13+7,12)
I4=IROTOR(4)
NY=LIMIT(8,14+6,18)
DO 10 I=1,30
   LI=CHI(I)
   IF(LI.EQ.0) LI=1
   GATE(I,1)=LIMIT(0,(CHI(I)-NF)*8/2**13,1023)
   GATE(2,1)=DATA(LI)/(2**14)*16
10 CONTINUE
RETURN
END
SUBROUTINE REED(ITYPE, FNAME, NEXT, EXIST)
C........SUBROUTINE TO READ DATA FROM TAPE FOR USE WITH IPK2
C.............AND SIMUL2
INTEGER DATA(1024), DATAD(4096), BKGN(1024)
REAL FNAME(2)
LOGICAL EXIST, BITEST
COMMON DDATA
EQUIVALENCE (DATA(I), DATAD(I025)), (BKGN(I), DATAD(2249))
CALL TOGGLS(IT)
IF(BITEST(IT, 15)) GO TO 3
CALL INPUT1(FNAME(1), HDNAME, 6)
CALL INPUT1(NEXT, 4HNEXT, 1)
CALL BCDEXT(FNAME, NEXT)
CALL FSTAT(tr, FNAME, EXIST)
IF(EXIST) GO TO 2
WRITE(6, l01) FNAME
IF(BITEST(IT, 15)) RETURN
GO TO 1
2 IF(ITYPE.EQ.1) CALL ZERO(DATA)
IF(ITYPE.EQ.1) WRITE(6, l01) FNAME
101 FORMAT(1HI, 12H RUN NUMBER , 2A5)
IF(ITYPE.EQ.2) CALL ZERO(BKGN)
CALL SEEK(I, FNAME)
IF(ITYPE.EQ.1) READ(I) TS, IRT, ILT, ND, (DATA(I), I=1, 1024)
IF(ITYPE.EQ.2) READ(I) TS, IRT, ILT, ND, (BKGN(I), I=1, 1024)
RETURN
100 FORMAT(IX, 6H FILE , 2A5, 12H NOT FOUND.)
END

SUBROUTINE MAXER(DATA, CHMAX)
INTEGER DATA(1024), CHMAX
CHMAX=450
DO 400 I=450, 1024
IF(DATA(I).GT.DATA(CHMAX)) CHMAX=I
400 CONTINUE
RETURN
END

SUBROUTINE SET1(CHMAX, IDAT, POINT)
C........ROUTINE TO SET UP CALL TO FITALL TO FIND HEIGHT OF C NORMALIZATION PEAK
INTEGER CHMAX, IDAT(1024), DATAD(4096), LIST(520)
REAL POINT(100), PARAM(15)
COMMON DDATA
EQUIVALENCE (LIST(I), DATAD(3073)), (PARAM(I), DATAD(4056))
IMAX=CHMAX+20
IMIN=CHMAX-20
BG2=IDAT(IMAX)
BG1=IDAT(IMIN)
DO 200 I=1, 41
ICO=IMIN+1-I
POINT(I)=IDAT(ICO)
200 CONTINUE
PARAM(2)=(BG1)
PARAM(1)=(BG2-BG1)/40.
PARAM(5)=6./1.665
PARAM(3) = FLOAT(IDAT(CHMAX)) - PARAM(2) - PARAM(1) * 20.
PARAM(4) = PARAM(4) + FLOAT(CHMAX - 21)
IF (LIST(4) .NE. 0) WRITE(6, 111) LIST(4)
111
ANORM = PARAM(3) * PARAM(5) * 1.7725
ABNORM = 40. * PARAM(2) + R00. * PARAM(1)
WRITE(6, 123) (PARAM(4), ANORM
WRITE(6, 124) ABNORM
124
FORMAT(*, X, 15 BACKGROUN DB HAS, F10. 3, 8H COUNTS.)
123
FORMAT(*, X, 29H NORMALIZATION PEAK IN CHANNE
1L, F10. 2, 4H HAS, F10. 2, 8H COUNTS.)
RETURN
END

SUBROUTINE OUTER(PARAM, LIST, ANORM, ABNORM, CHMAX)
INTEGER CHMAX, LIST(520)
REAL PARAM(15)
PARAM(4) = PARAM(4) + FLOAT(CHMAX - 21)
IF (LIST(4) .NE. 0) WRITE(6, 111) LIST(4)
111
ANORM = PARAM(3) * PARAM(5) * 1.7725
ABNORM = 40. * PARAM(2) + R00. * PARAM(1)
WRITE(6, 123) (PARAM(4), ANORM
WRITE(6, 124) ABNORM
124
FORMAT(*, X, 15 BACKGROUN DB HAS, F10. 3, 8H COUNTS.)
123
FORMAT(*, X, 29H NORMALIZATION PEAK IN CHANNE
1L, F10. 2, 4H HAS, F10. 2, 8H COUNTS.)
RETURN
END

