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**GRPANL: a program for
fitting complex peak groupings
for gamma and x-ray
energies and intensities**

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January, 1980

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Manuscript date: January, 1980

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GRPANL: a program for fitting complex peak groupings for gamma and x-ray energies and intensities

ABSTRACT

GRPANL is a general-purpose peak-fitting program that calculates gamma-ray and x-ray energies and intensities from a given spectral region. The program requires that the user supply input information such as the first and last channels of the region, the channels to be used as pre- and post-region background, the system gain and zero-intercept, and a list of approximate energy values at which peaks occur in the region. Because the peak position and peak-shape parameters enter nonlinearly into the peak-fitting algorithm, an iterative least-square procedure is used in the fitting process. The program iterates until either all convergence criteria are met or ten iterations have elapsed.

The code described here allows for twenty free parameters and a region as large as 240 data channels. This code runs on an LSI-11 computer with 32K memory and disk-storage capability.

INTRODUCTION

The program called GRPANL (GRouP ANaLysis) first developed in 1974, has evolved as an interactive program for use on minicomputers to analyze peak groupings of gamma and x rays in spectra taken with germanium detectors. Its purpose is to calculate peak positions, or energies, and peak intensities while allowing the operator control with respect to the initial parameters for analysis of the peak grouping. Recently, the program has been adapted by others to perform automatic, though prescribed, analyses of spectra.^{1,2}

We describe here the algorithm used by GRPANL and provide a Fortran listing of the source code. Although the program was originally written for use on a PDP-8 computer, the version given in the Appendix of this report operates on a PDP-11 under Digital Equipment Corporation's RT-11-V03 operating system. GRPANL, with its subprograms ULOAD2, ULFIT2, and ULOUT2,

is capable of analyzing a peak grouping spanning a region of up to 240 channels and allows up to 20 parameters to be freed, i.e. degrees of freedom allowed with respect to any combination of peak heights, positions, and peak shape parameters. The operator may tie any peak position or intensity to that of another designated peak within a region. X-rays, whose shapes differ from gamma rays, can also be fitted. The peak energies are determined either by specifying the exact gain and zero-intercept, or by allowing calculation of the energy scaling, using specified internal reference peaks. For exact energy determinations, the program accounts for system nonlinearity. Finally, GRPANL can calculate gamma emission rates from peak areas by means of efficiency algorithms, which are based on the same model used by the generalized computer program GAMANAL,^{3,4} which is a comprehensive program that not only reduces but interprets data.

FITTING TECHNIQUE AND MODEL

Accurate determination of peak positions and areas is one of the most important aspects of analyzing complex x- and gamma-ray spectra obtained with solid-state detectors. These measurements usually require a fitting procedure, particularly when two or more peaks overlap severely. Several methods of fitting have been developed.⁴⁻⁷ Each fitting technique is based on a supporting model or methodology. The methodology frequently grows out of such factors as experience, intended use of the analysis program, size and speed of the computer used, and accuracy that is required. In this section, we will discuss the methodology used in the GRPANL program.

PEAK SHAPE ALGORITHM

The most easily detected and intense portion of a gamma-ray peak may be described by a Gaussian function, as illustrated in Fig. 1. However, deviations from the Gaussian distribution known as tailing occur on the low-energy and occasionally on the high-energy side of a peak. The low-side tailing is a result of incomplete charge collection in the detector, though low-angle scattering in the sample source or in surrounding materials can also contribute to low-side tailing. Tailing on the high-energy side arises from signal distortion by the pulse electronics modules. This latter effect should be eliminated or reduced as much as possible.

The tailing portion of a peak can generally be described by means of one or more terms of exponential form. Some computer programs divide each peak into regions and apply a separate fitting function to each region.⁵ The boundary conditions are chosen so that the calculated response and, in most cases its first derivative, form a smooth curve. The analytical expression for the shape function used by GRPANL is adapted from the work of Sanders and Holmes⁸ and treats the entire peak region with a single expression:

$$y_i = y_0 [\exp \alpha (x_i - x_0)^2 + T(x)] \quad (1)$$

where

y_i = net counts in channel x_i for a single peak

y_0 = peak height

$\alpha = -1/2 \sigma^2 = -2.7726/(\text{FWHM})^2$, where FWHM is the variable containing the peak-width

x_0 = peak position

$T(x)$ = tailing function.

The tailing function is given by

$$T(x) = [A \cdot \exp B(x_i - x_0) + C \cdot \exp D(x_i - x_0)] \times [1 - \exp 0.4\alpha(x_i - x_0)^2]^\delta \quad (2)$$

where

A and C = the short- and long-term tailing amplitudes, as illustrated in Fig. 1.

B and D = the tailing slopes

and $\delta = 1$ for $x_i < x_0$; $\delta = 0$ for $x_i > x_0$.

The expression in the right-hand bracket of the tailing function smoothly reduces the tailing intensity to zero as the peak centroid is approached. The long-term tailing component is disregarded (i.e., $C = 0$) for many applications. However, inclusion of this component is desirable in order to obtain a more accurate fit of a large-peak multiplet having good counting statistics.

The peak-shape parameters in the above expression are y_0 , x_0 , α , A, B, and occasionally C and D. Peak positions and heights are generally the measurements of interest, and therefore x_0 and y_0 are the principal parameters in the fitting process. The other parameters may be treated as fixed or as free parameters, depending on whether they have been predetermined by calibration. We have found that the values of α , A, and B can be expressed by simple equations involving the gamma-ray energy.

For example, the peak width σ_T can be expressed as a function of the gamma-ray energy E by

$$\sigma_T^2 = \sigma_n^2 + \sigma_s^2 = k_1 + k_2 E \quad (3)$$

where σ_n is related to the system "noise," and σ_s is a term related to the statistical nature of the charge collection process. Hence, the measured width of

FIG. 1. The principal component of the peak distribution is described by a Gaussian function. The low-side tailing can be described by two additional functions.

two isolated peaks, preferably a low- and a high-energy peak, can be used to determine the values for coefficients k_1 and k_2 . The above expression can subsequently be used to calculate the width parameter for a peak of any other energy.

By experience we have found that the tailing slope B can generally be treated as a constant for a given detector system. For an accurate determination of B , a high-energy peak where the tailing is most severe should be used. The peak should be caused by a single gamma ray and have good counting statistics. Once B is determined and held constant, the tailing amplitude A can then be expressed by:

$$\ln A = k_3 + k_4 E \quad (4)$$

The same two peaks that were used to determine the values for k_1 and k_2 determine k_3 and k_4 .

There are now five basic peak-shape constants: k_1 , k_2 , k_3 , k_4 , and B , plus the two long-term tailing constants, C and D , required only in special cases. GRPANL allows entry of the name of a disk file of peak-shape constants. The operator may still control whether the parameters calculated using these shape constants will be fixed in the fitting process or whether they will only be used as a starting estimate toward improving its value. If a disk file containing shape constants is not constructed the operator must provide initial estimates of the parameters, that is, estimates for the peak width (FWHM), the tailing amplitude A and the tailing slope B .

The peak shapes of x rays differ from those of gamma rays of the same energies because atomic transitions have much shorter lifetimes than nuclear transitions. This difference becomes more pronounced with increasing energy. The intrinsic radiative width of heavy-element x rays at 100 keV is about 100 eV, whereas gamma-ray widths are typically a small fraction of an electron volt. Furthermore, the intrinsic distribution is Lorentzian in shape. When the broadened x-ray distribution is convoluted with the nearly Gaussian instrumental response, the result is a more complex peak shape than that produced by gamma rays.

The modification to the peak shape algorithm necessary to fit an x-ray distribution, illustrated in Fig. 2, is discussed in an earlier report.⁹ GRPANL uses this modified algorithm.

DELINEATION OF BACKGROUND

The peaks of any x- or gamma-ray spectrum lie on top of a background distribution resulting from the Compton scattering process. In GRPANL, this distribution must be removed before the peaks can be fitted. This is done by specifying regions on either side of the peak grouping that establish corresponding background levels. The operator may also specify the slopes of the background continuum preceding and following the peak grouping if a peak grouping rests on a sloping background.

An explicit function⁴ calculates the interpolated background values under the peak grouping. This function has the following form:

$$B_i = b_n + (b_m - b_n) \left(\frac{\sum_{j=i}^{j=n} y_j}{\sum_{k=m}^{k=n} y_k} \right) \quad (5)$$

where

- B_i = computed background at channel i ,
- y_i = spectrum count of channel i ,
- b_n = average background level of the low-energy side of the peak,
- b_m = average background level of the high-energy side of the peak.

This function produces smoothed steps in the background that occur at positions of greatest intensity. This procedure works equally well for single peaks and for complex peak groupings, an example of which is shown in Fig. 3. An examination of Eq. (5) shows that it is essentially equivalent to the error-function form⁶ for describing the background continuum. However, the function in Eq. (5) is used to remove the background before the fitting process commences, whereas the error-function method includes it in the fitting process. The latter method therefore requires more fitting parameters and greater calculational time.

If a background continuum slope has been specified, the steps in the background are superimposed on the specified slope, and the size of the steps is increased or decreased depending on the sign and steepness of the slope. If the two input

FIG. 2. The intrinsic x-ray energy distribution is Lorentzian in shape. This distribution convolutes with the instrumental line shape resulting in a modified peak shape.

FIG. 3. The background continuum for a complex multiplet as shown here may be accurately calculated by the explicit function given in Eq. (5).

slopes are different, the background continuum makes a gradual change from the one to the other.

The selection of the group boundary position is usually a matter of judgement, and it is frequently difficult to determine or define where a peak should start or end. This is particularly true if one is to include long-term tailing and/or x rays in the fitting process, since these distributions extend to considerable distances from the peak, as previously illustrated in Figs. 1 and 2.

Regardless of where the boundaries are chosen, the regions selected for measuring the average background levels usually contain small contributions from the peaks. GRPANL handles this problem by adjusting the measured levels according to the current value of the contribution of the peaks to the two background regions. The adjustment is refined after each iteration of the least-squares fitting process.

Although long-term tailing may be included in the fitting process, GRPANL does not include the area beneath the long-term tailing as part of the reported peak area. However, the area under the short-term tail is included. From experience, we recommend that a short-term tailing slope of $B = 1$ be used to distinguish the two forms of tailing. The

short-term tailing slope should usually have a value between 1.0 and 5.0. The tailing amplitude varies according to the slope value with high amplitude occurring with higher slope values. It also varies according to the magnitude of peak tailing with low energy peaks of good detectors exhibiting rather low values (0.01-0.1) and higher energy peaks exhibiting tailing amplitude values greater than 1.0.

FITTING PROCESS

Following the removal of the background continuum, the net counts in each channel of a peak multiplet are considered as a set of data values Y_i that have been measured with respect to an independent variable x_i and to which several overlapping single peaks may be contributing according to the expression

$$Y_i = \sum_{j=1}^n y_{ji} \quad (6)$$

where n is the number of peaks in the grouping.

We now must find a function which, when evaluated point by point, most closely approximates the original data values (Y_i). This evaluation is done by minimizing chi square (χ^2). However, because the equations describing the peak shape are not of a linear form, an iterative procedure is used to arrive at a solution to the fit. The method used in GRPANL is a non-linear least-squares technique based on linearizing the equations by performing a first-order, Taylor's series expansion about the trial values of the free parameters. This procedure is also known as the Gauss-Seidel or Newton-Raphson method. From Eqs. (1) and (2), we see that y_j is related to several peak parameters which we here designate simply as p_k .

That is,

$$y_{ij} = f(p_1, p_2, \dots, p_k) \quad (7)$$

By retaining only the first term of the Taylor's expansion of this equation, we derive

$$y_{ij} - f(p_1^0, p_2^0, \dots, p_k^0) = \sum_{k=1}^n \left(\frac{\partial f}{\partial p_k} \right) \delta p_k \quad (8)$$

where

- y_{ij} = the contribution of the j -th peak to channel i
- p_k^0 = current best estimate in the k -th peak parameter
- Δp_k = the change required in the current best estimate of the k -th parameter to obtain a better fit to the data.

The current "free" parameter values are updated following each iteration, and the process is continued until the current change in each parameter is less than the prescribed amount.

