Pivotal Regression Analysis of Gamma-Ray Spectra from NaI(Tl) Detector

G. W. Phillips et al.

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Program PREGA was developed at NRL to perform a fast and efficient regression analysis of a gamma-ray spectrum from an unknown source, taken with a NaI(Tl) detector. The analysis determines the best subset from a library of standard spectra to use in fitting the data. Output at each step includes relative intensities and uncertainties for each standard used in the fit, plus the partial F statistic for significance of each library element. Final output includes an analysis of variance (ANOVA) table, distribution of residuals, location of largest residuals, distribution of runs of consecutive residuals with the same sign, and the location of largest runs. The program was written for the Nuclear Data ND6620 computer and has been transferred to VAX II/780.
11. TITLE (Include Security Classification)

PROGRAM PREGA — Pivotal Regression Analysis of Gamma-Ray Spectra from NaI(Tl) Detectors for the ND6620 Computer
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Program PREGA
Pivotal Regression Analysis
of Gamma-Ray Spectra from
NaI(Tl) Detectors
for the ND6620 Computer

1. INTRODUCTION

Gamma-ray pulse-height spectra from NaI(Tl) detectors often contain few or no discernable peaks due to the source of interest, as a result of the poor intrinsic resolution of these detectors and a predominance of background gamma rays. Even after background subtraction, the resulting spectrum is often of too poor a quality to reveal characteristic peaks. Thus, one cannot do a peak analysis such as is usually performed on gamma-ray spectra from high-resolution germanium diode detectors (see Ref. 1).

However, there is often sufficient information contained in such spectra in the overall spectral shape to identify the source of the gamma rays by comparison to a library of standard source shapes. The situation becomes more complicated when the spectrum may be due to a superposition of gamma-ray spectra from two or more sources. To determine the relative contributions of the individual sources it is necessary to do a multiple least-squares fit of the unknown source spectrum to a library of standard source spectra using regression analysis techniques.

The ALPHA-M program was developed at Oak Ridge\(^2\) to perform such a fit and calculate the concentrations of each of the standards in the unknown.

However, if there are more than a very few standards in the library, such a procedure often gives an ambiguous result, due to correlations between library spectra. In such a case, it is necessary to do a systematic search for the subset of library standards which gives the best fit to the unknown spectrum. Program PREGA was developed at NRL to efficiently perform this search for the best subset. It works in one of two optional modes.

The first mode is similar to standard stepwise regression analysis methods. It begins with a subset containing only background, and performs a least-squares fit for the intensity of the background in the unknown spectrum. It then calculates the correlation of the residual spectrum, not accounted for by background, with each of the remaining standards in the library. That standard with the largest correlation is added to the fitting subset and a new least-squares fit is performed. This continues until no remaining standards are significantly correlated with the residuals.

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The second mode begins with a fit to the full library. From the results of this fit a test set of library members most correlated with the unknown spectrum is selected. Additional library members are then pivoted in and out of the test set, depending on their correlation with the residuals, until the subset which gives the best significant fit is obtained.

PREGA begins by calculating the matrix of cross-correlations of the library members with each other and with the unknown spectrum. It then operates on this matrix using a method by Garside to obtain the quantities of interest in the fit with a minimum of mathematical manipulations. At no time is it necessary to do a complete matrix inversion, and individual library members can be pivoted into and out of the fit quickly and simply. This method is thus tailor-made for either the stepwise mode or the full library mode of PREGA.

The program PREGA is implemented as an extensive modification of the program NAI supplied by Nuclear Data, Inc. and runs on the Nuclear Data ND 6620 system. It is written in DEC RT-11 FORTRAN and is currently being adapted to run on the Digital Equipment Corporation VAX 11/780.

2. SETUP FOR ANALYSIS

Preparation of Library

Library spectra should be taken for each source of interest under conditions as close as possible as those under which the unknown spectrum is taken. Backscattering of gamma rays by nearby materials can affect the shape of the spectrum as can attenuation due to intervening materials between the source and detector. This results in removal of counts from the full-energy peaks and the addition of counts with lower energy due to scattered gamma rays.

Background spectra taken before and after each library spectrum should be normalized by counting time and subtracted from the library spectrum. An energy calibration must be determined either from known peaks in the library or background spectra, or from a calibration source spectrum taken before and after each library spectrum. Program PKANAL is included in the PREGA package and may be used to determine the position of the peaks. At least two peaks are needed, well separated in energy, to determine a linear calibration of peak energy $E$ versus channel number $I$ in the form

$$E(I) = E_0 + I \cdot E_1.$$  

If more than two peaks are available a linear least squares fit can be used to determine the offset $E_0$ and slope $E_1$. These should be recorded with each library spectrum along with source type, configuration, strength, range, attenuation and any other pertinent information.

Preparation of Background

A background spectrum should be taken as close as possible in time and other conditions to the unknown, preferably immediately before and after. An energy calibration should be obtained in the same manner as for the
library spectra. Program GSHIFT can then be used to shift the slope and offset of each library member to match the slope and offset of the unknown spectrum. PREGA has the option of subtracting the background from the unknown before fitting. Nevertheless, the background spectrum should be included in the library, because background intensity changes could lead to over or under subtraction. If this happens, a negative intensity may result for the background. To allow for this PREGA has the option of not allowing the background to be pivoted out. (A negative intensity for any other library member is generally not physically allowable and should be rejected).

Preparation for PREGA

The library to be used in the fit is specified interactively in the program SEDIT. The standard name, file name, counting time and half-life activity are specified for each library member. A background spectrum, which may be subtracted from each library member, must be specified although this is generally not used.

The unknown and its background are specified interactively in the program UEDIT. This also allows the user to select various options to be used in the fit and to select which of the library members will be used. The information entered by the user in SEDIT and UEDIT are written to control files which are used by PREGA to perform the fit. Thus PREGA requires no direct input from the user and can be run as a batch job if desired. Output is usually to a file which can be listed later on the lineprinter.

Selection of Mode

If only one or two library members are expected to be present together in the unknown, the stepwise mode of PREGA is usually more efficient than the mode which begins by using the entire library in the fit. If multiple library members may be present, it is usually best to run both modes. They will generally, but not always, agree on the subset of library members which give the best fit. In cases where they do not agree, correlations between library members or linear combinations of library members will be found to cause ambiguities in the fit. Enough information is printed out at each step for the analyst to determine which library members are causing the ambiguity. They can either be eliminated from the library or accepted as doubtful contributions to the unknown spectrum.

3. ALGORITHMS

Partial F Test

The criterion used for selection or rejection of library members at each step is given by the partial F-test statistic $F_p$ defined in Chapter 4. For convenience, this is converted to an equivalent normally distributed parameter $X(F)$ which gives the value of $F_p$ in standard deviations (sigma units). This is compared to a threshold $F_0$ usually set at 2.5 sigma.
Full PREGA

The full PREGA algorithm begins with the fit to the complete library and selection of the trial subset C. It then goes directly to the regression on the trial subset C. PREGA then pivots library elements out (backward step) and in (forward step) successively, based on the partial F-values, until a best fit is found. The full PREGA algorithm proceeds as follows:

1. Do the fit to the complete library L.
2. Let the trial subset C include all library elements I with a relative intensity $B_I$ and error $\sigma_I(B)$ such that
   
   $$\frac{B_I}{\sigma_I(B)} > 1.$$ 

3. Let $E$ be the set containing all library elements included in the fit at each step. Initially let $E = C$.
4. Let $D$ be the set of elements not in the fit at the beginning of step 6, below. Initially let $D = 0$ (empty set).
   a. Let $C = E$.
   b. Calculate partial F to remove, $F_p(I)$, for all library elements $I$ in $C$.
   c. Let $F_p(J) = \text{min } F_p(I)$, for all $I$ in $C$, and convert to $X(F)J$ in sigma units.
   d. IF: $X(F)J < F_0$,
      THEN: remove $J$, let $E = E - J$;
      ELSE: continue.
   e. IF: $E = L - D$, (no change in trial subset)
      THEN: end regression (go to 7);
      ELSE: continue.
   a. Let $D = L - C$
   b. Calculate partial F to include, $F_p(I)$, for all library elements $I$ in $D$.
   c. Let $F_p(J) = \text{max } F_p(I)$, for all $I$ in $D$, and convert to $X(F)J$ in sigma units.
d. IF: \( X(F) J > F_0 \),
THEN: include \( J \), let \( E = E + J \);
ELSE: continue.

e. IF: \( E = C \), (no change in trial subset)
THEN: end regression (go to 7);
ELSE: repeat pivots, go to 5.

7. End regression: do analysis of variance, calculate residuals and runs, and print out results.

Stepwise PREGA

The stepwise PREGA mode is implemented as an option of program PREGA. It is run by setting the Background Regression (BR) parameter in UEDIT to
1: trial set = background only. The stepwise mode proceeds as follows:

1. Begin regression with fit to background only.
2. Let the trial subset \( C = \) (background).
3. Initially let \( E = C \).
4. Go to the forward pivot (step 6) of the full PREGA mode and proceed from there on as in the full PREGA.

4. FORMULAS AND DEFINITIONS

1. Let \( Y \) be the vector of the observed source data spectrum,
\[
Y = \{y(1), y(2), \ldots, y(N)\},
\]
and let \( X_I \) be a similar vector for the spectrum of library element \( I \).

2. Define the augmented cross-product matrix \( S_L \) of dimension \( K \), where the number of library elements is \( K-I \), by
\[
S_L = \begin{cases} S_{IJ} & \text{for } I, J = 1, \ldots, K \\
\end{cases}
\]
where
\[
S_{IJ} = (X_I \cdot S_J), \text{ for } I, J=1, \ldots, K-1 \\
S_{IK} = (X_I \cdot Y) \\
S_{KJ} = (Y \cdot X_J) \\
S_{KK} = (Y \cdot Y),
\]

5
and the dot product
\[ (x_i \cdot x_j) = \sum_{r=1}^{N} w(r) x_i(r) x_j(r) \]
The weights \( w(r) \) are calculated by the inverse Poisson variances of the data \( y(r) \).

3. The least squares solution for
\[
Y = B X + \epsilon,
\]
where \( \epsilon \) is the vector of random errors in the data, is given by
\[
B = (X^T X)^{-1} (X^T Y)
\]
where \( B \) is the vector of coefficients of the library elements in the fit,
\[
B = \{B_1, \ldots, B_{k-1}\}.
\]

4. The residual sum of squares is given by
\[
\text{RSS} = (Y - BX)^T (Y - BX) = (Y^T Y) - (X^T Y)(X^T X)^{-1}(X^T Y).
\]

5. The results of a regression of \( Y \) on a subset \( C \) of the library \( L \) can be completely determined from the matrix \( S^*_C \) obtained by successive pivots \( \phi \) on the matrix \( S_L \), for each library element in \( C \). The pivot operation used in PREGA is described by Garside. The results for \( N \) data points and \( P \) elements \( I \) in \( C \) are
\[
B_I = S^*_{IK}
\]
\[
\text{RSS}_C = S^*_K K
\]
\[
\hat{\sigma}_C^2 = \text{RSS}_C / (N-P)
\]
\[
\sigma_I(B)^2 = S^*_{II} \hat{\sigma}_C^2
\]
6. The partial F-test\(^4\) to remove library element \(I\) from \(C\) is given, for \(H = C - I\), by

\[
F_p^{-}(I) = \frac{RSS_H - RSS_C}{(RSS_C/(N-P))}
\]

\[
= \frac{B_i^2}{\sigma_i^2(B)}
\]

\[
= \frac{(N-P)(S_{IK}^*)^2}{(S_{II}^* S_{KK}^*)}
\]

then

\[
RSS_H = RSS_C (1 + F_p^{-}/(N-P)).
\]

7. The partial F test to include library element \(J\) not in \(C\) is given, for \(G = C + J\), by

\[
F_p^{+}(J) = \frac{RSS_C - RSS_G}{(RSS_G/(N-P-1))}
\]

where

\[
RSS_G = RSS_C(1 - R_{JK,C}^2)
\]

and the partial correlation coefficient of \(J\) and \(K\) given \(C\) is just\(^6\)

\[
R_{JK,C}^2 = \frac{(S_{JK})^2}{(S_{II}^* S_{ KK}^*)}.
\]

8. An approximate normal transformation for \(F\) with \(D,1\) degrees of freedom is used,\(^*\)

\[
X(F) \approx \sqrt{F} (1 - 1/4D)/(1 - F/2D)^{1/2}
\]

(note that for \(D \gg 1\) and \(D \gg F\) then \(X \approx \sqrt{F}\)).

9. An approximation for the probability of obtaining a random value greater than \(X\) is used,\(^*\)

\[
Q(X) \approx Z(X)(a_1 t + a_2 t^2 + a_3 t^3)
\]

where

\[
Z(X) = \exp(-X^2/2)/(2\pi)^{1/2},
\]

\[
t = 1/(1 + px),
\]

and

\[
a_1 = .436184, \ a_2 = -.120168, \ a_3 = .937298, \ p = .33267.
\]

5. PROGRAM PKANAL

Operation

Program PKANAL reads in data from ND spectral files and calculates a background, peak positions, width and area for selected regions.

Language

The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

Inputs

Diskfile
Logical unit (LU) 8, spectral data in ND format

Keyboard
LU 5, operator inputs first and last channels for up to 20 regions followed by one or more filenames containing spectra to be analyzed

Outputs
LU6, table of results for each spectrum

Input Variables

Record 1a,...
JL, JR lower and upper limits of each region to be analyzed, one pair of limits per record up to a maximum of twenty (20), terminated with a double carriage return

Record 2o,...
filenames for spectra to be analyzed, one per record, terminated with a double carriage return

Lineprinter Output

Heading
Contents
REGION LIMITS input limits (JL, JR) for region
PEAK LIMITS limits determined by the program for the peak
HEIGHT maximum peak height above background
AREA net peak area above background
BKGD background area beneath the peak
CENTROID calculated peak position (center of gravity)
VARIANCE calculated variance about centroid
FWHM peak full width at half maximum
ENERGY calibrated energy of centroid position
Subroutines Called
FREEFM  free field input routine
GET  reads spectrum from ND spectral files
PEAKNL  does peak analysis for each region

6. PROGRAM GSHIFT

Operation
Program GSHIFT reads in a spectrum and its energy calibration from disk, performs a specified gain shift and zero offset, and writes the shifted spectrum and its calibration back to disk.

Language
The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

Inputs
Diskfile  logical unit (LU) 8, spectral data in ND format
Keyboard  LU5, operator inputs filenames and selects new gain or desired shift

Outputs
Diskfile  LU8, shifted spectrum in ND format
CRT  LU5, prompts to operator, energy calibration from header, etc.

Input from Keyboard

<table>
<thead>
<tr>
<th>Rec.</th>
<th>Prompt</th>
<th>Response</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>FILENAME FOR SPECTRUM</td>
<td>FILE.ELEMENT (for input spectrum)</td>
</tr>
<tr>
<td>2a.</td>
<td>ENERGY CALIB. FROM HEADER GIVES ...</td>
<td>YES (go to 3a.), or NO (go to 2b), (default = NO)*</td>
</tr>
<tr>
<td>2b.</td>
<td>ENTER OLD SLOPE, OFFSET</td>
<td>slope, offset (for calibration of input spectrum)</td>
</tr>
</tbody>
</table>
3a. TO GET NEW SLOPE AND OFFSET... FILE ELEMENT
    (spectrum with desired slope and offset in header, go to 4),
    (default, go to 3b)*

3b. ENTER NEW SLOPE, OFFSET slope, offset
    (for desired calibration, go to 4),
    (default, go to 3c)*

3c. ENTER GAIN, ZERO SHIFT desired gain, zero shift

4. FILENAME FOR OUTPUT SPECTRUM FILE ELEMENT

*immediate carriage return gives default values

Subroutines Called
GET reads spectrum and energy calibration from ND spectral file
FREEFM free field input routine
REGAIN performs gain and zero shift
RECHAN restores proper channel offset after call to REGAIN
PUT writes spectrum and energy calibration to ND spectral file
7. PROGRAM PREGA

Operation

Program PREGA performs a stepwise or pivotal regression analysis in order to fit a data spectrum to the "best" subset of a library consisting of a background spectrum and several characteristic source spectra. The program is essentially a modification to the Nuclear Data Inc. ND6600 NAI Data Reduction Package, designed to make analysis more efficient for the user. Therefore, the basic package architecture used by Nuclear Data Inc. is still retained as far as program input, file structure and logical units used is concerned. The general flow of PREGA is given in the flow chart in Fig. 1. A more detailed flow chart is given in Appendix B.

Language

The program is written in DEC RT11 FORTRAN and runs on the Nuclear Data ND6620 computer under the MIDAS operating system.

The program PREGA does not accept information directly from the user to perform its calculations; parameters and calculation options are entered through, and edited by, the editor programs SEDIT and UEDIT. All spectral data acquired by the user are stored on disk files and automatically read by PREGA; the user has only to indicate, via the editor programs, the locations of the spectral data.

For the purposes of this discussion, all input data may be grouped into six categories:

(1) spectral data
(2) individual library standard parameters
(3) all library standard parameters and calculation options
(4) sample spectrum parameters
(5) sample background parameters and calculation options
(6) weighting factor calculation options

On the following pages are listed all the necessary input data for the PREGA Program; where user options are available, they are mentioned.

For a more complete description of the input data, the user is referred to the section containing the listings and descriptions of the programs UEDIT and SEDIT. The actual use of UEDIT and SEDIT by PREGA is referred to in the section on software organization.

(1) Spectral Data

Gamma-ray spectra are acquired by the user in the laboratory and written on a disk file in spectral data format.

(2) Individual Library Standard Parameters

a. (standard number: 1 to 10 assigned by SEDIT in sequential order)
b. standard name: 8 characters maximum

c. location of individual standard spectrum on disk file LU-8:
   FILE.ELEMENT(,DEVICE)

d. half-life

e. half-life units: Y,D,H,M or S

f. counting time in seconds

g. activity (concentration): usually set to 1, or may be set to
   convenient units

(3) All Library Standard Parameters and Calculation Options

a. number of channels per standard: maximum 512

b. initial channel number

c. final channel number

d. location of background spectrum on disk file LU-8:
   FILE.ELEMENT(,DEVICE)

e. counting time for background spectrum, in seconds

f. background subtracted from spectrum: Yes or No?

g. number of isotopes used from library

h. printout order of library standards

i. library standard rejection coefficient; usually \( B/\sigma \) < 1

j. rejection coefficient applied Yes or No?

k. F-test rejection coefficient; usually set to 2.5

(4) Sample Spectrum Parameters

a. location of sample spectrum on disk file LU-8:
   FILE.ELEMENT(,DEVICE)

b. counting time, in seconds

c. volume reduction factor; usually set = 1

d. decay time, in seconds; set = 1

e. result multiplication factor; usually set = 1

(5) Sample Background Parameters and Calculation Options

a. location of sample background spectrum on disk file LU-8:
   FILE.ELEMENT(,DEVICE)

b. background supplied: Yes or No

c. is background to be subtracted from the sample spectrum Yes or
   No

d. counting time of background spectrum, in seconds

(6) Weighting Factor Calculation Options

a. How determined; user has 2 options:
   option 1: based on original spectral counts and held
   constant
   option 2: based on least-squares spectrum counts

b. weighting factor calculation: user has 3 options
   \( p_i = \text{weighting factor, } y_i = \text{sample counts, } b_i = \text{normalized bkg counts} \)
   option 1: \( p_i = 1/y_i \)
   option 2: \( p_i = 1/(y_i+b_i) \)
   option 3: \( p_i = 1 \)
Outputs

The output device, usually a line printer, prints out the following items in the order indicated: (see examples in Appendix A).

1. sum of standards
2. sample spectrum counts in each channel
3. sum of background and sample counts
4. "BACKGROUND NOT INCLUDED AS A STANDARD"
5. "PIVOT ON BACKGROUND PERMITTED"
6. correlation matrix
7. "STARTING ANALYSIS WITH TRIAL SET=BACKGROUND ONLY"
8. Result of current regression
9. Final Result
10. LLNL R-STATISTIC
11. Final Statistics for eliminated standards
12. residuals/standard deviations per channel
13. suspicious channels
14. Distribution of residuals
15. Distribution of Runs
16. locations and sizes of large runs

*These items are intended as visual flags in the output for the analyst.

1. "SUM OF STANDARDS"

For each standard nuclide in the complete library, the program gives the total number of counts in all channels recorded during the counting time of the radionuclide. These sums are printed out in the same order as the nuclides appear in the library. For the example shown in Appendix A, the complete library contained five (5) standards. In fitting the sample spectrum only four (4) of these standards are actually used. This is the last stage of the program in which the complete library is handled. All subsequent calculations only use the library standards (in the order in which they are listed in variable OR) given in the program UEDIT.

2. "SAMPLE SPECTRUM"

On the first line is printed the disk file location (LU-8) of the sample spectrum FILE.ELEMENT(),DEVICE). The sample counts minus the background counts for each channel are then printed. The background counts are multiplied by the ratio of the counting time of the sample to the counting time of the background to correct for any differences in counting times. The printout should be read horizontally from left to right.

3. "BACKGD SUM" and "SAMPLE SUM"

These are the background and sample counts in each channel (see "SAMPLE SPECTRUM" listed above) summed from the initial channel for computation to the final channel for computation. See page 36, program lines 129 and 134.
(4) "BACKGROUND NOT INCLUDED AS A STANDARD"

This is an output flag that is printed only when the background is not included as one of the selected library standards. **NOTE** For this flag to be functional the background spectrum must be standard No. 1 in the complete library list. The user is referred to the section on the program SEDIT.

(5) "PIVOT ON BACKGROUND PERMITTED"

This flag is output when the variable BP in UEDIT is set equal to one (BP = 1). It means that the user wants to allow the program to perform pivot operations on the background if the calculation allows them. **NOTE** This flag requires the background spectrum to be standard No. 1 in the full library (see SEDIT).

(6) "CORRELATION MATRIX"

This matrix is calculated to show the correlation of the user chosen set of standards with themselves and the sample. The standards are output in the order given by the variable OR in UEDIT. The sample always occupies the last row and column of the matrix.

(7) "STARTING ANALYSIS WITH TRIAL SET = BACKGROUND ONLY"

This flag is output when the user wishes to begin the regression with the trial set chosen to be only the background spectrum (UEDIT variable BR = 1). In this case PREGA executes in a manner similar to a step-wise regression (STREGA). **NOTE** This option flag requires that the background spectrum is standard No. 1 in the full library set (see SEDIT).

(8) Results of current regression

This section of output contains several pieces of information. These are:

a) A title line stating the type of regression or pivot operation just completed;

b) The degrees of freedom, Regression Sum of Squares (RSS) and Mean Sum of Squares (MSR);

c) The name of the standard and its relative concentration and standard error;

d) The partial F-value to remove and associated Q-value and x-value, and the new MSR for each standard.

e) If the next operation to be performed is a forward pivot, the name, partial F to add and associated Q- and x-values, the square root of the partial correlation coefficient, RHO, and the new MSR, are output for each standard being considered.
(9) FINAL RESULT

This section of output is broken down as follows:

a) "FIT"

The "FIT" is the reduced $\chi^2$ statistic and gives an overall quantitative value for the fitting process. $\chi^2$ is computed by the program as follows. The residual $r_i$ in each channel (the difference between the sample spectrum and the least-squares spectrum) is computed: $\sum(y_i-f_i)$. The variance in channel $i$ for the least-squares spectrum $\sigma_i$ is then computed from the formula

$$\sigma_i = (f_i+0.1) + b_i t/t'(1+t/t'),$$

Then

$$\chi^2 = \sum_i r_i/\sigma_i$$

and reduced $\chi^2$ is $=(1/D_f)\sum_i r_i$

where $D_f =$ number of (channels - standards).

b) "RESULTS + CONCENTRATIONS AND EST STANDARD ERRORS"

The nuclide name, nuclide concentration, and the estimated standard error is printed out for each nuclide, in the "printout" order. The concentration is in the same units as the standards in the nuclide library, and is the "actual" concentration determined by multiplying the "relative" concentration computed by the program multiplied by factors that take into account sample decay, volume reduction and result multiplication, the activity of the standard, and sample and standard counting times. The relative standard error is multiplied by the same factors. Also included in this section of output are the final partial F-values and the corresponding Q- and x-values for each standard in the final set.

c) "ANALYSIS OF VARIANCE"

This table lists the contributions of the regression and residuals to the total variance. In it are given the degrees of freedom and sums of squares for the regression, residuals and total; the mean sums of square due to the regression and residuals, and the overall F-value. The Mean Square Residual has an expected value for a good fit of $1.0 \pm (2/D_f)^{1/2}$.

(10) "LLNL R-STATISTIC"

This output is the result of the analysis of the residuals from the least-squares fit. It gives the auto-correlation statistic, its expectation value, standard deviation and an approximate associated FAP.
low value of the auto-correlation coefficient means that the distribution of residuals is random. As this value approaches one (1) the residuals are becoming more correlated, indicating a poorer fit to the data.

(11) "FINAL STATISTIC FOR ELIMINATED STANDARDS"

This is a listing of the name and final partial F-value and associated Q- and X-value for each library standard eliminated from the set during the regression. It is useful to determine whether a standard was eliminated because it is truly uncorrelated with the sample or the threshold value for the F-test (variable FØ in UEDIT) was too high.

(12) "RATIO OF RESIDUALS OVER STD DEV PER CHANNEL"

The "residual" in each channel is the difference between the sample spectrum and the least-squares spectrum (yi-fi). The standard deviation for the least-squares spectrum is defined to be

\[
s_i = \left[ \left( f_i + 0.1 \right) + b_i t / t' \right]^{1/2}
\]

The program prints out one ratio for each channel in the least-squares spectrum; the printout should be read horizontally from left to right. These ratios, when squared, summed for all channels, and divided by the number of degrees of freedom Df, will be "reduced" \( \chi^2 \).

An examination of these ratios reveals where the least-squares spectrum \( f_i \) fits poorly the sample spectrum \( y_i \), since these ratios will be "large." Ratios > 10 or three consecutive ratios > 2 are flagged as "suspicous channels" and printed out in the next part of the output.

(13) "SUSPICIOUS CHANNELS"

The location and contents of any suspicious channels are given. These are the channels where the ratio of the residual to the standard deviation, \( r_i / \sigma_i \), is greater than 10 or the central channel of three consecutive channels that are all greater than +2. These are the same ratios that are printed out in the section "Residuals/Standard Deviation per Channel"; the "Suspicous Channels" indicates those channels where the least-squares fit is poor. The "suspicous channels" pointed out may or may not indicate the presence of an unexpected nuclide.

(14) "DISTRIBUTION OF RESIDUALS"

This is a histogram plot of the distribution of the residuals/standard deviation per channel. It is preceded by a moment analysis of the distribution of residuals giving the "MEAN," "VARIANCE," "SKEWNESS," and "EXCESS." The shape described by the moments as well as the visual identification of large residuals can be used in determining the "goodness of the fit" to the sample spectrum. In the present version of the subroutine RESID, residuals with \( r_i / \sigma > 5 \) are put in the first or last channel depending on the sign of the residual.
This is a histogram plot of the number of positive and negative runs in the residual spectrum. A run is a series of consecutive channels in the residual spectrum. For a good fit, the expected value for the number of runs, for these spectra, is $D_f/2 \times (D_f/4)^{1/2}$. The presence of large runs or a low number of runs can be an important aid in determining the randomness of the residuals and, hence, the goodness of the fit.

The last item in the PREGA output is the location (or starting channel) of the large runs, and the length of the run. The sign of the length denotes whether this is a run of positive or negative residuals. In the present version of the subroutine RUNS only runs of absolute length five or greater are output.