SUBROUTINE SUBTR(ANORM, ABNORM, CHMAX, OUTPT, GAM)
INTEGER DATA(1024), CHMAX, DATA(4096), BKGND(1024)
REAL PARAM(15)
LOGICAL OUTPT, BITEST
COMMON DATA
EQUIVALENCE (DATA(1), DATA(1025)), (BKGND(1), DATA(2049)),
1 (PARAM(1), DATA(4056))
PARAM(4) = PARAM(4) + FLOAT(CHMAX - 21)
CNORM = PARAM(3) * PARAM(5) * 1.7725
CBNORM = 40. * PARAM(2) + R00. * PARAM(1)
WRITE(6, 123) (PARAM(4), CNORM
WRITE(6, 124) CBNORM
124
FORMAT(*, X, 15 BACKGROUN DB HAS, F10. 3, 8H COUNTS.)
RAT = ABNORM / CBNORM
DO 5 I = 1, 1023
5 IS = I - 2
DATA(I) = FLOAT(DATA(I)) - RAT * FLOAT(BKGND(I - 1) + BKGND(I) +
1 BKGND(I + 1))/3.
BKGND(IS) = FLOAT(DATA(I)) + 2. * RAT * FLOAT(BKGND(I - 1) +
1 BKGND(I) + BKGND(I + 1))/3.
IF (DATA(1) .LT. 0) DATA(1) = 0
CONTINUE
BKGND(1023) = 0
BKGND(1024) = 0
CALL TOGLS(IT)
IF (BITEST(IT, 15)) RETURN
WRITE(6, 105)
CALL INPUTI(OUTPT, SHOUTPT, 4)
CALL INPUTI(GAM, SIIAGAM, 2)
SUBROUTINE MULT(IMAX, IMIN, J)
INTEGER CHB(30), DATAD(4096)
LOGICAL DOUBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD, QUIN, UNQUIN
COMMON/MUP/ DOUBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD, QUIN,
1 UNQUIN, JPEAK,
1 GAM, IDUB, ITRIP, IQUAD, IQUIN
COMMON DATAD
EQUIVALENCE (CHB(1), DATAD(4021))
DOUBLE=.FALSE.,
TRIPLE=.FALSE.,
QUAD=.FALSE.,
QUIN=.FALSE.,
I0=CHB(J),
IMAX=CHB(J)+IFIX(GAM)
IMIN=CHB(J)-IFIX(GAM)
IF(UND0UR) GO TO 82
IF(J.EQ.JPEAK) GO TO 82
IF(CHB(J+1).LT.(I0+IFIX(4.*GAM))) DOUBLE=.TRUE.
IDUB=CHB(J+1)
IF(UNTRIP) GO TO 82
IF(J.EQ.JPEAK-1) GO TO 82
IF(CHB(J+2).LT.(IDUB+IFIX(4.*GAM))) TRIPLE=.TRUE.
TRIPLE=DOUBLE.AND.TRIPLE
ITRIP=CHB(J+2)
IF(QUAD) GO TO 82
IF(J.EQ.JPEAK-2) GO TO 82
IQUAD=CHB(J+3)
IF(UNQUAD) GO TO 82
IF(J.EQ.JPEAK-3) GO TO 82
IQUAD=CHB(J+4)
82
UND0UR=.FALSE.,
UNTRIP=.FALSE.,
UNQUAD=.FALSE.,
UNQUIN=.FALSE.,
IF(DOUBLE) IMAX=IDUB+IFIX(GAM)
IF(TRIPLE) IMAX=ITRIP+IFIX(GAM)
IF(QUAD) IMAX=IQUAD+IFIX(GAM)
IF(QUIN) IMAX=IQUN+IFIX(GAM)
RETURN
END