The rate of convergence depends upon a number of factors. Among these are the complexity of the grouping, the number of free parameters, the convergence criteria, and the accuracy of the initial parameter estimates. In addition to slow convergence, poor parameter estimates may also lead to an ill-conditioned matrix or a fitting sequence that does not converge. GRPANL precludes or rectifies these conditions by including boundary constraints, damping or limiting the estimated changes in the free parameters and limiting the allowable number of iterations to 10.

Convergence is determined by comparing the magnitude of the last changes made in each of the parameters being determined with internally specified convergence criteria. Each convergence criterion value is calculated using an equation that contains a fixed and a variable component, the latter being related to the error associated with the parameter being determined. The use of the error component allows early convergence because the specification arising only from the fixed component would be needlessly tight when applied to statistically poor data.

Once convergence has been attained, final calculations are made for peak energies, intensities, and the respective errors. The latter are based on counting statistics and on the goodness-of-fit (the variable QFIT)* and are normally calculated using the formula

$$\text{ERROR}(j) = (\text{DM}(j) * \text{QFIT})^{1/2} \quad (9)$$

where

$\text{DM}(j)$ = diagonal error matrix element of parameter j

and

$$\text{QFIT} = \left(\sum_{i=1}^n R_i^2 \right) / \text{DOF} \quad (10)$$

R_i = the weighted residuals of the fit

and

DOF = degrees of freedom.

With this method, a poor fit in one region affects all the calculated errors, whereas intuitively we know that this is not necessarily true. We have therefore modified Eq. (10) so that a "localized" goodness-of-fit is calculated and applied to each peak in the multiplet. In the new expression, each R_k^2 value is appropriately weighted according to its proximity to the peak in question.

Thus

$$\text{QFIT}(j) = \frac{\sum_{i=1}^n R_i^2 [\exp(\alpha \cdot \Delta x_i^2)]^{1/2}}{\sum_{i=1}^n [\exp(\alpha \cdot \Delta x_i^2)]^{1/2}} \quad (11)$$

where

- α = peak width parameter
- Δx_i = distance from peak position.

*In this report, computer variable names of one or more letters are used to signify single-function variables.

GAMMA INTENSITY CALCULATIONS

GRPANL also calculates gamma emission rates from the determined peak areas. The instructions are based on the same efficiency model that is used in the GAMANAL program.^{3,10} A basic premise of the model is that the overall efficiency can be treated as the product of two components: the intrinsic efficiency of the detector, defined in Eq. (12), and the source-detector geometry. The latter is calculated after determining two hypothetical points in space, one at which the detector is said to reside and another at which all of the sample is said to be concentrated. To determine the efficiency for a particular source-detector geometry, the rule of physics is invoked; that the detection efficiency is inversely proportional to the square of the source-to-detector distance. The fundamental equation used by the model is

$$\epsilon_E \equiv \frac{C_E}{\gamma_E} \cdot d^2 \quad (12)$$

where

ϵ_E = counting efficiency for gamma ray of energy E, normalized to 1cm

C_E = net counts per unit time in peak

γ_E = source emission rate of gamma energy E

d = source-to-detector distance.

Once a calibration curve (ϵ as a function of E) has been determined, the equation can be transposed to yield photon emission rates, γ_E , for sources of unknown intensity.

A typical configuration for a cylindrical detector and a point source is shown in Fig. 4. To use Eq. (12), the parameter d must be assessed by using measured or calculated values shown in Fig. 4 for:

x = distance from source to detector window

w = distance from window to active detector surface

p = effective penetration of gamma ray into detector

r = effective interaction radius in the detector

r_0 = limiting value of r at low energy

d = distance from source to effective zone of interaction

T = detector thickness

R = detector radius.

FIG. 4. A point source and a cylindrical detector used to model the effects of geometry on photopeak counting efficiency. Distances shown are defined in the section, *Gamma Intensity Calculations*.

From simple geometry we have

$$d^2 = (x + w + p)^2 + r^2 \quad (13)$$

Of these, x is the only easily measured parameter. The others must be empirically determined, as discussed in Ref. 10. Our experience indicates that the geometry contribution to the counting efficiency for point sources can be calculated to within $\pm 1-2\%$ of the correct values for all energies and all usable source-to-detector distances.

The intrinsic detection efficiencies as defined in Eq. (12) are determined by counting absolute standards at relatively large distances and normalizing these efficiencies to a 1-cm distance. These values may be described by a fifth- or sixth-order polynomial equation of the form

$$\ln \epsilon_i = \sum_{j=1}^n a_j (\ln E_i)^{(j-1)} \quad (14)$$

where

- ϵ_i = efficiency at the i th energy
- E_i = gamma energy
- a_j = coefficients of the polynomial.

We have found that a single function cannot adequately describe the full range of energies of interest, 0.05–4.0 MeV. Thus, we use two polynomial equations that overlap in the 100–200 keV energy region. After the data are fitted by a least-squares analysis, the resulting curves are examined in the region of overlap, and a crossover energy is chosen that gives the same efficiency by either equation. In this way, the efficiency polynomial can be fitted to the calibration to within ± 1 –2%.

Many sources are not point sources. The model also contains formulae to account for the perturbations such as by source extension in two or three dimensions, gamma ray attenuation by the matrix of a volume sample, and by absorbers between the source and the detector. These corrections are also discussed in Ref. 10.

For many prospective users of GRPANL, the inclusion and use of the efficiency model may perhaps be ancillary to the principal purpose of the program, which is to obtain peak positions (energies) and areas. We will therefore not further describe in this report details on the use of the model.

GRPANL OPERATION: AN OVERVIEW

GRPANL is written in FORTRAN IV for use on PDP-11 systems operating with Digital Equipment Corporation's RT-11 V03 or RSTS/E V06B. Because of its size, the program is broken up into GRPANL and three subprograms: ULOAD2, ULFIT2, and ULOUT2. GRPANL begins the execution, and control to the other programs is transferred directly by the subroutine CHAIN, found in the above-named system's subroutine library. The size of common blocks GNL and PASS prevents them from being transferred automatically by the CHAIN subroutine. The transfer is accomplished by each subprogram which writes the contents of the common blocks into the files GNL.DAT and PASS.DAT on the system device before calling CHAIN. After transfer to the next subprogram is completed, the subprogram reads back into core the respective common blocks. The user must make available at least 24 blocks of contiguous disk space on the system device before starting GRPANL for this operation to succeed.

The input data for the program is contained in two disk files: the peak-shape parameter file and the spectral data file. The peak-shape parameter file contains the five basic peak-shape constants, k_1 , k_2 , k_3 , k_4 and B , and the two long-term tailing constants, C and D , which are necessary only in special cases. These constants may be calculated for a detector system by the program PKSHAP, listed in the Appendix. Input to PKSHAP requires the measured widths and tail amplitudes of two isolated peaks in a spectrum taken with the detector system. GRPANL may be used to initially determine these parameters. If a peak-shape parameter file does not exist, GRPANL requests the operator to provide initial estimates of the peak width (stored in variable FWHM), tailing amplitude (EXP1), and tailing slope (EXP2). The new values obtained by GRPANL are then used as input to PKSHAP, provided the value of QFIT, as defined in Eq. (10) is reasonable.

The user enters the shape constant results printed out by PKSHAP into a peak-shape parameter file, a file created and edited by the program FILES, which is also listed in the Appendix. FILES is a general-purpose program for preparing or editing unformatted sequential files. With FILES, the user enters the five shape constants sequentially into the first five locations of the

peak-shape parameter file. If the user wishes to use long-term tailing in the fitting process, then the two long-term tailing constants should be entered into locations 7 and 8 of the file. If a correction for system nonlinearity is to be made, the appropriate coefficients are entered into locations 11 through 15. These coefficients are determined by least-squares fitting a power-series polynomial to data where the dependent variable is energy, and the independent variable is the corresponding channel location. The user enters in location 11-15 the coefficients beyond first-order divided by the first-order coefficient, i.e., gain.

The spectral data file contains the pulse-height data which is stored in standard PDP-11 floating-point notation, two words per channel count. The ULOUT2 program, which uses the peak areas to calculate gamma emission rates, requires the livetime (seconds) for the count in the first location of the data file. The second location in this file stores the time of the count, in decimal days. This is for informational purposes only, and it is not necessary for the operation of the code. The spectral data for the region indicated to the GRPANL code is read into core by the subroutine RDSK, which is also listed in the Appendix.

GRPANL reads in the input parameters from the terminal and from the detector parameter disk file, if any. From this information the subprogram calculates the initial values for the peak-shape parameters and sets all the appropriate flags that indicate fixed or free parameters. Program control is transferred next to ULOAD2, which loads the spectral data for the region being fit. The subprogram ULOAD2 determines the net channel data by removing the background calculated by the subroutine BKGRD. From the net data, ULOAD2 determines the initial values for the peak positions and heights. After ULOAD2, ULFIT2 performs an iterative fit to the data. After each iteration, the program prints on the terminal the current peak positions and heights. The current values for the peak shape parameters are also printed if a complete output was initially requested by the user. The program continues its iteration until the current indicated change in each free parameter is less than a prescribed amount, or until 10 iterations have occurred.

When the fitting process is completed, program control is transferred to ULOUT2. The function of the subprogram ULOUT2 is to calculate the peak energies, peak areas, errors on the peak areas, and the value of the reduced chi-square. The program prints this information along with the input information given by the user and the values determined for the peak-shape parameters with their associated errors. If the user chose the option of a complete printout, ULOUT2 lists, channel by channel, the net counts to which the fit was made, the residuals (difference between net count and calculated count), and the standard deviation, as illustrated in Fig. 5, an abbreviated listing of the output.

The ULOUT2 subprogram can also calculate gamma emission rates from the determined peak areas. In the ULOUT2 listing in the Appendix, the FORTRAN statements necessary for this calculation are shown as comment statements. If ULOUT2 is used, a third disk file of detector-parameter data

is required. This file is also created using the formatting program FILES. Sixteen entries are needed for the detector-parameter file:

- (1-6) The high-energy portion of the detector's intrinsic efficiency curve.
- (7-11) The low-energy portion of the detector's intrinsic efficiency curve.
- (12) The crossover energy for the above two polynomial equations describing the efficiency vs energy curve for the detector.
- (13) The detector depth (cm).
- (14) The detector radius (cm).
- (15) Surface distance, window to detector (cm).
- (16) Germanium dead layer on the front surface of the detectors (g/cm^2).

These sixteen values are read into the array DCNST.

FILE NAME IAEAP1

PARAMETER FILE

LIVE TIME 4300.0 SECONDS

START DAY 0.000

KEV/CHANNEL 0.110457

GROUP STARTS AT CHANNEL 463
 GROUP ENDS AT CHANNEL 530
 BACKGROUND LOW ENERGY 5
 BACKGROUND HIGH ENERGY 5
 ZERO 107.6716

REFERENCE PK #1 ENERGY = 129.294

REFERENCE PK #2 ENERGY = 208.000

PARAMETER TABLE FREE
 ALPHA YES
 SHORT TAIL AMPLITUDE YES
 SHORT TAIL SLOPE NO

LONG TERM TAIL AMPLITUDE NO
 LONG TERM TAIL SLOPE NO

LOW ENERGY REGION BACKGROUND SLOPE 0.0000
 HIGH ENERGY REGION BACKGROUND SLOPE 0.0000

PEAK NUMBER	ENERGY KEV	WIDTH EV	UNCERTAIN ENERGY	FIXED TO	UNCERTAIN INTENSITY	RATIOED TO	RATIO
1	159.955	0.00	NO	5	YES	0	0.00000
2	160.190	0.00	NO	4	NO	4	-0.05170
3	160.280	0.00	YES	0	YES	0	0.00000
4	161.450	0.00	YES	0	YES	0	0.00000
5	164.580	0.00	YES	0	YES	0	0.00000
6	165.930	0.00	YES	0	YES	0	0.00000

ANALYSIS RESULTS

GFIT 1.0 FWHM 0.95927+-0.0011 KEV/CHANNEL 0.110457
 EXP1 0.18617+-0.0701 EXP2 1.99897+-0.0000
 EXP3 0.00000+-0.0000 EXP4 0.00000+-0.0000

CHANNEL	ENERGY	COUNTS	GAMMAS/MIN	PCTERR
1	473.341	159.955	4537. 0.0000E+00	6.6
2	475.753	160.222	42. 0.0000E+00	0.0
3	477.598	160.426	2553. 0.0000E+00	4.3
4	487.160	161.482	826. 0.0000E+00	12.7
5	515.212	164.580	28900. 0.0000E+00	1.0
6	524.431	165.599	289. 0.0000E+00	47.8

CHANNEL	ENERGY	INDEX	YNET	RESIDUALS	STD DEV
463	158.81	1	10.29	-8.28	-0.27
464	158.92	2	89.26	59.31	1.85
465	159.03	3	121.23	72.03	2.21
466	159.14	4	130.21	50.30	1.54
467	159.25	5	151.18	25.66	0.78
468	159.37	6	162.15	-25.90	-0.78
469	159.48	7	234.10	-32.44	-0.95

FIG. 5. Full output from GRPANL run.