**VARIABLES (PREGA)**

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(10,10)</td>
<td>Square matrix to be inverted</td>
</tr>
<tr>
<td>AC(10)</td>
<td>Activity of standards from library</td>
</tr>
<tr>
<td>ARR(10,64)</td>
<td>Matrix containing 64 channels of (max.) 10 standard spectra; for residual calculation</td>
</tr>
<tr>
<td>ASC(60)</td>
<td>Disk locations of standard spectra</td>
</tr>
<tr>
<td>B(1)</td>
<td>$C_j = \sum w_i a_{ij} x_i$</td>
</tr>
<tr>
<td>BA(512)</td>
<td>Spectrum for either standard background or sample background, depending on location in program</td>
</tr>
</tbody>
</table>
| BR                | User option to do regression with trial set consisting of;  
|                  | = 0 all standards chosen  
|                  | = 1 background only  
<p>|                  | NOTE: FOR BR=1; BACKGROUND MUST BE STANDARD No. 1 IN THE LIST |
| C                 | Bit pattern of standards currently in regression for present pivot |
| CC(10,10)         | Correlation matrix for standards and sample |
| CH                | $x^2$ value for least-square spectrum |
| CHDF              | $= CH/DN$; &quot;reduced&quot; $x^2$ for least-squares spectrum |</p>
<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>Bit pattern of standards removed from original set</td>
</tr>
<tr>
<td>DAY</td>
<td>Decay time of sample (seconds)</td>
</tr>
<tr>
<td>DEF(10)</td>
<td>Hollerith constant DEF 8,</td>
</tr>
<tr>
<td>DF</td>
<td>Degrees of freedom; NCH-P</td>
</tr>
<tr>
<td>DG</td>
<td>Regression degrees of freedom; N</td>
</tr>
<tr>
<td>DN</td>
<td>Degrees of freedom; the number of channels used in the least-squares fit minus the number of standard isotopes</td>
</tr>
<tr>
<td>DR</td>
<td>Residual degrees of freedom; MF-NZ-P+1</td>
</tr>
<tr>
<td>DT</td>
<td>Total degrees of freedom; DG+DR</td>
</tr>
<tr>
<td>E</td>
<td>Bit pattern integer for standards currently in regression analysis</td>
</tr>
<tr>
<td>EF(10)</td>
<td>Logical variable to keep track of standard status in subroutine PIVOT</td>
</tr>
<tr>
<td>F</td>
<td>Bit pattern integer of original set of standard nuclei used</td>
</tr>
<tr>
<td>FØ</td>
<td>F-test rejection coefficient</td>
</tr>
<tr>
<td>FAT</td>
<td>t/t'; counting time of standard divided by counting time of standard background</td>
</tr>
<tr>
<td>FD</td>
<td>Correction for decay of sample and standard</td>
</tr>
<tr>
<td>FF</td>
<td>Final F-statistic = XG/XR</td>
</tr>
<tr>
<td>FILE</td>
<td>Logical unit number 8 (disk file:spectra)</td>
</tr>
<tr>
<td>FMAX</td>
<td>Maximum F-value (I) in forward pivot</td>
</tr>
<tr>
<td>FMIN</td>
<td>Minimum F-value (I) in backward pivot</td>
</tr>
<tr>
<td>FP(10)</td>
<td>F-value (I) after doing pivot</td>
</tr>
<tr>
<td>FPM(10)</td>
<td>F-value (I) for &quot;F-to-remove&quot; or &quot;F-to-add&quot;</td>
</tr>
<tr>
<td>FPS</td>
<td>Partial F-value sent to subroutine XQCALC</td>
</tr>
<tr>
<td>FS</td>
<td>t/t'; counting time of sample divided by counting time of sample background</td>
</tr>
</tbody>
</table>
### VARIABLES (PREGA) (Cont'd)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>FX</td>
<td>$t/t'(1 + t/t')$; second order correction term for time difference</td>
</tr>
<tr>
<td>HA(10)</td>
<td>Half-life of standards from library: input library order</td>
</tr>
<tr>
<td>HAT(10)</td>
<td>Half-life of standards; printout order</td>
</tr>
<tr>
<td>HF(5)</td>
<td>Hollerith output variable for titles</td>
</tr>
<tr>
<td>HG</td>
<td>Hollerith output variable for titles</td>
</tr>
<tr>
<td>HH(6)</td>
<td>Hollerith output variable for titles</td>
</tr>
<tr>
<td>HR</td>
<td>Hollerith output variable for titles</td>
</tr>
<tr>
<td>HT</td>
<td>Hollerith output variable for titles</td>
</tr>
<tr>
<td>I</td>
<td>Index used for nuclide and channel number</td>
</tr>
<tr>
<td>I0</td>
<td>Beginning of loop over standards value</td>
</tr>
<tr>
<td>I1</td>
<td>End of loop over standards value</td>
</tr>
<tr>
<td>IDAT</td>
<td>Associated variable for logical units 9 and 11</td>
</tr>
<tr>
<td>IFORKL(30)</td>
<td>Variable format statement number associated with ENCODE statement</td>
</tr>
<tr>
<td>IFORN(20)</td>
<td>Variable format statement number associated with ENCODE statement</td>
</tr>
<tr>
<td>II</td>
<td>Index used in library standards read/write operations</td>
</tr>
<tr>
<td>IN</td>
<td>Integer resulting from checking if standard I is in the current list before a pivot</td>
</tr>
<tr>
<td>INEG</td>
<td>Integer used to check sign of partial correlation coefficient ($R^2=RHO\cdot RHO$)</td>
</tr>
<tr>
<td>IPO</td>
<td>Integer used to direct program in next step after output of a pivot result</td>
</tr>
<tr>
<td>IR(512)</td>
<td>Suspicious channel number</td>
</tr>
<tr>
<td>IS(10)</td>
<td>Printout order of standards; OR in UEDIT can change as program is executed</td>
</tr>
</tbody>
</table>
### VARIABLES (PREGA) (Cont'd)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>ISL(10)</td>
<td>Printout order of standards; OR in UEDIT never changes during execution</td>
</tr>
<tr>
<td>IT(10)</td>
<td>Serial order of standards to be used in least-squares fit</td>
</tr>
<tr>
<td>IVAR</td>
<td>Associated variable for logical units 8 and 10</td>
</tr>
<tr>
<td>J</td>
<td>Index used for nuclide and channel number</td>
</tr>
<tr>
<td>JJ</td>
<td>Index used with ASC for sample and background spectra</td>
</tr>
<tr>
<td>JJJ</td>
<td>Do loop counter</td>
</tr>
<tr>
<td>JDF</td>
<td>Standard set F minus standard set D, used at end of backward pivot</td>
</tr>
<tr>
<td>K</td>
<td>Index used for nuclide and channel number</td>
</tr>
<tr>
<td>KAC</td>
<td>Variable associated with ENCODE statement for format 916</td>
</tr>
<tr>
<td>KRO</td>
<td>Output residual (Yes = 1, No = 0)</td>
</tr>
<tr>
<td>LN</td>
<td>Number of standards used plus 1, N + 1</td>
</tr>
<tr>
<td>LOOP</td>
<td>Integer to read 64 channels from disk for residual calculation</td>
</tr>
<tr>
<td>LSK</td>
<td>Variable associated with ENCODE statement for format 916</td>
</tr>
<tr>
<td>LW</td>
<td>User option for weighting factor p_i; WF in UEDIT if based on actual counts</td>
</tr>
<tr>
<td></td>
<td>- 1 for p_i = 1</td>
</tr>
<tr>
<td></td>
<td>0 for p_i = 1/(sample counts + background counts)</td>
</tr>
<tr>
<td></td>
<td>- 1 for p_i = 1/(sample counts + 1.0)</td>
</tr>
<tr>
<td>M</td>
<td>Number of channels of standard and sample spectra (max = 512)</td>
</tr>
<tr>
<td>MF</td>
<td>Final channel number for computation</td>
</tr>
<tr>
<td>MI</td>
<td>Logical unit 9 (disk file: nuclide library)</td>
</tr>
<tr>
<td>MIU</td>
<td>Logical unit 11 (disk file: unknown sample)</td>
</tr>
<tr>
<td>MO</td>
<td>Logical unit 6 (line printer)</td>
</tr>
<tr>
<td>NAME (DIMENSIONS)</td>
<td>USAGE</td>
</tr>
<tr>
<td>------------------</td>
<td>-------</td>
</tr>
<tr>
<td>MP</td>
<td>= 6 logical unit number of line printer</td>
</tr>
<tr>
<td>MY(10)</td>
<td>Integer vector used to check bit pattern of current set of standards for a particular standard</td>
</tr>
<tr>
<td>N</td>
<td>Number of standard nuclides to be fit (max = 9)</td>
</tr>
<tr>
<td>N2</td>
<td>Maximum channel number minus two; used for suspicious channels calculation</td>
</tr>
<tr>
<td>N5</td>
<td>Used to represent one (specified by program) value from IS or IT array</td>
</tr>
<tr>
<td>N6</td>
<td>Used to represent one (specified by program) value from IS or IT array</td>
</tr>
<tr>
<td>NBA</td>
<td>User option for standard background subtraction; BS in UEDIT</td>
</tr>
<tr>
<td></td>
<td>= 1 for subtraction</td>
</tr>
<tr>
<td></td>
<td>= 0 for no subtraction</td>
</tr>
<tr>
<td>NBR</td>
<td>User option for background; BG in UEDIT</td>
</tr>
<tr>
<td></td>
<td>= 1 for background supplied</td>
</tr>
<tr>
<td></td>
<td>= 0 for no background supplied</td>
</tr>
<tr>
<td>NBS</td>
<td>User option for sample background subtraction</td>
</tr>
<tr>
<td></td>
<td>= 1 subtraction</td>
</tr>
<tr>
<td></td>
<td>= 0 no subtraction</td>
</tr>
<tr>
<td>NCH</td>
<td>Number of channels used for calculation; MF-NZ+1</td>
</tr>
<tr>
<td>NDE</td>
<td>= 0 dead time correction (0 = no, 1 = yes)</td>
</tr>
<tr>
<td>NEWST</td>
<td>User option for application of rejection coefficient; RC in UEDIT</td>
</tr>
<tr>
<td></td>
<td>= 1 for application</td>
</tr>
<tr>
<td></td>
<td>= 0 for no application</td>
</tr>
<tr>
<td>NIT</td>
<td>Carry over from old NAI program. To be eliminated when SEDIT and UEDIT are restructured</td>
</tr>
<tr>
<td>NNN</td>
<td>= 0 counter index used in calling subroutine DECAY</td>
</tr>
<tr>
<td>NS</td>
<td>Number of standard spectra in library (maximum = 40)</td>
</tr>
<tr>
<td>NW</td>
<td>User option for weighting factor ( p_i ); WD in UEDIT</td>
</tr>
</tbody>
</table>
### VARIABLES (PREGA) (Cont'd)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>NZ</td>
<td>Initial channel used for calculation</td>
</tr>
<tr>
<td>P</td>
<td>Number of standards currently in regression</td>
</tr>
<tr>
<td>Q</td>
<td>Rejection coefficient; RC in SEDIT</td>
</tr>
<tr>
<td>QF</td>
<td>Q(X) associated with F-values</td>
</tr>
<tr>
<td>QH</td>
<td>User defined threshold channel number, TC in UEDIT</td>
</tr>
<tr>
<td>R(512)</td>
<td>1. Standard spectra (up to line 493) then 2. Ratio of residual divided by standard deviation</td>
</tr>
<tr>
<td>R2</td>
<td>Concentration of standard squared divided by standard error of standard divided by residual sum of squares; used to calculate partial F-values for PIVOT; partial correlation coefficient</td>
</tr>
<tr>
<td>RE</td>
<td>Residual count; RE = Y(J) - SV</td>
</tr>
<tr>
<td>RHO</td>
<td>Square root of partial correlation coefficient, R2</td>
</tr>
<tr>
<td>RMSR</td>
<td>Residual sum of squares divided by DF</td>
</tr>
<tr>
<td>RSS</td>
<td>Residual sum of squares</td>
</tr>
<tr>
<td>RT</td>
<td>$x^2$ sum for least-squares spectrum</td>
</tr>
<tr>
<td>S(512)</td>
<td>Standard spectra counts; $a_{ij}$</td>
</tr>
<tr>
<td>S1</td>
<td>$\sum x_i$; sum of counts for the sample spectrum</td>
</tr>
<tr>
<td>S2</td>
<td>$S1 + SB \times FX$; sum of sample plus corrected background counts</td>
</tr>
<tr>
<td>SA</td>
<td>$b_{jk}$; least square sum coefficients for unknown concentrations $Z(I)$ and sample $Y(I)$; store in $A(L,K)$; total sum of squares</td>
</tr>
<tr>
<td>SB</td>
<td>Sum of counts for the sample background spectrum from the initial to the final channel</td>
</tr>
<tr>
<td>SG</td>
<td>Regression sum of squares</td>
</tr>
<tr>
<td>SIR(50)</td>
<td>Contents of suspicious channels</td>
</tr>
<tr>
<td>SNAM(2)</td>
<td>Sample file name used in output for identification</td>
</tr>
<tr>
<td>NAME (DIMENSIONS)</td>
<td>USAGE</td>
</tr>
<tr>
<td>-------------------</td>
<td>-------</td>
</tr>
<tr>
<td>SQUC</td>
<td>Used to check sign of number before taking square root</td>
</tr>
<tr>
<td>SR</td>
<td>Residual sum of squares</td>
</tr>
<tr>
<td>SRD1</td>
<td>$\sigma_{ii}$ for correlation coefficient $CC(I,J)$</td>
</tr>
<tr>
<td>SRD2</td>
<td>$\sigma_{jj}$ for correlation coefficient $CC(I,J)$</td>
</tr>
<tr>
<td>SS(10)</td>
<td>$\sum_{j}^{i} a_{ij} t_{j}$; sum of counts for standard isotopes from the initial to final channel</td>
</tr>
<tr>
<td>ST</td>
<td>Residual sum of squares</td>
</tr>
</tbody>
</table>
| STD(10)           | 1. Variance of the nuclide concentration; input library order  
|                   | 2. Corrected standard error of the nuclide concentration; input library order |
| SUM               | Relative nuclide concentration, $m_j$ |
| SUM W             | Sum of weighting factors, $p_i$, from initial channel to final channel |
| SV                | Least squares spectrum sum, $\sum_{i} f_i$ |
| SX                | $c_j$, least squares sums for constant terms |
| T                 | 1. $Y(I)BA(I)*FX$ defined at program line  
|                   | 2. Reciprocal of $p_i$ defined at program line  
|                   | 3. $r_j^2$; residual squared defined at program line 480 |
| TB                | Counting time for background |
| TE                | 1. $Y(J)BA(J)*FX$ used in calculation of CHDFS |
| TIS1              | Hollerith constant to store "SAMP" |
| TIS2              | Hollerith constant to store "LE" |
| TISO(20)          | Names of stored nuclides used in least squares fit; in printout order |
| TISO(40)          | standard nuclide names; input library order |
| TMO               | $= (0.1 + SV)$; reciprocal of $p_i$ based upon least-squares spectrum |

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### VARIABLES (PREGA) (Cont'd)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>TMP</td>
<td>TMP = TMO + BA(J)*FX; reciprocal of ( p_i ) based upon least-squares spectrum + corrected background; defined at program line 484. Redefined at program line 493 as the square root of TMP.</td>
</tr>
<tr>
<td>TNAME(36)</td>
<td>Original location of sample spectrum</td>
</tr>
<tr>
<td>TSA</td>
<td>Counting time for sample in seconds</td>
</tr>
<tr>
<td>TST(10)</td>
<td>Counting time of standard in seconds; from PREGA library</td>
</tr>
<tr>
<td>VM</td>
<td>User defined result multiplication factor; MF in UEDIT</td>
</tr>
<tr>
<td>VRED</td>
<td>User defined volume reduction factor; VR in UEDIT</td>
</tr>
<tr>
<td>VU</td>
<td>Sum of residuals squared</td>
</tr>
<tr>
<td>VVV</td>
<td>Sum of TMP</td>
</tr>
<tr>
<td>VY</td>
<td>Residual squared times ( p_i )</td>
</tr>
<tr>
<td>W(512)</td>
<td>Weighting factors ( p_i )</td>
</tr>
<tr>
<td>XF</td>
<td>X-value returned from subroutine XQCALC and checked against ( F_0 )</td>
</tr>
<tr>
<td>XG</td>
<td>Final regression sum of squares divided by degrees of freedom</td>
</tr>
<tr>
<td>XR</td>
<td>Final residual sum of squares divided by degrees of freedom</td>
</tr>
<tr>
<td>Y(513)</td>
<td>Sample spectrum ( X_i )</td>
</tr>
<tr>
<td>Z(10)</td>
<td>Library nuclide concentration</td>
</tr>
<tr>
<td>ZS</td>
<td>Nuclide concentration sent to subroutine XQCALC</td>
</tr>
</tbody>
</table>

### Program Calculations

PREGA is a FORTRAN language program consisting of approximately 638 lines and requiring ~ 52K words of memory for execution. The main calculation steps used by the program to calculate the best subset of standards using the pivotal regression technique, the nuclide concentration, residuals and the statistical analysis of accidental errors are listed on the following pages. This section is included to provide further understanding of the calculation and as a guide for future modifications that may become necessary or desirable.
<table>
<thead>
<tr>
<th>Program Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>70</td>
<td>FAT = TST(I)/TB</td>
<td>Counting time of standard i counting time of background</td>
<td>1</td>
</tr>
<tr>
<td>72</td>
<td>S(J) = S(J)-BA(J)*FAT</td>
<td>[Standard counts – corrected background counts] in each channel summed over all channels</td>
<td>2</td>
</tr>
<tr>
<td>103</td>
<td>FS = TSA/TB</td>
<td>Counting time of sample counting time of background</td>
<td>4</td>
</tr>
<tr>
<td>104</td>
<td>FX = FS + FS*2</td>
<td>Second order correction factor used in line 484</td>
<td>5</td>
</tr>
<tr>
<td>121</td>
<td>Y(I) = Y(I)-BA(I)*FS</td>
<td>[Sample counts – corrected background counts] in each channel i</td>
<td>6</td>
</tr>
<tr>
<td>124</td>
<td>SB = SB + BA(I)</td>
<td>Total background counts; this is the &quot;BACKGD SUM&quot; that is printed out</td>
<td>7</td>
</tr>
<tr>
<td>129</td>
<td>S1 = S1 + Y(I)</td>
<td>Total sample counts (corrected background subtracted); this is the &quot;SAMPLE SUM&quot; that is printed out</td>
<td>8</td>
</tr>
<tr>
<td>211</td>
<td>SS(L) = SS(L)*R(J)/W(J)</td>
<td>Weighted sum of standard counts in all channels i for nuclide j; this is the &quot;WEIGHTED SUM OF STANDARDS AND UNKNOWN&quot; that is printed out</td>
<td>3</td>
</tr>
</tbody>
</table>

***SET UP ARRAY A(N+1, N+1) AND CORRELATION MATRIX***
<table>
<thead>
<tr>
<th>Program Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>216</td>
<td>S(J) redefined as original standard spectra</td>
<td>FORTRAN S(J) here represents the standard spectra</td>
<td></td>
</tr>
<tr>
<td>219</td>
<td>SA=SA+S(I)*R(I)*W(I)</td>
<td>Standards cross product terms times weighting factor stored in A(L,K)</td>
<td>9</td>
</tr>
<tr>
<td>225</td>
<td>SA=SA+R(I)*Y(I)*W(I)</td>
<td>Cross product of standards and sample terms stored in A(N+1,L) and B(L)</td>
<td>10</td>
</tr>
<tr>
<td>233</td>
<td>SA=SA+Y(I)*Y(I)*W(I)</td>
<td>Stored in A(N+1, N+1); this location is the residual sum of squares during the pivot operations. Also stored in ST</td>
<td>11</td>
</tr>
<tr>
<td>244</td>
<td>SRD1=A(K,K)-SS(N6)**2/SUMW</td>
<td>Variance of standard K (or sample)</td>
<td>12</td>
</tr>
<tr>
<td>245</td>
<td>SRD2=A(L,L)-SS(N5)**2/SUMW</td>
<td>Variance of standard L (or sample)</td>
<td>13</td>
</tr>
<tr>
<td>246</td>
<td>CC(K,L)=(A(K,L)-SS(N6)<em>SS(N5)/SUMW)/SQRT(SRD1</em>SRD2)</td>
<td>Correlation coefficient: covariance of standards K and L divided by the square root of the product of their variances</td>
<td>14</td>
</tr>
</tbody>
</table>

***START PIVOTAL REGRESSION ANALYSIS***

<table>
<thead>
<tr>
<th>Program Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>329</td>
<td>FPM(I)=(NCH-P)*((A(I,LN)**2)/(-A(I,I)*A(LN,LN)))</td>
<td>Calculate partial F to remove; NCH-P = degrees of freedom</td>
<td>15</td>
</tr>
</tbody>
</table>
### PREGA Program Calculations (Cont'd)

<table>
<thead>
<tr>
<th>Program Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>381</td>
<td>FPM(I)=((NCH-P-1)*R2)/(1.0-R2)</td>
<td>Calculate pal F to add; NCH-P-1 =degrees of freedom</td>
<td>16</td>
</tr>
<tr>
<td>409</td>
<td>RSS = A(LN, LN)</td>
<td>Residual sum of squares</td>
<td></td>
</tr>
<tr>
<td>410</td>
<td>RMSR = RSS/DF</td>
<td>Residual sum of squares per degree of freedom</td>
<td></td>
</tr>
<tr>
<td>418</td>
<td>Z(J) = -A(I, LN)*TST(N5)/TSA</td>
<td>Relative concentration of standard J</td>
<td>17</td>
</tr>
<tr>
<td>422</td>
<td>STD(J) = SQRT(SQUC)<em>RMSR</em>TST(N5)/TSA</td>
<td>Relative standard error of standard J determined from the variance</td>
<td>18</td>
</tr>
<tr>
<td>448</td>
<td>SG = SG - A(I, LN)*B(I)</td>
<td>Regression sum of squares</td>
<td></td>
</tr>
<tr>
<td>475</td>
<td>SV = SV + ARR(JJ, JJJ)*(-A(I, LN))</td>
<td>Calculates the least-squares spectrum counts in each channel (because of memory limitations, this is done 64 channels at a time)</td>
<td>19</td>
</tr>
<tr>
<td>479</td>
<td>RE = Y(J) - SV</td>
<td>Residual = difference between sample and least-squares spectrum</td>
<td>20</td>
</tr>
<tr>
<td>480</td>
<td>T = RE**2</td>
<td>Squares the residual</td>
<td>21</td>
</tr>
<tr>
<td>481</td>
<td>VY = VY + W(J)*T</td>
<td>Residual sum of squares; stored in SR at line 472</td>
<td>22</td>
</tr>
<tr>
<td>482</td>
<td>VU = VU + T</td>
<td>Sum of residuals squared over all channels</td>
<td>23</td>
</tr>
<tr>
<td>483</td>
<td>TMO = ABS(0.1 + SV)</td>
<td>( f_i ) must ( \neq 0 ); zero divide prevention</td>
<td>24</td>
</tr>
</tbody>
</table>
PREGA Program Calculations (Cont'd)

<table>
<thead>
<tr>
<th>Program Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>484</td>
<td>TMP = TMO + BA(J)*FX</td>
<td></td>
<td>25</td>
</tr>
<tr>
<td>485</td>
<td>VVV = VVV + TMP</td>
<td>Accumulates TMP over all channels</td>
<td>26</td>
</tr>
<tr>
<td>491</td>
<td>RT = T/TMP</td>
<td>Residual squared TMP</td>
<td></td>
</tr>
<tr>
<td>492</td>
<td>CH = CH + RT</td>
<td>Accumulates RT over all channels; this is chi-squared for least-squares spectrum</td>
<td>27</td>
</tr>
<tr>
<td>493</td>
<td>TMP = SQRT(TMP)</td>
<td>Redefine TMP as square root of TMP</td>
<td></td>
</tr>
<tr>
<td>494</td>
<td>R(J) = RE/TMP</td>
<td>Calculates residuals over standard deviations; printed out as &quot;RATIO OF RESIDUALS OVER STD DEVIATION PER CHANNEL&quot;</td>
<td></td>
</tr>
<tr>
<td>498</td>
<td>DN = MF-P-NZ+1</td>
<td>Calculates the number of degrees of freedom for $x^2$, MF = end channel,</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NZ = start channel, P = number of standards in fit</td>
<td></td>
</tr>
<tr>
<td>501</td>
<td>DT = DR+DG</td>
<td>Total number degrees of freedom</td>
<td></td>
</tr>
<tr>
<td>502</td>
<td>CHDF = CH/DN</td>
<td>&quot;Reduced&quot; $x^2$ for the least-squares spectrum; this is the &quot;FIT&quot; that is</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>printed out</td>
<td></td>
</tr>
</tbody>
</table>
| 513                 | FD = EXP(0.693*DAY/HA(N5)) | Correction for decay of sample  
DAY = $t_{1/2} =$half-life of sample and  
HA = $T_{1/2} =$half-life of standard | 28              |
<p>| 514                 | STD(J)=SQRT(-A(I,I)*A(LN,LN)/DN) *TST(N5)/TSA | Relative standard error determined from variance of standard l |                 |</p>
<table>
<thead>
<tr>
<th>Line Number</th>
<th>FORTRAN Expression</th>
<th>Description</th>
<th>Equation Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>515</td>
<td>STU(J)=AC(N5)<em>FD</em>STD(J)*VM/VRED</td>
<td>Corrected standard error; AC is the activity of the sample; VM is result multiplication factor; VRED is volume reduction factor</td>
<td></td>
</tr>
<tr>
<td>516</td>
<td>Z(J)=(-A(I,LN)*(TST(N5)/TSA) *AC(N5)<em>FD</em>VM/VRED</td>
<td>Relative concentration m_j is converted to actual concentration level</td>
<td></td>
</tr>
<tr>
<td>526</td>
<td>XG = SG/DG</td>
<td>Reduced regression sum of squares</td>
<td></td>
</tr>
<tr>
<td>527</td>
<td>XR = SR/DR</td>
<td>Reduced residual sum of squares</td>
<td></td>
</tr>
<tr>
<td>528</td>
<td>FF = XG/XR</td>
<td>Final F-statistic</td>
<td></td>
</tr>
</tbody>
</table>
Equations Used in PREGA (FORTRAN variables are underlined)

1. \( \text{FAT} = t_j/t' \)

2. \( S(J) = \sum a_{ij} = \sum S_{ij} - b_i(t_j/t') \)

3. \( \text{SS(J)} = \sum c_{ij} \)

4. \( \text{FS} = t_s/t' \)

5. \( \text{FX} = (t_s/t')(1 + t_s/t') \)

6. \( Y(I) = x_i = z_i - b_i(t_s/t') \)

7. \( \text{SB} = \sum b_i \)

8. \( S1 = \sum x_i \)

9. \( A(L,K) = \sum a_{lk}a_{lj}w_i \)

10. \( S_A = \sum a_{il}x_iw_i \)

11. \( S_A = \sum x_iw_i \)

12. \( \text{SRD1} = \sigma_{kk} = A_{kk} - (\sum a_{ik}w_i)^2/\sum w_i \)

13. \( \text{SRD2} = \sigma_{11} = A_{11} - (\sum a_{ij}w_i)^2/\sum w_i \)

\[ A_{k1} = \left[ \sum_i a_{ik}w_i \frac{\sum_i a_{i1}w_i}{\sum w_i} \right] \]

14. \( \rho_{k1} = \frac{A_{k1}}{(\sigma_{kk} \sigma_{11})^{1/2}} \)

15. \( F_p^- = DF*R^2 = DF*A_{1,N+1}^2 / (-A_{IL}A_{N+1,N+1}) \)
Equations Used in PREGA (FORTRAN variables are underlined) (Cont'd)

16. \[ F_p^+ = DF*R^2/(1-R)^2 \]

17. \[ Z(j) = \sum_i a_{ij}^* t_j / t' = m_j \]

18. \[ STD(j) = (A(-I,I)*A(N+1,N+1)/DF)t_j / t' \]

19. \[ SV = f_i = \sum_j a_{ij} m_j \]

20. \[ r_i = (x_i - f_i) \]

21. \[ r_i^2 = (x_i - f_i)^2 \]

22. \[ VV = \sum_i r_i^2 w_i \]

23. \[ VU = \sum_i r_i^2 \]

24. \[ TMO = 0.1 + f_i \]

25. \[ TMP = (0.1 + f_i) + b_i FX \]

26. \[ VVV = \sum (0.1 + f_i) + b_i FX \]

27. \[ CH = \sum r_i^2 / (0.1 + f_i) + b_i FX \]

28. \[ FD = \exp(0.693 \ t_{1/2}^s / t_{1/2}^s) \]
Software Organization

(1) Logical Unit and Disk File Structure

The program PREGA and the two editor programs SEDIT and UEDIT have access to data stored in disk files via specific, user-defined logical units. The organization of these programs, disk files, and logical units is shown in figure 2.

The program PREGA uses logical units 6, 8, 9, 10, and 11. It shares logical unit 9 with the SEDIT editor program and shares logical unit 11 with the UEDIT editor program.

Logical unit 6 is used to print out the results of the program; it is usually a line printer.

Logical unit 8 is a disk file that stores spectral data that have been accumulated by the user in the laboratory. The program PREGA reads this data to perform its calculations. Each spectrum is stored in one disk file element. The data will include the sample spectrum, the background spectrum for the sample, the standard spectra (up to 9 standards are permitted at present) and the background spectrum for the standard. The background spectrum must be standard No. 1 in the library.

Logical unit 9 is the standard nuclide library file. The file contains information common to all nuclides in the library (the "header") as well as specific information about each nuclide (the "list of standards"). For each standard spectrum in logical unit 8 there will be a corresponding entry in the nuclide library file. The editor program SEDIT is used to add, delete, or make changes in this file.

Logical unit 10 is used by the program PREGA for temporary storage of large data arrays. This is a "scratch" file.

Logical unit 11 is a disk file that contains information about the unknown spectrum the user has acquired. The UEDIT editor program is used to add, delete or change the information in this file.

The file structures for logical units 8, 9, 10, and 11 are shown on the following pages. The file structures for logical units 9 and 11 show two columns of program parameter names. The editor programs use the names in the first column and the program PREGA uses the names in the second column.

The following relation exists among sectors, records, words, bytes, and bits for all files defined as logical units 8, 9, 10, and 11 in the program PREGA:

1 sector = 64 records = 128 words = 256 bytes
1 record = 2 words = 4 bytes = 32 bits
1 word = 2 bytes
1 byte = 8 bits
Logical Unit 8

The program PREGA uses the GET subroutine to read each spectrum through logical unit 8. Each file element contains one spectrum. The spectral data begins with record number 129 (decimal byte offset 512); the first 128 records (511 bytes) in each file element are not used by PREGA. The first 128 records comprise the Header section of Nuclear Data spectral files and contain information used by other programs (e.g. GSHIFT, GET, PUT).

The numbering system is illustrated below for the first 2 records.

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
<th>Record 129</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 515</td>
<td>byte 514</td>
<td></td>
</tr>
<tr>
<td>Word 2</td>
<td>Word 1</td>
<td>Record 130</td>
</tr>
<tr>
<td>byte 519</td>
<td>byte 518</td>
<td></td>
</tr>
</tbody>
</table>

Data type coding is as follows:

**Sptr** (Spectral data) The spectral data from each channel is stored in 4 bytes. Only 30 bits are used. The values are stored as double integers. Word 1 is the least significant word.

Regardless of the number of bits/channel assigned to an ADC, each channel is always written to disk as a 32-bit word.

If \( M \) = the number of channels of spectral data, the decimal byte length of the file element is \( 512 + 4 \times M \). The user can use this to determine how much disk space must be reserved for the spectral data. For example, the maximum number of channels a user can have in one spectrum is 512. This would require 2560 bytes or 10 sectors to be reserved for that file element. The maximum number of spectra accessible by SEDIT at any given time is currently 9. The number of spectra which can be stored on the disk in file DATA is determined by the size of file DATA. Because SEDIT is limited to 9 standards, the maximum number of spectra, or file elements a user can have on logical unit 8 is 12 (see below) so the upper limit of the size of this disk file is 120 sectors.

The total number of file elements will be the sum of:

1. to 9 file elements for the standard spectra
2. file element for the standard background spectrum
3. file element for the unknown sample spectrum
4. file element for the unknown sample background spectrum
NOTE - The program SEDIT can actually handle up to 40 standard spectra. The limitation of only 9 standard spectra is caused by PREGA. As stated earlier, PREGA was built on the framework of the Nuclear Data, Inc. NAI analysis program, which has some built-in inefficiency. The method for modifying PREGA and, hence the whole package is given in more detail below. At present, it was felt that 9 standards would be sufficient for the present analysis without making PREGA unnecessarily larger.
### Structure of PREGA File 8

<table>
<thead>
<tr>
<th>Record Number</th>
<th>Decimal Byte Offset</th>
<th>Decimal Byte Length</th>
<th>Parameter Description</th>
<th>Data Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>4</td>
<td>Not used</td>
<td>...</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>4</td>
<td>Not used</td>
<td>...</td>
</tr>
<tr>
<td>128</td>
<td>508</td>
<td>4</td>
<td>Not used</td>
<td>...</td>
</tr>
<tr>
<td>129</td>
<td>512</td>
<td>4</td>
<td>Number of counts in channel 1</td>
<td>Sptr</td>
</tr>
<tr>
<td>130</td>
<td>516</td>
<td>4</td>
<td>Number of counts in channel 2</td>
<td>Sptr</td>
</tr>
<tr>
<td>131</td>
<td>520</td>
<td>4</td>
<td>Number of counts in channel 3</td>
<td>Sptr</td>
</tr>
<tr>
<td>641</td>
<td>2560</td>
<td>4</td>
<td>Number of counts in channel 512</td>
<td>Sptr</td>
</tr>
</tbody>
</table>
(1b) Logical Unit 9

SEDIT writes the file to logical unit 9 and the program PREGA reads from logical unit 9.

The numbering system is illustrated below for the first 2 records.

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 3</td>
<td>byte 2</td>
</tr>
<tr>
<td></td>
<td>byte 1 byte 0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 7</td>
<td>byte 6</td>
</tr>
<tr>
<td></td>
<td>byte 5 byte 4</td>
</tr>
</tbody>
</table>

Data type coding is as follows:

- A  ASCII characters
- F  REAL*4 single precision floating point with 4 bytes
- I*2  INTEGER*2 with 2 bytes
- L*1  LOGICAL*1 with 1 byte

The number in the "offset" column is the address.