SUBROUTINE SIT2(IMAX, IMIN, J, ANORM)
C......TO PREPARE FINAL FIT TO DATA
REAL PARAM(15), POINT(102)
INTEGER DATA(1024), LIST(528), CHB(30), IR(5), DATAD(4096)
LOGICAL DOUBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD, QUIN, UNQUIN,
1 BITEST
COMMON/MUP/DOUBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD, QUIN,  
UNQUIN, JPEAK, GAM, IDUB, ITRIP, IQUAD, IQUIN
COMMON DATAD
EQUIVALENCE (DATA(1), DATAD(1025)), (LIST(1), DATAD(3073)),  
(CH(1), DATAD(2821)), (POINT(1), DATAD(3593)),  
(POINT(1), DATAD(3593)), (PARAM(1), DATAD(4056))
ITOT=IMAX-IMIN+1
DO 84 I=1, ITOT
IDOWN=IMIN+I-1
POINT(I)=FLOAT(DATA(IDOWN))
CONTINUE
I0=CH(1)
PARAM(14)=FLOAT(IQUIN-IMIN+1)
PARAM(15)=GAM/1.665
PARAM(13)=FLOAT(DATA(IQUIN))
PARAM(11)=FLOAT(IQUAD-IMIN+1)
PARAM(12)=GAM/1.665
PARAM(10)=FLOAT(DATA(IQUAD))
PARAM(7)=FLOAT(DATA(ITRIP))
PARAM(8)=FLOAT(ITRIP-IMIN+1)
PARAM(9)=GAM/1.665
PARAM(6)=FLOAT(IDUB)
PARAM(5)=FLOAT(IDUB-IMIN+1)
PARAM(4)=GAM/1.665
PARAM(3)=GAM/1.665
LIST(1)=ITOT
LIST(3)=3
LIST(4)=0
LIST(5)=12
LIST(6)=3
IF(.NOT.DOUBLE) GO TO 88
LIST(2)=6
LIST(6)=6
IF(.NOT.TRIPLE) GO TO 88
LIST(2)=9
LIST(6)=9
IF(.NOT.QUAD) GO TO 88
LIST(2)=12
LIST(6)=12
IF(.NOT.QUIN) GO TO 88
LIST(2)=15
LIST(6)=15
LIST(5)=15
CONTINUE
NPARAM=LIST(6)
CALL ZERO(IR)
ISUM=0
K=0
DO 95 I=1, NPARAM, 3
K=K+1
IF(PARAM(I).LT.0.0000300*ANORM) IR(K)=1
ISUM=ISUM+IR(K)
CONTINUE
LIST(2)=LIST(2)-3*ISUM
LIST(5)=LIST(5)-ISUM*3
LIST(6)=LIST(6)-3*ISUM
28
I=1
DO 97 I=1,K
IF(IR(I).NE.0) GO TO 97
PARAM(I)=PARAM(3*I-2)
PARAM(I+1)=PARAM(3*I-1)
PARAM(I+2)=PARAM(3*I)
I=I+3
97 CONTINUE
CALL TOGGLS(IT)
IF(DOUBLE.AND.(.NOT.TRIPLE).AND.BITEST(IT,14)) WRITE(6,115)
IF(TRIPLE.AND.(.NOT.QUAD).AND.BITEST(IT,14)) WRITE(6,116)
IF(QUAD.AND.(.NOT.QUIN).AND.BITEST(IT,14)) WRITE(6,118)
RETURN
115 FORMAT(1X,DIH DOUBLET)
116 FORMAT(1X,RH TRIPLET)
118 FORMAT(1X,DIH QUADRUPLET)
119 FORMAT(1X,DIH QUINTUPT)
END