EXECUTION

To begin execution of GRPANL, the user must have a file of spectral data on disk. An optional file of peak-shape parameters, and/or a detector parameter file may also be constructed prior to execution. A carriage return must follow all input messages. File names have a maximum of six characters, which may be preceded by the device name and a colon if they do not reside on the default device, e.g. *device:file*.

User: R GRPANL

Routine: COMPLETE PRINTOUT?

User: Y selects for inclusion in the output the position, net area, and error for each peak in the fit, and lists the net counts, calculated fit, residual (the difference between the net count and the calculated count), and standard deviation for each channel in the region of interest. An abbreviated sample of the output is shown in Fig. 5.

N deletes channel by channel results from the report.

Routine: SPECTRUM ID IS

User: *device:file*

specifies the file name of the spectral data file.

Routine: GROUP STARTS AT

User: *nnnn* specifies the first channel in the region of interest, for use by subroutine RDSK in filling array Y from spectral data.

Routine: GROUP ENDS AT

User: *nnnn* specifies the last channel in the region of interest. The number of channels between the starting and ending points may not exceed 240.

Routine: # OF BKG. CHANNELS IN FRONT OF GROUP

User: *nnnn* specifies the number of channels preceding the starting channel to be used to calculate the background level on the low-energy side of the region.

Routine: # OF BKG. CHANNELS IN BACK OF GROUP

User: *nnnn* specifies the number of channels following the ending channel to be used in calculating the background level on the high-energy side of the region.

Routine: GAIN (NEG. VALUE FOR ABSOLUTE)
IF = 0, PEAK AREA SIMPLY INTEGRATED

User: *xx.xxxxxx*

(positive value) specifies the "approximate" gain used in locating reference peaks to determine the gain and zero for the spectrum. The energies of two well-defined peaks in

the spectrum are then requested. The two peaks become calibration points for a two-point determination of the gain and zero. If zero is entered for peak No. 1 (PK #1), GRPANL assumes zero energy at channel zero.

0 terminates only the total net counts in the region. A zero entry signifies that a fit to the peaks in the designated region is not desired.

-xx.xxxxxx

(negative value) specifies "absolute gain," i.e., no internal peaks are used for energy reference, and the final energy values are based on this gain.

Routine: ENERGY OF ZERO CHANNEL

User: xxx.xxxx

specifies the energy of channel zero, information useful for those spectra which have a large zero offset.

Routine: LIST PK ENERGIES IN THIS GROUP (NEG. VALUE FOR X-RAYS)
TERMINATE WITH A ZERO

User: xxxxx.xxxx

specifies the energy for a peak in the region. Additional peak energies may be entered, each followed by a carriage return. Terminate the list of energies with a zero entry.

-xxxxx.xxxx

(negative value) signifies that the peak is an x ray. For negative values, the intrinsic width of the x-ray line of the form xxx.x is then entered after the prompt.

INTRINSIC WIDTH (EV)
IF ENTRY = 0, AN INTERNALLY ESTIMATED VALUE USED

The values to be entered are listed in Ref. 11. If zero is entered, an internal algorithm calculates an approximate width.

0 terminates the entry of peak energies.

Routine: PEAKS ENTERED FOR THIS REGION

(displays the number of peaks entered)

TYPE SEQUENCE # OF PEAKS WHOSE ENERGY ARE UNCERTAIN
TYPE 99 FOR ALL—
NEG. FOR FIXED RELATIONSHIP. END WITH 0.

User: 99 designates all peaks in the list as free in the fitting process.

nnn (sequence number) designates the centroid position of the peak as variable in the fitting process. Those not designated in this step are fixed in position to the channel corresponding to the energy of the peak entered, by the formula

$$\text{peak position} = (\text{peak energy} - \text{zero channel energy}) / \text{gain}$$

-nnn (negative sequence number) fixes the peak energy relative to another peak in the region. The sequence number of this other peak in the form nnn is entered in response to the prompt.

ENERGY FIXED RELATIVE TO PEAK #:

The centroid of the current peak is then varied as the centroid of the peak to which it has been fixed. This option is used for splitting close multiplets or for locating weak peaks.

^ terminates the entry of sequence numbers of peaks of uncertain energy.

Routine: SEQUENCE # OF PEAK WHOSE INTENSITY IS KNOWN

User: nnn (sequence number) indicates that the intensity of this peak is known. A zero entry indicates that all are unknown. The peak height is entered after the prompt.

PEAK HEIGHT (NEG. FOR RATIO) =

xxxxxxx.xxx

designates the peak height for the sequence-numbered peak named above.

-xxxxxxx.xxx

(negative entry) specifies that the peak height is to be ratioed to another peak in the region, a procedure useful when both peaks are from the same isotope and their branching ratios are well known. The absolute value of this entry is the ratio of the current peak height to the height of the reference peak.

Enter the sequence number of the reference peak in the form nnn following the prompt RATIOED TO PEAK #: .

Routine: IS THERE A PARAMETER FILE?

User: Y reads in a file of peak-shape parameters available on disk. Enter the file name in the form *device:file* after the prompt FILE NAME?

After the file name is entered, the routine asks

DO YOU WANT TO FREE ANY SHAPE PARAMETERS?

Y presents each shape parameter for a further Y or N decision.

- Y frees this shape parameter. The maximum number of free parameters, including peak positions and heights, that are allowed for fitting each peak grouping is 20.
- N fixes the parameter to the value determined from the parameter file, in accordance with Eqs. (3) and (4), above.
- N indicates there is no parameter file. If there is none, enter a value for each peak-shape parameter, as listed below. For each, a response to the prompt TO BE FREED? is required.
- Y frees the parameter.
- N fixes the parameter to the value entered.

The peak-shape parameters that can be freed for the entire peak grouping are:

FWHM (IN KEV)
 SHORT-TERM TAIL AMPLITUDE
 SHORT-TERM TAILING SLOPE
 LONG-TERM TAIL AMPLITUDE
 LONG-TERM TAIL SLOPE

The height and the position may be freed for each peak in the multiplet. A 20-peak multiplet may be fit if peak height is the only free parameter. A seven-peak multiplet can be fit if all parameters are free.

Routine: LOW ENERGY BKGRD SLOPE EXPRESSED IN %/CHAN =

User: x.xxx specifies the value for the slope before the region of interest, expressed as % change in counts per channel relative to the average counts per channel in the region. This option is useful for peaks which lie in a region where the Compton continuum is not flat, but has a nonzero slope.

Routine: HIGH ENERGY BKGRD SLOPE EXPRESSED IN %/CHAN =

User: x.xxx specifies a similar value for the slope following the region of interest.

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5. J. J. Routti and S. G. Prussin, "Photopeak Method for the Computer Analysis of Gamma-Ray Spectra from Semiconductor Detectors," *Nucl. Inst. and Methods* **72**, 125 (1969).
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9. R. Gunnink, "An Algorithm for Fitting Lorentzian-Broadened K-Series X-Ray Peaks of the Heavy Elements," *Nucl. Inst. and Methods* **143**, 145 (1977).
10. R. Gunnink and J. B. Niday, in: *ERDA Symposium on X- and Gamma-Ray Sources and Applications* (U. S. Energy Research and Development Administration, CONF-760539, Washington, D.C., GPO, 1976) p. 55.
11. S. I. Salom and P. L. Lee, "Experimental Widths of K and L X-Ray Lines," *Atomic Data and Nuclear Data Tables* **18**(3) 233 (1976).

APPENDIX: SOURCE LISTINGS

GRPANL
ULOAD2
ULFIT2
ULOUT2
FILES
PKSHAP

Subroutines:

RDSK
YESNO
MAXVAL
MINVAL
NCNTS
NCTS
AVE
BKGRD
GFIT
BWF
MLR
MLRA
MLRE
GPM
CALMU
CALGPM

```

C      PROGRAM GRPANL
C      LINK WITH RISK,YESNO,AVE,MAXVAL,GFIT,NCNTS,NCTS
C
C      THIS PROGRAM IS A GENERAL PURPOSE PROGRAM FOR FITTING
C      MULTIPLETS (GAMMA-RAYS AND X-RAYS).
C      IT WILL ACCOMMODATE UP TO 20 FREE PARAMETERS. THE PEAK
C      HEIGHTS (AREAS) ARE AUTOMATICALLY FREED. THE OTHERS
C      CAN BE SELECTED. UP TO 240 DATA POINTS ARE ALLOWED.
C
C      THIS PROGRAM READS IN GRPANL PARAMETERS
C      FROM TTY TERMINAL
C
0001      INTEGER*2 ULOAD2(4)
0002      LOGICAL YESNO
0003      DIMENSION AMATRX(5888),BMATRX(256)
0004      COMMON/GNL/NUMS,NUME,NDF1S,NF,NWRIS(6),NFLG(20),NYFLG(20),
1      NXFLG(20),FNAME(3),SP(2),GAIN,ZERO,START,ALPHA,FWHM,ATAIL,
2      BTAIL,EXP3,EXP4,STD(2),C1,C2,AVERG,SLF(2),EN(20),SHAPC(10),
3      CLINC5,HIGHT(20),GAMA(20),Y(240),DUM(4500)
0005      COMMON/PASS/ENJ(20),IST,IEND,NUMSJ,NUMEJ,GAINJ,ZEROJ,ST1J,
1      ST2J,STRJ(20),NENUM,ALPJ,STAMP,STSLF,TLAMP,TLSLF,BKGSPLF(2),
2      CFILE(3),SSS,YES,BK1,NGAIN,IREGG,LISTFG,PAME(3)
C
0006      EQUIVALENCE (NUMS,AMATRX(1)),(ENJ(1),BMATRX(1))
C      LISTFG = LISTING FLAG = 0 COMPLETE PRINTOUT
C      OF CALCULATIONS
C      = 1 SHORT PRINTOUT
C      THE FOLLOWING STATEMENT PROVIDES FOR CHAINING TO THE PROGRAM
C      ULOAD2 ON LOGICAL DEVICE RK3. IT MUST BE CHANGED ACCORDINGLY
C      IF THE PROGRAM RESIDES ELSEWHERE.
C
0007      DATA ULOAD2/3RRK3,3RUL0,3RAD2,3RSAY/
C
0008      LISTFG = 1
0009      IALGTH = 5888
0010      IBLGTH = 256
0011      TYPE 99
0012      99  FORMAT(' COMPLETE PRINTOUT? ',%)
0013      IF(YESNO())LISTFG = 0
0015      1   TYPE 100
0016      100 FORMAT(' SPECTRUM ID IS ',%)
0017      ACCEPT 101,FNAME
0018      101 FORMAT(3A4)
0019      TYPE 102
0020      102 FORMAT(' GROUP STARTS AT ',%)
0021      ACCEPT 106,IST
0022      TYPE 104
0023      104 FORMAT(' GROUP ENDS AT ',%)
0024      ACCEPT 106,IEND
0025      TYPE 105
0026      105 FORMAT(' # OF BKG. CHANNELS IN FRONT OF GROUP = ',%)
0027      ACCEPT 106,NUMS
0028      NUMSJ = NUMS
0029      106 FORMAT(I4)
0030      SUM(J) = 0.
0031      AMP1 = EXP1
0032      AMP2 = EXP3
0033      GAMMA = 0.
0034      XI = PKPOS(J)
0035      DO 300 L = 1,2
0036      CC = CX * XI
0037      IF(GAMA(J))201,201,100
0038      100 CALL BWFC(C)
0039      201 BG(L)=BG(L)+PKHT(J)*( .6366*GAMA(J)*CX*CC+AMP1*EXP(-EXP2*XI)
1      +AMP2*EXP(-EXP4*XI))