This file requires 256 bytes for the "header" section and 64 bytes for each nuclide in the library. If N represents the number of nuclides in the library, then a total of 256 + 64N bytes of storage are required; one sector = 256 bytes. For example, the maximum number of nuclides a user can have in the library is 9. This would require 256 + 576 = 832 bytes. An example printout of this file is given in the section about SEDIT. The example consists of two parts: the first part is the "PREGA LIBRARY HEADER" and the second part is the "PREGA LIBRARY STANDARDS".
### Structure of PREGA and SEDIT File 9

<table>
<thead>
<tr>
<th>Record Number Offset</th>
<th>Decimal Offset</th>
<th>Byte</th>
<th>SEDIT Name</th>
<th>PREGA Name</th>
<th>Parameter Description</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>M</td>
<td>NS</td>
<td>number of isotopes in standard library (max = 9)</td>
<td>I*2</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>2</td>
<td>NC</td>
<td>M</td>
<td>number of channels per standard library (max = 512)</td>
<td>I*2</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>2</td>
<td>IT</td>
<td>NIT</td>
<td>number of iterations for threshold and gain calculation (not used)</td>
<td>I*2</td>
</tr>
<tr>
<td>4</td>
<td>12</td>
<td>2</td>
<td>BS</td>
<td>NBA</td>
<td>background subtract l = yes, o = no</td>
<td>I*2</td>
</tr>
<tr>
<td>5</td>
<td>16</td>
<td>2</td>
<td>IS</td>
<td>NZ</td>
<td>initial channel for computation</td>
<td>I*2</td>
</tr>
<tr>
<td>6</td>
<td>20</td>
<td>2</td>
<td>IE</td>
<td>MF</td>
<td>final channel for computation</td>
<td>I*2</td>
</tr>
<tr>
<td>7</td>
<td>24</td>
<td>132</td>
<td></td>
<td></td>
<td>space reserved for file expansion</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>156</td>
<td>4</td>
<td>BT</td>
<td>TB</td>
<td>counting time for standard background</td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>160</td>
<td>4</td>
<td>RC</td>
<td>Q</td>
<td>rejection coefficient</td>
<td>F</td>
</tr>
<tr>
<td>42</td>
<td>164</td>
<td>30</td>
<td>BA</td>
<td>ASC</td>
<td>standard background location</td>
<td>L*1</td>
</tr>
<tr>
<td>49</td>
<td>194</td>
<td>2</td>
<td>word 2 of record 49 not used</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>196</td>
<td>60</td>
<td></td>
<td></td>
<td>space reserved for file expansion</td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>256</td>
<td>8</td>
<td>A</td>
<td>TISOT</td>
<td>first standard isotope name</td>
<td>A</td>
</tr>
<tr>
<td>67</td>
<td>264</td>
<td>30</td>
<td>A</td>
<td>ASC</td>
<td>first isotope location</td>
<td>L*1</td>
</tr>
<tr>
<td>74</td>
<td>294</td>
<td>2</td>
<td>word 2 of record 74 not used</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>75</td>
<td>296</td>
<td>4</td>
<td>HL</td>
<td>HA</td>
<td>half-life of first isotope</td>
<td>F</td>
</tr>
<tr>
<td>76</td>
<td>300</td>
<td>4</td>
<td>SEC</td>
<td>TST</td>
<td>counting time of first isotope</td>
<td>F</td>
</tr>
<tr>
<td>77</td>
<td>304</td>
<td>4</td>
<td>ACT</td>
<td>AC</td>
<td>activity of first isotope</td>
<td>F</td>
</tr>
<tr>
<td>78</td>
<td>308</td>
<td>12</td>
<td></td>
<td></td>
<td>not used</td>
<td></td>
</tr>
<tr>
<td>81</td>
<td>320</td>
<td>52</td>
<td></td>
<td></td>
<td>data for standard isotope two</td>
<td></td>
</tr>
<tr>
<td>94</td>
<td>372</td>
<td>12</td>
<td></td>
<td></td>
<td>not used</td>
<td></td>
</tr>
<tr>
<td>97</td>
<td>384</td>
<td>52</td>
<td></td>
<td></td>
<td>data for standard isotope three</td>
<td></td>
</tr>
<tr>
<td>110</td>
<td>436</td>
<td>12</td>
<td></td>
<td></td>
<td>not used</td>
<td></td>
</tr>
</tbody>
</table>

The second word of records 1, 2, 3, 4, 5 and 6 is not used.

---

through 65+ (NS*16) -3

where NS = number of isotopes in standard library
PREGA reads and writes to the file of the logical unit 10. This file, a "scratch" file, is used for temporary storage of the large data arrays manipulated by the Nal program.

The numbering system is illustrated below for the first 2 records.

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 3</td>
<td>byte 1</td>
</tr>
<tr>
<td>byte 2</td>
<td>byte 0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Word 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 7</td>
</tr>
<tr>
<td>byte 6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 5</td>
</tr>
<tr>
<td>byte 4</td>
</tr>
</tbody>
</table>

Data type coding is as follows:

Sptr (Spectral Data) The spectral data from each channel is stored in 4 bytes. Only 30 bits are used. The values are stored as double integers. Bits 14 and 15 have been set for 0 for word 2, which is the most significant word.
### Structure of PREGA File 10 ("Scratch" file)

<table>
<thead>
<tr>
<th>Record Number Offset</th>
<th>Decimal Byte Offset</th>
<th>Decimal Byte Length</th>
<th>PREGA Name</th>
<th>Parameter Description</th>
<th>DATA Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>4*M</td>
<td>S</td>
<td>storage for all channels of first standard spectrum</td>
<td>Sptr</td>
</tr>
<tr>
<td>M+1</td>
<td>4*M</td>
<td>4*M</td>
<td>S</td>
<td>storage for all channels of second standard spectrum</td>
<td>Sptr</td>
</tr>
<tr>
<td>2*M+1</td>
<td>2<em>4</em>M</td>
<td>4*M</td>
<td>S</td>
<td>storage for all channels of third standard spectrum</td>
<td>Sptr</td>
</tr>
<tr>
<td>3*M+1</td>
<td>3<em>4</em>M</td>
<td>4*M</td>
<td>S</td>
<td>storage for all channels of fourth standard spectrum</td>
<td>Sptr</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>NS*M+1</td>
<td>NS<em>4</em>M</td>
<td>4*M</td>
<td>S</td>
<td>storage for all channels of sample spectrum</td>
<td>Sptr</td>
</tr>
</tbody>
</table>

where M = number of channels per standard

NS = number of isotopes in standard library
Logical Unit 11

UEDIT writes the file to logical unit 11 and PREGA reads from logical unit 11.

The numbering system is illustrated for the first 2 records.

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 3</td>
<td>byte 1</td>
</tr>
<tr>
<td>byte 2</td>
<td>byte 0</td>
</tr>
</tbody>
</table>

Record 1

<table>
<thead>
<tr>
<th>Word 2</th>
<th>Word 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>byte 7</td>
<td>byte 5</td>
</tr>
<tr>
<td>byte 6</td>
<td>byte 4</td>
</tr>
</tbody>
</table>

Record 2

Data type coding is as follows:

- F REAL*4 single precision floating point with 4 bytes
- I*2 INTEGER*2 with 2 bytes
- L*1 LOGICAL*1 with 1 byte

The number in the "offset" column is the address.

An example of the printout of this file is given in the section on UEDIT with the heading "PREGA UNKNOWN SAMPLE PARAMETERS".
Structure of PREGA and UEDIT File II

<table>
<thead>
<tr>
<th>Record Number</th>
<th>Decimal Offset</th>
<th>Decimal Length</th>
<th>UEDIT Name</th>
<th>PREGA Name</th>
<th>Parameter Description</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>4</td>
<td>dummy</td>
<td></td>
<td></td>
<td>L*1</td>
</tr>
<tr>
<td>2-9</td>
<td>1</td>
<td>30</td>
<td>UN ASC</td>
<td></td>
<td>location of sample spectrum</td>
<td>L*1</td>
</tr>
<tr>
<td>9</td>
<td>34</td>
<td>2</td>
<td>GN FIT</td>
<td></td>
<td>gain shift ratio (not used)</td>
<td>F</td>
</tr>
<tr>
<td>10</td>
<td>36</td>
<td>4</td>
<td>TH SHCT</td>
<td></td>
<td>threshold shift (not used)</td>
<td>F</td>
</tr>
<tr>
<td>11</td>
<td>40</td>
<td>4</td>
<td>BG NBR</td>
<td></td>
<td>background supplied yes = 1 no = 0</td>
<td>I*2</td>
</tr>
<tr>
<td>12</td>
<td>44</td>
<td>2</td>
<td></td>
<td></td>
<td>background subtract yes = 1, no = 0</td>
<td>I*2</td>
</tr>
<tr>
<td>13</td>
<td>48</td>
<td>2</td>
<td>BS NBS</td>
<td></td>
<td>counting time for sample background (sec)</td>
<td>F</td>
</tr>
<tr>
<td>14</td>
<td>52</td>
<td>4</td>
<td>BT TB</td>
<td></td>
<td>counting time for sample background (sec)</td>
<td>F</td>
</tr>
<tr>
<td>15</td>
<td>56</td>
<td>4</td>
<td>CT TSA</td>
<td></td>
<td>sample concentration factor</td>
<td>F</td>
</tr>
<tr>
<td>16</td>
<td>60</td>
<td>4</td>
<td>VR VRED</td>
<td></td>
<td>decay (sec)</td>
<td>F</td>
</tr>
<tr>
<td>17</td>
<td>64</td>
<td>4</td>
<td>MF VM</td>
<td></td>
<td>sample dilution factor</td>
<td>F</td>
</tr>
<tr>
<td>18</td>
<td>68</td>
<td>4</td>
<td></td>
<td></td>
<td>location of sample background</td>
<td>L*1</td>
</tr>
<tr>
<td>19</td>
<td>72</td>
<td>30</td>
<td>BA ASC</td>
<td></td>
<td>word 2 of record 27 not used</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>104</td>
<td>2</td>
<td></td>
<td></td>
<td>weighting factor determination: I*2 = 0 if based on actual counts/channel = 1 if based on calculated counts/channel</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>108</td>
<td>2</td>
<td>WD NW</td>
<td></td>
<td>number of library spectra to be fitted to the sample</td>
<td>I*2</td>
</tr>
<tr>
<td>29</td>
<td>112</td>
<td>2</td>
<td>NS N</td>
<td></td>
<td>F-test rejection coefficient</td>
<td>R*4</td>
</tr>
<tr>
<td>30</td>
<td>116</td>
<td>2</td>
<td>Fθ Fφ</td>
<td></td>
<td>weighting factor</td>
<td>I*2</td>
</tr>
<tr>
<td>31</td>
<td>120</td>
<td>2</td>
<td>WF LW</td>
<td></td>
<td>apply rejection coefficient I*2 = 0 if 1 = yes only; 0 = no, 1 = yes</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>124</td>
<td>2</td>
<td>RC NEWST</td>
<td></td>
<td>start regression with background I*2 = 0 if 1 = yes only; 0 = no, 1 = yes</td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>128</td>
<td>2</td>
<td>BR BR</td>
<td></td>
<td>allow pivot on background I*2 = 0 if 1 = yes</td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>132</td>
<td>2</td>
<td>BP BP</td>
<td></td>
<td>output residuals I*2 = 0 if 1 = yes</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>136</td>
<td>2</td>
<td>RO KRO</td>
<td></td>
<td>ID of output file for residuals L<em>1 library standard number I</em>2</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>140</td>
<td>32</td>
<td>RS ASC</td>
<td></td>
<td>listed in the order of desired printout</td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>176</td>
<td>4*N</td>
<td>OR IS</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

N is the number of library nuclides to be fit to the sample.

The second word of records 12, 13, 27, 28, 29, 30, 32, 33, 34, and 35 through 43+N is not used.
Subroutines Called by the Program PREGA

The following eleven subroutines are used during the execution of PREGA. Figure 3 shows the hierarchy of subroutine calls. Brief descriptions of each subroutine are given below. Listings of the subroutines are given in Appendix B.

1. GET+(ASC, ARRAY, IVAR, FILE, M)

The subroutine GET is used by the NAI program to obtain spectral data from the various disk file/elements defined as logical unit 8. The program PREGA first obtains the location of the spectrum and sends this location, as an ASCII character string, to the GET subroutine. GET in turn calls CONCAT which concatenates the character string and LUNDEF subsequently sends the concatenated string to the operating system, MIDAS, which interprets the string and performs the command operation. GET is a FORTRAN language subroutine, while the other two, CONCAT and LUNDEF, are written in assembler language.

Listings or descriptions of the system routines CONCAT and LUNDEF are given in Appendix C.

<table>
<thead>
<tr>
<th>VARIABLES (GET)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NAME (DIMENSIONS)</strong></td>
</tr>
<tr>
<td>ARRAY(256)</td>
</tr>
<tr>
<td>ASC(60)</td>
</tr>
<tr>
<td>DEF(10)</td>
</tr>
<tr>
<td>FILE</td>
</tr>
<tr>
<td>IVAR</td>
</tr>
<tr>
<td>K</td>
</tr>
<tr>
<td>LSB</td>
</tr>
<tr>
<td>M</td>
</tr>
<tr>
<td>MSB</td>
</tr>
<tr>
<td>NAM(60)</td>
</tr>
<tr>
<td>RE1</td>
</tr>
<tr>
<td>RE2</td>
</tr>
</tbody>
</table>
The FORTRAN subroutine HISTO is called by the Subroutines RESID and RUNS. From the data received from these two subroutines it generates a labeled, scaled histogram which is output to logical unit 6. The two histograms are "DISTRIBUTION OF RESIDUALS" and "DISTRIBUTION OF RUNS". This routine was written by G. Phillips at NRL in June of 1981.

**VARIABLES (HISTO)**

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(50)</td>
<td>Data point character '*'</td>
</tr>
<tr>
<td>ASTAR</td>
<td>Data point character '*'</td>
</tr>
<tr>
<td>ACOLON</td>
<td>Data point character ':'</td>
</tr>
<tr>
<td>I</td>
<td>Loop index to skip 5 lines after histogram is output</td>
</tr>
<tr>
<td>IDIV</td>
<td>Scale factor for output histogram</td>
</tr>
<tr>
<td>IH(21)</td>
<td>Number of steps on x-axis (21 MAX)</td>
</tr>
<tr>
<td>IOUT</td>
<td>Logical unit = 6 for output</td>
</tr>
<tr>
<td>IT</td>
<td>$\sum x_i$ for output histogram</td>
</tr>
<tr>
<td>J</td>
<td>Y-value for each channel x</td>
</tr>
<tr>
<td>K</td>
<td>Loop over number of x-values in histogram</td>
</tr>
<tr>
<td>LABEL (4)</td>
<td>Title label for output histogram</td>
</tr>
<tr>
<td>MAX</td>
<td>Maximum Y-value allowed; used to determine scale factor (MAX/IDIV &lt; 50)</td>
</tr>
<tr>
<td>N</td>
<td>Number of x-values in histogram</td>
</tr>
<tr>
<td>X</td>
<td>First (or lowest) x-value</td>
</tr>
<tr>
<td>XD</td>
<td>Step size of x-values</td>
</tr>
<tr>
<td>XL</td>
<td>Lowest x-value from calling program</td>
</tr>
</tbody>
</table>
PIVOT (A,P,E,K)

PIVOT is a FORTRAN subroutine called by PREGA. Its purpose is to produce
the negative of the upper triangle of the inverse of a square symmetric
matrix by operating only on the upper triangle of the matrix. The procedure
by which this is accomplished is an adaptation of the Gauss-Jordon Method.
On each entry to PIVOT a specified diagonal element is used for one pivot
operation. To invert a kth order matrix the procedure must be called k
times. The order of which diagonal element is pivoted is unimportant. This
routine checks for a near-zero pivot. All pivots are done with
single-precision arithmetic with no significant loss of accuracy. The
routine was written in FORTRAN by G. Phillips and B.G. Glagola, NRL in July
1982 from Algorithm AS 37 by M.J. Garside.3

VARIABLES (PIVOT)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(10,10)</td>
<td>Array of standards and sample to be inverted</td>
</tr>
<tr>
<td>AA</td>
<td>Reciprocal of the element about which the pivot occurs (A(P,P))</td>
</tr>
<tr>
<td>AIP</td>
<td>A(I,P)*AA or A(P,I)*AA</td>
</tr>
<tr>
<td>E(10)</td>
<td>Variable to determine which standards are in the current subset</td>
</tr>
</tbody>
</table>
| I                 | Loop index over standards with array index less than that of
|                   | the pivoting standard (max P1 = P-1) |
| J                 | Loop index over standards and sample with array index greater
|                   | than that of the pivoting standard (min P2 = P+1) |
| K                 | Number of standards in original set plus one (in PREGA K = LN
|                   | = N+1) |
| P                 | Index of the pivoting standard |
| P1                | P1 = P-1; loop maximum |
| P2                | P2 = P+1; loop minimum |
(4) PUT (ASC, ARRAY, IVAR, FILE, M)

The FORTRAN subroutine PUT was written by G. Phillips, NRL in June 1981. PREGA uses PUT to write the residual spectrum on disk using logical unit 8. This routine also uses CONCAT and LUNDEF to send a character string to the MIDAS operating system and perform the command.

**VARIABLES (PUT):**

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARRAY (256)</td>
<td>Spectrum to be output to disk</td>
</tr>
<tr>
<td>ASC (60)</td>
<td>Disk location of spectrum (File. Name (, Device))</td>
</tr>
<tr>
<td>DEF (10)</td>
<td>Hollerith constant DEF 8, used to create a command in CONCAT and LUNDEF</td>
</tr>
<tr>
<td>FILE</td>
<td>Logical unit number 8</td>
</tr>
<tr>
<td>IVAR</td>
<td>Associated variable for logical unit 8</td>
</tr>
<tr>
<td>K</td>
<td>Loop index over number of channels in output spectrum</td>
</tr>
<tr>
<td>LSB</td>
<td>Least significant byte of data word ARRAY(K)</td>
</tr>
<tr>
<td>M</td>
<td>Number of channels in output spectrum</td>
</tr>
<tr>
<td>MSB</td>
<td>Most significant byte of data word ARRAY(K)</td>
</tr>
<tr>
<td>NAM</td>
<td>Concatenated character string ASC sent to LUNDEF</td>
</tr>
<tr>
<td>V</td>
<td>Data word ARRAY(K)</td>
</tr>
</tbody>
</table>

(5) RESID (R, NZ, MF)

The FORTRAN subroutine RESID was written by G. Phillips, NRL in June 1981. It is used by PREGA to generate a distribution of residuals from the residual/standard deviation spectrum and perform a moment analysis of this distribution. The output from RESID is the "MEAN RESIDUAL", "VARIANCE", "SKEWNESS", and "EXCESS" of the distribution. RESID also calls HISTO to generate and output the histogram of the distribution of residuals.
<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(10)</td>
<td>Moments of the residual distribution</td>
</tr>
<tr>
<td>C(10)</td>
<td>Constants for the moment calculations</td>
</tr>
<tr>
<td>EX</td>
<td>Excess of the residual distribution</td>
</tr>
<tr>
<td>I</td>
<td>Index for loop over the number of channels in the residual spectrum</td>
</tr>
<tr>
<td>IH(21)</td>
<td>Number of steps on the x-axis for SUBROUTINE HISTO</td>
</tr>
<tr>
<td>IOUT</td>
<td>Logical unit for output = 6</td>
</tr>
<tr>
<td>J</td>
<td>Index for the loop to calculate Cj</td>
</tr>
<tr>
<td>K</td>
<td>Index for yield at each step on x-axis for HISTO</td>
</tr>
<tr>
<td>LABEL (4)</td>
<td>Title for histogram sent to HISTO</td>
</tr>
<tr>
<td>M</td>
<td>Number of channels used in calculation plus 1</td>
</tr>
<tr>
<td>MF</td>
<td>Initial channel used in calculations</td>
</tr>
<tr>
<td>N</td>
<td>Number of data points sent to HISTO</td>
</tr>
<tr>
<td>NZ</td>
<td>Final channel used in calculations</td>
</tr>
<tr>
<td>R(256)</td>
<td>Residual/standard error spectrum</td>
</tr>
<tr>
<td>SD</td>
<td>Second moment of residual distribution</td>
</tr>
<tr>
<td>SQ</td>
<td>Third moment of residual distribution, skewness</td>
</tr>
<tr>
<td>U</td>
<td>Mean residual</td>
</tr>
<tr>
<td>U2</td>
<td>Mean squared residual</td>
</tr>
<tr>
<td>U3</td>
<td>Mean cubed residual</td>
</tr>
<tr>
<td>U4</td>
<td>Mean fourth power residual</td>
</tr>
<tr>
<td>V</td>
<td>Variance of residual distribution</td>
</tr>
<tr>
<td>XD</td>
<td>Step size for HISTO</td>
</tr>
<tr>
<td>XL</td>
<td>Lowest x-value for HISTO</td>
</tr>
</tbody>
</table>
RSTAT (NCH, P, R, NZ, MF)

The subroutine RSTAT analyzes the residual/standard deviation spectrum from PREGA to compute an auto-correlation coefficient, its expectation value, standard deviation and an approximate associated FAP. RSTAT uses an entry to the subroutine XQCALC to calculate the associated FAP. This version of RSTAT is an adaptation to PREGA by B.G. Glagola, NRL, 20 July 1982 of the original routine written by T.B. Gosnell, LLNL, 22 June 1982.

VARIABLES (RSTAT)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH</td>
<td>Number of channels in residual spectrum</td>
</tr>
<tr>
<td>DF</td>
<td>Number of degrees of freedom</td>
</tr>
<tr>
<td>EP</td>
<td>Number of standards in final set</td>
</tr>
<tr>
<td>EXRES</td>
<td>Expectation value of residual auto correlation coefficient</td>
</tr>
<tr>
<td>I</td>
<td>Index for loop over number of channels minus one</td>
</tr>
<tr>
<td>MF</td>
<td>Final channel in spectrum</td>
</tr>
<tr>
<td>MF1</td>
<td>MF-1</td>
</tr>
<tr>
<td>NCH</td>
<td>Number of channels in spectrum from PREGA</td>
</tr>
<tr>
<td>NRMR</td>
<td>Equivalent normal standard deviations</td>
</tr>
<tr>
<td>NZ</td>
<td>Initial channel in spectrum</td>
</tr>
<tr>
<td>P</td>
<td>Number of standards in final set from PREGA</td>
</tr>
<tr>
<td>Q</td>
<td>Residual statistic &quot;False Alarm Probability&quot; returned from XQCALC</td>
</tr>
<tr>
<td>R(512)</td>
<td>Residual/standard error spectrum from PREGA</td>
</tr>
<tr>
<td>RSTT</td>
<td>Auto-correlation coefficient</td>
</tr>
<tr>
<td>SIGRES</td>
<td>Standard deviation of R-statistic</td>
</tr>
</tbody>
</table>
The FORTRAN subroutine RUNS analyzes the residual/standard deviation spectrum from PREGA for runs of consecutive channels with the same sign. It outputs the location (starting channel of a run) and the size of the run. The sign of the size indicates a run of positive or negative residuals. RUNS also calls HISTO to generate and output a histogram of the distribution of runs. This routine was written by G. Phillips, NRL, June, 1981.

VARIABLES (RUNS)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Index used for channel counting</td>
</tr>
<tr>
<td>ICH</td>
<td>Beginning channel of a particular run</td>
</tr>
<tr>
<td>IH(21)</td>
<td>Counter for the number of times a particular run length occurs</td>
</tr>
<tr>
<td>J</td>
<td>Output index over location and number of large runs</td>
</tr>
<tr>
<td>K</td>
<td>Index for x-axis of number of runs histogram</td>
</tr>
<tr>
<td>KSI(12)</td>
<td>Storage variable for length of long runs</td>
</tr>
<tr>
<td>LABEL(4)</td>
<td>Identification label for histogram, sent to HISTO</td>
</tr>
<tr>
<td>MF</td>
<td>Last channel of spectrum used for calculations</td>
</tr>
<tr>
<td>N</td>
<td>Number of data points sent to HISTO</td>
</tr>
<tr>
<td>NCH(50)</td>
<td>Initial channel of long runs for output</td>
</tr>
<tr>
<td>NRS(50)</td>
<td>Length of long runs for output</td>
</tr>
<tr>
<td>NZ</td>
<td>Initial channel of spectrum used for calculation</td>
</tr>
<tr>
<td>R(256)</td>
<td>Residual/standard error spectrum from PREGA</td>
</tr>
<tr>
<td>XD</td>
<td>Step-size of x-axis of output histogram</td>
</tr>
<tr>
<td>XL</td>
<td>Lowest value on x-axis of output histogram</td>
</tr>
</tbody>
</table>
Future Modifications of PREGA

The program SEDIT, as received originally from Nuclear Data, Inc., is capable of handling up to 40 standard nuclides in the library. At the present PREGA limits the number of standards that are allowed to be in the library. This is because PREGA was built on the framework of the Nuclear Data, Inc. NAI Analysis Package. In this package, the analysis program (called PREGA now) reads control parameters first from SEDIT and then from UEDIT. Hence, PREGA reads all of the standards listed by SEDIT from disk, and computes their sums and does background corrections before it reads from UEDIT which standards and in which order they are to be used in the regression analysis. To keep PREGA from becoming unnecessarily large, it was decided that nine standards would be sufficient to fit a sample spectrum. To increase the maximum number of standards allowed several variable dimensions in PREGA and subroutine PIVOT have to be modified. Currently these have the dimension (10) or (10,10) for arrays. These variables are listed below along with their identification, with \( N \) = maximum number of standards in the library.

PREGA

\[
A(N+1, N+1) \quad \text{The matrix that the pivot operations are carried out on}
\]

\[
AC(N) \quad \text{Activity of standards from library in SEDIT}
\]

\[
ARR(N,64) \quad \text{Matrix containing 64 channels of } N \text{ standard spectra for residual calculation}
\]

\[
B(N) \quad C_j = \sum_{i} w_{ij} x_i
\]

\[
CC(N+1, N+1) \quad \text{Correlation matrix for standards and sample}
\]

\[
EF(N) \quad \text{Logical variable to keep track of standard status in subroutine PIVOT}
\]

\[
FP(N) \quad \text{Partial F-value for output after pivot}
\]

\[
FPM(N) \quad \text{Partial F-to-add or F-to-remove}
\]

\[
HA(N) \quad \text{Half-life of standards from library in SEDIT}
\]

\[
HAT(N) \quad \text{Half-life of standard; printout order}
\]

\[
IS(N) \quad \text{Printout order of standards; OR in UEDIT can change during execution}
\]

\[
ISL(N) \quad \text{Printout order of standard; never changes during execution}
\]

\[
IT(N) \quad \text{Serial order of standards to be used in least-squares fit}
\]
PREGA (Cont'd)

**MY(N)**  
Integer vector used to check bit pattern of current set of standards for a particular standard; NOTE - values must also be added to DATA statement for **MY**

**SS(N)**  
Sum of counts over channels of standard spectra

**STD(N)**  
Standard error of nuclide concentration

**TISO(2*N),TISOT(2*N)**  
Names of standard nuclides

**TST(N)**  
Counting time of standard in seconds, from SEDIT

**Z(N)**  
Standard nuclide concentration

NOTE: For neatness of output, if the number of standards is increased the I/O statements for the correlation matrix at PREGA lines 204-208 and 248-252 must also be modified.

**PIVOT**

**A(N+1, N+1)**  
Matrix to be pivoted

**E(N)**  
Logical variable to determine which standards are in the current subset
8. PROGRAM SEDIT

Operation

The standards editor program, SEDIT, is used to prepare a file that contains control parameters for the standards and the standard library for use by PREGA. The library contains information about the name, disk location, half-life, etc., about each standard spectrum. SEDIT writes to a file assigned to logical unit 9. SEDIT allows the user to build, change or list the standard control parameters, and to also create a new library, insert or delete a standard, append new standards or list the present library. The structure of the output file on logical unit 9 is given in the section under PREGA software organization. A listing of SEDIT is given in Appendix B.

LANGUAGE

The program is written in DEC RT-11 FORTRAN.

INPUTS

Keyboard Logical unit 5, all operator interaction and input is from keyboard
Logical Unit 11 Output file of UEDIT used for reading number of standards wanted for fit, for one standard library listing option
Logical Unit 9 For modifying an existing SEDIT output file

OUTPUT

Logical Unit 6 Record of operator interaction with SEDIT. This is usually defined as the keyboard unit the operator is using for input
File.Element Logical unit 9 output file for SEDIT saved on disk for use with PREGA

A sample copy of the output from SEDIT is given in Appendix A.
<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(32)</td>
<td>Isotope name or file.element disk location</td>
</tr>
<tr>
<td>ACT</td>
<td>Activity of standard</td>
</tr>
<tr>
<td>ANS</td>
<td>Alphanumeric answer to SEDIT prompt (e.g. Y, N)</td>
</tr>
<tr>
<td>BA</td>
<td>Background spectrum location FILE.ELEMENT (.DEVICE)</td>
</tr>
<tr>
<td>BB</td>
<td>= B, for build new header containing standard control parameters</td>
</tr>
<tr>
<td>BS</td>
<td>Background subtract option</td>
</tr>
<tr>
<td>BT</td>
<td>Counting time for background spectrum in seconds</td>
</tr>
<tr>
<td>CC</td>
<td>= C, to change one of the header parameters</td>
</tr>
<tr>
<td>D</td>
<td>Days, half-life unit</td>
</tr>
<tr>
<td>EDT</td>
<td>Program pointer</td>
</tr>
<tr>
<td>FNUM</td>
<td>REAL*4 I/O variable</td>
</tr>
<tr>
<td>H</td>
<td>Hours, half-life unit</td>
</tr>
<tr>
<td>HL</td>
<td>Standard half-life</td>
</tr>
<tr>
<td>I</td>
<td>Index for program control</td>
</tr>
<tr>
<td>IE</td>
<td>Final channel for computation</td>
</tr>
<tr>
<td>INT(26)</td>
<td>Used to rewrite library when inserting or deleting a standard</td>
</tr>
<tr>
<td>IS</td>
<td>Initial channel for computation</td>
</tr>
<tr>
<td>IT</td>
<td>Number of iterations</td>
</tr>
<tr>
<td>NOTE - no longer used, set = 1</td>
<td></td>
</tr>
<tr>
<td>IVAR</td>
<td>Record number for direct-access I/O</td>
</tr>
<tr>
<td>K</td>
<td>Check time units of half-life and program pointer</td>
</tr>
<tr>
<td>L</td>
<td>Defines logical unit for output</td>
</tr>
<tr>
<td>LA</td>
<td>Switch program to append library mode</td>
</tr>
<tr>
<td>LD</td>
<td>Switch program to delete standard mode</td>
</tr>
</tbody>
</table>
## VARIABLES (SEEDIT), (cont'd)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>LENGTH</td>
<td>Check for answer being carriage return only (to switch from header to library section or exit program)</td>
</tr>
<tr>
<td>LI</td>
<td>Switch program to insert standard mode</td>
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<tr>
<td>LN</td>
<td>Switch program to create a new library mode</td>
</tr>
<tr>
<td>LP</td>
<td>Switch program to list mode</td>
</tr>
<tr>
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<td>Logical unit to read UEDIT variables NR and OR</td>
</tr>
<tr>
<td>LU</td>
<td>Logical unit for output file of SEEDIT</td>
</tr>
<tr>
<td>M</td>
<td>Total number of standards in library</td>
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<tr>
<td>MLA</td>
<td>NS from UEDIT for list standard option</td>
</tr>
<tr>
<td>MLI</td>
<td>OR from UEDIT for list standard option</td>
</tr>
<tr>
<td>MM</td>
<td>Months, half-life unit</td>
</tr>
<tr>
<td>N</td>
<td>Counter for number of standards in library</td>
</tr>
<tr>
<td>NC</td>
<td>Number of channels per standard</td>
</tr>
<tr>
<td>NUM</td>
<td>I*2 I/O variable</td>
</tr>
<tr>
<td>RC</td>
<td>Rejection coefficient no longer used, set = 1</td>
</tr>
<tr>
<td>SEC</td>
<td>Counting time of standard in seconds</td>
</tr>
<tr>
<td>Y</td>
<td>YES, I/O answer to SEEDIT prompt</td>
</tr>
</tbody>
</table>
9. PROGRAM UEDIT

Operation

The unknown sample editor program, UEDIT, is used to prepare a file that contains control parameters and information about the sample for use by PREGA. UEDIT writes to a file assigned to logical unit 11. The program SEDIT also reads the UEDIT output file to control an operator option for listing the standard library. UEDIT allows the user to Build, Change, or List the output file with prompting questions. The structure of the output file on logical unit 11 is given in the section under PREGA software organization.