SUBROUTINE IDENT(ELE,ENORM,BNORMX,DR,JPEAK,FNAME,NEXT)
C..........SUBROUTINE TO MAKE FINAL IDENTIFICATION OF ELEMENTS,
C..........AND MAKE CORRECTIONS FOR BETA PEAKS.
REAL ELE(30),ENORM(30),BNORMX(30),DR(30),FNAME(2),
1 ESI(24),ES2(24),ATOR(24),NAM(24),EFF(4)
LOGICAL BITEST,BETA
DATA ESI(1),ES2(1),ATOR(1),NAM(1)/2.62,2.81,0.2,HCL/,
1 ESI(2),ES2(2),ATOR(2),NAM(2)/2.96,3.19,0.2,HAR/,
2 ESI(3),ES2(3),ATOR(3),NAM(3)/3.13,3.58,0.1141HK/,
3 ESI(4),ES2(4),ATOR(4),NAM(4)/3.69,4.02,0.0092HCA/,
4 ESI(5),ES2(5),ATOR(5),NAM(5)/4.09,4.46,0.1052HSC/,
5 ESI(6),ES2(6),ATOR(6),NAM(6)/4.51,4.93,0.1052HT/,
6 ESI(7),ES2(7),ATOR(7),NAM(7)/4.95,5.42,0.1052HV/
DATA ESI(8),ES2(8),ATOR(8),NAM(8)/5.41,5.94,0.1142HCP/,
1 ESI(9),ES2(9),ATOR(9),NAM(9)/5.89,6.49,0.1082HNN/,
2 ESI(10),ES2(10),ATOR(10),NAM(10)/6.40,7.05,0.1062HFE/,
3 ESI(11),ES2(11),ATOR(11),NAM(11)/6.93,7.64,0.1182HCO/,
4 ESI(12),ES2(12),ATOR(12),NAM(12)/7.47,8.26,0.1052HNI/,
5 ESI(13),ES2(13),ATOR(13),NAM(13)/8.04,8.80,0.1132HCU/
DATA ESI(14),ES2(14),ATOR(14),NAM(14)/8.63,9.57,0.1172HZN/,
1 ESI(15),ES2(15),ATOR(15),NAM(15)/10.54,11.72,0.2832HAs/,
2 ESI(16),ES2(16),ATOR(16),NAM(16)/11.22,12.49,0.13,2HSe/,
3 ESI(17),ES2(17),ATOR(17),NAM(17)/11.92,13.29,0.1362HBr/,
4 ESI(18),ES2(18),ATOR(18),NAM(18)/14.64,15.83,0.1512HSh/,
5 ESI(19),ES2(19),ATOR(19),NAM(19)/15.77,17.66,0.1722HZn/
DATA ESI(20),ES2(20),ATOR(20),NAM(20)/17.48,19.60,0.182HMg/,
1 ESI(21),ES2(21),ATOR(21),NAM(21)/8.39,9.67,0.7752Hw/,
2 ESI(22),ES2(22),ATOR(22),NAM(22)/10.26,12.21,0.6722Ht/,
3 ESI(23),ES2(23),ATOR(23),NAM(23)/12.54,12.61,0.6452HPd/,
4 ESI(24),ES2(24),ATOR(24),NAM(24)/12.96,12.22,0.5532HTh/
DATA EPS,UNKNW/8.060,2H--/
DATA EFF(1),EFF(2),EFF(3),EFF(4)/1.775,1.66,1.66,2.02/
NEXT= NEXT+1
CALL BCDEXTC(FNAME,NEXT)
DO 4 I=3,JPEAK
ELEC(I)=UNKNW
DO 2 J=1,24
IF(ABS(ENORM(I)-ESI(I)).LT.EPS) GO TO 1

GO TO 2
BETA=.FALSE.
DO 3 K=I, JPEAK
IF(BNORMX(K) .GT. 0.3*RNOFMX(I)) BETA=.TRUE.
BNORMX(K)=BNORMX(K)-ATOR(J)*BNORMX(I)
IF(BNORMX(K) .LT. 0.) BNORMX(K)=0.
3 CONTINUE
IF(J.LT.21) ELE(I)=NAM(J)
IF(J.GE.21 .AND. BETA) GO TO 6
GO TO 2
ELE(I)=NAM(J)
BNORMX(I)=BNORMX(I)*EFF(J-20)
DR(I)=DR(I)*EFF(H-20)
2 CONTINUE
4 CONTINUE
CALL Toggls(IT)
IF(.NOT.BITEST(IT,13)) GO TO 5
CALL ENTER3(FNAME)
WRITE(3,100) (ELE(I),BNORMX(I),DR(I),I=3,JPEAK)
100 FORMAT(1X,IA5,2E11.5)
CALL CLOSE(3)
5 CALL Toggls(IT)
IF(.NOT.BITEST(IT,12)) RETURN
WRITE(6,103) FNAME
C........WRITE(6,104) G
C........FORMAT(1X,2HG=9F6.4)
WRITE(6,101)
WRITE(6,102) (ELE(I),BNORMX(I),DR(I),I=3,JPEAK)
RETURN
101 FORMAT(1X,7HELEMENT,ZX,13HCONCENTRATION,9H ERROR)
102 FORMAT(4X,IA5,E12.6,E12.6)
103 FORMAT(1HI,5X,2A5)
END