```

```

0040      AMP1 = 0.
0041      AMP2 = 0.
0042      XI = XPTS - PKPOS(J)
0043 300    CONTINUE
0044 400    CONTINUE
0045      YP = 0.
0046      BRG = BG(2) - BG(1)
0047      CALL AVE(1,NDPTS,YSUM,AV,YNET)
      C      ZERO COEFFICIENT ARRAY
0048      DO 2 J=1,20
0049      DO 2 I=1,NDPTS
0050 2      ACOEF(I,J)=0.
      C      FORM MATRIX OF LINEAR EQUATIONS
0051      DO 30 I = 1,NDPTS
0052      XI = I
0053      FX = 0.0
0054      FXY=0.0
0055      DALFA = 0.0
0056      DBETA = 0.0
0057      DGAMA = 0.0
0058      DBELT = 0.0
0059      DCHI = 0.0
      C      DETERMINE WEIGHTING FACTOR
0060      WT = 1.0 / SQRT (YNET(I) + AVERG)
0061      K = KK
      C      CALCULATE COEFFICIENTS FOR EACH OF "NP" PEAKS
0062      DO 20 J = 1,NP
0063      DLTAX = XI - PKPOS(J)
0064      DX = DLTAX
0065      DLX = DLTAX
0066      DLXSQ = DLTAX * DLTAX
0067      EXPN1 = 0.0
0068      PHT = PKHT(J)
0069      ALFA = -2.7726 / (ASLP * PKPOS(J) + S6)
0070      EXPNT = ALFA * DLXSQ
0071      EXPN3 = 0.
0072      IF (EXPNT + 14.) 4,3,3
      C      CALCULATE GAUSSIAN COMPONENT OF PEAK
0073 3      EXPN1 = EXP (EXPNT)
0074 4      IF (DLTAX)53,54,54
0075 53      EXPN3 = EXP (0.4 * EXPNT)
0076 54      FXX = EXPN1
0077      IF (GAMA(J))52,52,51
      C      COMPUTE MODIFIED SHAPE FOR X-RAY PEAK
0078 51      WL = GAMA(J) * CX
0079      CX = SQRT(-ALFA)
0080      CD = CX * DLTAX
0081      C1 = 1. - .5642 * WL
0082      C2 = .15915 * WL
0083      C3 = .25 * WL * WL
0084      C4 = .6366 * WL
0085      RT = C1 + C3
0086      CC = ABS(CD)
0087      CALL BWF(CC)
0088      AA = (C1 - C2 * EXPNT + C3 * (1. + 2. * EXPNT)) * EXPN1 + C4 * CC
0089      CU = AA/RT
0090      FXX = CD
0091 52      IF (NFLG1) 6,6,5
      C      PEAK WIDTH PARAMETER FREE
0092 5      DALFA = DALFA + PHT * DLXSQ * EXPN1
0093 6      IF (DLTAX) 7,14,14
0094 7      EXPN = EXP2 * DLTAX
0095      IF (EXPN + 10.) 12,8,8
0096 8      EXPN2 = EXP (EXPN)
0097      CB = EXPN2 * (1.0 - EXPN3)

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0098      FXX = FXX + EXP1 * CB
0099      IF (NFLG3) 10,10,9
          SHORT TERM TAILING SLOPE FREE
0100      9      DGAMA = DGAMA + DLTAX * EXP1 * PHT * CB
0101      10     IF (NFLG2) 12,12,11
          C      SHORT TERM TAILING AMPLITUDE FREE
0102      11     DBETA = DBETA + CB * PHT
0103      12     EXPN = EXP4 * DLTAX
0104      IF(EXPN + 10.)14,18,18
0105      18     CB = EXP(EXPN) * (1. - EXPN3)
0106      CY = PHT * EXP3
0107      FXY = FXY + CY * CB
0108      IF(NFLG4)28,28,27
          C      LONG TERM TAILING AMPLITUDE FREE
0109      27     DBELT = DBELT + CB * PHT
0110      28     IF(NFLG5)14,14,29
          C      LONG TERM TAILING SLOPE FREE
0111      29     DCHI = DCHI + DLTAX * CY * CB
0112      14     IF(NYFLG(J))161,16,15
0113      161    IF(HIGHT(J))162,16,16
0114      162    LPK = -NYFLG(J)-1
0115      L = KK
0116      DO 166 M=1,LPK
0117      IF(NYFLG(M))164,164,163
0118      163    L = L+1
0119      164    IF(NXFLG(M))166,166,165
0120      165    L=L+1
0121      166    CONTINUE
0122      L = L+1
0123      VALU=-HIGHT(J)*EXPN1*WT
0124      GOTO 114
          C      PEAK HEIGHT FREE
0125      15     K = K + 1
0126      L=K
0127      VALU=EXPN1*WT
0128      114    ACOEF(I,L) =VALU + ACOEF(I,L)
0129      16     IF (NXFLG(J)) 19,19,17
          C      PEAK POSITION FREE
0130      17     K = K + 1
0131      ACOEF(I,K) = -2. *ALFA *PHT * DX *EXPN1 * WT
0132      19     FX = FX +FXY + FXX * PHT
0133      SUM(J) = SUM(J) + FXX * PHT
0134      20     CONTINUE
0135      L = 0
0136      IF (NFLG1) 22,22,21
0137      21     L = L + 1
0138      ACOEF(I,L) = DALFA * WT
0139      22     IF (NFLG2) 24,24,23
0140      23     L = L + 1
0141      ACOEF(I,L) = DBETA * WT
0142      24     IF (NFLG3) 38,38,25
0143      25     L = L + 1
0144      ACOEF(I,L) = DGAMA * WT
0145      38     IF(NFLG4)37,37,36
0146      36     L = L + 1
0147      ACOEF(I,L) = DBELT * WT
0148      37     IF(NFLG5)39,39,26
0149      26     L = L + 1
0150      ACOEF(I,L) = DCHI * WT
0151      39     YP = YP + YNET(I)
0152      DELY(I) = (YNET(I) + BG(I) +YP * DBG/(YSUM -FX) * WT
0153      30     CONTINUE
0154      LFLG = 1
0155      CALL ASSIGN(1,'RKO:AMTRX.DAT',0,'NEW',.CC)
0156      DO 101 J = 1,K

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0157      WRITE(1) (ACDEF(I,J), I = 1,240)
0158 101    CONTINUE
0159      CALL CLOSE(1)
      C    PERFORM LEAST-SQUARES CALCULATION
0160      CALL MLR(240,NDPTS,K,DELY,DEL,ACDEF,RM,WM,VM,LFLG)
0161      IF(LFLG,ER,2)GOTO 102
0163      CALL MLRA(240,NDPTS,K,DELY,DEL,ACDEF,RM,WM,VM,LFLG)
0164 102    CONTINUE
0165      FWHM= GAIN * SQRT(-2.7726/ALPHA)
0166      EX2 = EXP2/GAIN
0167      EX4 = EXP4/GAIN
0168      TYPE 9040
0169 7040   FORMAT(/,' ITERATION FWHM      EXP1      EXP2      EXP3      EXP4')
0170      TYPE 9030,ITER,FWHM,EXP1,EX2,EXP3,EX4
0171 9030   FORMAT(I3,6X,F9.5,4F8.4)
0172      IF(LISTFG,ER,1) GOTO 301
0174      TYPE 9010
0175 9010   FORMAT(/,' CHANNEL KEV      PEAK HEIGHT ')
0176      DO 200 J=1,NP
0177      PKP=PKPOS(J)+START
0178      PKE =(PKP - REFCH)*GAIN + REFEN
0179      TYPE 9020,PKP,PKE,PKHT(J)
0180 200    CONTINUE
0181 9020   FORMAT(2F9.2,F14.3)
0182      GOTO(301,302,303)LFLG
0183 302    TYPE 305
0184 305    FORMAT(' MATRIX IS SINGULAR')
0185      STOP
0186 303    TYPE 306
0187 306    FORMAT(' SUM OF SQUARES OF R > THAN THOSE OF Y')
0188 310    STOP ' RETRN2 310'
0189 301    CALL MLRE(DM,240,K,ACDEF,WM)
0190      DO 304 J =1,K
0191 304    DM(J) = SQRT(DM(J))
0192      DO 307 J = 1,7
0193 307    ERR(J) = 0.
      C    INCREMENT THE TRIAL VALUES AND CHECK FOR COMPLETION OF ITERATIVE
      C    PROCESS.
0194 1000   L = 0
0195      LFLG = 0
0196      IF (NFLG1) 43,43,41
      C    INCREMENT PEAK WIDTH PARAMETER
0197 41     L = L + 1
0198      ERR(3) = DM(L)
0199      ADEL = ABS(DEL(L))
0200      IF(ADEL + .01 * ALPHA)430,430,42
0201 42     ALPHA = ALPHA + DEL(L) * (1. +0.8* ADEL/(ALPHA - ADEL))
0202      LFLG = 1
0203      GOTO 43
0204 430    ALPHA = ALPHA +DEL(L)
0205 43     IF (NFLG2) 46,46,44
0206 44     L = L + 1
0207      ERR(4) = DM(L)
0208      IF(ITER -NFLG1)45,45,115
      C    INCREMENT SHORT TERM TAILING AMPLITUDE
0209 115    IF (EXP1 + DEL(L)) 116,116,117
0210 116    DEL(L) =- .5 * EXP1
0211 117    ADEL = ABS(DEL(L))
0212      IF(ADEL - DM(L) - 0.1*EXP1)460,460,45
0213 45     EXP1 = EXP1 + DEL(L) * (1. -0.8* ADEL / (EXP1 + ADEL))
0214      LFLG = 1
0215      GOTO 47
0216 460    EXP1 = EXP1 + DEL(L)
0217 46     IF (NFLG3) 49,49,47
0218 47     L = L + 1

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0219      ERR(5) = DM(L)
0220      IF (ITER-NFLG1-NFLG2)480,480,119
      C      INCREMENT SHORT TERM TAILING SLOPE
0221 119      IF (EXP2 + DEL(L)) 120,120,118
0222 120      DEL(L) = -.5 * EXP2
0223 118      ADEL = ABS(DEL(L))
0224      IF(ADEL - DM(L) - .02*EXP2)490,490,48
0225 48      EXP2 = EXP2 + DEL(L) * (1. -0.8* ADEL / (EXP2 + ADEL))
0226 480      LFLG = 1
0227      GOTO 49
0228 490      EXP2 = EXP2 + DEL(L)
0229 49      IF(NFLG4)126,126,121
      C      INCREMENT LONG TERM TAILING AMPLITUDE
0230 121      L = L + 1
0231      ERR(6) = DM(L)
0232      ADEL=ABS(DEL(L))
0233      IF(ADEL - DM(L) - .01*EXP3)1260,1260,125
0234 125      EXP3 = EXP3 +DEL(L) * ABS(1. -0.8* ADEL/(EXP3 + ADEL))
0235      LFLG = 1
0236      GOTO 126
0237 1260      EXP3 = EXP3 + DEL(L)
0238 126      IF(NFLG5)132,132,127
      C      INCREMENT LONG TERM TAILING SLOPE
0239 127      L = L + 1
0240      ERR(7) = DM(L)
0241      ADEL=ABS(DEL(L))
0242      IF(ADEL - DM(L) - .02*EXP4)131,131,130
0243 130      EXP4 = EXP4 +DEL(L)*ABS(1. -0.8*ADEL/(EXP4+ADEL))
0244      LFLG = 1
0245      GOTO 132
0246 131      EXP4 = EXP4 + DEL(L)
0247 132      K = L
0248      DO 60 J = 1,NP
0249      IF (NYFLG(J)) 152,152,150
      C      INCREMENT PEAK HEIGHTS
0250 150      K = K + 1
0251      ADEL = ABS(DEL(K))
0252      PKHT(J) = PKHT(J) + DEL(K) * (1. - ADEL / (PKHT(J) + ADEL))
0253      IF (ADEL - DM(K) - .001 * PKHT(J)) 152,152,151
0254 151      LFLG = 1
0255 152      IF (NXFLG(J)) 60,60,153
      C      INCREMENT PEAK POSITIONS
0256 153      K = K + 1
0257      ADEL = ABS(DEL(K))
0258      IF(ADEL - 1.)56,55,55
0259 55      DEL(K) = DEL(K)/ADEL
0260 56      PKPOS(J) = PKPOS(J) + DEL(K)
0261      IF(ADEL - DM(K) - .01 * PKPOS(J))60,60,154
0262 154      LFLG = 1
0263 60      CONTINUE
      C      REESTABLISH PEAK ENERGY AND INTENSITY RELATIONSHIPS
      C      SPECIFIED IN INPUT.
0264      DO 65 J = 1,NP
0265      IF(NYFLG(J))61,63,63
0266 61      PKHT(J) = HIGHT(J)
0267      IF(HIGHT(J))62,63,63
0268 62      L = -NYFLG(J)
0269      PKHT(J) = -HIGHT(J) * PKHT(L)
0270 63      IF(NXFLG(J))64,65,65
0271 64      L = -NXFLG(J)
0272      PKPOS(J) = PKPOS(L) -(EN(L) - EN(J))/GAIN
0273 65      CONTINUE
0274      IF(LFLG) 70,79,70
0275 70      ITER = ITER + 1
0276      IF (ITER - 10)78,78,77

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```

C      ITERATE CALCULATION AGAIN
0277 78 DO 90 I = 1,5
0278 IF(NFLG(I))91,90,90
0279 91 NFLG(I) = - NFLG(I)
0280 90 CONTINUE
0281 GOTO 1
0282 77 TYPE 105
0283 105 FORMAT ('MAXIMUM ITERATIONS EXCEEDED.')
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      TERMINATE ITERATIONS. OUTPUT RESULTS.
0284 79 CALL ASSIGN(NDEV,'SY:GNL.DAT')
0285 WRITE (NDEV) (AMATRX(I), I = 1,IALGTH)
0286 CALL CLOSE(NDEV)
0287 CALL ASSIGN(NDEV,'SY:PASS.DAT')
0288 WRITE (NDEV) (BMATRX(I), I = 1,IBLGTH)
0289 CALL CLOSE(NDEV)
0290 CALL CHAIN(ULOUT2,0,0)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0291 END

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C      PROGRAM ULOAD2
C      THIS SUBPROGRAM IS THE SECOND PART TO THE PROGRAM "GRANL"
C      LINK WITH RDSK,MAXVAL,MINVAL,AVE,BKGRJ,GFIT
C
0001      INTEGER*2 ULFIT2(4)
0002      DIMENSION AMATRIX(5888),BMATRIX(256),XC(2),REFCH(2)
0003      COMMON/GNL/ NUMS,NUME,NDPTS,NP,ITER,NWRDS(5),NFLG(20),
1      NYFLG(20),NXFLG(20),FNAME(3),SP(2),
2      GAIN,ZERO,START,ALPHA,FWHM,ATAIL,BTA',EXP3,EXP4,
3      STD(2),C1,C2,AVERAGE,SLP(2),EN(20),SHAPC(10),CLIN(5),
4      HIGHT(20),GAMA(20),Y(240),PKPOS(20),PKHT(20),IUM(4460)
0004      COMMON/PASS/ENJ(20),IST,IEND,NUMSJ,NUMEJ,GAINJ,ZEROJ,ST1J,ST2J,
1      STRJ(20),NENUM,ALPJ,STAMP,STSLP,TLAMP,TLSLP,BGSLP(2),FILE(3),
2      SSS,YES,BK1,NGAIN,IREGG,LISTFG,FAME(3)
0005      EQUIVALENCE (NUMS,AMATRIX(1)),(ENJ(1),BMATRIX(1))
C      THIS PROGRAM CHAINS TO THE PROGRAM ULFIT2 WHICH RESIDES
C      ON PHYSICAL DEVICE RK3. THIS DATA STATEMENT MUST BE
C      CHANGED ACCORDINGLY IF THE PROGRAM RESIDES ELSEWHERE.
0006      DATA ULFIT2/3RRK3,3PULF,3RIT2,3RSBV/
C      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      THE FOLLOWING STATEMENTS READ THE COMMON BLOCKS BACK INTO CORE
0007      NDEV = 1
0008      CALL CLOSE(NDEV)
0009      CALL ASSIGN(NDEV,'SY:GNL.DAT')
0010      IALGTH = 5888
0011      READ (NDEV) (AMATRIX(I), I = 1,IALGTH)
0012      CALL CLOSE(NDEV)
0013      IBLGTH = 256
0014      CALL ASSIGN(NDEV,'SY:PASS.DAT')
0015      READ (NDEV) (BMATRIX(I), I = 1,IBLGTH)
0016      CALL CLOSE(NDEV)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      4 NEGATIVE NGAIN IS A FLAG TO INDICATE THAT INTERNAL
C      REFERENCE PEAKS ARE TO BE USED TO ESTABLISH ENERGY SCALING.
C      TWO PEAKS ARE USED. IF FIRST PEAK ENERGY=0, INTERPRETED
C      TO MEAN CHANNEL ZERO =0 KEV.
0017      IF(NGAIN) 29,29,54
0018      29 DO 50 J=1,2
0019          REFCH(J)=0.
0020          XC(J)=0.
0021          IF(STD(J)) 32,50,32
0022      32 REF=(STD(J)- ZERO)/GAIN
0023          ST1=REF-30.
0024          NX = ST1
0025          ST1 = FLOAT(NX)
0026          IST1 = ST1 + 1.
0027          CALL RDSK(IST1,60,FNAME,Y)
0028          CALL MAXVAL (20,40,JPK,YMAX,Y)
0029          CALL MINVAL (1,JPK,MS,BG1,Y)
0030          CALL MINVAL (JPK,60,ME,BG2,Y)
0031          CALL AVE (MS,ME,SUM,AV,Y)
0032          YS = 0.0
0033          DBG = BG2 - BG1
0034          DO 35 I = MS,ME
0035              YS = YS + Y(I)
0036          Y(I) = Y(I) - BG1 - DBG * YS/SUM
0037      35 CONTINUE
0038      IF(SHAPC(1).EQ.0)GOTO 33
0039      GSD = GAIN * GAIN
0040      SG = SHAPC(1)/GSD + SHAPC(2) *(ST1/GAIN +ZERO/GSD)+.462
0041      ALFA=-2.7726/SG
0042      EXP1=EXP(SHAPC(3) +STD(J) *SHAPC(4))
0043      EXP2=BTAIL
0044      GOTO 34
0045      C      NO PARAMETER FILE; FOLLOWING VALUES ARE ONLY APPROXIMATE

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0046 33 ALFA=-2.7726*GSQ/FWHM**2
0047 EXP1=ATAIL
0048 EXP2=BTAIL
0049 34 NUM = 9
0050 IF (ALFA +.2) 36,36,37
0051 36 NUM = 7
C DETERMINE PEAK POSITIONS OF REFERENCE PEAKS
0052 37 CALL GFIT (JPK,PKP0,PHT,NUM,ALFA,EXP1,EXP2,Y)
0053 REFCH(J) = ST1 + PKP0 - 1.
0054 PP = REFCH(J)
0055 PKP = PP
0056 DO 38 I = 1,4
0057 PKP = PKP * REFCH(J)
0058 38 PP = PP + CLIN(I) * PKP
0059 XC(J) = PP
0060 50 CONTINUE
0061 GAIN = (STD(2) - STD(1)) / (XC(2) - XC(1))
0062 GAINJ = GAIN
0063 ZERO = STD(1) - GAIN * XC(1)
0064 ZEROJ = ZERO
C CALCULATE AFFECT OF SYSTEM NONLINEARITY ON ENERGY MEASUREMENT.
C CLIN(I) VALUES = 0 FOR LINEAR RESPONSE.
0065 54 AVECH= 0.5 * (IST+IEND)
0066 PP = AVECH
0067 PKP = PP
0068 DO 52 I = 1,4
0069 PKP = PKP * AVECH
0070 52 PP = PP + CLIN(I) * PKP
0071 STD(1) = ZERO + GAIN * PP
0072 STD(2) = AVECH
0073 REFEN = STD(1)
0074 REFCH = STD(2)
C DETERMINE PEAK GROUPING LOCATION AND READ IN DATA
0075 NDPTS = IEND - IST + 1
0076 NDATA = NDPTS + NUMS + NUME
0077 IST2= IST-NUMS+1
0078 CALL RDSK(IST2,NDATA,FNAME,Y)
0079 START = IST -1
0080 XN = 0.
0081 40 NE1 = NDPTS + NUMS
C DETERMINE AVERAGE BACKGROUND LEVEL IN FRONT AND BACK OF
C PEAK GROUPING
0082 CALL AVE (1,NUMS,BGD,AVBG1,Y)
0083 CALL AVE (NE1,NDATA,YSUM,AVBG2,Y)
0084 BGD = BGD - YSUM
0085 K = NUMS + 1
0086 KK = NE1 - 1
0087 CALL AVE (K,KK,YSUM,BD,Y)
C REMOVE BACKGROUND CONTINUUM FROM PEAK GROUPING. PRESERVE
C ENTERING AND EXITING BACKGROUND SLOPES.
0088 SLP(1) = SLP(1) * .01 * AVBG1
0089 SLP(2) = SLP(2) * .01 * AVBG2
0090 CALL BKGRD (NUMS,NE1,AVBG1,AVBG2,SLP(1),SLP(2),YSUM,NDPTS,Y,Y)
C TEST TO SEE IF TOO MANY CHANNELS
0091 IF (NDPTS - 240) 44,44,43
0092 43 CONTINUE
0093 TYPE 100,NDPTS
0094 100 FORMAT ('TOO MANY CHANNELS. NDPTS = ',I4)
0095 TYPE 101
0096 101 FORMAT(' NEW STARTING CHANNEL = ',I4)
0097 ACCEPT 102,IST
0098 102 FORMAT(I4)
0099 IF(IST)47,46,47
0100 CALL BKGRD (NUMS,NE1,AVBG1,AVBG2,SLP(1),SLP(2),YSUM,NDPTS,Y,Y)
0101 46 IST = START + 1.
0101 47 ST1 = IST

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0162      CALL CLOSE(NDEV)
0163      CALL CHAIN(ULFIT2,0,0)
0164      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      END

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C      PROGRAM ULFIT2
C      LINK WITH BWF,AVE,MLR,MLRA,MLRE
C      THIS SUBPROGRAM IS THE THIRD PART TO THE PROGRAM "GRFANL".
C      IT PERFORMS A TAYLOR'S EXPANSION ABOUT THE TRIAL VALUES
C      TO OBTAIN A SET OF LINEAR EQUATIONS, WHICH ARE SOLVED BY
C      THE METHOD OF LEAST SQUARES. THE TRIAL VALUES ARE THEN
C      INCREMENTED BY THE RESULTS OF THE FIT. IF THE INCREMENT(S)
C      EXCEEDS A SPECIFIED VALUE, THE SET OF EQUATIONS IS REFORMED,
C      SOLVED AND INCREMENTED. THE PROCESS CONTINUES UNTIL ALL
C      TESTS ARE SATISFIED OR 10 ITERATIONS HAVE BEEN MADE,
C      WHICHEVER OCCURS FIRST.
0001      INTEGER*2 ULOUT2(4)
0002      DIMENSION AMATRIX(5888),BMATRIX(256)
0003      COMMON/GNL/ K,KK,NDFTS,NP,ITER,NWRDS(5),NFLG1,NFLG2,NFLG3,
1      NFLG4,NFLG5,NXF,MWRDS(14),NYFLG(20),NXFLG(20),FNAME(3),ATAIL,
2      BTAIL,GAIN,ALFA,START,ALPHA,FWHM,EXP1,EXP2,EXP3,EXP4,REFEN,
3      REFCB,BG(2),AVEBG,ASLP,SLF,EN(20),SHAPC(10),CLIN(5),
4      HIGHT(20),GAMA(20),YNET(240),PKPDS(20),PKHT(20),DELY(240),
5      DEL(20),RM(240),VM(20),ACDEF(240,20),DM(20),ERR(7)
0004      COMMON/PASS/ENJ(20),IST,IEND,NUMSJ,NUMEJ,GAINJ,ZEROJ,ST1J,ST2J,
1      STRJ(20),NENUM,ALFJ,TAMP,TSLP,TLAMP,TLSLP,BKGS(2),TLE(3),SSS,
2      YES,BK1,NGAIN,IREGG,LISTFG,FAME(3),SUM(20)
0005      DIMENSION WM(20),NFLG(5)
0006      EQUIVALENCE (K,AMATRIX(1)),(ENJ(1),BMATRIX(1)),(NFLG(1),NFLG1)
C      THIS PROGRAM CHAINS TO THE SUBPROGRAM ULOUT2 ON RK3
0007      DATA ULOUT2/3RRK3,3RULO,3RUT2,3RSAV/
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      READ IN THE COMMON BLOCKS FROM THE SYS DEVICE
0008      IALGTH = 5888
0009      IBLGTH = 256
0010      NDEV = 1
0011      CALL ASSIGN(NDEV,'SY:GNL.DAT')
0012      READ (NDEV) (AMATRIX(I), I = 1,IALGTH)
0013      CALL CLOSE(NDEV)
0014      CALL ASSIGN(NDEV,'SY:PASS.DAT')
0015      READ (NDEV) (BMATRIX(I), I = 1,IBLGTH)
0016      CALL CLOSE(NDEV)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0017      1  KK = NFLG1 + NFLG2 + NFLG3 + NFLG4 + NFLG5
0018      IF(ITER - NFLG4 -NFLG5)/32,33,33
0019      32  KK = KK -NFLG2
0020      NFLG2 = -NFLG2
0021      33  IF(ITER - NFLG3 -NFLG4 - NFLG5)/34,35,35
0022      34  KK = KK - NFLG3
0023      NFLG3 = - NFLG3
0024      35  SG = -2.7726 / ALPHA
0025      CX = SQRT(-ALPHA)
0026      XPTS = NDFTS
C      CALCULATE PEAK TAILING INTENSITIES AT THE GROUP BOUNDARIES.
C      THESE VALUES USED LATER TO ADJUST NET COUNTS OF PEAK
C      GROUPING.
0027      BG(1) = 0.
0028      BG(2) = 0.
0029      DO 400 J = 1,NP
0030      TYPE 107
0031      107  FORMAT(' # OF BKG. CHANNELS IN BACK OF GROUP = ',%)
0032      ACCEPT 106,NUME
0033      NUMEJ = NUME
0034      TYPE 108
0035      108  FORMAT(' GAIN (NEG. VALUE FOR ABSOLUTE' /
1      ' IF =0, PEAK AREA SIMPLY INTEGRATED) = ',%)
0036      ACCEPT 109,GAIN
0037      109  FORMAT(F9.6)
0038      NGAIN = 0
0039      TYPE 110

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0040 110  FORMAT(' ENERGY OF ZERO CHAN =',%)
0041      ACCEPT 111,ZERO
0042      ZEROJ=ZERO
0043 111  FORMAT(F8.4)
0044      IF(GAIN)60,59,61
0045 59    C  IF GAIN=0, SIMPLY INTEGRATE NET COUNTS ABOVE BACKGROUND
0046      NDPTS=IEND-IST+1
0047      NDATA=NDPTS+NUMS+NUME
0048      XNUMS=NUMS
0049      ST2=ST-XNUMS
0050      IST2=ST2+1.
0051      CALL RDSK(IST2,NDATA,FNAME,Y)
0052      NE1=NDPTS+NUMS
0053      CALL MAXVAL(1,NDATA,JPK,YMAX,Y)
0054      CALL GFIT(JPK,PKPO,PHT,5,0.,0.,0.,Y)
0055      PKPO=PKPO+ST2 - 1.
0056      CALL NCNTS(1,NUMS,NE1,NDATA,ND,BGI,SUM,ER,AVEBG,Y,Y)
0057      ER=ER/SUM*100.
0058      PRINT 1089,PKPO
0059 1089  FORMAT(' PEAK POSITION:',F8.3)
0060      PRINT 1090,SUM,ER
0061 1090  FORMAT(' NET COUNTS FOR GIVEN REGION:',F8.0,'+ ',F7.2,'%')
0062      CALL EXIT
0063  C  GAIN IS ABSOLUTE
0064 60    GAIN = - GAIN
0065      GAINJ = GAIN
0066      NGAIN = 1
0067      RKEV = GAIN
0068      GOTO 62
0069  C  GET REFERENCE PEAKS FOR REDETERMINATION OF GAIN AND ZERO
0070 61    TYPE 112
0071 112  FORMAT(' REFERENCE PK #1 ENERGY = ',%)
0072      ACCEPT 113,STD(1)
0073      ST1J = STD(1)
0074 113  FORMAT(F8.3)
0075      TYPE 114
0076 114  FORMAT(' REFERENCE PK #2 ENERGY = ',%)
0077      ACCEPT 113,STD(2)
0078      ST2J = STD(2)
0079 62    TYPE 115
0080 115  FORMAT(' LIST PK ENERGIES IN THIS GROUP (NEG. VALUES FOR XRAYS)'
0081      1 / ' TERMINATE WITH A 0')
0082      I = 0
0083 2    I = I + 1
0084      TYPE 1150,I
0085 1150 FORMAT(I3,' ',%)
0086      NXFLG(I) = 0
0087      GAMA(I) = 0.
0088      ACCEPT 116,EN(I)
0089 116  FORMAT(F10.4)
0090      NYFLG(I) = 1
0091      ENJ(I) = EN(I)
0092      STRJ(I) = AND
0093      IF(EN(I))3,4,2
0094 3    TYPE 117
0095 117  FORMAT(' INTRINSIC WIDTH (EV) = ',/
0096      1 / ' IF ENTRY=0, ESTIMATED VALUE USED ',%)
0097      ACCEPT 118,GAMA(I)
0098 118  FORMAT(F6.1)
0099      EN(I)=-EN(I)
0100      IF(GAMA(I).NE.0)GOTO 1181
0101      GAMA(I)=-0.4+0.4*EN(I)
0102      F(EN(I),GT,2B,)GAMA(I)=GAMA(I)-27.22+.972*EN(I)
0103 1181 GAMA(I) = GAMA(I) * .001/GAIN
0104      GOTO 2

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0102 4      NP = I -1
0103      NENUM = NP
0104      TYPE 1190,NP
0105 1190    FORMAT(//,I3,' PEAKS WERE ENTERED FOR THIS REGION')
0106      TYPE 119
0107 119     FORMAT(' TYPE SEQUENCE # OF PEAKS WHOSE ENERGY ARE UNCERTAIN' /
1 ' TYPE 99 FOR ALL -- NEG. FOR FIXED RELATIONSHIP. END WITH 0')
0108 12      ACCEPT 120,N
0109 120     FORMAT(I3)
0110      IF(N)5,10,6
0111 5        N = -N
0112      TYPE 121
0113 121     FORMAT(' ENERGY FIXED RELATIVE TO PEAK #: ',%)
0114      ACCEPT 120,M
0115      NXFLG(N) = -M
0116      GOTO 12
0117 6        IF(N-99)7,8,7
0118 7        NXFLG(N) = 1
0119      STRJ(N) = AYES
0120      GOTO 12
0121 8        DO 9 N = 1,NP
0122      STRJ(N) = AYES
0123 9        NXFLG(N) = 1
0124 10       TYPE 122
0125 122     FORMAT(' SEQUENCE # OF PEAK WHOSE INTENSITY IS KNOWN /
1 ' 0 FOR NONE')
0126 40      ACCEPT 120,N
0127      IF(N)41,48,41
0128 41       NYFLG(N) = -1
0129      TYPE 123
0130 123     FORMAT(' PEAK HEIGHT (RED FOR PAID) = ',%)
0131      ACCEPT 124,HIGHT(N)
0132 124     FORMAT(E12,4)
0133      IF(HIGHT(N))42,43,43
0134 42       TYPE 125
0135 125     FORMAT(' RATIODEED TO PEAK #: ',%)
0136      ACCEPT 120,M
0137      NYFLG(N) = -M
0138 43       GOTO 40
0139 48       DO 133 I = 1,5
0140      SHAPC(I)=0.
0141 133      CLIN(I) = 0.
0142      TYPE 126
0143 126     FORMAT(' IS THERE A PARAMETER FILE? ',%)
0144      IF(.NOT.YESNO()) IVAL = 1
0146      IF(IVAL.EQ.1)GOTO 135
0148      TYPE 150
0149 150     FORMAT(' FILE NAME? ',%)
0150      ACCEPT 101,CFILE
0151 11       CALL ASSIGN(1,CFILE,10)
0152      READ (1) (NUM,SHAPC(I), I =1,NUM)
0153      CALL CLOSE(1)
0154      EXP3 = SHAPC(8)
0155      EXP4 = SHAPC(9)*GAIN
0156 135     ALPJ = AND
0157      STAMP = AND
0158      STSLP = AND
0159      TLAMP = AND
0160      TLSLP = AND
0161      NFLG(1) = 0
0162      NFLG(2) = 0
0163      NFLG(3) = 0
0164      NFLG(4) = 0
0165      NFLG(5) = 0
0166      IF(IVAL.EQ.1)GOTO 25

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0168      TYPE 127
0169 127  FORMAT(' DO YOU WANT TO FREE ANY SHAPE PARAMETERS? ', $)
0170      IF(.NOT.YESNO())GOTO 24
0172      TYPE 128
0173 128  FORMAT(' ALPHA? ', $)
0174      IF(.NOT.YESNO())GOTO 15
0176      NFLG(1) = 1
0177      ALPJ = AYES
0178      TYPE 129
0179 129  FORMAT(' SHORT TERM TAIL AMPLITUDE? ', $)
0180      IF(.NOT.YESNO())GOTO 17
0182      NFLG(2) = 1
0183      STAMP = AYES
0184 17   TYPE 130
0185 130  FORMAT(' SHORT TERM TAIL SLOPE? ', $)
0186      IF(.NOT.YESNO())GOTO 22
0188      NFLG(3) = 1
0189      STSLP = AYES
0190 22   TYPE 140
0191 140  FORMAT(' LONG TERM TAIL AMPLITUDE? ', $)
0192      IF(.NOT.YESNO())GOTO 23
0194      NFLG(4) = 1
0195      TLAMP = AYES
0196 23   TYPE 141
0197 141  FORMAT(' LONG TERM TAIL SLOPE? ', $)
0198      IF(.NOT.YESNO())GOTO 24
0200      NFLG(5) = 1
0201      TLSLP = AYES
0202      GOTO 24
0203 25   TYPE 142
0204 142  FORMAT(' FWHM (IN KEV) = ', $)
0205      ACCEPT 143,FWHM
0206 143  FORMAT(F7.4)
0207      TYPE 144
0208 144  FORMAT(' TO BE FREED? ', $)
0209      IF(.NOT.YESNO())GOTO 26
0211      NFLG(1) = 1
0212      ALPJ = AYES
0213 26   TYPE 145
0214 145  FORMAT(' SHORT TERM TAIL AMPLITUDE = ', $)
0215      ACCEPT 143,ATAIL
0216      TYPE 144
0217      IF(.NOT.YESNO())GOTO 27
0219      NFLG(2) = 1
0220      STAMP = AYES
0221 27   TYPE 146
0222 146  FORMAT(' SHORT TERM TAILING SLOPE = ', $)
0223      ACCEPT 143,BTAIL
0224      BTAIL = BTAIL * GAIN
0225      TYPE 144
0226      IF(.NOT.YESNO())GOTO 28
0228      NFLG(3) = 1
0229      STSLP = AYES
0230 28   TYPE 147
0231 147  FORMAT(' LONG TERM TAILING AMPLITUDE = ', $)
0232      ACCEPT 143,EXP3
0233      TYPE 144
0234      IF(.NOT.YESNO())GOTO 29
0236      NFLG(4) = 1
0237      TLAMP = AYES
0238 29   TYPE 148
0239 148  FORMAT(' LONG TERM TAILING SLOPE = ', $)
0240      ACCEPT 143,EXP4
0241      EXP4 = EXP4 * GAIN
0242      TYPE 144

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0243      IF(.NOT.YESNO())GOTO 30
0245      NFLG(5) = 1
0246      TSLF = AYES
0247 30     SG = FWHM ** 2
0248      ALPHA = -2.7726 * GAIN * GAIN / SG
0249      SHAPC(2) = .0017!THIS IS AN APPROXIMATE VALUE USED FOR ASLP
0250      GOTO 31
0251 24     GSQ = GAIN * GAIN
0252      AVECH = 0.5 * (IST + IEND)
0253      AVEN = AVECH * GAIN + ZERO
0254      SG = SHAPC(1)/GSQ + SHAPC(2) * (IST/GAIN+ZERO/GSQ) + .462
0255      FWHM = SQRT(SG)
0256      ATAIL = EXP(SHAPC(3) + AVEN * SHAPC(4))
0257      BTAIL = SHAPC(5) * GAIN
0258      ALPHA = -2.7726/ SG
0259 31     TYPE 131
0260 131    FORMAT(' LOW ENERGY BKGRD SLOPE EXPRESSED IN %/CHAN =',%)
0261      ACCEPT 132,SLF(1)
0262      BKGSFP(1) = SLP(1)
0263      TYPE 1331
0264 1331   FORMAT(' HIGH ENERGY BKGRD SLOPE EXPRESSED IN %/CHAN =',%)
0265      ACCEPT 132,SLF(2)
0266      BKGSFP(2)=SLF(2)
0267 132    FORMAT(F5,3)
C        THE FOLLOWING STATEMENTS WRITE THE COMMON BLOCKS TO
C        THE SYSTEM DEVICE.  THESE FILES ARE THEN READ BY ULOAD2
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0268      NDEV = 1
0269      CALL ASSIGN(NDEV,'SY:GNL,DAT')
0270      WRITE (NDEV) (AMATRX(I), I = 1,IALGTH)
0271      CALL CLOSE(NDEV)
0272      CALL ASSIGN(NDEV,'SY:PASS,DAT')
0273      WRITE (NDEV) (BMATRX(I), I = 1,IBLGTH)
0274      CALL CLOSE(NDEV)
0275      CALL CHAIN(ULOAD2,0,0)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0276      END

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C      PROGRAM ULOUT2
C      LINK WITH RISK,AVE
C      ALSO LINK WITH CALMU,CALGPM,GPM IF
C      GAMMA EMISSIONS ARE INCLUDED
0001     LOGICAL*1 DTE(10),YESNO
0002     REAL*8 STIME,COFNU
0003     DIMENSION B(20),AMATRX(5888),BMATRX(256)
0004     COMMON/GNL/ K,KK,NDPTS,NP,NWRDS(26),NYFLG(20),NXFLG(20),
1       FNAME(3),ATAIL,BTAIL,GAIN,ALFA,START,ALPHA,FWHM,EXP1,EXP2,
2       EXP3,EXP4,REFEN,REFCH,BG(2),AVERG,ASLP,SLP,EN(20),SHAPC(10),
3       CLIN(5),HIGHT(20),GAMA(20),YNET(240),
4       PKPOS(20),PKHT(20),RES(240),DEL(20),RM(240),VM(20),
5       BM(4800),DM(20),ERR(7)
0005     COMMON/PASS/ENJ(20),IST,IEND,NUMSJ,NUMEJ,GAINJ,ZEROJ,ST1J,
1       ST2J,STRJ(20),NENUM,ALPJ,TAMP,TSLF,TLAMP,TLSP,BKGSFP(2),
2       CFILE(3),SSS,YES,BK1,NGAIN,IREGG,LISTFG,DFILE(3),
3       YSUM(20),QFT(100),SDOF(20),SUMR(20),EDGE(20),NSMBL(20),
4       COFNU(8,20),MTLZ(5),CMPOS(5),NARS(5),ABSRB(5),DCNST(16),
5       N1,N2,GEOM,SURFC,SMPWT,DEPTH
0006     EQUIVALENCE (K,AMATRX(1)),(ENJ(1),BMATRX(1))
0007     DATA Y/4HYES /
0008     DATA ANO/4HNO /
0009     DATA BL/4H /
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      READ IN COMMON BLOCKS FROM SYS DEVICE
0010     IALGTH = 5888
0011     IBLGTH = 256
0012     NDEV = 1
0013     CALL ASSIGN(NDEV,'SY:GNL.DAT')
0014     READ (NDEV) (AMATRX(I), I = 1,IALGTH)
0015     CALL CLOSE(NDEV)
0016     CALL ASSIGN(NDEV,'SY:PASS.DAT')
0017     READ (NDEV) (BMATRX(I), I = 1,IBLGTH)
0018     CALL CLOSE(NDEV)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0019     CALL DATE(DTE)
0020     SG = -2.7726/ ALPHA
0021     ALFA = -2.7726/SG
0022     FWHM = SQRT(SG)
0023     BTAIL = EXP2/GAIN
0024     EXP4 = EXP4/GAIN
0025     DO 4 I=1,100
0026 4     QFT(I)=0.0
0027     QFT(50)=1.
0028     DX=0.
0029     L=50
0030     DO 6 I=51,100
0031     DX=DX+1.
0032     L=L-1
0033     QFT(I)=SQRT(EXP(ALFA*DX*DX))
0034     QFT(L)=QFT(I)
0035     IF(QFT(I)-.01)8,6,6
0036 6     CONTINUE
0037 8     DO 9 J=1,NP
0038     SDOF(J)=0.0
0039 9     SUMR(J)=0.0
0040     SUM=0.0
0041     DO 11 I = 1,NDPTS
0042     RES(I) = RM(I) * SQRT (YNET(I) + AVERG)
0043     RR = RM(I)**2
0044     SUM = SUM + RR
0045     DO 10 J=1,NP
0046     NPK=PKPOS(J)+0.5
0047     K=I-NPK+50
0048     IF(K.LT.0)GOTO 10

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0050      IF(K.GT.100)GOTO 10
0052      SDOF(J)=SDOF(J)+QFT(K)
0053      SUMR(J)=SUMR(J)+QFT(K)*RR
0054 10     CONTINUE
0055 11     CONTINUE
0056      DOF = NDPIS - KK - NP
0057      QFIT = SUM / DOF
0058      FWHM = FWHM * GAIN
0059      CALL RDSK(1,20,FNAME,B)
0060      TIME = B(1)
0061      TOC = B(2)
0062      CALL GTIM(TIME)
0063      CALL CUTTIM(STIME,IHR,IMIN,ISEC,ITIC)
0064      WRITE(6,9010)(DTE(J),J=1,9),IHR,IMIN,FNAME,CFILE,
1TIME,TIMOC,GAIN
0065 9010  FORMAT('1 PROGRAM GRFANL LLL VERSION 1',10X,9A1,I4,';',I2,/,
1' FILE NAME',2X,3A4,20X,' PARAMETER FILE',2X,3A4,/,
1' LIVE TIME',F8.1,' SECONDS',/,
1' START DAY ',F7.3,/,
1' KEV/CHANNEL',F10.6,/)
0066      WRITE(6,9020)IST,IEND,NUMSJ,NUMEJ,ZEROJ,ST1J,ST2J,ALPJ,TAMP,
1 TSLP,TLAMP,TLSP,BKGS(1),BKGS(2)
0067 9020  FORMAT(/
1' GROUP STARTS AT CHANNEL ',I5/
1' GROUP ENDS AT CHANNEL ',I5/
1' BACKGROUND LOW ENERGY ',I5/
1' BACKGROUND HIGH ENERGY ',I5/
1' ZERO ',13X,F8.4//
1' REFERENCE PK #1 ENERGY =',F8.3/
1' REFERENCE PK #2 ENERGY =',F8.3//
1' PARAMETER TABLE FREE'//
1' ALPHA ',12X,A4/
1' SHORT TAIL AMPLITUDE',6X,A4/
1' SHORT TAIL SLOPE ',6X,A4//
1' LONG TERM TAIL AMPLITUDE',2X,A4/
1' LONG TERM TAIL SLOPE',6X,A4//
1' LOW ENERGY REGION BACKGROUND SLOPE ',F8.4/
1' HIGH ENERGY REGION BACKGROUND SLOPE ',F8.4/)
0068      WRITE (6,9030)
0069 9030  FORMAT(/
1' PEAK ENERGY WIDTH UNCERTAIN FIXED UNCERTAIN RATIOED
1' RATIO'//
1' NUMBER KEV EV ENERGY TO INTENSITY TO'//)
0070      DO 500 I=1,NUMUM
0071      GAMA(I)=GAMA(I)*GAINJ/.001
0072      IF(GAMA(I).EQ.0)GAMA(I) = BL
0073      NX = BL
0074      IF(NXFLG(I).LT.0)NX=-NXFLG(I)
0075      ANY = Y
0076      NYY = BL
0077      IF(NYFLG(I).LT.0)ANY = AND
0078      IF(NYFLG(I).LT.0)NYY = - NYFLG(I)
0079      IF(HIGHT(I).EQ.0)HIGHT(I)=BL
0080      WRITE (6,9040) I,ENJ(I),GAMA(I),STRJ(I),NX,ANY,NYY,HIGHT(I)
0081 9040  FORMAT(I6,F9.3,F7.2,5X,A4,3X,I4,9X,A4,3X,I4,9X,F8.5)
0082      CONTINUE
0083      WRITE(6,9050) QFIT,FWHM,ERR(3),GAIN,EXP1,ERR(4),BTAIL,ERR(5),
1 EXP3,ERR(6),EXP4,ERR(7)
0084 9050  FORMAT('/// ANALYSIS RESULTS',/,
1' QFIT',F6.1,' FWHM',F8.5,'+',F6.4,' KEV/CHANNEL',F10.6,/,33X,
1' EXP1',F9.5,'+',F6.4,' EXP2',F9.5,'+',F6.4,/,33X,
1' EXP3',F9.5,'+',F6.4,' EXP4',F9.5,'+',F6.4,/)
0090      IF(EXP3.GE.0.)GOTO 38
0091      PRINT 9060
0092 9060  FORMAT(' EXP3 IS NEGATIVE---CHECK BACKGROUND')