LANGUAGE

The program is written in DEC RT-11 FORTRAN

INPUTS

Keyboard Logical unit 5, all operator interaction and input is from keyboard
Logical Unit 11 For modifying an existing UEDIT output file

OUTPUTS

Logical Unit 6 Record of operator interaction with UEDIT. This is usually defined as the keyboard unit the operator is using for input
FILE.ELEMENT Logical unit 11 output file for UEDIT saved on disk for use with SEDIT and PREGA

A sample copy of the output from UEDIT is given in Appendix A.
<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(32)</td>
<td>FILE.ELEMENT location on disk of the unknown sample spectrum, background spectrum or residual spectrum</td>
</tr>
<tr>
<td>ANS</td>
<td>Alpha-numeric I/O variable</td>
</tr>
<tr>
<td>BA</td>
<td>Background spectrum disk location (FILE.ELEMENT (DEVICE))</td>
</tr>
<tr>
<td>BG</td>
<td>Background supplied option</td>
</tr>
<tr>
<td>BP</td>
<td>Pivot on background allowed option</td>
</tr>
<tr>
<td>BR</td>
<td>Start analysis with background only option</td>
</tr>
<tr>
<td>BS</td>
<td>Subtract background from sample option</td>
</tr>
<tr>
<td>BT</td>
<td>Counting time for background in seconds</td>
</tr>
<tr>
<td>CC</td>
<td>Switch program to change parameter mode</td>
</tr>
<tr>
<td>CRT</td>
<td>In logical unit number = 5</td>
</tr>
<tr>
<td>CT</td>
<td>Counting time of sample in seconds</td>
</tr>
<tr>
<td>DT</td>
<td>Decay time of sample, set = 1</td>
</tr>
<tr>
<td>EDT</td>
<td>Program pointer</td>
</tr>
<tr>
<td>F$\phi$</td>
<td>Rejection coefficient for partial F test</td>
</tr>
<tr>
<td>FNUM</td>
<td>R*4 I/O variable</td>
</tr>
<tr>
<td>GN</td>
<td>Gain shift ratio no longer used, set = 1</td>
</tr>
<tr>
<td>I</td>
<td>Index for loop over location of spectra</td>
</tr>
<tr>
<td>II</td>
<td>Index for program control</td>
</tr>
<tr>
<td>ITT</td>
<td>Upper bound of loop for output</td>
</tr>
<tr>
<td>IVAR</td>
<td>Record number for direct-access I/O to logical unit 11 file</td>
</tr>
<tr>
<td>K</td>
<td>Program control variable</td>
</tr>
<tr>
<td>LENGTH</td>
<td>Used as check for carriage return to exit current mode of program or exit program</td>
</tr>
<tr>
<td>LL</td>
<td>Switch program to list mode</td>
</tr>
</tbody>
</table>
## VARIABLES (UEDIT)

<table>
<thead>
<tr>
<th>NAME (DIMENSIONS)</th>
<th>USAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>LUN</td>
<td>Logical unit 11 for output</td>
</tr>
<tr>
<td>M</td>
<td>First record of LU 11 file</td>
</tr>
<tr>
<td>MF</td>
<td>Result multiplication factor option (usually set = 1)</td>
</tr>
<tr>
<td>NN</td>
<td>Switch program to create a new file mode</td>
</tr>
<tr>
<td>NO</td>
<td>N, the answer no to UEDIT prompt question</td>
</tr>
<tr>
<td>NS</td>
<td>Number of standards from library to be used in least-squares fit by PREGA</td>
</tr>
<tr>
<td>NUM</td>
<td>I*2 I/O variable</td>
</tr>
<tr>
<td>NUM1</td>
<td>Control variable for record number in LU-11 file</td>
</tr>
<tr>
<td>OR</td>
<td>Number of library standard in order of desired printout</td>
</tr>
<tr>
<td>RC</td>
<td>Rejection coefficient for rejection of standards used. No longer used.</td>
</tr>
<tr>
<td>RO</td>
<td>Output residuals option</td>
</tr>
<tr>
<td>RS</td>
<td>Residual spectrum disk location (FILE.ELEMENT (,DEVICE))</td>
</tr>
<tr>
<td>SB</td>
<td>Subtract background from standards option</td>
</tr>
<tr>
<td>TH</td>
<td>Threshold shift, no longer used. Set = 1</td>
</tr>
<tr>
<td>UN</td>
<td>Unknown spectrum disk location (FILE.ELEMENT (,DEVICE))</td>
</tr>
<tr>
<td>VR</td>
<td>Volume reduction factor option, usually set = 1</td>
</tr>
<tr>
<td>WD</td>
<td>Weighting factor determination option</td>
</tr>
<tr>
<td>WF</td>
<td>Weighting factor calculation option</td>
</tr>
<tr>
<td>YES</td>
<td>Y, the answer to a UEDIT prompt question</td>
</tr>
</tbody>
</table>
PREGA - GENERAL OUTLINE

SET UP (SEDIT & UEDIT)

REGRESSION WITH ALL LIBRARY STANDARDS

SELECT TRIAL SUBSET

BACKWARD PIVOT

CHANGE IN SUBSET?

FORWARD PIVOT

OUTPUT FINAL RESULTS AND RESIDUALS AND RUNS TESTS

Figure 1. Summary flow chart of the program PREGA showing the major sections of the code.
Figure 2. Logical unit and disk file structure for the program PREGA.
Figure 3. Hierarchy of subroutines called by the program PREGA.
REFERENCES


5. ND6600 NAI Data Reduction Package Operational Instruction Documentation (Nuclear Data, Inc. publication, March 1978).


7. T. Gosnell, Lawrence Livermore National Laboratory, Livermore, CA, private communication.
APPENDIX A: Sample Output for PREGA

Sample Output for Least Squares Analysis

The following pages contain sample outputs from the editor programs UEDIT and SEDIT, and from the program PREGA. The listing from UEDIT and SEDIT are provided to show the various options used in PREGA. The least squares analysis method used is the full PREGA mode. This mode uses a trial set of standards comprised of those standards which are most highly correlated with the unknown spectrum, as determined from a fit to the complete library.
PREGA UNKNOWN SAMPLE PARAMETERS

(UN) UNKNOWN SPECTRUM: FILE.ELEMENT(,DEVICE)
    : PREGA.G12161

(GN) GAIN SHIFT RATIO : 1.00000

(TH) THRESHOLD SHIFT : 1.00000

(BG) BACKGROUND SUPPLIED ? : Y

(BS) SUBTRACT BACKGROUND ? : Y

(BT) COUNTING TIME FOR BACKGROUND (SECS) : 300.000

(CT) COUNTING TIME FOR UNKNOWN SAMPLE : 430.000

(VR) VOLUME REDUCTION (OR INVERSE OF DILUTION) FACTOR : 1.00000

(DT) DECAY TIME : 0.000000

(MF) RESULT MULTIPLICATION FACTOR : 1.00000

(BA) BACKGROUND SPECTRUM: FILE.ELEMENT(,DEVICE)
    : PREGA.B12161

(WD) HOW ARE WEIGHTING FACTORS TO BE DETERMINED ?
    0: BASED ON ACTUAL COUNTS/CHANNEL.
    1: BASED ON CALCULATED COUNTS/CHN : 0

(NS) NUMBER OF ISOTOPES USED FROM THE STANDARD LIBRARY?: 6

(F0) F-TEST REJECTION COEFFICIENT : 2.50000

(WF) WEIGHTING FACTOR CALCULATION.
    -1: (COUNTS)**-1
    0: (SIGMA)**2
    1: 1 : 0

(RC) REJECTION COEFFICIENT APPLIED ? : Y

(BR) BACKGROUND REGRESSION ?
    0: TRIAL SET = CHOSEN STANDARDS
    1: TRIAL SET = BACKGROUND ONLY : 1

(BP) PIVOT ON BACKGROUND SPECTRUM ALLOWED?
    0: NO PIVOT ON BACKGROUND ALLOWED
    1: ALLOW PIVOT ON BACKGROUND SPECTRUM : 0

(RD) OUTPUT RESIDUALS ?: N

(RS) RESIDUAL SPECTRUM: FILE.ELEMENT(,DEVICE)
    : DDTAB.R31828

(OR) NUMBER OF LIBRARY STANDARD IN ORDER OF DESIRED PRINTOUT
    : 1 2 3 4 5 7
PREGA LIBRARY HEADER

(NC) NUMBER OF CHANNELS PER STANDARD (MAX-512) : 255
(IT) NUMBER OF ITERATIONS FOR THRESHOLD & GAIN CALC. : 1
(BS) BACKGROUND SUBTRACT ? : N
(IS) INITIAL CHANNEL FOR COMPUTATION : 19
(IE) FINAL CHANNEL FOR COMPUTATION : 242
(BT) COUNTING TIME OF BACKGROUND (SECS.) : 388.800
(RC) REJECTION COEFFICIENT : 1.00000
(BA) BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))
   : PREGA.B12161
PREGA LIBRARY STANDARDS USED

STANDARD * 1 : B12161
FILE.ELEMENT(,DEVICE) : PREGA.B12161
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  3.8000E 02
ACTIVITY:  1.0000E 00

STANDARD * 2 : 226RA
FILE.ELEMENT(,DEVICE) : NAI.RAD45
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  1.4000E 03
ACTIVITY:  1.0000E 00

STANDARD * 3 : TH232
FILE.ELEMENT(,DEVICE) : NAI.TH232
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  1.0000E 03
ACTIVITY:  1.0000E 00

STANDARD * 4 : K40
FILE.ELEMENT(,DEVICE) : NAI.K40
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  1.0000E 03
ACTIVITY:  1.0000E 00

STANDARD * 5 : PC060
FILE.ELEMENT(,DEVICE) : NAI.PC060
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  3.8000E 02
ACTIVITY:  1.0000E 00

STANDARD * 7 : CS137
FILE.ELEMENT(,DEVICE) : NAI.CS137
HALF-LIFE (SECS):  1.0000E 09
COUNTING TIME OF STANDARD (SECS):  1.0000E 03
ACTIVITY:  1.0000E 00
### Output for Prega Analysis Program

**Sample Spectrum: PREGA.G12161**

<p>| | | | | | | | |</p>
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BACKGD SUM = 1.732E 05  SAMPLE SUM = 4.606E 04

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WEIGHTED SUMS OF STANDARDS AND UNKNOWN

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9.4290E 01  1.0245E 02  8.8000E-01
### RESULTS OF FULL SET REGRESSION ON G12161

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226RA   F= 1.2789E 01  0= 1.4521E-04  X= 3.6256E 00  RMSR= 2.1816E 00
TH232   F= 1.4523E-01  0= 3.5171E-01  X= 3.0072E 00  RMSR= 2.0621E 00
K40     F= 2.9365E-01  0= 7.0589E-01  X= -5.4146E-01  RMSR= 2.0635E 00
PC060   F= 5.3934E 02  0= 6.0000E-01  X= 9.9999E 09  RMSR= 7.1591E 00
CS137   F= 1.5861E 00  0= 1.0378E-01  X= 1.2603E 00  RMSR= 2.0757E 00

### RESULTS OF TEST SET REGRESSION ON G12161

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226RA   F= 1.9334E 01  0= 3.5809E-06  X= 4.4918E 00  RMSR= 2.2271E 00
PC060   F= 5.5820E 02  0= 8.0000E-01  X= 9.9999E 09  RMSR= 7.1671E 00
CS137   F= 1.8771E 00  0= 8.5109E-02  X= 1.3714E 00  RMSR= 2.0647E 00
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MSR = 2.065E 00

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CALCULATED PARTIAL F-, Q- AND X-VALUES TO ADD:

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FINAL RESULT FOR G12161

FIT = 2.073E 00

RESULTS = CONCENTRATIONS AND EST STANDARD ERRORS

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**** LLNL R-STATISTIC ****

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EXPECTATION VALUE............................. -1.3393E-02
STANDARD DEVIATION........................... 6.7722E-02
EQUIVALENT NORMAL STANDARD DEVIATIONS........ 1.4513E 01
R-STAT FAP.................................. 0.0000E-01

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### Suspectious Channels

97  4.10 108  4.79 109  4.91 110  5.24

Mean Residual = -0.004, Variance = 2.045, Skewness = 0.376, Excess = 1.87
DISTRIBUTION OF RESIDUALS

SCALE FACTOR= 1

-5.00 1 *
-4.50 0 :
-4.00 1 *
-3.50 0 :
-3.00 3 ****
-2.50 4 ****
-2.00 8 ********
-1.50 18 **************
-1.00 33 ********____________________
-0.500 28 ____________________________
0.000 37 ______________________________
0.500 42 ______________________________
1.00 17 ______________________________
1.50 7 ********
2.00 14 ********
2.50 4 ****
3.00 1 *
3.50 2 **
4.00 1 *
4.50 0 :
5.00 3 ****

TOTAL = 224

DISTRIBUTION OF RUNS

SCALE FACTOR= 1

-10.0 0 :
-9.00 0 :
-8.00 1 *
-7.00 2 **
-6.00 2 **
-5.00 0 :
-4.00 6 ********
-3.00 6 ********
-2.00 6 ********
-1.00 26 ______________________________
0.000 0 :
1.00 28 ______________________________
2.00 14 _____________________________
3.00 6 ********
4.00 3 ***
5.00 2 **
6.00 0 :
7.00 2 **
8.00 1 *
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10.0 0 :

TOTAL = 97

LOCATIONS AND SIZES OF LARGE RUNS

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71
Appendix B: FORTRAN Listings, DEC RT-11

1. PKANAL
2. PEAKNL
3. FREEFM
4. GSHIFT
5. REGAIN
6. RECHAN
7. SEDIT
8. UEDIT
9. PREGA
10. GET
11. HISTO
12. PIVOT
13. PUT
14. RESID
15. RSTAT
16. RUNS
17. XQCALC
PROGRAM PKANAL
WRITTEN BY G.W.PHILLIPS, JULY 1981

READS IN DATA FROM NUCLEAR DATA SPECTRAL FILES
AND CALCULATES PEAK POSITIONS, WIDTHS AND AREAS
FOR SELECTED REGIONS

INPUT: JL,JR - LOWER AND UPPER CHANNELS FOR PEAK REGIONS
ASC - FILENAME FOR SPECTRUM TO BE ANALYZED

OUTPUT: JL,JR - INPUT LIMITS FOR PEAK REGIONS
KL,KR - PEAK LIMITS (POSITIVE NET COUNT)
AMAX - PEAK MAXIMUM (NET COUNTS)
AREA - PEAK NET AREA
BKGD - BACKGROUND AREA BENEATH PEAK
CG - PEAK CENTROID
VAR - PEAK VARIANCE ABOUT CENTROID
FWHM - PEAK FULL WIDTH AT HALF MAXIMUM
ENERGY - CALIBRATED PEAK ENERGY

PROCEDURES CALLED:
PEAKNL - DOES PEAK ANALYSIS
GET - READS SPECTRUM AND ENERGY CALIBRATION FOR DISK
C

0001 COMMON ARRAY ARRAY(512)
0002 INTEGER CRT, DATA, PERIOD, BLANK, JL(20), JR(28)
0003 COMMON DATA DATA(60), FREE INTEG(16), REALX16, ALPHA(16)
0004 REAL*8 ALPHA, ABLANK, AHEAD(11)
0005 LOGICAL*1 ASC(60)
0006 DATA ABLANK=8H
0007 DATA CRT/5L,LP/6L,IN/5L,OUT/6L,PERIOD/1L,BLANK/1H,LUF/8H
0008 DATA AHEAD/8H REGION 8H LIMITS 8H PEAK 8H LIMITS ,
   1 8H HEIGHT 8H AREA 8H BKGD.,
   2 8H CENTROID 8H VARIANCE 8H FWHM ,
   3 8H ENERGY /

C

0009 100 WRITE(CRT,110)
0010 110 FORMAT(1X,"ENTER REGIONS BY FIRST LAST CHANNEL")
0011 DO 160 I=1,20
0012 READ(CRT,120)LEN,DATA
0013 120 FORMAT(Q,00A1)
0014 IF(LEN.LT.1) GOTO 100
0016 NX=2
0017 MX=1
0018 NA=1
0019 CALL FREEFM(NX, MX, NA, 1)
0020 JL(I)=INTEG(1)
0021 JR(I)=INTEG(2)
0022 160 CONTINUE
0023 I=21
0024 180 N=I-1
0025 IF(N.LT.1) GOTO 990

C
C
C
0027 200  IFORM=1
0028
0029 210  WRITE(CRT,210)
0030
0031 220  FORMAT(IHB,'FILENAME FOR SPECTRUM'
0032 230  READ(CRT,230)LEN,ASC
0033 240  FORMAT(Q,80A1)
0034
0035 250  IF(LEN.LT.1) GOTO 990
0036
0037 260  WRITE(IOUT,240) IFORM,(ASC(I),I=1,LEN)
0038
0039 270  FORMAT(I1,80A1)
0040 280  IFORM=0
0041
0042 290  WRITE(IOUT,250) AHEAD
0043
0044 300  IF(LEN.LT.1) GOTO 990
0045
0046 310  CALL GET(ASC.ARRAY,IVAR.LUF,MI,A0,B0,C0)
0047
0048 320  WRITE(CRT,260) MI
0049
0050 330  DO 360 I=1,N
0051 340  KL=JL(I)
0052 350  KR=JR(I)
0053
0054 360  CALL PEAKNL(KL,KR,ML,MR,MLX,KLX,KR)
0055
0056 370  IFORM=1
0057
0058 380  WRITE(IOUT,320) JL(I),KR(I),ML,MR,MLX,KLX,KL,KR,AMAXPAREA,BKGD,CG.VAR,FHWM,ENERGY
0059
0060 390  CONTINUE
0061
0062 400  GOTO 220
0063
0064 410  WRITE(IOUT,399)
0065
0066 420  FORMAT(IHB)'CHANNELS READ IN'
0067
0068 430  CONTINUE
0069
0070 440  GOTO 220
0071
0072 450  WRITE(IOUT,499)
0073
0074 460  FORMAT(IHB)'END'
0075
0076 470  STOP
0077  END
### MIDAS FORTRAN IV STORAGE MAP

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**COMMON BLOCK /ARRAY/**  
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**ARRAY**  
000000 REAL*4 ARRAY (512)

**COMMON BLOCK /DATA/**  
LENGTH 000240

**DATA**  
000000 INTEGER*2 ARRAY (90)

**COMMON BLOCK /FREE/**  
LENGTH 000340

**INTEG**  
000000 INTEGER*2 ARRAY (16)

**REALX**  
000040 REAL*4 ARRAY (16)

**ALPHA**  
000140 REAL*8 ARRAY (16)
SUBROUTINE PEAKNL(KL, KR, ML, MR, MX, XR,
   IAL, BL, AMAX, AREA, BKGD, CG, VAR, FWHM)
C WRITTEN BY G.W. PHILLIPS, JULY 1981
C
C FINDS THE AREA, CENTER OF GRAVITY, VARIANCE AND FWHM
C FOR A PEAK IN A REGION BETWEEN KL AND KR
C AFTER SUBTRACTING A BACKGROUND CALCULATED
C AS A STRAIGHT LINE DRAWN BETWEEN
C THE MINIMUM BELOW THE PEAK AND THE MINIMUM
C ABOVE THE PEAK.
C IF THE DATA IS FLAT WITHIN STATISTICS AT THE MINIMUM
C THE AVERAGE OF THE THREE CHANNELS
C INCLUDING THE MINIMUM IS USED.
C
INPUT: KL, KR - INITIAL LIMITS FOR PEAK REGION
C
OUTPUT: KL, KR - FINAL LIMITS FOR PEAK (POSITIVE NET COUNT)
ML, MR - MINIMUM CHANNELS BELOW AND ABOVE PEAK
MX - PEAK MAXIMUM CHANNEL
XL, XR - HALF MAXIMUM POINTS BELOW AND ABOVE PEAK
AL, BL - SLOPE AND OFFSET (FROM ML)
FOR BACKGROUND
AMAX - PEAK MAXIMUM (NET COUNTS)
AREA - PEAK NET AREA
BKGD - BACKGROUND AREA BENEATH PEAK
CG - PEAK CENTROID
VAR - PEAK VARIANCE ABOUT CENTROID
FWHM - PEAK FULL WIDTH AT HALF MAXIMUM
C
0002 COMMON ARRAY AX(512)
D DATA ICRT/5/
C
C LOOK FOR MAXIMUM IN THE REGION
C
0003 100 AMAX=0.
0004 MX=0
0005 DO 110 I=KL,KR
0006 IF(AMAX.GT.AX(I)) GOTO 110
0008 AMAX=AX(I)
0009 MX=I
0010 110 CONTINUE
C
C LOOK FOR LOWER AND UPPER MINIMA
C
0011 AMINL=AX(KL)
0012 ML=KL
0013 DO 130 I=KL,MX
0014 IF(AX(I).GT.AMINL) GOTO 130
0016 AMINL=AX(I)
0017 ML=I
0018 130 CONTINUE
0019 AMINR=AX(MX)
0020 MR=MX
0021 DO 140 I=MX,KR
0022 IF(AX(I).GE.AMINR) GOTO 140
0024 AMINR=AX(I)
0025 MR=I
0026 140 CONTINUE
DETERMINE BACKGROUND PARAMETERS

IF(ML.EQ.KL) ML=ML+1
J=ML-1
K=ML+1
SUML=0.
SQL=0.
DO 210 I=J,K
FL=AX(I)
SUML=SUML+FL
SQL=SQL+FL**2
CONTINUE

IF(MR.EQ.KR) MR=MR-1
J=MR-1
K=MR+1
SUMR=0.
SOR=0.
DO 220 I=J,K
FR=AX(I)
SUMR=SUMR+FR
SOR=SOR+FR**2
CONTINUE

DL=AMAX1(ABS(AX(ML-1)-AX(ML)),ABS(AX(ML+1)-AX(ML)))
DR=AMAX1(ABS(AX(MR-1)-AX(MR)),ABS(AX(MR+1)-AX(MR)))
AL=SUML/3.
IF(DL.LT.2.*SOL) GOTO 248
IF(AX(ML).GT.AX(ML-1)) ML=ML-1
AL=AX(ML)

AR=SUMR/3.
IF(DR.LT.2.*SQR) GOTO 250
IF(AX(MR).GT.AX(MR-1)) MR=MR+1
AR=AX(MR)
BL=(AR-AL)/FLOAT(MR-ML)
WRITE(ICRT,260)ML,MR,AL,BL
D260 FORMAT(1X,’BACKGROUND PARAMETERS: ML MR AL BL’/
1X,21.2G12.4)

LOOK FOR MAXIMUM IN NET COUNTS

AMAX=AX(ML)-AL
DO 270 I=ML,MR
A=AX(I)-AL-BL*FLOAT(I-ML)
IF(A.LT.AMAX) GOTO 270
AMAX=A
CONTINUE
C DEFINE PEAK LIMITS
C
0073 300 KL=ML-1
0074  DO 310 I=ML,MX
0075 IF(A(I).LT.AL+BL*FLOAT(I-ML)) KL=I
0077 310 CONTINUE
0078 KL=MINO(KL+1,MX)
0079 KR=MX
0080  DO 328 I=MX,MR
0081 IF(A(I).LT.AL+BL*FLOAT(I-ML)) GOTO 330
0083 KR=I
0084 328 CONTINUE
C CALCULATE PEAK PARAMETERS
C
0085 330 AI=0.
0086 AISO=0.
0087 AREA=0.
0088 BKGD=0.
0089 CG=0.
0090 VAR=0.
0091 FWHM=0.
D WRITE(ICRT,340)
D340 FORMAT(4X,'I',3X,'COUNTS ',3X,'BKGD ',3X,'NET ',
D I ',3X,'AREA ',3X,'AI ',3X,'AISO ',)
0092  DO 360 I=KL,MR
0093 B=AL+BL*FLOAT(I-ML)
0094 BKGD=BKGD+B
0095 A=A(I)-B
0096 AREA=AREA+A
0097 AISO=AISO+A*FLOAT(I)
0098 AREA=AREA*CG**2+2.*AI*CG/AREA
D WRITE(ICRT,350)I,A(I),B,A,AREA,AISO
D350 FORMAT(1X,I4,6G11.3)
0099 360 CONTINUE
0100 IF(AREA.EQ.0.) RETURN
0102 CG=AI/AREA
0103 VAR=(AISO+AREA*CG**2-2.*AI*CG)/AREA
C
C  FIND FWHM
C
0104  400   AHALF=AMAX/2.
0105   B=AL+BL*FLOAT(KL-ML-1)
0106   AO=AX(KL-1)-B
0107   DO 410  I=KL,MX
0108     IL=I
0109     B=B+BL
0110   A=AX(I)-B
0111   IF(A.GT.AHALF) GOTO 420
0113   AO=A
0114  410   CONTINUE
0115  420   DA=AO-A
0116   IF(DA.EQ.0.) DA=2.*(A-AHALF)
0118   X=(A-AHALF)/DA
0119   XL=FLOAT(IL)-X
C
0120   B=AL+BL*FLOAT(MX-ML-1)
0121   AO=AX(MX-1)-B
0122   DO 430  I=MX,KR
0123     IR=I
0124     B=B+BL
0125   A=AX(I)-B
0126   IF(A.LT.AHALF) GOTO 440
0128   AO=A
0129  430   CONTINUE
0130   IR=IR+1
0131  440   DA=AO-A
0132   IF(DA.EQ.0.) DA=2.*(AHALF-A)
0134   X=(AHALF-A)/DA
0135   XR=FLOAT(IR)-X
0136   FWHM XR-IXL
D   WRITE(I CRT, 450) MX, IL, IR, XL, XR, FWHM
D450  FORMAT(5X, 'WIDTH PARAMETERS: MX IL IR XL XR FWHM'/
D        1X, 318, 3G12.4/)  
C
0137   RETURN
0138   END
**MIDAS FORTRAN IV STORAGE MAP**

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<td>X</td>
<td>000172</td>
<td>REAL*4 VARIABLE</td>
</tr>
<tr>
<td>IR</td>
<td>000176</td>
<td>INTEGER*2 VARIABLE</td>
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</tbody>
</table>

**COMMON BLOCK ARRAY**  LENGTH 004000

82
SUBROUTINE FREEFM(NM,NAPITYPE)

LAST REVISED AUGUST 1981 BY G.W.P.