SUBROUTINE ERR0(J,IMIN,DP)
REAL ELE(30),BNORMX(30),DP(15),PARAM(15)
INTEGER LIST(520),DATAD(4096),IR(5),CH0(30)
LOGICAL DOUBLE,UNDOUB,TRIPLE,UNTRIP,QUAD,UNQUAD,QUIN,UNQUIN,
1 BITEST
COMMON /MUP/DouBLE,UNDOUB,TRIPLE,UNTRIP,QUAD,UNQUAD,QUIN,
1 UNQUIN,JPEAK,GAM,IDUB,ITRIP,IQUAD
COMMON DATAD
COMMON/FINOUT/ELE,A1,A2
EQUIVALENCE (LIST(1),DATAD(3073)),(BNORMX(1),DATAD(3861)),
1 (DB(1),DATAD(3921)),(IR(1),DATAD(4051)),(DATAD(4021),
2 CH0(1),PARAM(I),DATAD(4056))
DATA RNONE/4HNONE/
CALL Toggls(IT)
IF(BITEST(IT,14)) WRITE(6,111) LIST(4)
111 FORMAT(1H ERROR,TYPE,12)
IF(.NOT.DOUBLE) GO TO 89
IF(.NOT.TRIPLE) GO TO 90
IF(.NOT.QUAD) GO TO 91
IF(.NOT.QUIN) GO TO 92
UNQUIN=.TRUE.
RETURN
92 UNQUAD=.TRUE.
RETURN
91 UNTRIP=.TRUE.
RETURN
90 UNDOUB=.TRUE.
RETURN
89 PARAM(1)=0.
PARAM(3)=0.
PARAM(2)=FLOAT(CHO(J)-IMIN+1)
DP(1)=0.
DP(2)=0.
DP(3)=0.
RETURN
END

SUBROUTINE ENERG(IMIN,A1,A2,J,DP)
REAL PARAM(15),ENORM(30),DP(15)
INTEGER DATAD(4096),LIST(520),IR(5),CHO(30)
COMMON DATAD
EQUIVALENCE (DATAD(3R00),ENORM(1)),(LIST(1),DATAD(3073)),
1 (CH0(1),DATAD(4021)),(IR(1),DATAD(4051))
2 (PARAM(1),DATAD(4056))
K=J
ISUM=0
DO 2 I=1,5
IF(IR(I).EQ.0) GO TO 2
ISUM=ISUM+IR(I)
2 CONTINUE
KI=0
NPPEAK=LIST(6)/3
NPEAK=NPPEAK+ISUM
DO 3 I=1,NPEAK
MPEAK=NPEAK-1+I
M3PEAK=3*MPEAK
IF(IR(M3PEAK).EQ.0) GO TO 4
JMPEAK=J+MPEAK-1
PARAM(M3PEAK)=0.
DP(M3PEAK)=0.
PARAM(M3PEAK-1)=FLOAT(CH0(JMPEAK)-FLOAT(IMIN-1)
DP(M3PEAK-1)=0.
PARAM(M3PEAK-2)=0.
DP(M3PEAK-2)=0.
GO TO 3
4 N3PEAK=3*(NPPEAK-KI)
PARAM(M3PEAK)=PARAM(N3PEAK)
DP(M3PEAK)=DP(N3PEAK)
PARAM(M3PEAK-1)=PARAM(N3PEAK-1)
DP(M3PEAK-1)=DP(N3PEAK-1)
PARAM(M3PEAK-2)=PARAM(N3PEAK-2)
DP(M3PEAK-2)=DP(N3PEAK-2)
KI=KI+1
3 CONTINUE
LIST(6)=LIST(6)+3*ISUM
NPARAM=LIST(6)
DO 5 I=1,NPARAM,3
IP2=I+1
PARAM(IP2)=PARAM(IP2)+FLOAT(IMIN-1)
ENORM(CHO)=A1*PARAM(IP2)+A2
K = K + 1
5 CONTINUE
RETURN
END