```

```

C      THIS PORTION OF CODING FOR THE CALCULATION OF ABSOLUTE
C      GAMMA INTENSITIES
C      EFLG=0                !INITIALIZE FLAG
C      TYPE 110
C110  FORMAT (' DO YOU WANT PHOTON EMISSION RATES CALCULATED? ',%)
C      IF(.NOT.YESNO())GOTO 29
C      EFLG=1
C      TYPE 111
C111  FORMAT (' FILE NAME FOR DETECTOR CONSTANTS IS ',%)
C      ACCEPT 9111,DFILE
C9111  FORMAT(3A4)
C      CALL ASSIGN(1,DFILE,16)
C      READ(1)(NUM,DCNST(I),I=1,NUM)
C      CALL CLOSE(1)
C      TYPE 113
C113  FORMAT (' SAMPLE DISTANCE FROM DETECTOR =',%)
C      ACCEPT 9113,GEOM
C9113  FORMAT(F6.2)
C      WRITE(6,8113)GEOM
C8113  FORMAT(' SAMPLE DISTANCE FROM DETECTOR =',F6.2)
C      GEOM = GEOM + DCNST(15)
C      TYPE 114
C114  FORMAT (' SAMPLE AREA =',%)
C      ACCEPT 9113,SURFC
C      WRITE(6,8114)SURFC
C8114  FORMAT(' SAMPLE SURFACE AREA =',F6.2)
C      IF (SURFC) 21,22,21
C21  TYPE 115
C115  FORMAT (' SAMPLE WEIGHT =',%)
C      ACCEPT 9115,SMPWT
C9115  FORMAT(F8.3)
C      WRITE(6,8115)SMPWT
C8115  FORMAT(' SAMPLE WEIGHT =',F8.3)
C22  DEPTH = .00001
C      N1 = 0
C      IF (SMPWT) 24,25,24
C24  TYPE 116
C116  FORMAT (' SAMPLE DEPTH =',%)
C      ACCEPT 9116,DEPTH
C9116  FORMAT(F6.3)
C      WRITE(6,8116)DEPTH
C8116  FORMAT(' SAMPLE DEPTH =',F6.3)
C      TYPE 117
C117  FORMAT (' SPECIFY SAMPLE COMPOSITION (TERMINATE WITH 0 AMOUNT)'
C      1 // ELEMENT AMOUNT(Z)')
C      WRITE(6,117)
C      K = 0
C26  K = K + 1
C      READ(5,118)MTLZ(K),CMPOS(K)
C118  FORMAT (A2,F10.2)
C      WRITE(6,8118)MTLZ(K),CMPOS(K)
C8118  FORMAT(1X,A2,F10.2)
C      CMPOS(K) = 0.005 * CMPOS(K) * SMPWT / SURFC
C      IF (CMPOS(K)) 26,27,26
C27  N1 = K - 1
C25  TYPE 119
C119  FORMAT (' SPECIFY ABSORBERS USED',// ELEMENT AMOUNT (G/SQ-CM)')
C      WRITE(6,119)
C      K = 0
C28  K = K + 1
C      READ (5,118) NABS(K),ABSRB(K)
C      WRITE(6,8118)NABS(K),ABSRB(K)
C      IF (ABSRB(K)) 28,29,28
C29  N2 = K - 1
C      IF (N1 + N2) 37,38,37