GENERAL SUBROUTINE TO DECODE DATA READ IN FREE FIELD FORMAT
DELIMITERS ARE EITHER A BLANK OR A COMMA
THE ROUTINE ASSUMES THE DATA HAS BEEN READ INTO ARRAY IDATA WITH
THE FORMAT (88A1)
N IS THE NUMBER OF DATA ELEMENTS, MAXIMUM=16
N IS RETURNED AS THE NUMBER OF DATA ELEMENTS FOUND
M IS THE LOCATION IN THE ARRAY FOR STORING THE FIRST DATA ELEMENT
M IS RETURNED AS THE LOCATION FOLLOWING THE NTH DATA ELEMENT
NA IS THE BEGINNING COLUMN OF THE DATA
NA IS RETURNED AS THE COLUMN FOLLOWING THE NTH DATA ELEMENT
ITYPE IS THE TYPE OF DATA,
1=INTEGER
2=REAL
3=ALPHANUMERIC

COMMON/DATA/IDATA(88)
COMMON/FREE/INTEG(16),REALX(16),ALPHA(16)
INTEGER SEMI,E,COMMA
REAL*8 ALPHA,BLANK
DIMENSION ITEMP(20),AFORM(2)

DATA SEMI,E,IBLK1,COMMA,IBLK2,BLNK4,BLANK

L=M
M=M+N-1
DO 300 I=L,M
IF(NA.GT.88) GO TO 400

LOOK FOR START OF CURRENT FIELD

DO 210 J=NA,00
JQQ=J
IF(IDATA(J).NE.IBLK1) GO TO 215
210 CONTINUE
NA=81
GO TO 400

IF(IDATA(JQQ).NE.COMMA) GO TO 220
NA=JQQ+1
GO TO 290
C LOOK FOR END OF CURRENT FIELD
C
  0024  220  IL=JQQ
  0025     ILQ = IL
  0026  221  DO 230 J=ILQ,88
  0027     JQQ=J
  0028     IF(IDATA(J).EQ.IBLK1) GO TO 235
  0029     IF(IDATA(J).NE.COMMA) GO TO 230
  0030     IR=J-1
  0031     NA=J+1
  0032     GO TO 250
  0033  230  CONTINUE
  0034     IR=88
  0035     NA=81
  0036     GO TO 250
C CHECK FOR EXPONENT
C
  0039  235  IF((ITYPE.NE.2).OR.(IDATA(JQQ-1).NE.E)) GO TO 236
  0040     ILQ = JQQ + 1
  0041     GO TO 221
  0042  236  IR=JQQ - 1
  0043     IJ=JQQ+1
C SET NA TO START OF NEXT FIELD
C
  0045  240  DO 248 J=IJ,88
  0046     IF(IDATA(J).EQ.IBLK1) GO TO 248
  0047     NA=J
  0048     IF(IDATA(J).EQ.COMMA) NA=NA+1
  0049     GO TO 250
  0050  248  CONTINUE
  0051     NA=81
C ENCODE DATA IN CURRENT FIELD
C
  0054  250  NI=IR-IL+1
  0055     IF(NI.LT.1) GO TO 290
  0056     ENCODE(NI,255,ITEMP) (IDATA(J),J=IL,IR)
  0057  255  FORMAT(83A1)
C
0059     GO TO (260,270,280),IYPE
C
C DECODE INTEGER DATA
C
0060   260 ENCODE(8,265,AFORM) NI
0061   265 FORMAT(('I'12/'))
0062     DECODE(NI,AFORM,ITEMP) INTEG(I)
0063     GO TO 300
C
C DECODE REAL DATA
C
0064   270 ENCODE(8,275,AFORM) NI
0065   275 FORMAT(('E'12,'.8'))
0066     DECODE(NI,AFORM,ITEMP) REALX(I)
0067     GO TO 300
C
C DECODE ALPHANUMERIC DATA
C
0068   280 IF(NI.GT.8) NI=8
0070     DO 287 J=1,NI
0071     IF(ITEMP(J).EQ.SEMI) ITEMP(J)=COMMA
0073   287 CONTINUE
0074   288 ENCODE(8,288,AFORM)NI
0075   289 FORMAT(('A',I1.''))
0076     DECODE(8,AFORM,ITEMP) ALPHA(I)
0077     GO TO 300
C
C BLANK OUT REMAINING DATA
C
0078   290 INTEG(I)=IBLK2
0079     REALX(I)=BLNK4
0080     ALPHA(I)=BLANK
0081   300 CONTINUE
0082     M=M+1
0083     RETURN
C
C BLANK INPUT, BLANK OUT ALL DATA
C
0084   410 DO 418 J=1,M
0085     INTEG(J)=IBLK2
0086     REALX(J)=BLNK4
0087     ALPHA(J)=BLANK
0088   418 CONTINUE
0089     M=1
0090     M=M-L
0091     RETURN
0092     END
### MIDAS FORTRAN IV STORAGE MAP

**NAME** | **OFFSET** | **ATTRIBUTES**
---|---|---
ITEMP | 000024 | INTEGER*2 ARRAY (20)
AFORM | 000074 | REAL*4 ARRAY (2)
N | 000114 | INTEGER*2 PARAMETER VARIABLE
M | 000116 | INTEGER*2 PARAMETER VARIABLE
NA | 000200 | INTEGER*2 PARAMETER VARIABLE
ITYPE | 000022 | INTEGER*2 PARAMETER VARIABLE
SEMI | 000104 | INTEGER*2 VARIABLE
E | 000106 | INTEGER*2 VARIABLE
COMMA | 000112 | INTEGER*2 VARIABLE
BLANK | 000122 | REAL*8 VARIABLE
IBLK1 | 000110 | INTEGER*2 VARIABLE
IBLK2 | 000114 | INTEGER*2 VARIABLE
BLNK4 | 000116 | REAL*4 VARIABLE
L | 000210 | INTEGER*2 VARIABLE
I | 000212 | INTEGER*2 VARIABLE
J | 000214 | INTEGER*2 VARIABLE
JQQ | 000216 | INTEGER*2 VARIABLE
IL | 000220 | INTEGER*2 VARIABLE
ILQ | 000222 | INTEGER*2 VARIABLE
IR | 000224 | INTEGER*2 VARIABLE
IJ | 000226 | INTEGER*2 VARIABLE
NI | 000230 | INTEGER*2 VARIABLE

**COMMON BLOCK /DATA/**  LENGTH 000240

IDATA | 000000 | INTEGER*2 ARRAY (80)

**COMMON BLOCK /FREE/**  LENGTH 000340

INTEG | 000000 | INTEGER*2 ARRAY (16)
REALX | 000040 | REAL*4 ARRAY (16)
ALPHA | 000140 | REAL*8 ARRAY (16)
PROGRAM GSHIFT
WRITTEN BY G.W.PHILLIPS, AUGUST 1981

READS IN DATA FROM NUCLEAR DATA SPECTRAL FILES
AND PERFORMS A GAIN AND ZERO OFFSET ADJUSTMENT

0001 DIMENSION S(256),R(256)
0002 INTEGER CRT,DATA,P ERIOD, BLANK
0003 COMMON/DATA/DATA(80)/FREE/INTEGR(16),REALX(16),ALPHA(16)
0004 COMMON/HEAD/IDR.TITLE(32),ID(8),ELTIME,ELTIME,ERTIME,ERTIME
0005 INTEGER*2 TITLE,ID,DUMT(32),DUMID(8)
0006 REAL*8 :ALPHA,AB LANK, AHEAD(10)
0007 LOGICAL*1 ASC(60),YES
0008 DATA CRT/5/,LP/6/,IN/5/,IDOUT/6/,PERIOD/1H./,BLANK/1H./,LUF/8/
0009 DATA AHEAD/8H REGION,8H LIMITS ,8H PEAK,8H LIMITS ,
1 8H HEIGHT,8H AREA,8H BKGD.
2 8H CENTROID,8H VARIANCE,8H FWHM /
0010 DATA BLNK4/4H/AB LANK/8H/,YES/1HY/
C  
C
0011 100 WRITE(CRT,110)
0012 110 FORMAT(1H0,'FILENAME FOR SPECTRUM'/) 
0013 READ(CRT,120)LEN,ASC
0014 120 FORMAT(0.80A1) 
0015 IF(LEN.LT.1) GOTO 990 
0017 LUF=8
0018 NCH=256
0019 CALL GET(ASC,R.IVAR,LUF,NCH,A0,A0,C0)
0020 WRITE(CRT,130) NCH
0021 130 FORMAT(IX,IS,' CHANNELS READ IN'/)
D  WRITE(IOUT,140)(R(I),I=1,NCH)
D140 FORMAT(1H1.18G12.3/(1X,18G12.3)) 
D  WRITE(IOUT,150) 
D150 FORMAr(1HI)
0022 WRITE(CRT,160)A0,A0,C0 
0023 160 FORMAT(IX,'ENERGY CALIBRATION FROM HEADER GIVES SLOPE,OFFSET,' 
1     ,'CURVATURE:'/3G12.4/ 
2     IX,'USE THIS FOR OLD SLOPE AND OFFSET, YES OR NO?'/) 
0024 READ(CRT,170)LEN,ASC
0025 170 FORMAT(0.80A1) 
0026 IF(LEN.LT.1) GOTO 200 
0028 IF(ASC(1).EQ.YES) GOTO 300 
C  
C
0030 200 A0=0. 
0031 A0=1. 
0032 C0=0. 
0033 WRITE(CRT,210) 
0034 210 FORMAT(IX,'ENTER OLD SLOPE,OFFSET'/) 
0035 READ(CRT,220)LEN,DATA 
0036 220 FORMAT(0.80A1) 
0037 IF(LEN.LT.1) GOTO 300 
0039 NX=2 
0040 NX=1 
0041 NA=1 
0042 CALL FREEFM(NX,NX,NA,2) 
0043 IF(REALX(1).NE.BLNK4) A0=REALX(1) 
0044 IF(REALX(2).NE.BLNK4) A0=REALX(2) 
0045 300 DO 230 I=1,32 
0046 DUMT(I)=TITLE(I) 
0048 DUM(1)=ID(1) 
0049 230 CONTINUE 
0050 DO 235 I=1,8 
0051 DUM(1)=ID(I) 
0052 235 CONTINUE 
0053 IDEL=ELTIME 
0054 IPPLT=PLTIME 
0055 IDERT=ERTIME 
0056 IDPRT=PRTIME
C
  WRITE(CRT,310)
  FORMAT('TO GET NEW SLOPE AND OFFSET FROM SPECTRAL FILE')
  READ(CRT,320)LEN,ASC
  IF(LEN.LT.1) GOTO 350
  KUF=0
  MCH=256
  CALL GET(ASC,S,JVAR,KUF,MCH,A1,B1,C1)
  WRITE(CRT,330)B1,A1,C1
  FORMAT(' HEADER GIVES SLOPE,OFFSET,CURVATURE')
  IF(LEN.LT.1) GOTO 350
  IF(ASC1).EO.YES) GOTO 488
  GOTO 378
C
  A1=0.
  B1=1.
  C1=0.
  WRITE(CRT,355)
  FORMAT(1X,'ENTER NEW SLOPE,OFFSET')
  READ(CRT,360)LEN,DATA
  IF(LEN.LT.1) GOTO 998
  NX=2
  MX=1
  NA=1
  CALL FREEFM(NX,MX,NA,2)
  IF(REALX(1).NE.BLNK4) G-REALX(1)
  IF(REALX(2).NE.BLNK4) EPS-REALX(2)
  GOTO 411
C
  G=1.
  EPS=0.
  WRITE(CRT,380)
  FORMAT(1X,'ENTER GAIN,ZERO SHIFT')
  READ(CRT,390)LEN,DATA
  IF(LEN.LT.1) GOTO 990
  NX=2
  MX=1
  NA=1
  CALL FREEFM(NX,MX,NA,2)
  IF(REALX(1).NE.BLNK4) G-REALX(1)
  IF(REALX(2).NE.BLNK4) EPS-REALX(2)
  GOTO 411
PERFORM GAIN SHIFT

G = G0 / B1
EPS = (A0 - A1) / B1
WRITE (CRT, 410) G, EPS
FORMAT (1H0, 'RESULTING GAIN AND ZERO SHIFT ARE:' / 2G12.4/)
MF = 1
MR = NCH
CALL REGAIN (R, S, G, EPS, MR, MF, NCH)
CALL RECHAN (R, S, MR, MF, NCH)
WRITE (IOUT, 412) (R(I), I = 1, NCH)
FORMAT (1H0, 'RESULTING GAIN AND ZERO SHIFT ARE:' / 2G12.4/)
WRITE (CRT, 420)
FORMAT (1H0, 'FILENAME FOR OUTPUT SPECTRUM'/)
READ (CRT, 430) LEN, ASC
FORMAT (Q, 8B1)
IF (LEN.LT.1) GOTO 998
DO 440 I = 1, 32
CONTINUE
DO 445 I = 1, 6
CONTINUE
PLTIME = IDPLT
ERTIME = IDERT
PRTIME = IDPRT
CALL PUT (ASC, R, IYAR, LUF, NCH, A1, B1, C1)

CONTINUE
CONTINUE

998 STOP
END
### MIDAS FORTRAN IV STORAGE MAP

<table>
<thead>
<tr>
<th>Name</th>
<th>Offset</th>
<th>Attributes</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
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<td>REAL*4 array</td>
<td>(256)</td>
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<td>(32)</td>
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<td>(8)</td>
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### COMMON BLOCK /DATA/ LENGTH 000240

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### MIDAS FORTRAN IV STORAGE MAP

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</table>


MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS MK-4
SUBROUTINE REGAIN(R,S,G,EPS,MR,MF,NCH)

C WRITTEN BY G.W. PHILLIPS
C NAVAL RESEARCH LABORATORY
C LAST REVISED AUGUST 1981 BY G.W.P.
C PERFORMS DIGITAL GAIN AND ZERO SHIFT
C ON SPECTRAL DATA

DIMENSION R(1),S(1)

THE EFFECT OF THIS SUBROUTINE IS TO FIRST ADJUST THE
GAIN BY G, AND THEN TO SHIFT THE DATA BY EPS

R=INITIAL DATA ARRAY, S=SHIFTED DATA ARRAY
G=GAIN SHIFT, EPS=ZERO SHIFT, MF=OFFSET FOR CHANNEL 1
MR=NUMBER OF DATA CHANNELS, NCH=MAXIMUM NUMBER OF CHANNELS

IF(G.NE.1.0.OR.EPS.NE.0.0) GOTO 100
DO 50 J=1,NCH
S(J)=R(J)
RETURN

MI=MF-1
AT=G*(MR+MI)+EPS
MT=INT(AT)
MT=MIN(MT,NCH)
MRI=MR
MJ=INT(G*MI+EPS)
MJ=MAX(MJ,8)
MF=MJ+1
MR=MT-MJ
GINV=1./G
IF(G.GT.1) GO TO 300
DISTRIBUTE COUNTS (REBIN)

DO 200 I=1, MRI
   A=G*(I+MI)+EPS
   IF(A.LT.0) GOTO 200
   J=INT(A)
   DJ=A-J
   J=J-MJ
   IF(J.LT.0.OR.J.GT.MR) GOTO 200
   IF(J.LT.MR) S(J+1)=S(J+1)+R(I)
   GOTO 200
   DJ=AJ*GINV*R(I)
   IF(J.LT.MR) S(J+1)=S(J+1)+DR
   IF(J.GT.0) S(J)=S(J)+R(I)-DR
CONTINUE
JM=J+1
DJM=DJ

EXTRAPOLATE ENDS

A0=G*MI+EPS
IF(A0.LE.0) GOTO 240
J=INT(A0)
DJ=A0-J
J=J-MJ
IF(J.LT.0) GOTO 240
S(J+1)=S(J+1)+DJ*GINV*R(I)
IF(J.LT.) GOTO 240
JO=J
DO 220 J=1,JO
S(J)=GINV*R(I)
RETURN

240 IF(JM.GT.MR) RETURN
S(JM)=S(JM)+(1-DJM)*GINV*R(MR)
JM=JM+1
IF(JM.GT.MR) RETURN
DO 260 J=JM, MR
S(J)=GINV*R(MR)
RETURN
C
C    INTERPOLATE BETWEEN MIDPOINTS
C
0067    300  DO 400  J=1,MR
0068       A=FLOAT(J+MJ)-0.5
0069       I=INT((A-EPS)*GINV)
0070       B=G*(I-0.5)+EPS
0071       I=I-MI
0072   340  IF(A-B.LE.G) GOTO 340
0073       I=I+1
0074       B=B+G
0075   340  IF(I.GT.M) GOTO 350
0076       S(J)=R(I)*GINV
0077   350  IF(I.LT.MRI) GOTO 360
0078       S(J)=R(MRI)*GINV
0079   360  DG=(A-B)*GINV
0080       S(J)=DG*R(I+1)*GINV+(1.-DG)*R(I)*GINV
0081   400  CONTINUE
0082    RETURN
0083    END
<table>
<thead>
<tr>
<th>NAME</th>
<th>OFFSET</th>
<th>ATTRIBUTES</th>
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SUBROUTINE RECHAN(R,S,MR,MF,NCH)
C WRITTEN BY G.W.PHILLIPS, AUGUST 1981
C
C SHIFTS DATA IN ARRAY S BY MF-1 CHANNELS
C AND STORES THE SHIFTED DATA IN ARRAY R
DIMENSION R(256),S(256)

K=MF-1
MF=1
MR=MR+K
IF(MF LT.8) MR=8
IF(MR.GT.NCH) MR=NCH
J=1
IF(K.LT.1) GOTO 120
J=K+1
DO 110 I=1,K
110 R(I)=S(I-K)
DO 136 I=J,MR
136 R(I)=S(I-K)
L=MR+1
IF(L.GT.NCH) RETURN
DO 146 I=L,NCH
146 R(I)=0.
RETURN
END
## MIDAS FORTRAN IV STORAGE MAP

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EDIT MOD 44-0436-81 10 MAR 77 L.HOLMES
THIS IS THE PREGA LIBRARY FILE EDITOR
IT BUILDS A LIST OF THE STANDARD ISOTOPE SPECTRA
TO BE USED FROM THE DISK.

FILE STRUCTURE

RECORD : PARAMETER

1 NUMBER OF STANDARDS IN LIBRARY
2 NUMBER OF CHANNELS PER STANDARD
3 NUMBER OF ITERATIONS FOR GAIN THRESHOLD SHIFT
4 BACKGROUND SUBTRACT ?
5 INITIAL CHANNEL FOR COMPUTATION
6 FINAL CHANNEL FOR COMPUTATION
7-39 SPACE RESERVED FOR FILE EXPANSION
40 COUNTING TIME FOR BACKGROUND
41 REJECTION COEFFICIENT.
42-49 ID FOR LIBRARY BACKGROUND
50-64 SPACE RESERVED FOR FILE EXPANSION

65-96,97-128,... LIST OF STANDARDS WITH ASSOCIATED PARAMETERS
I.E.

RECORD : PARAMETER

65 CHARACTER NAME OF STANDARD
66-73 FILE ELEMENT ID
74 HALF-LIFE
75 COUNTING TIME OF SAMPLE
76 ACTIVITY OF SAMPLE

0001 INTEGER ANSWER
0002 DATA YES,NO/1HY,1HN/
0003 INTEGER INT(26), MLI(40)
0004 LOGICAL*1 A(32)
0005 DATA LN/1HN/
0006 DATA LI, LD, LA, LP/1HI, IHA, 1HL/
0007 INTEGER BB, CC
0008 DATA BB, CC/1HB, 1HC/
0009 INTEGER BS, BT, RC, BA
0010 DATA NC, IT, BS, IS, IE, LL, LS, BT, RC, BA
0011 INTEGER Y, D, H
0012 DATA Y, D, H/1HY, 1HD, 1HH/
0013 INTEGER EDT
0014 EDT=0
0015 L=5
0016 N=0
0017 LUN=9
0018 LUI=11
0019 DO 1200 I=1, 40
0020 1200 MLI(I)=I
0021 DEFINE FILE LUN(4096, 2, UIVAR)
0022 DEFINE FILE LUI(496, 2, UIVAR)
0023 IVAR=1
0024 READ(LUN', END-508, ERR-688) M
0025 LRITE(5, I)
0026 FORMAT(1X, 'PREGA LIBRARY FILE EDITOR', /)
0027 CONTINUE
0028 WRITE(5, 2000)
0029 2000 FORMAT(IX, 'HEADER: BUILD(B), CHANGE(C), LIST(L)', $)
0030 READ(5, 5000) LENGTH, ANS
0031 IF(LENGTH.LE.0) GO TO 15
0032 IF(ANS.EQ.BB) GO TO 2801
0033 IF(ANS.EQ.CC) GO TO 2500
0034 GO TO 18888
0035 ASSIGN 2060 TO K
0036 WRITE(5, 2061)
0037 2061 FORMAT(' ', '(BS) BACKGROUND SUBTRACT ?', $)
0038 READ(5, 5001) LENGTH, FNUM
0039 IF(LENGTH.LE.0) GO TO 10000
0040 IF(FNUM.GT.512.) FNUM=512.
0041 IF(FNUM.LE.1.8) FNUM=1.8
0042 GO TO 6500
0043 GO TO 10000
0044 ASSIGN 2050 TO K
0045 WRITE(5, 2051)
0046 2051 FORMAT(' ', '(IT) NUMBER OF ITERATIONS FOR THRESHOLD & GAIN CALC.
0047      I ', $)
0048 READ(5, 5001) LENGTH, FNUM
0049 IF(LENGTH.LE.0) GO TO 10000
0050 IF(FNUM.GT.512.) FNUM=512.
0051 IF(FNUM.LE.1.0) FNUM=1.0
0052 NUM=FNUM
0053 WRITE(LUN', 2) NUM
0054 GO TO K
0055 ASSIGN 2050 TO K
0056 WRITE(5, 2051)
0057 2051 FORMAT(' ', '(NC) NUMBER OF CHANNELS PER STANDARD (MAX-512)', $)
0058 READ(5, 5001) LENGTH, FNUM
0059 IF(LENGTH.LE.0) GO TO 10000
0060 IF(FNUM.GT.512.) FNUM=512.
0061 IF(FNUM.LE.1.0) FNUM=1.0
0062 NUM=FNUM
0063 WRITE(LUN', 3) NUM
0064 GO TO K
0065 ASSIGN 2070 TO K
0066 WRITE(5, 2061)
0067 2061 FORMAT(' ', '(BS) BACKGROUND SUBTRACT ?', $)
READ(5,5000) LENGTH, ANS
IF(LENGTH.LE.0) GO TO 10000
NUM = 0
IF(ANS.EQ.YES) NUM = 1
WRITE(LUN'4') NUM
GO TO K
ASSIGN 2000 TO K
WRITE(5,2071)
FORMAT('''IS) INITIAL CHANNEL FOR COMPUTATION ',S)
READ(5,5001) LENGTH, FNUM
IF(LENGTH.LE.0) GO TO 10000
IF(FNUM.GT.512.) FNUM = 512.
IF(FNUM.LE.1.0) FNUM = 1.0
NUM = FNUM
WRITE(LUN'5') NUM
GO TO K
ASSIGN 2000 TO K
WRITE(5,2081)
FORMAT('''IE) FINAL CHANNEL FOR COMPUTATION ',S)
READ(5,5001) LENGTH, FNUM
IF(LENGTH.LE.0) GO TO 10000
IF(FNUM.GT.512.) FNUM = 512.
IF(FNUM.LE.1.0) FNUM = 1.0
NUM = FNUM
WRITE(LUN'6') NUM
GO TO K
ASSIGN 2110 TO K
WRITE(5,2111)
FORMAT('''BT) COUNTING TIME OF BACKGROUND (SECS.) ',S)
READ(5,5001) LENGTH, FNUM
IF(LENGTH.LE.0) GO TO 10000
WRITE(LUN'48') FNUM
GO TO K
ASSIGN 2120 TO K
WRITE(5,2121)
FORMAT('''RC) REJECTION COEFFICIENT ',S)
READ(5,5001) LENGTH, FNUM
IF(LENGTH.LE.0) GO TO 10000
WRITE(LUN'41') FNUM
GO TO K
ASSIGN 2130 TO K
WRITE(5,2131)
FORMAT('''BA) BACKGROUND SPECTRUM (FILE, ELEMENT [, DEVICE]) ',/
READ(5,4) LENGTH, (A(1), I=1, 32)
IVAR = 42
DO 2133 I = 1, 32, 4
WRITE(LUN'4VAR') A(I), A(I+1), A(I+2), A(I+3)
GO TO K
ASSIGN 2140 TO K
READ(5.2581)
FORMAT('''WHICH PARAMETER DO YOU WISH TO MODIFY ? ',S)
READ(5,5007) LENGTH, ANS
IF(LENGTH.LE.0) GO TO 10000
IF(ANS.EQ.NO) GO TO 6000
0138 IF(ANS.EQ.IT)GO TO 6001
0140 IF(ANS.EQ.BS)GO TO 6002
0142 IF(ANS.EQ.IS)GO TO 6003
0144 IF(ANS.EQ.1E)GO TO 6004
0146 IF(ANS.EQ.RT)GO TO 6007
0148 IF(ANS.EQ.RC)GO TO 6008
0150 IF(ANS.EQ.BA)GO TO 6009
0152 GO TO 2500
0153 6000 READ(LUN'2')NUM
0154 WRITE(L,2044)
0155 WRITE(L,5004)NUM
0156 IF(EDT.EQ.1)GO TO 7000
0158 GO TO 2042
0159 6001 READ(LUN'3')NUM
0160 WRITE(L,2051)
0161 WRITE(L,5004)NUM
0162 IF(EDT.EQ.1)GO TO 7000
0164 GO TO 2052
0165 6002 READ(LUN'4')NUM
0166 WRITE(L,2061)
0167 ANS=NO
0168 IF(NUM.EQ.1)ANS=YES
0170 WRITE(L,5008)ANS
0171 IF(EDT.EQ.1)GO TO 7000
0173 GO TO 2062
0174 6003 READ(LUN'5')NUM
0175 WRITE(L,2071)
0176 WRITE(L,5004)NUM
0177 IF(EDT.EQ.1)GO TO 7000
0179 GO TO 2072
0180 6004 READ(LUN'6')NUM
0181 WRITE(L,2081)
0182 WRITE(L,5004)NUM
0183 IF(EDT.EQ.1)GO TO 7000
0185 GO TO 2082
0186 6005 READ(LUN'48')FNUM
0187 WRITE(L,2111)
0188 WRITE(L,5005)FNUM
0189 IF(EDT.EQ.1)GO TO 7000
0191 GO TO 2112
0192 6006 READ(LUN'49')FNUM
0193 WRITE(L,2121)
0194 WRITE(L,5005)FNUM
0195 IF(EDT.EQ.1)GO TO 7000
0197 GO TO 2122
0198 6007 IVAR=42
0199 DO 2600 I=1,32,4
0200 2600 READ(LUN'IVAR')A(I),A(I+1),A(I+2),A(I+3)
0201 WRITE(L,2131)
0202 WRITE(L,5006)(A(I),I=1,32)
0203 IF(EDT.EQ.1)GO TO 7000
0205 GO TO 2132
C HEADER LISTER
0206 6500 CONTINUE
0207 L=6
0208 EDT=1
0209 WRITE(L,6501)
FORMAT('1', 'PREGA LIBRARY HEADER', '/', ')

I=0
I=I+1
IF(I.GT.8) GO TO 6010
GO TO (6000, 6001, 6002, 6003, 6004, 5007, 5008, 6009), !
L=5
EDIT=0
WRITE(6,411)
WRITE(6,411)
GO TO 1999
CONTINUE
WRITE(5,16)
16 FORMAT('LIST OF STANDARDS')
WRITE(5,111)
111 FORMAT('1X.*LIST OF STANDARDS')
WRITE(5, 111)
FORMAT(1X.NEU FILECN).INSERTCI).DELETE(DX.APPENDCA).LIST(L)
IVAR-1
N=0
EDT-8
WRITEC5,28)
28 FORMAT('1X.*ISOTYPE NAME (8 CHARACTERS MAX) ', $)
READ(5,2) LENGTH, ANS
2 FORMAT(Q, A(1))
IF(LENGTH.EQ.0) GO TO 1000
IF(ANS.EQ.LN) GO TO 25
IF(ANS.EQ.LI) GO TO 100
IF(ANS.EQ.LD) GO TO 200
IF(ANS.EQ.LA) GO TO 300
IF(ANS.EQ.LP) GO TO 400
GO TO 15
CONTINUE
IVAR=65+H*16
WRITE(5,20)
20 FORMAT('1X.ISOTOPE NAME (8 CHARACTERS MAX) ', $)
READ(5,21) LENGTH, (A(I), I=1, 8)
21 FORMAT(Q, A(1))
IF(LENGTH.EQ.0) GO TO 15
DO 22 I=1, 8, 4
WRITE(LUN'IVAR), A(I), A(I+1), A(I+2), A(I+3)
22 FORMAT(S, 3)
WRITE(5,3)
3 FORMAT('1X.FILE ELEMENT (DEVICE) ', $)
READ(5,4) LENGTH, (A(I), I=1, 32)
4 FORMAT(Q, 32A1)
4 FORMAT(Q, 32A1)
IF(LENGTH.EQ.0) GO TO 15
DO 10 I=1, 32, 4
WRITE(LUN'IVAR), END=500, ERR=600), A(I), A(I+1), A(I+2), A(I+3)
10 FORMAT(S, 5)
WRITE(5, 5)
5 FORMAT('1X.HALF-LIFE. UNITS (Y, D, H, M, S) ', $)
READ(5,6) LENGTH, HL, K
6 FORMAT(Q, E12.0, A(1))
IF(LENGTH.EQ.0) GO TO 15
IF(K.EQ.Y)HL=HL*31536000.
IF(K.EQ.D)HL=HL*86400.
IF(K.EQ.H)HL=HL*3600.
IF(K.EQ.MM)HL=HL*60.
WRITE(LUN'IVAR), HL
7 FORMAT(S, 7)
WRITE(5,7)
WRITE(5,5)
7 FORMAT('1X.COUNTING TIME OF STANDARD (SECS.) ', $)
READ(5,5001) LENGTH, SEC
7
IF(LENGTH.EQ.0)GO TO 15
IF(SEC.LE.1.8)SEC=1.0
WRITE(LUN',IVAR)SEC
WRITE(5,9)
FORMA1(9,ACTIVITY (MAY BE SET TO 1),$)
READ(5,5001)LENGTH,ACT
IF(LENGTH.EQ.0)GO TO 15
WRITE(LUN',IVAR)ACT
IF(EDT.EQ.1)GO TO 15
N=N+1
WRITE(LUN',1)M
GO TO 25
WRITE(5,101)
FORMAT(1X,'NUMBER OF ENTRY TO BE INSERTED ',$)
READ(5,102)FNUN
NUM=FNUN
N=M
IF(N.LT.NUM)GO TO 15
M=M+1
N=M
EDT=1
IF(N.LT.NUM)GO TO 25
IVAR=65+(N-1)*16
DO 104 I=1,26,2
READ(LUN',IVAR)INT(I),INT(I+1)
IVAR=IVAR+3
DO 105 I=1,26,2
WRITE(LUN',IVAR)INT(I),INT(I+1)
N=N-1
GO TO 103
C
WRITE(5,201)
FORMAT(1X,'NUMBER OF ENTRY TO BE DELETED ',$)
READ(5,202)FNUN
NUM=FNUN
IF(NUM.GT.M)GO TO 15
IF(NUM.EQ.M)GO TO 206
IF(M.LE.6)GO TO 206
CONTINUE
IVAR=NUM*16+65
DO 204 I=1,26,2
READ(LUN',IVAR,END=500,ERR=600)INT(I),INT(I+1)
IVAR=IVAR-29
DO 205 I=1,26,2
WRITE(LUN',IVAR,END=500,ERR=600)INT(I),INT(I+1)
NUM=NUM+1
IF(NUM.LT.M)GO TO 203
CONTINUE
M=M-1
GO TO 15
3843 300 N=M
GO TO 25
400 IF(M.EQ.0)GO TO 15
C

**F. P. MIDAS FORTRAN IV 11 AUG 1983 2:13:03 PM PAGE 007**

**0347** 1000 WRITE(5,1010)
**0348** 1010 FORMAT(' ', 'DO YOU WISH TO PRINT FULL STANDARD LIST?', $)
**0349** READ(5,2) LENGTH, ANS
**0350** IF (LENGTH .LE. 0) GO TO 1000
**0352** IF (ANS.EQ.YE$) GO TO 1020
**0354** READ(LUI'29) MLA
** D WRITE(6,7100) MLA
** D7100 FORMAT(' ', 'MLA=', I6)
** D WRITE(5,7105)
** D7105 FORMAT(' ', 'IVAR=', $)
** D READ(LUN'84) MLA
** D7106 FORMAT(12)
** I4 VAR=44
**0355** DO 1014 I=1, MLA
**0357** READ(LUN'IVAR) MLI(I)
** D WRITE(6,7110) IVAR, I, MLI(I)
** D7110 FORMAT(' ', 'MLA-M=', I4)
**0358** 1014 CONTINUE
**0359** WRITE(6,1016)
**0360** 1016 FORMAT('1', ' PREGA LIBRARY STANDARDS USED', '/
**0361** GO TO 1024
**0362** 1020 MLA=M
** D WRITE(6,7120) MLA
** D7120 FORMAT(' ', 'MLA=M=', I4)
**0363** WRITE(6,401)
**0364** 401 FORMAT('1', ' PREGA LIBRARY STANDARDS', '/
**0365** 1024 DO 1090 JI=1, MLA
**0366** IVAR=65+16*(MLI(JI)-1)
**0367** DO 415 I=1, 8, 4
**0368** 415 READ(LUN'IVAR) A(I), A(I+1), A(I+2), A(I+3)
**0369** WRITE(6,425) MLI(JI), (A(I), I=1, 8)
**0370** 425 FORMAT(1X, 'STANDARD *', 12, ' :', 8A1)
**0371** DO 484 I=1, 32, 4
**0372** 484 READ(LUN'IVAR) A(I), A(I+1), A(I+2), A(I+3)
**0373** WRITE(6,3)
**0374** WRITE(6,405) (A(I), I=1, 32)
**0375** 405 FORMAT('+', 13, 32A1)
**0376** READ(LUN'IVAR) SEC
**0377** WRITE(6,406) SEC
**0378** 406 FORMAT(1X, 'HALF-LIFE (SECS):', 1PE12.4)
**0379** READ(LUN'IVAR) HL
**0380** WRITE(6,407) HL
**0381** 407 FORMAT(1X, 'COUNTING TIME OF STANDARD (SECS):', 1PE12.4)
**0382** READ(LUN'IVAR) ACT
**0383** WRITE(6,408) ACT
**0384** 408 FORMAT(1X, 'ACTIVITY:', 1PE12.4, '/
**0385** 1090 CONTINUE
**0386** C
**0388** 410 WRITE(6,411)
**0387** WRITE(6,411)
**0388** WRITE(6,411)
**0389** WRITE(6,411)
**0390** WRITE(6,411)
**0391** WRITE(6,411)
**0392** WRITE(6,411)
**0393** WRITE(6,411)
**0394** 411 FORMAT('+', $