SUBROUTINE LOCUM
C.....TO LOCATE PEAKS IN X-RAY FLUORESCENT ENERGY SPECTRA...
C.....TO BE USED WITH IPK3, AS PART OF AN EXECUTE FILE..SAVLOC
INTEGER DATA(1024), GATE(5,30), CH0(30), DATAD(4096), CHMAX,
1 CH1, CH2, CH3, CH4, CH5, RKGND(1024), GATI(140)
REAL C(36), R(36), PHI2, PHI
LOGICAL DOUBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD,
1 QUIN, UNQUIN
COMMON/STUFF/GATE
COMMON/MP5/DUDBLE, UNDOUB, TRIPLE, UNTRIP, QUAD, UNQUAD,
1 QUIN, UNQUIN, JPEAK, GAM, IDUR, ITIRP, IQUAD, IQUN
COMMON DATAD
COMMON/DIFF/C, P, M
EQUIVALENCE (DATA(1), DATAD(1025)), (CH0(1), DATAD(4021)),
1 (RKGND(1), DATAD(2049)), (GATI(1), GATE(1, 3))
CALL ZERO(GATI)
NHMAX = 470
M = IFIX((0.6 * GAM - 1.0) / 2.0)
IF(M.EQ.0) M = 1
C.....COMPUTE COEFFICIENT C(J)
CALL ZERO(C)
CALL ZERO(B)
C(1) = -0.2
C(2) = 0.1
C(3) = 0.
DO 31 L = 1, 5
DO 30 J = 1, 36
B(J) = C(J)
DO 30 K = 1, M
KI = J + K
K2 = J - K
IF(J = K, LE, P) K2 = K - J + 2
B(J) = B(J) + C(KI) + C(K2)
IF(KI.GT.36) R(J) = 0
30 CONTINUE
DO 31 J = 1, 36
C(J) = B(J)
31 CONTINUE

C.....COMPUTE GENERALIZED SECOND DIFFERENCE, S
C.....COMPUTE STANDARD DEVIATIONS IN S
PHI = C(1)**2
M1 = 5 * M + 2
DO 50 J = 2, M1
PHI = PHI + 2.0 * C(J)**2
50 CONTINUE
PHI2 = SQRT(PHI)
C.....COMPUTE CRITERIA FOR PEAK LOCATION
C.....NI = EXPECTED NUMBER OF CHANNELS IN NEGATIVE PEAK
NI = IFIX((1.22 * (GAM + 0.5))
NI = NI + 4
NI MIN = NI - 2
C.....BEGIN TO SEARCH FOR PEAKS
CH5 = 25
JPEAK=2
JPEAK=JPEAK+1
ICHNL=CH5
IF(ICHNL.EQ.NHMAX) GO TO 70
ICHNL=ICHNL+1
IF(S(ICHNL).GE.-1.6*PHI2*SORT(FLOAT(BKGND(ICHNL-2)+1))) GO TO 60
GO TO 62
IF(ICHNL.EQ.NHMAX) GO TO 70
ICHNL=ICHNL+1
IF(S(ICHNL+1).LT.(ICHNL).OR.(ICHNL-1).LT.(ICHNL)) GO TO 61
IF(S(ICHNL).LT.-1.6*PHI2*SORT(FLOAT(BKGND(ICHNL-2)+1))) GO TO 62
CH5=ICHNL
GO TO 59
CH4=ICHNL
GO TO 64
IF(ICHNL.EQ.NHMAX) GO TO 70
ICHNL=ICHNL+1
CH5=ICHNL-1
ICHNL=ICHNL+1
IF(ICHNL.LE.0.8*S(CH4)) GO TO 63
CH3=ICHNL+1
GO TO 67
IF(ICHNL.EQ.1) GO TO 59
ICHNL=ICHNL-1
IF(S(ICHNL).LT.0.) GO TO 65
CH2=ICHNL
GO TO 69
IF(ICHNL.EQ.1) GO TO 59
ICHNL=ICHNL-1
IF(S(ICHNL).LT.PHI2*SORT(FLOAT(BKGND(ICHNL-2)+1))) GO TO 66
CH1=ICHNL+1
C....COMPUTE EXPECTED WIDTHS
N2 MIN=IFIX((PHI2*SORT(FLOAT(DATA(CH4)+1)))/ABS(S(CH4)))+0.5
N2 MAX=IFIX((PHI2*SORT(FLOAT(DATA(CH4)+1)))/ABS(S(CH4)))+0.5
N3 MIN=IFIX(FLOAT(N1 MIN)*(1.-2.*PHI2*SORT(FLOAT(DATA(CH4)+1)))/
ABS(S(CH4)))+0.5
N3 MAX=IFIX(FLOAT(N1 MAX)*(1.-2.*PHI2*SORT(FLOAT(DATA(CH4)+1)))/
ABS(S(CH4)))+0.5
C........IF(CH5-CH3+1.LT.N1 MIN) GO TO 59
C........IF(CH5-CH3+1.GT.N1 MAX) GO TO 59
C........IF(N2 MAX.EQ.0) GO TO 72
C........IF(CH3-CH2-1.GT.N2 MAX) GO TO 59
GO TO 73
72 IF(CH3-CH2-1.GT.1) CONTINUE
73 IF(CH2-CH1+1.LT.N3 MIN) CONTINUE
CH0(JPEAK)=CH4
GATE(1,JPEAK)=CH4
GATE(2,JPEAK)=DATA(CH4)
GATE(3,JPEAK)=0
GATE(4,JPEAK)=128
GATE(5,JPEAK)=-10
CALL SCAL1(NX,NY,NF)
GO TO 58
70 JPEAK=JPEAK-1
RETURN
REFERENCES