```

```

C37  CALL ASSIGN(1,'SY:ABSCOF.DAT','OLD')
C    READ(1,120)(NSMBL(J),EDGE(J),(COFNU(I,J),I=1,8),J=1,20)
C120 FORMAT(1X,A2,F7.3,4F12.9/10X,4F12.9)
0094 38  L = KK
0095    WRITE (6,121)
0096 121  FORMAT (/3X,' CHANNEL      ENERGY COUNTS GAMMAS/MIN  PCTERR')
0097    DO 122 J = 1,NP
0098      SG = -2.7726/ALPHA + ASLP * PKPOS(J)
0099      ALFA = -2.7726/SG
C    CALCULATE PORTION OF PEAK AREAS OUTSIDE BOUNDARIES
0100      FRACT1 = 0.
0101      FRACT2 = 0.
0102      IF(GAMA(J))48,48,50
0103 50  GAMA(J)=GAMA(J)*.001/GAIN
0104      FRAC1 = ATAN(2. * PKPOS(J)/GAMA(J))
0105      FRACT1 = 1. - .6366 * FRAC1
0106      DELT = NDPTS - PKPOS(J)
0107      FRAC2 = ATAN(2. * DELT/GAMA(J))
0108      FRACT2 = 1. - .6366 * FRAC2
0109 48  CTS = YSUM(J) + YSUM(J) * (FRACT1 + FRACT2)
0110      PCERR = 0.0
0111      IF(NYFLG(J))36,36,31
0112 31  L = L+1
0113      QFTL=SUMR(J)/(SIOF(J)-1.)
0114      PCERR = (100. * IM(L) * SQRT(QFTL))/PKHT(J)
0115 36  CHAN = PKPOS(J) + START
0116      EPK = REFIN + (CHAN - REFC) * GAIN
C    THIS PORTION OF CODING FOR CALCULATION OF ABSOLUTE
C    GAMMA INTENSITIES
C    GAMAS =0.
C    VALUE=CTS
C    IF(EFLG.EQ.0)GOTO 40
C    CALL CALGPM(EPK,VALUE)
C    GAMAS=VALUE
C    GAMAS = GAMAS / TIME * 60.
0117 40  WRITE (6,102) J,CHAN,EPK,CTS,GAMAS,PCERR
0118 102  FORMAT (I3,F9.3,F10.3,F9.0,E11.4,F6.1)
0119      IF (NXFLG(J)) 122,122,90
0120 90  L = L + 1
0121 122  CONTINUE
0122      IF(LISTFG.EQ.1) RETURN
0124      WRITE(6,9100)
0125 9100  FORMAT(' CHANNEL ENERGY INDEX YNET RESIDUALS STD DEV')
0126      YP=0.
0127      DO 103 I=1,NDPTS
0128        DBG = BG(2)-BG(1)
0129        CALL AVE(1,NDPTS,TAREA,AV,YNET)
0130        IICH=I+START
0131        EENG = (FLOAT(IICH) - REFC)* GAIN + REFIN
0132        YP = YP + YNET(I)
0133        YNET(I) = YNET(I) + DBG(1) + DBG * YP/TAREA
0134        WRITE(6,9110) IICH,EENG,I,YNET(I),RES(I),RM(I)
0135 9110  FORMAT(I5,F11.2,I5,3F10.2)
0136 103  CONTINUE
0137      CALL CLOSE(6)
0138      STOP 'END OF JOB'
0139      END