105
GO TO 15
500 WRITE(5,501)
501 FORMAT(IX,'FILE NOT LARGE ENOUGH')
GO TO 1000
600 WRITE(5,601)
601 FORMAT(IX,'FILE SET UP NOT CORRECT')
GO TO 1000
5000 FORMAT(Q,A1)
5001 FORMAT(Q,E12.8)
5003 FORMAT(Q,32A1)
5004 FORMAT('+',' ',/)
5005 FORMAT('+',' ',/)
5006 FORMAT(IX,':',/)
5007 FORMAT(Q,A2)
5008 FORMAT(+/','/,)
1000 IF(M.GE.40)M=40
1010 WRITE(LUN')M
END
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C PROGRAM UEDIT
C MODIFIED 8 JUNE 1981 BY G.PHILLIPS
C
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SCHAUMBURG, ILLINOIS 60196
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C
C UEDIT MOD 44-0435-81 10 MAR 77 L.HOLMES
C THIS IS THE NAI UNKNOWN LIBRARY EDITOR.
C IT SETS UP THE ANALYSIS PARAMETERS FOR
C THE UNKNOWN SAMPLE SPECTRUM.
C
C FILE STRUCTURE
C
C RECORD : PARAMETER
C
C 1-8 ID OF SAMPLE
C 10 GAIN SHIFT RATIO
C 11 THRESHOLD SHIFT
C 12 BACKGROUND SUPPLIED ?
C 13 BACKGROUND SUBTRACT ?
C 14 COUNTING TIME FOR BACKGROUND
C 15 COUNTING TIME FOR UNKNOWN SAMPLE
C 16 VOLUME REDUCTION FACTOR
C 17 DECAY TIME
C 18 RESULT MULTIPLICATION FACTOR
C 19-27 ID OF SAMPLE BACKGROUND
C 28 WEIGHTING FACTOR DETERMINATION
C 29 NUMBER OF STANDARDS USED
C 30 F-TEST REJECTION COEFFICIENT
C 31 WEIGHTING FACTOR CALCULATION
C 32 LIBRARY REJECTION COEFFICIENT APPLIED ?
C 33 BACKGROUND REGRESSION?
C 34 PIVOT ON BACKGROUND?
C 35 OUTPUT RESIDUALS?
C 36-42 ID OF OUTPUT FILE
C 43,44,... ORDER OF OUTPUT FILE
C
C 108
C
C
0001 INTEGER CC
0002 INTEGER EDT
0003 INTEGER UN, OP, CB, BG, BS, BT, UT, VR, DT, MF, SB, WD, NS, F0, UF, RC, BR, BP, ANS,
YES, CRT, RO, RS
0004 DATA UN, OP, CB, BG, BS, BT, UT, VR, DT, MF, SB, WD, NS, F0, UF, RC, BR, BP, RO, RS
1/2HUN, 2HOP, 2HCB, 2HBS, 2HBR, 2HVT, 2HDR, 2HDF, 2HMF, 2HSD, 2HJD, 2HNS, 2HF0,
2HUF, 2HRC, 2HBR, 2HBP, 2HRD, 2HRS/
0005 INTEGER GN, TH
0006 DATA GN, TH/2HGN, 2HTH/
0007 INTEGER OR
0008 DATA OR/2HOR/
0009 DATA UT/2HUT/
0010 DATA NN, CC, LL, YES, NO/1HN, 1HC, 1HL, 1HY, 1HN/
0011 INTEGER CT
0012 DATA CT/2HCT/
0013 INTEGER BA
0014 DATA BA/2HBA/
0015 LOGICAL*1 A(32)
0016 LUN=11
0017 DEFINE FILE LUN(4096, 2, U, IVAR)
0018 CRT=5
0019 READ(LUN'1')M
0020 WRITE(CRT, I)
0021 1 FORMAT(1X, 'PREGA UNKNOWN FILE EDITOR', //)
0022 10000 CONTINUE
0023 1500 WRITE(5, 4)
0024 4 FORMAT(1X, 'NEW FILE(N), CHANGE(C), LIST(L) ', $)
0025 READ(CRT, 1002)LENGTH, ANS
0026 IF (LENGTH.LE.0) GO TO 11000
0028 IVAR=2
0029 IF (ANS.EQ.CC) GO TO 450
0031 IF (ANS.EQ.LL) GO TO 900
0033 IF (ANS.EQ.NH) GO TO 9
0035 GO TO 1500
C BUILD INDIVIDUAL FILES

C

0036 49 CONTINUE
0037 50 WRITE(CRT,51)
0039 51 FORMAT(1X,"(UN) UNKNOWN SPECTRUM: FILE.ELEMENT (.DEVICE) ",/
0040 52 READ(CRT,1001)LENGTH,(A(I),I=1,32)
0041 53 IF(LENGTH.LE.0)GO TO 10000
0043 55 DO 55 I=1,32,4
0044 56 WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0045 57 GO TO K
0046 60 ASSIGN 70 TO K
0047 61 WRITE(CRT,61)
0048 62 FORMAT(1X,'(GN) GAIN SHIFT RATIO ",$
0049 63 READ(CRT,1003)LENGTH,FNUM
0050 64 IF(LENGTH.LE.0)GO TO 10000
0052 66 IF(FNUM.LE.(1.8E-5))FNUM=1.0
0054 67 WRITE(LUN'IVAR)FNUM
0055 68 GO TO K
0056 70 ASSIGN 80 TO K
0057 71 WRITE(CRT,71)
0058 72 FORMAT(1X,'(TH) THRESHOLD SHIFT ",$
0059 73 READ(CRT,1003)LENGTH,FNUM
0060 74 IF(LENGTH.LE.0)GO TO 10000
0062 76 WRITE(LUN'IVAR)FNUM
0063 77 GO TO K
0064 80 ASSIGN 90 TO K
0065 81 WRITE(CRT,81)
0066 82 FORMAT(1X,'(BG) BACKGROUND SUPPLIED ? ",$
0067 83 READ(CRT,1002)LENGTH,ANS
0068 84 IF(LENGTH.LE.0)GO TO 10000
0070 86 NUM=0
0071 87 IF(ANS.EQ.YES)NUM=1
0073 89 WRITE(LUN'IVAR)NUM
0074 90 GO TO K
0075 98 ASSIGN 100 TO K
0076 99 WRITE(CRT,91)
0077 91 FORMAT(1X,'(BS) SUBTRACT BACKGROUND ? ",$
0078 92 READ(CRT,1002)LENGTH,ANS
0079 94 IF(LENGTH.LE.0)GO TO 10000
0081 96 NUM=0
0082 97 IF(ANS.EQ.YES)NUM=1
0084 99 WRITE(LUN'IVAR)NUM
0085 100 GO TO K
C
0086 100 ASSIGN 110 TO K
0087 WRITE(CRT,101)
0088 101 FORMAT(IX,'(BT) COUNTING TIME FOR BACKGROUND (SECS) ',$)
0089 102 READ(CRT,1003) LENGTH,FNUM
0090 IF(LENGTH.LE.0)GO TO 10000
0091 IF(FNUM.LE.1.0)FNUM=1.0
0092 WRITE(LUN'IVAR)FNUM
0093 GO TO K
0095 110 ASSIGN 120 TO K
0096 WRITE(CRT,111)
0097 111 FORMAT(IX,'(CT) COUNTING TIME FOR UNKNOWN SAMPLE ',$)
0098 112 READ(CRT,1003) LENGTH,FNUM
0100 IF(LENGTH.LE.0)GO TO 10000
0101 IF(FNUM.LE.1.0)FNUM=1.0
0102 WRITE(LUN'IVAR)FNUM
0103 GO TO K
0105 120 ASSIGN 130 TO K
0106 WRITE(CRT,121)
0107 121 FORMAT(IX,'(VR) VOLUME REDUCTION (OR INVERSE OF DILUTION) ',$,I1
1 ' FACTOR ',$)
0109 122 READ(CRT,1003) LENGTH,FNUM
0110 IF(LENGTH.LE.0)GO TO 10000
0111 IF(FNUM.LE.(1.0E-5))FNUM=1.0
0112 WRITE(LUN'IVAR)FNUM
0113 GO TO K
0115 130 ASSIGN 140 TO K
0116 WRITE(CRT,131)
0117 131 FORMAT(IX,'(DT) DECAY TIME ',$)
0119 132 READ(CRT,1003) LENGTH,FNUM
0120 IF(LENGTH.LE.0)GO TO 10000
0121 WRITE(LUN'IVAR)FNUM
0122 GO TO K
0123 140 ASSIGN 150 TO K
0124 WRITE(CRT,141)
0125 141 FORMAT(IX,'(MF) RESULT MULTIPLICATION FACTOR ',$)
0127 142 READ(CRT,1003) LENGTH,FNUM
0128 IF(LENGTH.LE.0)GO TO 10000
0130 WRITE(LUN'IVAR)FNUM
0131 GO TO K
0132 150 ASSIGN 180 TO K
0133 WRITE(CRT,151)
0134 151 FORMAT(IX,'(BA) BACKGROUND SPECTRUM: FILE.ELEMENT(/))$)
0135 152 READ(CRT,1001) LENGTH,(A(I),I=1,32)
0136 IF(LENGTH.LE.0)GO TO 10000
0138 DO 153 I=1,32,4
0139 153 WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0140 GO TO K
C
0141 160  ASSIGN 170 TO K
0142 162  WRITE(CRT,161)
0143 161  FORMAT(1X,"ANALYSIS OPTIONS ")
0144  GO TO K
0145 170  ASSIGN 190 TO K
0146  WRITE(CRT,171)
0147 171  FORMAT(1X,"(SB) SUBTRACT BACKGROUND ? ",S)
0148 172  READ(CRT,1002)LENGTH,ANS
0149   IF(LENGTH.LE.0)GO TO 10000
0150   WRITE(LUN,'IVAR)ANS
0151   GO TO K
0152 180  ASSIGN 190 TO K
0153 181  IVAR=IVAR+1
0154  WRITE(CRT,181)
0155 181  FORMAT(1X,"(WD) HOW ARE WEIGHTING FACTORS TO BE DETERMINED ?",/1X
0156 182  1: 
0157 182  2: BASED ON ACTUAL COUNTS/CHANNEL.",/1X.
0158 182  3: BASED ON CALCULATED COUNTS/CHN ",/)
0159 182   READ(CRT,1003)LENGTH,FNUM
0160   IF(LENGTH.LE.0)GO TO 10000
0161   NUM=0
0162   IF(FNUM.EQ.1.0)NUM=1
0163   WRITE(LUN,'IVAR)NUM
0164   GO TO K
0165 190  ASSIGN 200 TO K
0166  WRITE(CRT,191)
0167 191  FORMAT(1X,"(NS) NUMBER OF ISOTOPES USED FROM THE STANDARD LIBRARY
0168 192  1?"S)
0169 192   READ(CRT,1003)LENGTH,FNUM
0170   IF(LENGTH.LE.0)GO TO 10000
0171   NUM=FNUM
0172   IF(NUM.GE.15)NUM=15
0173   IF(NUM.LE.1)NUM=1
0174 195  WRITE(LUN,'IVAR)NUM
0175 195   GO TO K

112
C
0178 200 ASSIGN 210 TO K
0179 WRITE(CRT,201)
0180 201 FORMAT(1X,'(F0) F-TEST REJECTION COEFFICIENT.',$)
0181 202 READ(CRT,1003)LENGTH,FNUM
0182 IF(LENGTH.LE.0)GO TO 10000
0184 WRITE(LUN'IVAR)FNUM
0185 GO TO K
0186 210 ASSIGN 220 TO K
0187 WRITE(CRT,211)
0188 211 FORMAT(1X,'(WF) WEIGHTING FACTOR CALCULATION.'
1./,1X,' 1: (COUNTS)**-1'
2./,1X,' 0: (SIGMA)**-2'
3./,1X,' 1: 1 **,$)
0189 212 READ(CRT,1003)LENGTH,FNUM
0190 IF(LENGTH.LE.0)GO TO 10000
0194 NUM=1
0195 IF(FNUM.EQ.0.0)NUM=0
0196 IF(FNUM.EQ.(-1.0))NUM=-1
0197 NUM=FNUM
0198 WRITE(LUN'IVAR)NUM
0199 GO TO K
0200 220 ASSIGN 230 TO K
0201 WRITE(CRT,221)
0202 221 FORMAT(1X,'(RC) REJECTION COEFICIENT APPLIED?',$)
0203 222 READ(CRT,1002)LENGTH,ANS
0204 IF(LENGTH.LE.0)GO TO 10000
0205 NUM=0
0206 IF(ANS.EQ.YES)NUM=1
0207 WRITE(LUN'IVAR)NUM
0209 GO TO K
0210 230 ASSIGN 240 TO K
0211 231 FORMAT(1X,'(BR) BACKGROUND REGRESSION ?'
1./,6X,' 0: TRIAL SET = CHOSEN STANDARDS'
2./,6X,' 1: TRIAL SET = BACKGROUND ONLY',$)
0214 232 READ(CRT,1003)LENGTH,FNUM
0215 IF(LENGTH.LE.0)GO TO 10000
0217 NUM=FNUM
0218 WRITE(LUN'IVAR)NUM
0219 GO TO K
C
0220 248 ASSIGN 243 TO K
0221 WRITE(CRT.241)
0222 241 FORMAT(IX,'(BP) PIVOT ON BACKGROUND SPECTRUM ALLOWED?'
1,/,6X,'0: NO PIVOT ON BACKGROUND ALLOWED'
2,/,6X,'1: ALLOW PIVOT ON BACKGROUND SPECTRUM',$)
0223 242 READ(CRT.1003)LENGTH,FNUM
0224 IF(LENGTH.LE.0)GO TO 10000
0225 NUM=FNUM
0227 WRITE(LUN'IVAR)NUM
0228 GO TO K
0229 243 ASSIGN 246 TO K
0230 WRITE(CRT.244)
0231 244 FORMAT(IX,'(RO) OUTPUT RESIDUALS ?',$)
0232 245 READ(CRT.1002)LENGTH,ANS
0233 IF(LENGTH.LE.0) GOTO 10000
0235 NUM=0
0236 IF(ANS.EQ.YE) NUM=1
0238 WRITE(LUN'IVAR)NUM
0239 GOTO K
0240 246 ASSIGN 250 TO K
0241 WRITE(CRT.247)
0242 247 FORMAT(IX,'(RS) RESIDUAL SPECTRUM: FILE.ELEMENT(,DEVICE)'
0243 248 READ(CRT.1001)LENGTH,(A(I),I=1,32)
0244 IF(LENGTH.LE.0) GOTO 10000
0246 DO 249 I=1,32.4
0247 249 WRITE(LUN'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0248 GOTO K
0249 250 ASSIGN 10000 TO K
0250 IVAR=IVAR-6
0251 READ(LUN'IVAR)NUM
0252 IIT=NUM
0253 IVAR=IVAR+5
0254 WRITE(CRT.251)
0255 251 FORMAT(IX,'(OR) NUMBER OF LIBRARY STANDARD IN ORDER OF DESIRED ','PRINTOUT ')
0256 252 DO 253 I=1,IIT
0257 253 WRITE(CRT.254)
0258 254 FORMAT(IX,' STANDARD NUMBER : ',$)
0259 READ(CRT.1003)LENGTH,FNUM
0260 IF(LENGTH.LE.0)GO TO 10000
0262 NUM=FNUM
0263 WRITE(LUN'IVAR)NUM
0264 253 CONTINUE
0265 GO TO K
0266 450 IVAR=1
0267 IVAR=2
0268 ASSIGN 450 TO K
C THIS SECTION ENABLES MODIFICATION OF AN EXISTING FILE

0269 500 WRITE(CRT,501)
0270 501 FORMAT(1X,'WHICH PARAMETER DO YOU WISH TO MODIFY ? ',$)
0271  READ(CRT,1000)LENGTH,ANS
0272   IF(LENGTH.LE.0)GO TO 10000
0274   IF(ANS.EQ.UN)GO TO 600
0276   IF(ANS.EQ.GN)GO TO 610
0278   IF(ANS.EQ.TH)GO TO 620
0280   IF(ANS.EQ.BG)GO TO 630
0282   IF(ANS.EQ.BS)GO TO 640
0284   IF(ANS.EQ.BT)GO TO 650
0286   IF(ANS.EQ.DT)GO TO 660
0288   IF(ANS.EQ.MF)GO TO 670
0290   IF(ANS.EQ.BA)GO TO 680
0292   IF(ANS.EQ.NM)GO TO 690
0294   IF(ANS.EQ.BA)GO TO 700
0296   IF(ANS.EQ-UA)GO TO 710
0298   IF(ANS.EQ.NA)GO TO 720
0300   IF(ANS.EQ.F0)GO TO 730
0302   IF(ANS.EQ.UF)GO TO 740
0304   IF(ANS.EQ.FC)GO TO 750
0306   IF(ANS.EQ.BR)GO TO 760
0308   IF(ANS.EQ.BP)GO TO 770
0310   IF(ANS.EQ.WR)GOTO 780
0312   IF(ANS.EQ.RS)GOTO 790
0314   IF(ANS.EQ.MT)GO TO 790
0316   DO 681 I=1,32,4
0318   681 READ(LUN'IVAR',A(I),A(I+1),A(I+2),A(I+3)
0319   WRITE(CRT,51)
0320   WRITE(CRT,1004')(A(I),I=1,32)
0321   IF(EDT.EQ.1)GO TO 2000
0323   IVAR=IVAR+8
0324   GO TO 52
0325   610 IVAR=IVAR+8
0326   READ(LUN'IVAR',FNUM
0327   WRITE(CRT,61)
0328   WRITE(CRT,1007')FNUM
0329   IF(EDT.EQ.1)GO TO 2000
0331   IVAR=IVAR-1
0332   GO TO 62
C
0333  620  IVAR=IVAR+9
0334  READ(LUN*IVAR)FNUM
0335  WRITE(CRT,71)
0336  WRITE(CRT,1007)FNUM
0337  IF(EDT.EQ.1)GO TO 2000
0338  IVAR=IVAR-1
0339  GO TO 72
0340  IVAR=IVAR+10
0341  READ(LUN*IVAR)NUM
0342  WRITE(CRT,81)
0343  ANS=NO
0344  IF(NUM.EQ.1)ANS=YES
0345  WRITE(CRT,1006)ANS
0346  IF(EDT.EQ.1)GO TO 2000
0347  IVAR=IVAR-1
0348  GO TO 82
0349  IVAR=IVAR+11
0350  READ(LUN*IVAR)NUM
0351  WRITE(CRT,91)
0352  ANS=NO
0353  IF(NUM.EQ.1)ANS=YES
0354  WRITE(CRT,1006)ANS
0355  IF(EDT.EQ.1)GO TO 2000
0356  IVAR=IVAR-1
0357  GO TO 92
0358  IVAR=IVAR+12
0359  READ(LUN*IVAR)FNUM
0360  WRITE(CRT,101)
0361  WRITE(CRT,1007)FNUM
0362  IF(EDT.EQ.1)GO TO 2000
0363  IVAR=IVAR-1
0364  GO TO 102
0365  IVAR=IVAR+13
0366  READ(LUN*IVAR)FNUM
0367  WRITE(CRT,111)
0368  WRITE(CRT,1007)FNUM
0369  IF(EDT.EQ.1)GO TO 2000
0370  IVAR=IVAR-1
0371  GO TO 112
0372  IVAR=IVAR+14
0373  READ(LUN*IVAR)FNUM
0374  WRITE(CRT,121)
0375  WRITE(CRT,1007)FNUM
0376  IF(EDT.EQ.1)GO TO 2000
0377  IVAR=IVAR-1
0378  GO TO 122
C
0387 680  IVAR=IVAR+15
0388  READ(LUN 'IVAR)FNUM
0389  WRITE(CRT, 131)
0390  WRITE(CRT, 1007)FNUM
0391  IF (EDT.EQ.1) GO TO 2000
0393  IVAR=IVAR-1
0394  GO TO 132
0395  690  IVAR=IVAR+16
0396  READ(LUN 'IVAR)FNUM
0397  WRITE(CRT, 141)
0398  WRITE(CRT, 1007)FNUM
0399  IF (EDT.EQ.1) GO TO 2000
0401  IVAR=IVAR-1
0402  GO TO 142
0403 700  IVAR=IVAR+17
0404  DO 701 I=1,32,4
0405 701  READ(LUN 'IVAR)A(I),A(I+1),A(I+2),A(I+3)
0406  WRITE(CRT, 151)
0407  WRITE(CRT, 1004)(A(I),I=1,32)
0408  IF (EDT.EQ.1) GO TO 2000
0409  IVAR=IVAR-8
0410  GO TO 152
0411  710  IVAR=IVAR+25
0412  READ(LUN 'IVAR)NUM
0413  WRITE(CRT, 171)
0414  ANS=NO
0415  IF (NUM.EQ.1) ANS=YES
0416  WRITE(CRT, 1006)ANS
0417  IF (EDT.EQ.1) GO TO 2000
0418  IVAR=IVAR-1
0419  GO TO 172
0420  720  IVAR=IVAR+26
0421  READ(LUN 'IVAR)NUM
0422  WRITE(CRT, 181)
0423  WRITE(CRT, 1005)NUM
0424  IF (EDT.EQ.1) GO TO 2000
0425  IVAR=IVAR-1
0426  GO TO 182
0427  730  IVAR=IVAR+27
0428  READ(LUN 'IVAR)NUM
0429  WRITE(CRT, 191)
0430  WRITE(CRT, 1005)NUM
0431  IF (EDT.EQ.1) GO TO 2000
0432  IVAR=IVAR-1
0433  GO TO 192
C
0439 740  IVAR=IVAR+28
0440  READ(LUN' IVAR)FNUM
0441  WRITE(CRT.201)
0442  WRITE(CRT.1007)FNUM
0443  IF(EDT.EQ.1)GO TO 2000
0445  IVAR=IVAR-1
0446  GO TO 202
0447  750  IVAR=IVAR+29
0448  READ(LUN' IVAR)NUM
0449  WRITE(CRT.211)
0450  WRITE(CRT.1005)NUM
0451  IF(EDT.EQ.1)GO TO 2000
0453  IVAR=IVAR-1
0454  GO TO 212
0455  760  IVAR=IVAR+30
0456  READ(LUN' IVAR)NUM
0457  WRITE(CRT.221)
0458  ANS=NO
0459  IF(NUM.EQ.1)ANS=YES
0461  WRITE(CRT.1006)ANS
0462  IF(EDT.EQ.1)GO TO 2000
0464  IVAR=IVAR-1
0465  GO TO 222
0466  770  IVAR=IVAR+31
0467  READ(LUN' IVAR)NUM
0468  WRITE(CRT.231)
0469  WRITE(CRT.1005)NUM
0470  IF(EDT.EQ.1)GO TO 2000
0472  IVAR=IVAR-1
0473  GO TO 232
0474  780  IVAR=IVAR+32
0475  READ(LUN' IVAR)NUM
0476  WRITE(CRT.241)
0477  WRITE(CRT.1005)NUM
0478  IF(EDT.EQ.1)GO TO 2000
0480  IVAR=IVAR-1
0481  GO TO 242
C
0482 782  IVAR=IVAR+33
0483  READ(LUN*IVAR)NUM
0484  WRITE(CRT,244)
0485  ANS=NO
0486  IF(NUM.EQ.1) ANS=YES
0488  WRITE(CRT,1006)ANS
0489  IF(EDIT.EQ.1) GOTO 2000
0491  IVAR=IVAR-1
0492  GOTO 245
0493  784  IVAR=IVAR+34
0494  DO 785 I=1,32,4
0495  785 READ(LUN*IVAR)A(I),A(I+1),A(I+2),A(I+3)
0496  WRITE(CRT,247)
0497  WRITE(CRT,1004)(A(I),I=1,32)
0498  IF(EDIT.EQ.1) GOTO 2000
0500  IVAR=IVAR-8
0501  GOTO 240
0502  790  IVAR=IVAR+27
0503  READ(LUN*IVAR)NUM1
0504  ITT=NUM1
0505  WRITE(CRT,251)
0506  IVAR=IVAR+14
0507  796  WRITE(CRT,792)
0508  792 FORMAT(IX,'$')
0509  795 DO 793 I=1,ITT
0510  793 READ(LUN*IVAR)NUM
0511  WRITE(CRT,794)NUM
0512  794 FORMAT('+I3,$')
0513  IF(I.LT.18) GO TO 793
0515  IF(ITT.EQ.18) GO TO 793
0517  ITT=ITT-18
0518  G0 TO 796
0519  793 CONTINUE
0520  IF(EDIT.EQ.1) GO TO 2000
0522  ITT=NUM1
0523  IVAR=IVAR-NUM1
0524  WRITE(CRT,797)
0525  797 FORMAT('')
0526  G0 TO 252
C
0527 900 CONTINUE
0528   CRT=6
0529   EDT=1
0530   WRITE(CRT,901)
0531   901 FORMAT('I',:'PREGA UNKNOWN SAMPLE PARAMETERS',/)
0532   II=0
0533   2000 II=II+1
0534   IVAR=2
0535   IF(II.GT.21)GO TO 2881
0536   GO TO (688,618,628,638,648,658,668,678,688,698,788,728,738,748
0537       1,750,760,770,780,790,784,790) II
0538   2001 CONTINUE
0539   EDT=0
0540   WRITE(CRT,1009)
0541   WRITE(CRT,1008)
0542   WRITE(CRT,1008)
0543   WRITE(CRT,1008)
0544   WRITE(CRT,1008)
0545   WRITE(CRT,1008)
0546   WRITE(CRT,1008)
0547   WRITE(CRT,1008)
0548   CRT=5
0549   GO TO 1500
0550   1000 FORMAT(Q, A2)
0551   1001 FORMAT(Q,32A1)
0552   1002 FORMAT(Q,1A1)
0553   1003 FORMAT(Q,E12.0)
0554   1004 FORMAT(X, ':', 32A1, /)
0555   1005 FORMAT('+', ':', I5, /)
0556   1006 FORMAT('+', ':', 1A1, /)
0557   1007 FORMAT('+', ':', G14.6, /)
0558   1008 FORMAT('+', ':', *
0559   1009 FORMAT(' ')
0560   1100 CONTINUE
0561   END
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PURPOSE OF THE PROGRAM:
THIS PROGRAM DETERMINES THE ACTIVITY OF EACH NUCLIDE IN A SPECTRUM CONTAINING SEVERAL NUCLIDES WHOSE IDENTITIES ARE KNOWN BUT WHOSE ACTIVITIES ARE UNKNOWN. THE PROGRAM ASSUMES SPECTRAL DATA HAS BEEN ACQUIRED VIA A SODIUM IODIDE DETECTOR.