### TABLE I. - ELEMENTS RECOGNIZED BY SAVLOC

**(a) K series**

<table>
<thead>
<tr>
<th>Element</th>
<th>K₂ energy, keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorine</td>
<td>2.62</td>
</tr>
<tr>
<td>Argon</td>
<td>2.96</td>
</tr>
<tr>
<td>Potassium</td>
<td>3.313</td>
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<td>Calcium</td>
<td>3.691</td>
</tr>
<tr>
<td>Scandium</td>
<td>4.090</td>
</tr>
<tr>
<td>Titanium</td>
<td>4.510</td>
</tr>
<tr>
<td>Vanadium</td>
<td>4.952</td>
</tr>
<tr>
<td>Chromium</td>
<td>5.414</td>
</tr>
<tr>
<td>Manganese</td>
<td>5.898</td>
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<tr>
<td>Iron</td>
<td>6.403</td>
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<tr>
<td>Cobalt</td>
<td>6.930</td>
</tr>
<tr>
<td>Nickel</td>
<td>7.477</td>
</tr>
<tr>
<td>Copper</td>
<td>8.047</td>
</tr>
<tr>
<td>Zinc</td>
<td>8.638</td>
</tr>
<tr>
<td>Arsenic</td>
<td>10.543</td>
</tr>
<tr>
<td>Selenium</td>
<td>11.221</td>
</tr>
<tr>
<td>Bromine</td>
<td>11.923</td>
</tr>
<tr>
<td>Strontium</td>
<td>14.164</td>
</tr>
<tr>
<td>Zirconium</td>
<td>15.774</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>17.478</td>
</tr>
</tbody>
</table>

**(b) L series**

<table>
<thead>
<tr>
<th>Element</th>
<th>L₂α energy, keV</th>
<th>L₂β energy, keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tungsten</td>
<td>8.396</td>
<td>9.670</td>
</tr>
<tr>
<td>Thallium</td>
<td>10.266</td>
<td>12.210</td>
</tr>
<tr>
<td>Lead</td>
<td>10.549</td>
<td>12.611</td>
</tr>
<tr>
<td>Thorium</td>
<td>12.966</td>
<td>16.200</td>
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</table>

### TABLE II. - PARAMETERS USED TO DESCRIBE X-RAY EFFICIENCY FUNCTION F(E)

<table>
<thead>
<tr>
<th>I</th>
<th>P(I)</th>
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<tr>
<td>1</td>
<td>0.855</td>
</tr>
<tr>
<td>2</td>
<td>54.874</td>
</tr>
<tr>
<td>3</td>
<td>-705.322</td>
</tr>
<tr>
<td>4</td>
<td>5499.011</td>
</tr>
<tr>
<td>5</td>
<td>-22895.21</td>
</tr>
<tr>
<td>6</td>
<td>48343.26</td>
</tr>
<tr>
<td>7</td>
<td>-40357.17</td>
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</tbody>
</table>
Figure 1. - X-ray fluorescence facility.
Figure 2. - Typical X-ray spectrum.
Figure 3. - Functional control panel.

Figure 4. - Typical X-ray spectrum after background subtraction.
RUN NUMBER SEPT 01

NORMALIZATION PEAK IN CHANNEL 580.93 HAS 52878.78 COUNTS.
BACKGROUND HAS 52878.78 COUNTS.

NEXT(I) = 0

NORMALIZATION PEAK IN CHANNEL 580.93 HAS 52878.78 COUNTS.
BACKGROUND HAS 52878.78 COUNTS.

DO YOU WISH EXTRA OUTPUT?