```



```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C   PROGRAM FILES
C
C   THIS IS A GENERAL PURPOSE ROUTINE FOR THE PREPARATION OR EDITING
C   UNFORMATTED SEQUENTIAL DISK FILES
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001   COMMON CON(1000)
0002   DIMENSION FNAME(5)
C
0003   DATA MY,MC,MI,MD/'Y','C','I','D'/
C
0004   TYPE 100
0005   100   FORMAT(' FILE NAME IS ',%)
0006   ACCEPT 200,FNAME
0007   200   FORMAT(5A4)
0008   NDEV =1
0009   TYPE 102
0010   102   FORMAT(' IS THIS A NEW FILE? ',%)
0011   ACCEPT 202,NM
0012   202   FORMAT(A1)
0013   IF(NM.EQ.MY) GOTO 10
C
C   FETCH EXISTING FILE
C
0015   CALL ASSIGN(NDEV,FNAME)
0016   27   READ(NDEV)(LENGTH,CON(I), I= 1,LENGTH)
0017   CALL CLOSE(NDEV)
0018   TYPE 125,LENGTH
0019   125   FORMAT(' FILE LENGTH =',I5)
0020   TYPE 106
0021   106   FORMAT(' HOW MANY VALUES DO YOU WANT LISTED? ',%)
0022   ACCEPT 206,NUM
0023   206   FORMAT(I4)
0024   IF(NUM)29,29,28
0025   28   TYPE 107
0026   107   FORMAT(' STARTING AT ',%)
0027   ACCEPT 206,NM
0028   NUM = NUM + NM - 1
0029   PRINT 208, FNAME(1),FNAME(2),NDEV
0030   208   FORMAT(' FILE NAME IS ',2A4,' ON DEVICE # ',I1)
0031   WRITE(6,108)(I,CON(I), I = NM,NUM)
0032   108   FORMAT(/(I4,1PE14.6))
0033   CALL CLOSE(6)
0034   29   TYPE 110
0035   110   FORMAT(' DO YOU WANT TO EDIT THE FILE? ',%)
0036   ACCEPT 202,NM
0037   IF(NM.NE.MY)GOTO 30
0039   2   TYPE 111
0040   111   FORMAT(' CHANGE(C),INSERT(I), OR DELETE(D)? ',%)
0041   ACCEPT 202,JD
0042   IF(JD.EQ.MC)GOTO 4
0044   IF(JD.EQ.MI)GOTO 6
0046   IF(JD.EQ.MD)GOTO 15
0048   GOTO 20
C   CHANGE VALUES IN EXISTING FILE
0049   4   TYPE 112
0050   112   FORMAT(' WHICH VALUE? ',%)
0051   ACCEPT 206,N
0052   IF(N) 7,B,B
C   A NEGATIVE VALUE INDICATES ENTRY POSITION IN THE FILE FOR A
C   SEQUENCE OF CHANGES
0053   7   N = -N -1
0054   TYPE 121
0055   121   FORMAT(' HOW MANY VALUES WILL YOU CHANGE? ',%)