METHOD:
THE PROGRAM MAKES A CHANNEL BY CHANNEL COMPARISON BETWEEN THE UNKNOWN SPECTRUM AND A SERIES OF STANDARD SPECTRA. IT DETERMINES ACTIVITIES BY LEAST SQUARES RESOLUTION OF THE SAMPLE DATA AND USES PIVOTAL REGRESSION ANALYSIS TECHNIQUES TO CALCULATE AND LIST THE ACTIVITY OF EACH NUCLIDE WITH ESTIMATED ERROR AND OTHER INFORMATION ABOUT THE ANALYSIS.
VARIABLE DEFINITIONS

GENERAL CONTROL PARAMETERS
(USER DEFINED)
NS   = NUMBER OF ISOTOPES IN STANDARD LIBRARY (MAX=88)
M   = NUMBER OF CHANNELS PER STANDARD (MAX=512)
NIT  = NUMBER OF ITERATION FOR THRESHOLD & GAIN CALC.
NBA  = BACKGROUND SUBTRACT (1=YES,0=NO)
NZ  = INITIAL CHANNEL FOR COMPUTATION
MF  = FINAL CHANNEL FOR COMPUTATION
TB  = COUNTING TIME FOR BACKGROUND
Q   = REJECTION COEFFICIENT
ASC(I) = STANDARD BACKGROUND SPECTRUM (FILE.ELEMENT(,DEVICE))

CONTROL PARAMETERS FOR EACH LIBRARY ELEMENT
TISOT(JJ) = ISOTOPE NAME (8 CHARACTERS MAX)
HA(I) = HALF-LIFE (SECS.)
TST(I) = COUNTINUE TIME OF STANDARD
AC(I) = ACTIVITY
ASC(I) = STANDARD SPECTRUM (FILE.ELEMENT(,DEVICE))
CONTROL PARAMETERS FOR UNKNOWN SAMPLE
(USER DEFINED)

NBR = BACKGROUND SUPPLIED? (YES=1, NO=0)

NBS = BACKGROUND SUBTRACT? (YES=1, NO=0)

TB = COUNTING TIME FOR BACKGROUND (SECS)

TSA = COUNTING TIME FOR UNKNOWN SAMPLE (SECS)

VRED = VOLUME REDUCTION FACTOR (INVERSE OF DILUTION FACTOR)

DAY = DECAY TIME (SECS)

VM = RESULT MULTIPLICATION FACTOR

ASC(JJ) = SAMPLE & BACKGROUND SPECTRUM (FILE.ELEMENT(/DEVICE))

UNKNOWN SAMPLE OPTION VARIABLES
(USER DEFINED)

NW = WEIGHTING FACTOR DETERMINATION (BASED ON ACTUAL
     COUNTS/CHANNEL=0, BASED ON CALCULATED COUNTS/CHN=1)

N = NUMBER OF LIBRARY SPECTRA TO BE FITTED TO SAMPLE

F0 = F-TEST REJECTION COEFFICIENT

LW = WEIGHTING FACTOR CALCULATION (((COUNTS)**-1)**-1,
     (SIGMA)**-2=0, I=1)

NEWST = APPLY REJECTION COEFFICIENT? (YES=1, NO=0)

BR = BACKGROUND REGRESSION (TRIAL SET, CHOSEN STANDARDS=0,
     BACKGROUND ONLY=1)

BP = PIVOT ON BACKGROUND ALLOWED? (0=NO, 1=YES)

IS(I) = NUMBER OF LIBRARY STANDARD USED DURING BUILDUP REGRESSION

ISL(I) = NUMBER OF LIBRARY STANDARD TO BE FIT IN ORDER OF
        DESIRED PRINTOUT
COMMON/X,FUD
DIMENSION A(10,10),Y(513),Z(10),S(512),STD(10),B(10),
 1 R(512),U(512),IR(512),MY(10),FPM(10),FP(10),
 2 BA(512),SS(10),AC(10),HA(10),IS(10),TST(10),HAT(10),
 3 TNAME(36),TISO(40),TISO(20),IT(10),SNAM(2),
 4 R(10,64),HH(6),SIR(50),ISL(10),HF(4),
SIFORM(20),IFORKL(30),CC(10,10)
DOUBLE PRECISION HG,HR,HT,HH
DATA HF/0.0,HFFULL,SET,BHFTEST,BHBACKWARD,BHFORWARD/
DATA HG/0.0,HGREPSN,/,HR/0.0,HRRESIDUAL,/,HT/0.0,HTTOTAL/
DATA HH/0.0,HHSOUR,/,4H,DF,4H,SS,4H,MS,4H,F/
EQUIVALENCE (BA,IR),CARR,S)A(ThAME(Th,SNAM(1))
LOGICAL*1 ASC(68),DEF(18),EF(18)
LOGICAL*1 TNAME
INTEGER C,D,E,F,MY,P,BR,BP
DATA E/0/
DATA MY/1,2,4,8,16,32,64,128,256,512/
DATA TISO/4NSAMP/,TIS2/4NL/
DEF(9)=.FALSE.
DEF(10)=.FALSE.
ASC(33)=.FALSE.
ASC(34)=.FALSE.
INTEGER FILE
FILE=8
DEFINE FILE 9(4896,2.U.IDAT)
DEFINE FILE 11(4896,2.U.IDAT)
DEFINE FILE 18(8,2.U.IDAT)
0025  MI=9
0026  MIU=11
0027  MO=6
0028  WRITE(MO,900)
0029  900 FORMAT('I,' , OUTPUT FOR PREGA ANALYSIS PROGRAM',///)
C CHANGE RANGE OF NEXT DO LOOP TO MAX NR OF CHANNELS
0030  DO 1 I=1,512
0031 1 BA(I)=0.0
0032  IPO=0
0033  
C GENERAL CONTROL PARAMETERS
C
0034  2 READ(MI'1)NS
0035  READ(MI'2)M
0036  READ(MI'3)NIT
0037  READ(MI'4)NBA
0038  READ(MI'5)NZ
0039  READ(MI'6)MF
0040  READ(MI'48)T3.
0041  READ(MI'41)Q
0042  NCH=MF-NZ+1
C (USER DEFINED)
C NS = NUMBER OF ISOTOPES IN STANDARD LIBRARY (MAX=80)
C M = NUMBER OF CHANNELS PER STANDARD (MAX=512)
C NIT = NUMBER OF ITERATION FOR THRESHOLD & GAIN CALC.
C NIT IS TO BE REMOVED IN FUTURE STREAMLINING OF PROGRAM
C NBA = BACKGROUND SUBTRACT (1=YES, 0=NO)
C NZ = INITIAL CHANNEL FOR COMPUTATION
C MF = FINAL CHANNEL FOR COMPUTATION
C TB = COUNTING TIME FOR BACKGROUND
C Q = REJECTION COEFFICIENT
C
C
D WRITE (MO,981)NS,NIT,NBA,NZ,MF
0043  IF(NS)897,897,3
C
C
C
0044  3 JJ=1
0045  DO 10 I=1,NS
0046  IDAT=65+(I-1)*16
CONTROL PARAMETERS FOR EACH LIBRARY ELEMENT

C
0047 READ(MI'IDAT)TISOT(JJ)
0048 JJ=JJ+1
0049 READ(MI'IDAT)TISOT(JJ)
0050 JJ=JJ+1
0051 IDAT=IDAT+8
0052 READ(MI'IDAT)HA(I)
0053 READ(MI'IDAT)TST(I)
0054 READ(MI'IDAT)AC(I)
C
C TISOT(JJ) = ISOTOPE NAME (8 CHARACTERS MAX)
C HA(I)    = HALF-LIFE (SECS.)
C TST(I)   = COUNTINUE TIME OF STANDARD
C AC(I)    = ACTIVITY
C
0055 10 CONTINUE
IF (NBA) 50,50.40
DO 45 J=1,32.4
C
ASC(I) = STANDARD BACKGROUND SPECTRUM (FILE ELEMENT DEVICE)
C
45 READ(MI,IDAT)ASC(J),ASC(J+1),ASC(J+2),ASC(J+3)
WRITE(M0,902)(ASC(I),I=1,32)
902 FORMAT(1X'STANDARD BACKGROUND: ',32A1)
CALL GET(ASC,BA,IVAR,FILE,M)
WRITE (M0,903)(BA(I),I=1,M)

DO 130 I=1,NS
IDAT=65+(I-1)×16+2
DO 52 J=1,32.4
C
ASC(I) = STANDARD SPECTRUM (FILE ELEMENT DEVICE)
C
52 READ(MI,IDAT)ASC(J),ASC(J+1),ASC(J+2),ASC(J+3)
CALL GET(ASC,SA,IVAR,FILE,M)
C
SUBTRACT BACKGROUND (MULTIPLIED BY COUNT TIME OF STANDARD/ COUNT
TIME OF BACKGROUND) FROM STANDARD
C
IF(NBA) 70,70.60
C
60 FAT=TST(I)/TB
DO 65 J=1,M
S(J)=S(J)-BA(J)*FAT
65 CONTINUE
C
C DON'T LET STANDARD COUNTS BE LESS THAN .01
C
0074 70 DO 75 J=1,M
0075   IF(S(J).LT.0.0)S(J)=.01
0077 75 CONTINUE
0078   IF(NBA)100,100,880
0079 880 WRITE(M0,904)(ASC(II),II=1,32)
0080 904 FORMAT('O',"BACKGROUND SUBTRACTED STANDARD: ",32A1)
0081 WRITE(M0,903)(S(J),J=1,M)
0082 100 CONTINUE
C
C SAVE STANDARD SPECTRUM IN VIRTUAL MEMORY OUT ON DISK
C
0083   IVAR=I-1+1
0084 120 DO 130 K=1,M
0085 130 WRITE(10,'IVAR')S(K)
0086 130 CONTINUE
0087 170 WRITE (M0,908)
C
C
CONTROL PARAMETERS FOR UNKNOWN SAMPLE

IDAT=12
READ(MIU,IDAT)NBR
READ(MIU,IDAT)NBS
READ(MIU,IDAT)TB
READ(MIU,IDAT)TSA
READ(MIU,IDAT)VRED
READ(MIU,IDAT)DAY
READ(MIU,IDAT)VM

(USER DEFINED)

NBR = BACKGROUND SUPPLIED? (YES=1,NO=0)
NBS = BACKGROUND SUBTRACT? (YES=1,NO=0)
TB = COUNTING TIME FOR BACKGROUND (SECS)
TSA = COUNTING TIME FOR UNKNOWN SAMPLE (SECS)
VRED = VOLUME REDUCTION FACTOR (INVERSE OF DILUTION FACTOR)
DAY = DECAY TIME (SECS)
VM = RESULT MULTIPLICATION FACTOR
0096 100 IF (VM) 190,190,200
0097 190 VM=1.0
0098 200 IF (VRED) 210,210,220
0099 210 VRED=1.0
0100 220 IF (TB) 230,230,240
0101 230 FS=0.0
0102 GO TO 250
0103 240 FS=TSA/TB
0104 250 FX=FS+FS**2
0105 IF(NBR) 270,270,260
0106 260 CONTINUE
C
C
ASC(JJ) = SAMPLE & BACKGROUND SPECTRUM (FILE,ELEMENT,.DEVICE)
C
0107 DO 265 JJ=1,32,4
0108 265 READ(MIU,IDAT)ASC(JJ),ASC(JJ+1),ASC(JJ+2),ASC(JJ+3)
C
C
WRITE(MD,910)(ASC(I),I=1,32)
C910 FORMAT(1H1,'SAMPLE BACKGROUND: ',32A1)
C
0109 CALL GETASCBAIVAR.FILE.M)
C
WRITE (MD,903)(BA(I),I=1,M)
0110 270 CONTINUE
0111 IDAT=2
C
0112 DO 280 JJ=1,32,4
0113 280 READ(MIU,IDAT)ASC(JJ),ASC(JJ+1),ASC(JJ+2),ASC(JJ+3)
C
0114 WRITE(MO,911)(ASC(I),I=1,32)
0115 911 FORMAT(' ',SAMPLE SPECTRUM: ',32A1)
C
0116 DO 290 I=1,32
0117 290 TNAME(I)=ASC(I)
0118 CALL GET(ASC,Y,IVAR,FILE,M)
C
   ***********************************************************************
0119 IF (NBS) 310,318,300
0120 300 DO 305 I=1,M
0121 305 Y(I)=Y(I)-BA(I)*FS
0122 310 SB=0.0
0123 DO 320 I=NZ,MF
0124 320 SB=SB+BA(I)
0125 WRITE (MO,903)(Y(I), I=1,M)
0126 S1=0.0
0127 S2=0.0
0128 DO 330 I=NZ,MF
0129 330 S1=S1+Y(I)
0130 330 S2=S1+SB*FX
0131 WRITE (MO, 912)SB,S1
C
C SAVE ORIGINAL SAMPLE SPECTRUM OUT ON DISK
C
0132 IVAR=(NS+2)*M+1
0133 DO 340 I=1,M
0134 340 WRITE(10,IVAR)Y(I)
MIDAS FORTRAN IV  5 OCT 1983   1:36:04 PM  PAGE 012

C
C 0135  IDAT=IDAT+18
C
C  UNKNOWN SAMPLE OPTION VARIABLES
C
0136  MB=0
0137  READ(MIU,IDAT)NW
0138  READ(MIU,IDAT)N
0139  READ(MIU,IDAT)F0
0140  READ(MIU,IDAT)LW
0141  READ(MIU,IDAT)NEUST
0142  READ(MIU,IDAT)BR
0143  READ(MIU,IDAT)BP
0144  READ(MIU,IDAT)KRO
0145  DO 350 I=1,32,4
0146  350 READ(MIU,IDAT) ASC(I),ASC(I+1),ASC(I+2),ASC(I+3)
0147  NDET=0

C
C (USER DEFINED)

C  NW  =  WEIGHTING FACTOR DETERMINATION (BASED ON ACTUAL
C        COUNTS/CHANNEL=0, BASED ON CALCULATED COUNTS/CHN=1)
C  N   =  NUMBER OF LIBRARY SPECTRA TO BE FITTED TO SAMPLE
C  F0  =  F-TEST REJECTION COEFFICIENT
C  LW  =  WEIGHTING FACTOR CALCULATION ((COUNTS)**2-1, i=1)
C        (SIGMA)**2=0, i=1)
C  NEUST = APPLY REJECTION COEFFICIENT ? (YES=1,NO=0)
C  BR   =  BACKGROUND REGRESSION? (TRIAL SET, CHOSEN SET
C        OF STANDARDS=0, BACKGROUND ONLY=0)
C  BP   =  PIVOT ON BACKGROUND ALLOWED?
C        =0 NO PIVOT ON BACKGROUND ALLOWED
C          =1 ALLOW PIVOT ON BACKGROUND
C  KRO  =  OUTPUT RESIDUALS ? (YES=1,NO=0)
C  ASC  =  FILENAME FOR RESIDUALS
C  IS(I) =  NUMBER OF LIBRARY STANDARD TO BE FIT IN ORDER OF
C          DESIRED PRINTOUT
C 0148 DO 360 J=1,NS
0149 360 ISL(I)=0
0150 DO 370 I=1,N
0151 READ(MIU,IDAT)IS(I)
0152 370 ISL(I)=IS(I)
C 0153 DO 380 J=1,N
0154 DO 375 I=1,NS
0155 IF(IS(J)=I) 372,372,375
0156 372 II=2*I-1
C 0157 JJ=2*J-1
0158 TISO(JJ)=TISOT(I)
0159 II=II+1
0160 JJ=JJ+1
0161 TISO(JJ)=TISOT(I)
C 0162 GO TO 300
0163 375 CONTINUE
0164 380 CONTINUE
0165 TISO((N+I)*2-1)=SNAM(1)
0166 TISO((N+1)*2)=SNAM(2)
0167 IS(N+I)=N+1
0168 LN=N+1
DO 390 J=1,N

IT(J)=J

DO 395 I=1,N

IF(IS(I).EQ.1) GO TO 400

CONTINUE

WRITE(M0,913)

FORMAT('8',5X,45('*')/5X7'*.45X /'SX..'*',4X. 'XBACKGROUND NOT INCLUDED AS A STANDARD',4X. '*'/
X*','*',45X,'*',5X,45('*')/)

400 CONTINUE

IF(BP.EQ.0) GO TO 401

WRITE(M0,936)

401 DO 402 I=1,N

402 EF(I)=.FALSE.

C

C SET UP ARRAY A(N+1,N+1)

C

DO 405 I=1,M

IF(LU) 422,412,418

410 W(I)=1.0

DO 420 GO TO 420

412 T*Y(I)+BA(I)*FX

414 W(I)=1.0

DO 420 GO TO 420

416 W(I)=1.0/T

DO 420 CONTINUE

DO 422 I=1,M

423 W(I)=1.0/(Y(I)+1.0)
C
C COMputed weighted sumS of standard spectra
C
0209 436 J=NZ,MF
0211 436 SS(L)=SS(L)+R(J)*w(J)
0212 444 K=L,N
0213 437 READ(10*IVAR)*S(J)
0217 442 SA=0.
C GET LEAST SQUARES SUM COEFFICIENTS FOR UNKNOWN CONCENTRATIONS Z(i)
C AND SAMPLE Y(i)

DO 443 I=NZ,MF
SA=SA+S(I)*R(I)*W(I)
A(K,L)*SA
A(L,K)*A(K,L)
443 CONTINUE

SA=0.
DO 445 I=NZ,MF
SA=SA+R(I)*Y(I)*W(I)
445 CONTINUE
B(L)=SA
A(N+1,L)*SA
A(L,N+1)*A(N+1,L)
446 CONTINUE
SA=0.
DO 450 I=NZ,MF
SA=SA+Y(I)*Y(I)*W(I)
450 CONTINUE
A(LN,LN)=SA
ST=SA

C COMPUTE WEIGHTED SUM OF UNKNOWN

SS(LN)=0.
DO 460 J=NZ,MF
SS(LN)=SS(LN)+Y(J)*W(J)
460
C
C CALCULATE CORRELATION MATRIX

DO 468 L=1,LN
N5=IS(L)
DO 465 K=L,LN
N6=IS(K)
SRD1=A(K,K)-SS(N6)***2/SUMW
SRD2=A(L,L)-SS(N5)***2/SUMW
CC(K,L)=(A(K,L)-SS(N6)*SS(N5)/SUMW)/SQRT(SRD1*SRD2)
CONTINUE
LSK=(L-1)*18+2
KAC=LN-L+1
ENCODE(25,916,IFORKL) LSK,KAC
916 FORMAT('(2X.2A4.',I2.'X,',122C(F8.4.2X)/)')
WRITE(MO,985) TISO(L*2-1),TISO(L*2),CC(K,L),K=L,LN
CONTINUE

C PRINT OUT WEIGHTED SUMS OF STANDARDS AND UNKNOWN

WRITE(MO,985)
WRITE(MO,986) (SS(I),I=1,LN)
DO PIVOTAL REGRESSION ANALYSIS

REGRESSION WITH ALL REQUESTED STANDARDS

E=0
P=N
IF(BR.EQ.0) GO TO 479
WRITE(MO,938)
DO 479 I=1,N
IF(ISL(I).EQ.1) GO TO 471
CONTINUE
N5=ISL(I)
E=E+MY(N5)
CALL PIVOT(A,I,EF,LN)
IPO=1
P=1
GO TO 700
DO 480 I=1,P
E=E+MY(IS(I))
CALL PIVOT(A,I,EF,LN)
CONTINUE
IPO=1
GO TO 700
C
C SELECT TRIAL SUBSET OF MATRIX A
C
0277 500 F=E
0278 D=0
0279 IF(BR.EQ.0) GO TO 502
0281 F=0
0282 DO 501 I=1,N
0283 NS=ISL(I)
0284 P=P+MY(NS)
0285 501 CONTINUE
0286 GO TO 689
0287 582 P=N
0288 588 DO 518 I=1,N
0289 NS=ISL(I)
0290 IF(BP.EQ.1) GO TO 589
0292 IF(NS.EQ.1) GO TO 518
0294 IF(STD(I).LE.0.0) GO TO 511
0296 IF(Z(I)/STD(I).GE.1.0) GO TO 510
0298 511 CALL PIVOT(A1,EFLN)
0299 E=E-MY(NS)
0300 P=P-1
0301 510 CONTINUE
0302 IF(E.EQ.1.AND.Z(I).LT.0.8) GO TO 898
0304 IF(E.GT.8) GO TO 548
C
C FIND LARGEST F-VALUE AND USE THAT STANDARD AS THE TRIAL SET
C
0306 FPS=0.0
0307 DO 530 I=1,N
0308 IF(Z(I)) 530,530,520
0309 J=I
530 FP=FPS
0311 FP=FP(I)
0312 530 CONTINUE
0313 530 CONTINUE
0314 P=1
0315 E=E.AND.MY(ISL(J))
0316 540 IPO=2
0317 540 GO TO 788
C  BACKWARD PIVOT
C
0318  550  C=E
0319     IF(E.EQ.1.AND.BP.EQ.0) GO TO 800
0321  551  FMIN=10000.
0322     DO 555 I=1,N
0323     FPM(I)=1000.
0324     N5=ISL(I)
0325     IF(BP.EQ.1) GO TO 552
0327     IF(N5.EQ.1) GO TO 555
0329  552  IN=C.AND.MY(N5)
0330     IF(IN) 555,555,554
0331     554  FPM(I)=(NCH-P)*((A(ILN)*A(LN,LN))/(-A(I,I)*A(LN,LN)))
0332     IF(A(ILN).GT.@.0) FPM(I)--FPM(I)
0334     IF(FMIN(I).GE.FMIN) GO TO 555
0336     FMIN=FMIN(I)
0339     J=1
0338  555  CONTINUE
0339     DF=NCH-P
0340     ZS=A(J,LN)
0341     IF(FMIN.LT.8.@) FMIN=FMIN
0343     CALL XQCALC(DF,FMIN,ZS,XF,QF,8)
0344     IF(XF.GE.F@) GO TO 560
0346     CALL PIVOT(A,J,EF,LN)
0347     E=E-MY(ISL(J))
0348     P=P-1
0349  560  IPO=3
0350     GO TO 700
0351  600  JDF=F-D
0352     IF(E.EQ.JDF) GO TO 800
C
C FORWARDED PIVOT
C
0354       609 IF(BR.EQ.1) C=E
0356       D=F-C
0357       IF(D.EQ.0) GO TO 630
0359       FMAX=0.0
0360       DF=NCH-P-1
0361       WRITE(MO,932)
0362       DO 620 I=1,N
0363       FPM(I)=0.0
0364       N5=ISL(I)
0365       IF(NP.EQ.1) GO TO 610
0367       IF(N5.EQ.1) GO TO 620
0369       610 IN=D.AND.MY(N5)
0370       IF(IN) 620,628,615
0371       615 INEG=0
0372       SQUC=A(I,I)*A(LN,LN)
0373       IF(SOUC.GT.0.0) GO TO 616
0375       SQUC=-1.0*SQUC
0376       INEG=1
0377       616 RHO=A(I,LN)/SORT(SOUC)
0378       IF(INEG.EQ.1) RHO=-1.0*RHO
0380       R2=RHO**2
0381       IF(INEG.EQ.1) R2=-1.0*R2
0383       FPM(I)=DF*R2/(1.0-R2)
0384       ZS=A(I,LN)
0385       FPS=FPM(I)
0386       CALL XQCALC(DF,FPS,ZS,XF,QF,0)
0387       RMSR=A(LN,LN)**(1.0-R2)/DF
0388       WRITE(MO,933) TISO(I*2-1),TISO(I*2),FPS,QF,XF,RHO,RMSR
0389       IF(XF.LT.0.0) FPM(I)=FPM(I)
0391       IF(FPM(I).LE.FMAX) GO TO 620
0393       FMAX=FPM(I)
0394       J=1
0395       620 CONTINUE
0396       ZS=A(J,LN)
0397       CALL XQCALC(DF,FMAX,ZS,XF,QF,0)
0398       IF(XF.LT.F0) GO TO 630
0400       CALL PIVOT(A,J,EF,LN)
0401       E=EFMY(ISL(J))
0402       P=P+1
0403       IP0=4
0404       BR=0
0405       GO TO 700
0406       630 IF(E.EQ.C) GO TO 800
0408       GO TO 550
C
C OUTPUT SECTION FOR PARTIAL F.O.X AND ANALYSIS OF VARIANCE
C
0409 J=0
0410 DF=NCH-P
0411 RSS=A(LN.LN)
0412 RMSR=RSS/DF
0413 DO 730 I=1,N
0414 NS=ISL(I)
0415 IF(NS.EQ.0) 728
0416 NS=1
0417 J=J+1
0418 TISOT(2*J-1)=TIS0(2*I-1)
0419 TISOT(2*J)=TIS0(2*I)
0420 Z(J)=A(LN.I)*TST(N5)/TSA
0421 SQUC=A(I.I)
0422 IF(SQUC.LT.0.0) SQUC=-1.0*SQUC
0423 STD(J)=SORT(SQUC*RMSR)*TST(N5)/TSA
0424 FP(J)=(Z(J)/STD(J))**2
0425 730 CONTINUE
0426 WRITE(MO,918) TISOT(1*2-1),TISOT(1*2),Z(1),STD(1),FPS,OF,RMSR
0427 918 FORMAT(2X,'RESULTS OF '1', '2A4.'1',' REGRESSION ON '1', ,2A4.'1')
0428 WRITE(MO,919) DF,RSS,RMSR
0429 919 FORMAT(2X,'DEGREES OF FREEDOM=',F11.0/
0430 X13X,'RSS=',1PE11.3/13X,'RMSR=',1PE11.3'/)
0431 DO 740 I=1,P
0432 FPS=FPS(I)
0433 ZS=Z(I)
0434 CALL XOCCALC(DF,FPS,ZS,OF,QF,0)
0435 FP(I)=X
0436 RMSR=A(LN.LN)*((1.0+FPS/DF)/(DF+1)
0437 738 WRITE(MO,920) TISOT(1*2-1),TISOT(1*2),Z(1),STD(1),FPS,OF,RMSR
0438 920 FORMAT(2X,'2X,2A4,1PE13.4,2X,'+-',1PE11.2,3X,'F=',
0439 X1PE12.4,3X,'Q=',1PE12.4,3X,'X=',1PE12.4,3X,'RMSR=',1PE12.4)
0439 740 CONTINUE
0440 GO TO (500,550,600,630),IP0
C
C     FINAL RESULT SECTION
C
500 SG=0
J=0
IF(E.EQ.1.AND.Z(1).LT.0.0) GO TO 890
DO 828 I=1,N
N5=ISL(I)
IN=E.AND.MY(N5)
IF(IN) 820,820,815
815 J=J+1
SG=SG-A(I,LN)*8(I)
TISOT(J*2-1)=TISO(I*2-1)
TISOT(J*2)=TISO(I*2)
820 CONTINUE
THIS LOOP READS FROM A SCRATCH FILE INTO CORE UP TO 15
STANDARDS, 64 CHANNELS AT A TIME SO THAT RESIDUALS AND STANDARD
ERRORS MAY BE DETERMINED

DO 835 J=NZ,MF
JJJ=JJJ+1
SV=0.
JJ=0
DO 820 I=1,N
N5=ISL(I)
IN=E.AND.MY(N5)
IF(IN) 820,828,822
822 JJ=JJ+1
IF(JJJ.GT.I.AND.JJJ.LT.65)GO TO 827
JJJ=1
LOOP=(MF+I)-J
IF(LOOP.GT.64)LOOP=64
IVAR=(N5-1)*M+J
DO 826 II=1,LOOP
826 READ(10*IVAR)ARR(JJ,II)
WRITE(1030)(ARR(JJ,II),II=1,LOOP)
SV=SV+ARR(JJ,JJJ)*(-A(I,LH))
IF(JJ.EQ.P) JJ=0
828 CONTINUE
C
0481 RE=Y(J)-SV
0482 T=RE**2
0483 VY=VY+W(J)*T
0484 VU=VU+T
0485 TMO=ABS(0.1+SY)
0486 TMP=TMO+BA(J)*FX
0487 VV=VV+TMP
0488 IF (NW) 833,833,838
0489 830 IF (LW) 832,831,833
0490 831 U(J)=1.0/TMP
0491 GO TO 933
0492 832 U(J)=1.0/TMO
0493 833 RT=T/TMP
0494 CH=CH+RT
0495 TMP=SQRT(TMP)
C
C CALCULATES RESIDUALS OVER STANDARD DEVIATION, R(J)
C
0496 R(J)=RE/TMP
0497 TE=Y(J)+BA(J)**FX
0498 835 CONTINUE
0499 SR=VY
C
C CALCULATES NUMBER OF DEGREES OF FREEDOM, DN
C
0500         DN=M-P-NZ+1
0501         DR=DN
0502         DG=P
0503         DT=DR+DG
0504         CHDF=CH/DN
0505         VY=VY/DN
0506         WRITE(MO,896)
0507         WRITE(MO,934) SNAM(1),SNAM(2)
0508         WRITE (MO,921)CHDF
0509         J=0
0510     840 DO 844 I=1,N
0511         NS=ISL(I)
0512         IF(IN) 844,844,841
0513     841 J=J+1
C
C DECAY CORRECTION DONE HERE
C
0515         FD= EXP(0.693*DAY/HA(NS))
CORRECTED STANDARD ERROR DETERMINED FROM THE VARIANCE

\[
\text{STD}(J) = \text{SQRT}(-A(I, I) \times A(LN, LN) / D(N) \times \text{TST}(N5) / \text{TSA})
\]

RELATIVE CONCENTRATION IS CONVERTED TO ACTUAL CONCENTRATION LEVEL

\[
Z(J) = -A(I, LN) \times (\text{TST}(N5) / \text{TSA}) \times \text{AC}(N5) \times FD \times \text{VM} / \text{VRED}
\]

CONTINUE

\[
\text{WRITE (MO,922)}
\]

\[
\text{DO } 847 \text{ I}=1,P
\]

\[
\text{FPS} = (Z(I) / \text{STD}(I)) \times 2
\]

\[
\text{ZPS} = Z(I)
\]

\[
\text{CALL XOCALC(DN, FPS, ZPS, XF, QF, 0)}
\]

\[
\text{RMSR} = A(LN, LN) \times (1.0 + \text{FPS} / \text{DR}) / (\text{DR} + 1)
\]

\[
\text{WRITE(MO,926)} \text{TISOT(I*2-1), TISOT(I*2), Z(I), STD(I), FPS, QF, XF, RMSR}
\]

CONTINUE

WRITE ANALYSIS OF VARIANCE TABLE

\[
\text{WRITE (MO,924) HH}
\]

\[
\text{WRITE(MO,925) HG, DG, SG, XG, FF}
\]

\[
\text{WRITE(MO,925) HR, DR, SR, XR}
\]

\[
\text{WRITE(MO,925) HT, DT, ST}
\]

\[
\text{CALL RSTAT(NCH,P,R,NZ, MF)}
\]
C COMPUTE FINAL STATISTICS FOR STANDARDS ELIMINATED
C DURING PIVOTAL REGRESSION

C
0536   WRITE(MO,935)
0537   DF=NCH-P-1
0538   J=0
0539   DO 850 I=1,N
0540   NS=ISL(I)
0541   IF(NS) 858,856,848
0542   IN=D.AND.MY(N5)
0543   848 J=J+1
0544   TISO(J*2-1)=TISO(I*2-1)
0545   TISO(J*2)=TISO(I*2)
0546   ZS=A(I,LN)
0547   INEG=0
0548   SQUC=A(I,I)*A(LN,LN)
0549   IF(SQUC.GT.8.8) GO TO 849
0551   SQUC=-1.0*SQUC
0552   INEG=1
0553   849 RHO=A(I,LN)/SORT(SQUC)
0554   IF(INEG.EQ.1) RHO=-1.0*RHO
0556   R2=RHO**2
0557   IF(INEG.EQ.1) R2=-1.0*R2
0559   FPS=DF*R2/(1.0-R2)
0560   CALL XOCALC(DN,FPS,ZS,XF,QF,0)
0561   RMSR=A(LN,LN)*(1.0-R2)/DF
0562   WRITE(MO,933) TISO(J*2-1),TISO(J*2),FPS,QF,XF,RHO,RMSR
0563   850 CONTINUE
0564   WRITE (MO,926) SNAM(1),SNAM(2)
0565   DO 851 II=1,NZ-1
0566   851 R(II)=0.0
0567   WRITE (MO,927) (R(J),J=1,MF)
0568   853 K=0
0569   N2=M-2
C
C
C FIND SUSPICIOUS CHANNELS. THESE ARE DEFINED AS CHANNELS WHERE
C STD/RESIDUAL IS GREATER THAN 10 OR WHERE STD/RESIDUAL IS GREATER
C THAN 2 FOR THE CHANNELS ON EITHER SIDE OF THE ONE CONSIDERED.
C
0570    DO 870 J=NZ,N2
0571          T=ABS(R(J))
0572      IF(T-10.) 860,860,866
0573 860 IF(R(J-1)<-2.) 870.862,862
0574 862 IF(R(J-2)<-2.) 870.864,864
0575 864 IF(R(J+1)<-2.) 870.866,866
0576 866 K=K+1
0577          IR(K)=J
0578          SIR(K)=R(J)
0579      IF(K.GT.50) GO TO 872
0581      870 CONTINUE
0582 872 WRITE (1O,928)
0583          WRITE (1O,929)(IR(I),SIR(I),I=1,K)
0584      CALL RESID(R,NZ,MF)
0585      CALL RUNS(R,NZ,MF)
0586      IF(KRO.NE.1) GO TO 880
0588      DO 876 I=NZ,MF
0592      IF(R(I).LT.0.) R(I)=0.
0594      876 CONTINUE
0595      CALL PUT(ASCJR,IVARFILE,M)
0596 880 GO TO 895
C
0597 901 FORMAT("",1X,6I4)
0598 903 FORMAT(2X,7F8.0)
0599 905 FORMAT('8",1X,"WEIGHTED Sums OF STANDARDS AND UNKNOWNS",/)
0600 906 FORMAT(1X,1PE11.4,1PE11.4,1PE11.4,1PE11.4,1PE11.4,/
0601 908 FORMAT(1H0)
0602 909 FORMAT(3A2,2X, 12,15,13,12,110, 5E10.3)
0603 912 FORMAT(1H1,"BACKG S SUM",1PE12.3,"  SUM",1PE12.3,/
0604 921 FORMAT("",1X,"FIT",1PE11.3)
0605 922 FORMAT(1H0,"RESULTS=CONCENTRATIONS AND EST STANDARD ERRORS",/
0606 926 FORMAT(1H1," RATIO OF RESIDUALS OVER STD DEV PER CHANNEL FOR",
   1X,2A4,/
0607 927 FORMAT (1X,F7.1, 6F8.1)
0608 928 FORMAT(1H0,"SUSPICIOUS CHANNELS",/)
0609 929 FORMAT (5(14,2X,F5.2,/)  
0610 924 FORMAT(1H0,12X,"ANALYSIS OF VARIANCE"/1X,2A4,6X,4.4X,3(A4,7X))
0611 925 FORMAT(1X,98,F11.8,1PE11.3)
0612 930 FORMAT(1X,14X,40(""*/15X,"*/8X,
   1"STARTING ANALYSIS WITH",8X,"*/15X,"*/5X.
   2"TRIAL SET = BACKGROUND ONLY",6X,"*/15X.
   340(""*/)
0613 932 FORMAT("",/)/)/)/)/)/)/)/)/)/)
0614 933 FORMAT(1X,2A4,3X,"F=",1PE12.4,3X,"Q=",1PE12.4,
   13X,"X=",1PE12.4,3X,"RHO=",1PE12.4,3X,"AMSTR=",1PE12.4)
0615 934 FORMAT(1X,50(""*/13X,"FINAL RESULT FOR",2A4,50(""*/)
0616 935 FORMAT(1X,"/)/)/)/)/)/)/)
0617 936 FORMAT(1X,10X,41(""*/11X,"*/5X.
   1"PIVOT ON BACKGROUND PERMITTED",5X,"*/11X,41(""*/
0618 898 WRITE(M0,940)
0619  WRI TE(7,940)
0620 940 FORMAT(1X,"NONE OF THE CHOSEN STANDARDS RESULT","/
   X"IN A SIGNIFICANT CONTRIBUTION TO THE",/
   X"BACKGROUND SUBTRACTED SAMPLE SPECTRUM")
0621 895 WRITE(M0,896)
0622 896 FORMAT(1")
0623 897 CONTINUE
0624  END
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- **TRANSFER ADDRESS** = 020004
- **STACK SIZE** = 001000
SUBROUTINE HISTO(LABEL, IH, XL, XD, N)
C WRITTEN BY G.PHILLIPS JUNE 1981
C
REAL*8 LABEL(4)
LOGICAL*1 A(50), ASTAR, ACOLON
DIMENSION IH(21)
DATA A/50*1H*/. IOUT/6/
DATA ASTAR/1H*/.ACOLON/1H:

MAX=0
DO 200 K=1, N
IF (MAX.LE.IH(K)) MAX=IH(K)
DIV=1
L=5
200 IF (MAX/IV.LE.50) GO TO 300
DIV=DIV*2
IF (DIV.LT.L) GO TO 250
DIV=L*2
GO TO 250
300 IDELT=DIV/2
WRITE(IOUT,310) LABEL
310 FORMAT(IHI,4A8)
WRITE(IOUT,320) DIV
320 FORMAT(IHO,'SCALE FACTOR=',I6/
X=XL
IT=0
DO 400 K=1, N
IT=IT+IH(K)
400 CONTINUE
J=(IH(K)+IDELT)/DIV
IF (J.LT.1) A(1)=ACOLON
WRITE(IOUT,360) X, IH(K), (A(I), I=1,J)
360 FORMAT(IHX.G11.3,I8,2X,50A1)
A(1)=ASTAR
X=X+XD
CONTINUE
WRITE(IOUT,410) IT
410 FORMAT(IHO,4X,'TOTAL=',I8)
DO 500 I=1,5
500 WRITE(IOUT,510)
510 FORMAT(IHO)
RETURN
END

IF(REI.LT.0.)REI=32768.+REI
IF(REI.GE.16384.)REI=REI-16384.
ARRAY(K)=REI/65536.+RE2
CONTINUE
K=M+1
END FILE FILE
RETURN
END
### MIDAS FORTRAN IV STORAGE MAP

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**COMMON BLOCK HEAD**  
LENGTH 000143
SUBROUTINE PIVOT(A,P,E,K)

C
C WRITTEN BY: G. W. PHILLIPS AND B. G. GLAGOLA JULY, 1982 NRL
C
C REFERENCE: M. J. GARSIDE, APPL. STAT. 20(1971) 111-112
C
INTEGER P1,P2,P
REAL A(10,10)
LOGICAL*1 E(10)

C DIMENSION N MUST BE GREATER THAN OR EQUAL K.
C ARRAY E MUST BE INITIALIZED *.FALSE.* BEFORE
C FIRST CALL TO PIVOT.
C
AA=1.0/A(P,P)
A(P,P)=AA
P1=P-1
P2=P+1
IF(P.EQ.1) GO TO 350
DO 300 I=1,P1
AIP=A(I,P)*AA
DO 166 J=I,P1
A(I,J)=A(I,J)-AIP*A(J,P)
CONTINUE
300
DO 280 J=P2,K
A(I,J)=A(I,J)-AIP*A(J,P)
CONTINUE
200
DO 350 I=1,P2,K
AIP=A(I,P)*AA
DO 586 J=I,K
A(I,J)=A(I,J)-AIP*A(J,P)
CONTINUE
500
DO 400 I=P1,K
AIP=A(P,I)*AA
DO 486 J=I,K
A(I,J)=A(I,J)-AIP*A(J,P)
CONTINUE
400
DO 500 I=P1,K
A(IP)=AIP
IF(E(P)) A(IP)=AIP
CONTINUE
500
E(P)=.NOT.E(P)
RETURN
END

IF(RE1.LT.0.)RE1=32768.+RE1
IF(RE1.GE.16384.)RE1=RE1-16384.
ARRAY(K)=RE1*65536.+RE2
CONTINUE
K=M+1
END FILE FILE
M>K-1
RETURN
END
### MIDAS FORTRAN IV STORAGE MAP

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SUBROUTINE GET(ASC, ARRAY, IVAR, FILE, M)

C LAST MODIFIED OCTOBER 1982 BY G.W.P.

COMMON/HEAD/HDRTITLE(32), ID(9), ELTIME, PLTIME, ERTIME, PRTIME
INTEGER*2 TITLE, ID
DIMENSION ARRAY(256), ITIME(4)
LOGICAL*1 ASC(60), DEF(10), NAM(60)
INTEGER FILE
DEFINE FILE FILE(0,2,U,IVAR)
ENCODE(8,10,DEF)FILE
FORMAT('DEF ',12).
DEF(9)=.FALSE.
DEF(10)=.FALSE.
CALL CONCAT(DEF, ASC, NAM, 59)
CALL LUNDEF(NAM,E)
IVAR=12
DO 12 I=1,4
READ(FILE*IVAR)MLT, ITIME(1)
PLTIME=ITIME(1)
ELTIME=ITIME(2)
PRTIME=ITIME(3)
ERTIME=ITIME(4)
IVAR=84
DO 20 I=1,31,2
READ(FILE*IVAR)TITLE(I), TITLE(I+1)
DO 30 I=1,7,2
READ(FILE*IVAR)ID(I), ID(I+1)
IHDR=1
IVAR=28
READ(FILE*IVAR)A0
READ(FILE*IVAR)B0
READ(FILE*IVAR)C0
IVAR=193
DO 32 K=1,M
READ(FILE*IVAR,END=200)MSB, LSB
RE1=MSB
RE2=LSB
IF(RE2.LT.0.)RE2=65536.+RE2
IF(RE1.LT.0.)RE1=32768.+RE1
IF(RE1.GE.16384.)RE1=RE1-16384.
ARRAY(K)=RE1*65536.+RE2
CONTINUE
K=M+1
END FILE FILE
M=K-1
RETURN
END
### MIDAS FORTRAN IV STORAGE MAP

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**COMMON BLOCK /HEAD/**

*LENGTH 000142*

| IHDR | 000000 | INTEGER*2 VARIABLE |
| TITLE | 000002 | INTEGER*2 ARRAY (32) |
| ID | 000102 | INTEGER*2 ARRAY (8) |
| ELTIME | 000122 | REAL*4 VARIABLE |
| PLTIME | 000126 | REAL*4 VARIABLE |
| ERTIME | 000132 | REAL*4 VARIABLE |
| PRTIME | 000136 | REAL*4 VARIABLE |
SUBROUTINE PUT(ASC.ARRAY,IVAR,FILE,M)

C WRITTEN BY G. PHILLIPS, JUNE 1981

DIMENSION ARRAY(256)

LOGICAL*1 ASC(60),DEF(10),NAM(60)

INTEGER FILE

DEFINE FILE FILE(448,2,U,IVAR)

ENCODE(8,10,DEF)FILE

FORMAT('DEF ',12.', ')

DEF(9)=.FALSE.

DEF(10)=.FALSE.

CALL CONCAT(DEF,ASC,NAM,59)

CALL LUNDEF(NAM,E)

IVAR=193

M=IVAR-193

DO 100 K=1,M

V=ARRAY(K)

IF(V.LT.0.) V=0.

IF(V.LT.65536.) GOTO 50

V=V/65536.

IF(V.GT.16383.) V=16383.

MSB=V

LSB=0

GOTO 80

50 IF(V.GT.32767.) V=V-65536.

LSB=V

MSB=0

WRITE(FILE,IVAR)MSB,LSB

CONTINUE

ENDIF FILE

CALL CLOSEU(FILE)

RETURN

IF(REI.LT.0.)REI=32768.+REI

IF(RE1.GE.16384,;)REI=REI-16384.

ARRAY(K)=REI*65536.+RE2

CONTINUE

K=M+1

END FILE FILE

M=K-1

RETURN

END
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SUBROUTINE RESID(R,NZ,MF)
C
WRITTEN BY G.PHILLIPS JUNE 1981
C
DIMENSION R(256),A(4),C(4),IH(21)
DATA IOUT/6/
DATA LABEL/8H DIST,BRIBUTION,8H OF RESI,8HDUALS /
DO 100 K=1,21
  100 IH(K)=0.
DO 200 I=NZ,MF
  200 IH(K)=IH(K)+1
M=MF-NZ+1
DO 220 J=1,4
  220 C(J)=C(J)/M
U=C(1)
A(1)=U
U2=U*U
U3=U*U2
U4=U*U3
V=C(2)-U2
A(2)=V
A(3)=C(3)-3*U*C(2)+2*U3
A(4)=C(4)-4*U*C(3)+6*U2*C(2)-3*U4
SD=SQRT(V)
SQ=A(3)/SD**3
EX=A(4)/V**2-3.
WRITE(IOUT,1000)(I,A(I),C(I),I=1,4)
1000 FORMAT(1H6,'NUMBER OF ELEMENTS =',14/
  1 ) (I5.2G11.3))
WRITE(IOUT,300)U,V,SD,EX
300 FORMAT(1H6,'MEAN RESIDUAL =',F8.3,', VARIANCE =',F8.3.
  1 ' , SKEWNESS =',G11.3,' , EXCESS =',G11.3)
XL=5.0
XD=0.5
N=21
CALL HISTO(LABEL,IH,XL,XD,N)
RETURN
END
### MIDAS FORTRAN IV STORAGE MAP

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SUBROUTINE RSTAT(NCH,PRNZ,MF)
C WRITTEN BY T. B. GOSNELL 22 JUNE, 1982 LLNL
C MODIFIED FOR PREGA BY B. G. GLAGOLA 28 JULY, 1982 NRL
C
C THIS PROGRAM ANALYSES RESIDUALS FROM PREGA, COMPUTES A
C RESIDUAL STATISTIC, ITS EXPECTATION VALUE, STANDARD
C DEVIATION AND AN APPROXIMATE ASSOCIATED FAP.
C
C REFERENCE: A. AARNIO, M. J. KOSKELO AND P. ZOMBORI,
C NUCLEAR INSTR. AND METH. 184(487)1981.
C
DIMENSION R(512)
REAL NRMR
INTEGER P
CH=NCH
EP=P
DF=CH-EP
MF=MF-1
RSTT=0
DO 10 I=NZMFI
RSTT=RSTT+R(I)*R(I+I)
10 CONTINUE
RSTT=RSTT+R(I)*R(MF)
RSTT=RSTT/DF
EXRES=EP/CH
SIGRES=SORT(CH)/DF
NRMR=(RSTT-EXRES)/SIGRES
CALL XOCALC(DF,0.,1.,NRMR,Q,1)
WRITE(6,50)
50 FORMAT( '**** LLNL R-STATISTIC ****' )
WRITE(6,51) RSTT,EXRES,SIGRES,NRMR,Q
51 FORMAT('0.' , 'AUTO-CORRELATION COEFFICIENT',17(''),1PE12.4/
'1' EXPECTATION VALUE',28(''),1PE12.4/
'2' STANDARD DEVIATION',27(''),1PE12.4/
'3' EQUIVALENT NORMAL STANDARD DEVIATIONS',8(''),1PE12.4/
'4' R-STAT FAP',35(''),1PE12.4)
RETURN
END
<table>
<thead>
<tr>
<th>NAME</th>
<th>OFFSET</th>
<th>ATTRIBUTES</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>000020</td>
<td>REAL*4 PARAMETER ARRAY (512)</td>
</tr>
<tr>
<td>NCH</td>
<td>000014</td>
<td>INTEGER*2 PARAMETER VARIABLE</td>
</tr>
<tr>
<td>P</td>
<td>000016</td>
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</tr>
<tr>
<td>NZ</td>
<td>000022</td>
<td>INTEGER*2 PARAMETER VARIABLE</td>
</tr>
<tr>
<td>MF</td>
<td>000024</td>
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</tr>
<tr>
<td>NRMR</td>
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<tr>
<td>CH</td>
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<tr>
<td>EP</td>
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<tr>
<td>DF</td>
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</tr>
<tr>
<td>MF1</td>
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</tr>
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<td>EXRES</td>
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<td>SIGRES</td>
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<td>SORT</td>
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<tr>
<td>Q</td>
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<tr>
<td>LE</td>
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<td></td>
</tr>
<tr>
<td>EX</td>
<td>000052</td>
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</tr>
<tr>
<td>XL</td>
<td>000055</td>
<td>REAL*4 VARIABLE</td>
</tr>
<tr>
<td>XD</td>
<td>000062</td>
<td>REAL*4 VARIABLE</td>
</tr>
<tr>
<td>N</td>
<td>000066</td>
<td>INTEGER*2 VARIABLE</td>
</tr>
<tr>
<td>HISTO</td>
<td>000000</td>
<td>REAL*4 PROCEDURE</td>
</tr>
</tbody>
</table>
SUBROUTINE RUNS(R,NZ,MF)
C
URITEN BY G.PHILLIPS JUNE 1981
C
DIMENSION R(256),IH(21),NCH(50),KSI(12),NRS(50)
REAL*8 LABEL(4)
DATA LABEL/8H DISTRIBUTION OF R, 8HNS /
DATA KSI/-10,-9,-8,-7,-6,-5,5,6,7,8,9,10/
C
DO 100 K=1,21
100 IH(K)=0
I=NZ
J=0
C
K=0
ICH=I
210 IF(R(I).LT.8.) GOTO 300
K=K+1
I=I+1
IF(I.GT.MF) GOTO 400
IF(R(I).GE.8.) GOTO 210
GOTO 400
300 K=K-1
I=I+1
IF(I.GT.MF) GOTO 400
IF(R(I).LE.8.) GOTO 300
K=K+11
IF(K.LT.1) K=11
IF(K.GT.21) K=21
IH(K)=IH(K)+1
IF(K.GT.6.AND.K.LT.16) GO TO 450
IF(K.GT.6) K=K-9
J=J+1
NCH(J)=ICH
NRS(J)=KSI(K)
450 IF(I.LE.MF) GOTO 200
C
XL=-10.0
XD=1.0
N=21
CALL HISTO(LABEL,IH,XL,XD,N)
WRITE(6,500)
WRITE(6,501) (NCH(I),NRS(I),I=1,J)
501 FORMAT(’5s(5x,i4,16)')
RETURN
END
<table>
<thead>
<tr>
<th>NAME</th>
<th>OFFSET</th>
<th>ATTRIBUTES</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
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<tr>
<td>IH</td>
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<tr>
<td>NCH</td>
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<td>INTEGER*2 ARRAY (50)</td>
</tr>
<tr>
<td>KSI</td>
<td>00240</td>
<td>INTEGER*2 ARRAY (12)</td>
</tr>
<tr>
<td>NRS</td>
<td>00270</td>
<td>INTEGER*2 ARRAY (50)</td>
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<tr>
<td>LABEL</td>
<td>00434</td>
<td>REAL*8 ARRAY (4)</td>
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<td>NZ</td>
<td>00016</td>
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</tr>
<tr>
<td>MF</td>
<td>00020</td>
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</tr>
<tr>
<td>K</td>
<td>00564</td>
<td>INTEGER*2 VARIABLE</td>
</tr>
<tr>
<td>I</td>
<td>00566</td>
<td>INTEGER*2 VARIABLE</td>
</tr>
<tr>
<td>J</td>
<td>00570</td>
<td>INTEGER*2 VARIABLE</td>
</tr>
<tr>
<td>ICH</td>
<td>00572</td>
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<tr>
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<tr>
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<td>XL</td>
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</tr>
<tr>
<td>HISTO</td>
<td>00000</td>
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</tr>
</tbody>
</table>
SUBROUTINE XOCALC(DF,F,ZS,X,Q,IEN)

C 0!
C
C THIS ROUTINE CALCULATES X(F) AND Q(X) GIVEN F
C
0002 IF(IEN.EQ.1) GO TO 40
0004 DF2=2.*DF-1
0005 IF(F.GT.DF2) GO TO 50
0007 X=(SQRT(F)*((1.1-1./(4.*DF)))/(SQRT(1.-F/(2.*DF))))
0008 40 IF(X.GT.12.9) GO TO 60
0010 Z=0.398942*EXP(-X**2/2.)
0011 T=1.0/(1.0+0.33267*X)
0012 Q=Z*(.436184*T-.128168*T**2+.937298*T**3)
0013 GO TO 70
0014 50 X=9.9999E09
0015 60 Q=0.00
0016 70 IF(ZS.LT.0.0) Q=1.-Q
0019 80 IF(ZS.LT.0.0) X=-X
0020 RETURN
0021 END
0027 400 K=K+11
0029 IF(K.LT.1) K=1
0030 IF(K.GT.21) K=21
0032 IH(K)=IH(K)+1
0033 IF(K.GT.6.AND.K.LT.16) GO TO 450
0035 IF(K.GT.6) K=K-9
0037 J=J+1
0039 NCH(J)=ICH
0039 NRS(J)=KSI(K)
0040 450 IF,J
0049 501 FORMAT(",5(SX,14.I6))
0050 RETURN
0051 END
<table>
<thead>
<tr>
<th>NAME</th>
<th>OFFSET</th>
<th>ATTRIBUTES</th>
</tr>
</thead>
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<tr>
<td>DF</td>
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<tr>
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<td>REAL*4 PARAMETER VARIABLE</td>
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<td>INTEGER*2 PARAMETER VARIABLE</td>
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<tr>
<td>EXP</td>
<td>000090</td>
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</tr>
<tr>
<td>T</td>
<td>000074</td>
<td>REAL*4 VARIABLE</td>
</tr>
</tbody>
</table>
Flow Chart for the Program PREGA showing details of the Major Sections Given in Figure 1.
SELECT TRIAL SUBSET

1a

F = E; D = ∅

START WITH BKGD ONLY?

NO

P = N
BEGIN LOOP FOR I = 1, N

B(I)/σ(I) < 1?

NO

PIVOT I OUT
LET E = E AND NOT MY(I)
P = P - 1

END OF LOOP?

YES

E > 0?

NO

LOOP FOR I = 1, N TO FIND LARGEST Fp

P = 1
E = E AND MY(I)

PRINT OUT RESULTS OF REGRESSION B ± σ, Fp, 0, X FOR ALL P STANDARDS IN SET E

YES

END OF LOOP?

3

NO

F = F + MY(I)

END OF LOOP?

YES

2
BACKWARD PIVOT

1. LET C = E

2. FIND $F_p^-(J) = \min F_p^-(I)$ FOR STANDARD I IN SET C

3. IF $F_p^-(J) \leq F_\phi$ THEN PIVOT J OUT
   LET E = E AND NOT. MY(J)
   P = P - 1

4. PRINT OUT RESULTS $\theta, F_p, Q, X$ FOR ALL P STANDARDS IN SET E

5. IF E = F - D THEN
   IF YES THEN GO TO 3
   IF NO THEN GO TO 4
FORWARD PIVOT

1. LET D = F - C
2. IF D ≠ ∅ THEN
   2.1. CALCULATE $F_p^+$ FOR ALL STANDARDS I IN SET D
   2.2. PRINTOUT RESULTS $F_p^+, Q, X$ FOR STANDARDS IN SET D
   2.3. FIND $F_p^+(J) = \text{MAX } F_p^+(I)$ FOR ALL STANDARDS I IN SET D
   2.4. IF $F_p^+(J) < F_p^+$ THEN
         2.4.1. PIVOT J IN
         2.4.2. LET E = E OR MY (J)
         2.4.3. P = P + 1
         2.4.4. PRINT OUT RESULTS $B, F_p, Q, X$ FOR ALL P STANDARDS IN SET E
3. E = C
4. IF E = C THEN
   4.1. END
   4.2. ELSE
         4.2.1. GOTO 1
FINAL RESULTS

CALCULATE:
1. RESIDUALS/STANDARD DEVIATIONS
2. ACTUAL CONCENTRATION AND STANDARD ERROR
3. DEGREES OF FREEDOM

PRINT OUT RESULTS OF REGRESSION $B \pm \sigma, F_p, Q, X$ FOR ALL $P$ STANDARDS IN SET $E$ AND ANALYSIS OF VARIANCE TABLE

COMPUTE AUTO-CORRELATION COEFFICIENT AND OUTPUT RESULTS

COMPUTE AND PRINT OUT FINAL STATISTICS FOR ALL STANDARDS ELIMINATED DURING REGRESSION

PRINT OUT RESIDUAL SPECTRUM AND FIND SUSPICIOUS CHANNELS

DO ANALYSIS OF RESIDUALS AND RUNS PRINT OUT RESULTS

STORE RESIDUAL SPECTRUM ON DISK IF DESIRED

END
Appendix C: MIDAS System Subroutines

1. ATIME
2. MTAPEF
3. CLOSEU
4. CONCAT
5. LUNDEF
ATIME (ASCII Date/Time) Subroutine

The ATIME subroutine is used to return the ASCII date and time to the FORTRAN user. This subroutine is written in assembler.

Form

CALL ATIME (string)

String is the name of the 24 byte string to receive the ASCII date/time. The returned string is 24 bytes in length in the following format:

```
dd-mmm-yyyy hh:mm:ss xx
```

where:

- **dd**: Day (number)
- **mmm**: First three letters of the month
- **yyyy**: Year (number)
- **hh**: Hour of the day (12 hours)
- **mm**: Minutes after the hour
- **ss**: Seconds after the minute
- **xx**: AM or PM

**NOTE:** If the parameter count is <1 or >1, then a return is made to MIDAS.

**Example**

```
LOGICAL*1 STRING(24)

CALL ATIME(STRING)
```

181
MTAPEF (FORMATTED MAGNETIC TAPE) SUBROUTINE

The MTAPEF subroutine controls the magnetic tape and its related functions. The subroutine is compatible with either 7 or 9 track magnetic tape. This subroutine is written in Assembler.

Form

CALL MTAPEF (a,b,c,d,e)

where:

a = Command: INTEGER*2 variable (required argument).
   = 1 - Initialize control formatter (a,b).
   = 2 - Transport off-line (a,b).
   = 3 - Rewind (a,b).
   = 4 - Search for logical EOT (a,b).
   = 5 - Search for file (a,b,c).
   = 6 - Search for record (a,b,c).
   = 7 - Read one record (a,b,c,d,e).
   = 8 - Verify one record (a,b,c,d,e).
   = 9 - Write one record (a,b,c,d).
   = 10 - Not used.
   = 11 - Overwrite one record (a,b,c,d).
   = 12 - Dump one record (a,b,c,d).
   = 13 - Write one filemark (a,b).
   = 14 - Write a logical EOT (a,b).
   = 15 - Open transport (a,b,c).
   = 16 - Close transport (a,b).
   = 17 - Tagword (a,b,c,d)

b = Error Number: INTEGER*2 variable (required).
   = 1 - No error.
   = 2 - Transport assigned to other/or no user.
   = 3 - Magnetic tape transport number error.
   = 4 - Segment is read only.
   = 5 - Segment is not accessible for I/O.
   = 6 - Memory is not contiguous.
   = 7 - Cross segments have different status.
   = 8 - No filemark detected for last operation.
   = 9 - Filemark detected during last operation.
   = 10 - Located on or past physical EOT.
   = 11 - Record read less than list word #14.
   = 12 - Record read greater than list word #14.
   = 13 - Invalid or undefined OP code.
   = 14 - Data late.
   = 15 - Invalid password.
   = 16 - Motion error.
   = 17 - Verification error.
   = 18 - Write protect error.
   = 19 - Parity CRC or LRC error during read.
   = 20 - Operation attempt on off-line transport.
   = 21 - No logical EOT detected during operation.
= 22 - Logical EOT detected during operation.
= 23 - Magnetic tape not off-line.
= 24 - Undefined error bit in status.
= 25 - Executive error during operation.
= 26 - Illegal number of arguments.
= 27 - Illegal command number.
= 28 - Record length greater than 513 bytes for 7 track transport.

c = Command Parameter 1: INTEGER*2 variable.

<table>
<thead>
<tr>
<th>Command Number</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td># files to skip</td>
</tr>
<tr>
<td>6</td>
<td># records to skip</td>
</tr>
<tr>
<td>7</td>
<td># bytes to skip</td>
</tr>
<tr>
<td>8</td>
<td># bytes to skip</td>
</tr>
<tr>
<td>9</td>
<td># bytes to write</td>
</tr>
<tr>
<td>11</td>
<td># bytes to write</td>
</tr>
<tr>
<td>12</td>
<td># bytes to write</td>
</tr>
<tr>
<td>15</td>
<td># transport to open</td>
</tr>
<tr>
<td>17</td>
<td>Subcommand code (c)</td>
</tr>
<tr>
<td></td>
<td>c = 1 - Get tagword</td>
</tr>
<tr>
<td></td>
<td>c = 2 - Increment tagword</td>
</tr>
<tr>
<td></td>
<td>c = 3 - Put tagword</td>
</tr>
</tbody>
</table>

d = Command Parameter 2: INTEGER*2 variable or array name.

<table>
<thead>
<tr>
<th>Command Number</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td># bytes to read</td>
</tr>
<tr>
<td>8</td>
<td># bytes to verify</td>
</tr>
<tr>
<td>9</td>
<td>Array name to write</td>
</tr>
<tr>
<td>11</td>
<td>Array name to write</td>
</tr>
<tr>
<td>12</td>
<td>Array name to write</td>
</tr>
<tr>
<td>17</td>
<td>Get, Increment, or Put tagword</td>
</tr>
</tbody>
</table>

e = Command parameter 3: Integer variable.

<table>
<thead>
<tr>
<th>Command Number</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>Array name to read</td>
</tr>
<tr>
<td>8</td>
<td>Array name to verify</td>
</tr>
</tbody>
</table>

The following is a test program for MTAPEF. The program does the following things:

1. Opens transport.
2. Initializes magnetic tape controller.
3. Reads from the disk and writes to the tape 4096 channels in groups of 128 channels.
4. Writes logical end of tape (of double filemark).
5. Rewinds tape.
6. Reads from tape and writes to disk 4096 channels in groups of 128 channels.
7. Rewinds tape.

C PROGRAM TO TEST MAG TAPE OPERATIONS
C USING FORTRAN EXTENSION LIBRARY SUBROUTINE
C
INTEGER ARRAY (513) A,B,C,D
DEFINE FILE 12(4096,2,U,IVAR)
C
OPEN FILE
C
A=15
C=1
CALL MTAPEF(A,B,C)
IF (B.NE.1) WRITE (6,110) B
C
INITIALIZE MAG TAPE
C
A=1
CALL MTAPEF(A,B)
IF (B.NE.1) WRITE (6,100) B
C
NOW READ THE DISK & WRITE TO MAG TAPE
C
A=9
C=513
IVAR=129
DO 200 I=1,16
DO 300 J=1,512,2
300 READ (12,IVAR) ARRAY(J), ARRAY(J+1)
CALL MTAPEF(A,B,C,ARRAY)
IF (B.NE.1) WRITE (6,120) B
200 CONTINUE
C
WRITE A DOUBLE FILEMARK
C
A=14
CALL MTAPEF(A,B)
IF (B.NE.1) WRITE (6,130) B
C
REWIND TAPE
C
A=3
CALL MTAPEF(A,B)
IF (B.NE.1) WRITE (6,140) B
NOW READ FROM TAPE & WRITE TO DISK

A=7
C=0
D=513
IVAR=129
DO 400 I=1,16
CALL MTAPEF(A,B,C,D,ARRAY)
IF(B.NE.1)WRITE(6,150)B
DO 500 J=1,512,2
500 READ(12'IVAR)ARRAY(J),ARRAY(J+1)
400 CONTINUE

C
REWIND TAPE

A=3
CALL MTAPEF(A,B)
IF(B.NE.1)WRITE(6,160)B

C
DO A CLOSE

A=16
CALL MTAPEF(A,B)
IF(B.NE.1)WRITE(6,170)B

100 FORMAT(' 'ERROR ',I3,' IN MAG TAPE INITIALIZE')
110 FORMAT(' 'ERROR ',I3,' IN MAG TAPE OPEN')
120 FORMAT(' 'ERROR ',I3,' IN MAG TAPE WRITE')
130 FORMAT(' 'ERROR ',I3,' IN SETTING FILE MARK')
140 FORMAT(' 'ERROR ',I3,' IN FIRST REWIND')
150 FORMAT(' 'ERROR ',I3,' IN MAG TAPE READ')
160 FORMAT(' 'ERROR ',I3,' IN SECOND MAG TAPE REWIND')
170 FORMAT(' 'ERROR ',I3,' ERROR IN MAG TAPE CLOSE')
END
CLOSEU (Close with Update) Subroutine

This subroutine closes a file with update and moves the current end sector to the current end of the file. This subroutine is written in assembler.

Form

CALL CLOSEU(lun)

where:

lun = Logical unit number associated with the file.
System Subroutines

CONCAT

The CONCAT subroutine is used to concatenate character strings.

Form: \[ \text{CALL CONCAT (a, b, out, len, err))} \]

Where:

- \(a\) is the array containing the left string.
- \(b\) is the array containing the right string.
- \(\text{out}\) is the array into which the concatenated result is placed. This array must be at least one element longer than the maximum length of the result string (i.e., one greater than the value of \(\text{len}\), if specified).
- \(\text{len}\) is the integer number of characters representing the maximum length of the output string. The effect of \(\text{len}\) is to truncate the output string to a given length, if necessary.
- \(\text{err}\) is the Logical error flag set if the output string is truncated to the length specified by \(\text{len}\).

The string in array "a" immediately followed on the right by the string in array "b" and a terminating null character replaces the string in array "out". Any combination of string arguments is allowed so long as "b" and "out" do not specify the same array. Concatenation stops either when a null character is detected in "b" or when the number of characters specified by "len" have been moved.

If whether the left or right string is a null string, the other string is copied to "out". If both are null strings, then "out" is set to a null string. The old contents of "out" are lost when this routine is called.
Errors:

Error conditions are indicated by "err", if specified. If "err" is given and the output string would have been longer than "len" characters, then "err" is set to .TRUE.; otherwise, "err" is unchanged.

Example:

The following example concatenates the string in array STR and the string in array IN and stores the resultant string in array OUT. OUT cannot be larger than 29 characters.

```
LOGICAL*1 IN(30), OUT(30), STR(7)
.
.
.
CALL CONCAT(STR, IN, OUT, 29)
```
LUNDEF  MOD 44-8437-02  25 AUG 77  L.HOLMES

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.TITLE LUNDEF
.CSECT LUND
.MCALL EXEC
.MCALL RESTORE,SAVE,.REGDEF
.GLOBL LUNDEF
.REGDEF
LUNDEF: SAVE R0,R1,R2,R3,R4,R5
TST (R5)+
MDV (R5)+,R2
EXEC CLIS,R2
BCC RET
MDV @1,(R5)
CLC
RET: RESTORE R5,R4,R3,R2,R1,R8
RTS PC
.END

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