OUTPT(I) = F

ENERGIES FOR CALIBRATION:

El(R): 16.403
E2(R): 112.611

ENERGIES CONCENTRATION ERROR (UGRAMS/IH)*P>

<table>
<thead>
<tr>
<th>CHANNEL</th>
<th>STRENGTH</th>
<th>ENERGY</th>
<th>CONCENTRATION</th>
<th>ERROR</th>
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</thead>
<tbody>
<tr>
<td>3</td>
<td>78.035</td>
<td>3.701</td>
<td>.29701+02</td>
<td>.19374+01</td>
</tr>
<tr>
<td>4</td>
<td>91.404</td>
<td>4.516</td>
<td>.49822+02</td>
<td>.38400+01</td>
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</table>

DOUBLET

<table>
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<tr>
<th>CHANNEL</th>
<th>STRENGTH</th>
<th>ENERGY</th>
<th>CONCENTRATION</th>
<th>ERROR</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>128.084</td>
<td>5.912</td>
<td>.22555+01</td>
<td>.78361+00</td>
</tr>
<tr>
<td>6</td>
<td>148.871</td>
<td>6.483</td>
<td>.28154+03</td>
<td>.24637+01</td>
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</table>

QUADRUPELT

<table>
<thead>
<tr>
<th>CHANNEL</th>
<th>STRENGTH</th>
<th>ENERGY</th>
<th>CONCENTRATION</th>
<th>ERROR</th>
</tr>
</thead>
<tbody>
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<td>7</td>
<td>157.888</td>
<td>7.048</td>
<td>.22282+02</td>
<td>.15199+01</td>
</tr>
<tr>
<td>8</td>
<td>168.686</td>
<td>7.461</td>
<td>.23297+01</td>
<td>.94850+00</td>
</tr>
<tr>
<td>9</td>
<td>183.969</td>
<td>8.047</td>
<td>.40854+01</td>
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DOUBLET

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<th>CONCENTRATION</th>
<th>ERROR</th>
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Figure 5. - Sample of first page of teletype output.

SEPT 011

ELEMENT CONCENTRATION ERROR ELEMENT CONCENTRATION ERROR

| CA     | .259807+00 | .193737+01 |
| TI     | .498054+00 | .380084+01 |
| MN     | .255552+01 | .785055+00 |
| FE     | .220912+03 | .246371+01 |
| WI     | .151919+01 | .380084+01 |
| Cu     | .498054+00 | .380084+01 |
| ZN     | .397109+00 | .151919+01 |
| PR     | .341605+00 | .246371+01 |
| BR     | .008675+00 | .246371+01 |
| ZR     | .397109+00 | .151919+01 |
| MO     | .163229+02 | .29195+00 |

Figure 6. - Sample of second page of teletype output.
RUN NUMBER SEPT 011

NORMALIZATION PEAK IN CHANNEL 501.93 HAS 526878.78 COUNTS.
NORMALIZATION PEAK IN CHANNEL 501.48 HAS 648537.67 COUNTS.

DO YOU WISH EXTRA OUTPUT?

ENERGIES FOR CALIBRATION:
\( E_1^{(R)} = 36.403 \)  
\( E_2^{(R)} = 72.611 \)  
\( G = 0.0000 \)

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<td>6.546</td>
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<tr>
<td>3</td>
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<td>0.04439</td>
<td>4.516</td>
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QUADRUPELET

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DOUBLET

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<th>CONCENTRATION</th>
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<tr>
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<td>14.757</td>
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</tbody>
</table>

Figure 7. - Sample of augmented page 1 teletype output.
1. Exist = T
   Set data = 0
   Start ADC

2. Next > nlast?
   Yes
   Read file name and number (teletype)
   Set data = 0
   Start ADC
   Exist = T?
   Yes
   Up
   Timed out?
   No
   Down
   Yes
   Is ADC on?
   Yes
   Stop ADC
   Write data (dectape)
   Next = next + 1
   Up
   T15
   Down
   No
   B2
   P
   B1
   P
   B4
   P
   Timed out?
   Yes
   No
   Change sample

Figure 8. - Flow
Write results (dectape)

Down T13

Write page 2 of results (teletype)

Down T12

Write page 1 of results (teletype)

Up T14

Do least-squares fit to data

Up T16

Do new calibration based on peaks 1 and 2

Down T11

Locate peaks automatically

Up T11

Set exist = F

Up T15

Does file exist?

Yes

Read data (dectape)

N = N + 1

Fit rhodium peak

Down T15

No

Reading background file name, number (teletype)

Read background file exist?

Yes

Read background data (dectape)

No

Read background data (dectape)

B64

Ignore last peak selected

B32

B128

Select peak with light pen

Subtract background

Fit rhodium peak

chart for program.
"The aeronautical and space activities of the United States shall be conducted so as to contribute ... to the expansion of human knowl-
edge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."
—National Aeronautics and Space Act of 1958

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