```

```

0056      ACCEPT 206,NUM
0057      GOTO 13
0058  8      TYPE 114
0059  114     FORMAT(' NEW VALUE = ',%)
0060      ACCEPT 214,AA
0061  214     FORMAT(E12.5)
0062      CON(N)= AA
0063      TYPE 116
0064  116     FORMAT(' MORE CHANGES? ',%)
0065      ACCEPT 202,NM
0066      IF(NM.EQ.MY)GOTO 2
0068      GOTO 20
      C      INSERT A NEW VALUE
0069  6      TYPE 118
0070  118     FORMAT(' INSERT BEFORE WHICH VALUE? ',%)
0071      ACCEPT 206,N
0072      L = LENGTH
0073      DO 9 I = N,LENGTH
0074      CON(L + 1)=CON(L)
0075  9      L = L - 1
0076      LENGTH = LENGTH + 1
0077      GOTO 8
      C      DELETE A VALUE FROM THE FILE
0078  15     TYPE 112
0079      ACCEPT 206,N
0080      LENGTH = LENGTH - 1
0081      DO 17 I = N,LENGTH
0082  17     CON(I) = CON(I+1)
0083      GOTO 2
      C      PREPARE FOR FORMATION OF A NEW FILE
0084  10     TYPE 117
0085  117     FORMAT(' FILE LENGTH = ',%)
0086      ACCEPT 206,LENGTH
      C      ZERO OUT THE ARRAY BEFORE ENTERING VALUES
0087      NUM = LENGTH
0088      DO 11 I = 1,LENGTH
0089  11     CON(I) = 0.
0090      N = 0
0091  13     NUM = NUM + N
0092      TYPE 120
0093  120     FORMAT(' TYPE VALUES IN SEQUENCE. ')
0094  12     N = N + 1
0095      TYPE 122,N
0096  122     FORMAT(I4,2X,%)
0097      ACCEPT 214,CON(N)
0098      IF(N.NE.NUM)GOTO 12
0099      CALL ASSIGN(NDEV,FNAME)
0100  20     WRITE (NDEV) (LENGTH,CON(I), I = 1,LENGTH)
0101      CALL CLOSE(NDEV)
0102      STOP 'ALL DONE'
0103  30
0104      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      Program PKSHAP
C
C      This program determines a set of parameters used to describe the
C      peak shapes of a gamma spectrum. Input comes from SHAPE
C      characteristics of a low and high energy peak, each from the
C      GRPANL program.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      DIMENSION EN(2),CH(2),FWHM(2),ATAIL(2),WP(2),TP(2),SHAPC(10)
C
0002      TYPE 100
0003      100  FORMAT( ' Peakshape V1...use parameters from GRPANL,/'
+ ' Gain (keV./ch) = ',%)
0004      ACCEPT 102, GAIN
0005      PRINT 200, GAIN
0006      200  FORMAT ( ' Gain = 'F5.3,' keV./channel' )
0007      TYPE 201
0008      201  FORMAT ( ' Low energy peak (keV.) = ',%)
0009      ACCEPT 101, EN(1)
0010      101  FORMAT (F8.3)
0011      TYPE 202
0012      202  FORMAT ( ' FWHM = ',%)
0013      ACCEPT 102, FWHM(1)
0014      102  FORMAT (F5.3)
0015      TYPE 203
0016      203  FORMAT ( ' EXP1 = ',%)
0017      ACCEPT 103, ATAIL(1)
0018      103  FORMAT (F5.3)
0019      TYPE 204
0020      204  FORMAT ( ' Hi energy peak (keV.) = ',%)
0021      ACCEPT 101, EN(2)
0022      TYPE 202
0023      ACCEPT 102, FWHM(2)
0024      TYPE 203
0025      ACCEPT 103, ATAIL(2)
0026      TYPE 206
0027      206  FORMAT ( ' EXP2 = ',%)
0028      ACCEPT 102, BTAIL
0029      GSQ = GAIN * GAIN
0030      DO 1 J = 1,2
0031          WP(J) = FWHM(J) * FWHM(J) - 0.462 * GSQ
0032          TP(J) = ALOG (ATAIL(J))
0033      1      CONTINUE
0034      DO 2 I = 1,10
0035          SHAPC(I) = 0.0
0036      2      CONTINUE
C      Calculate the area / peak-height ratio for a 100 keV. peak.
0037      DEN = 1. / (EN(1) - EN(2))
0038      SA = (WP(1) - WP(2)) * DEN
0039      SHAPC(1) = WP(1) - EN(1) * SA
0040      SHAPC(2) = SA
0041      SA = (TP(1) - TP(2)) * DEN
0042      SHAPC(3) = TP(1) - EN(1) * SA
0043      SHAPC(4) = SA
0044      SHAPC(5) = BTAIL
C
0045      WRITE (6,110) SHAPC(1),SHAPC(2),SHAPC(3),SHAPC(4),SHAPC(5)
0046      110  FORMAT ( ' Shape parameters are :',/// S(1) =',F8.5,/' S(2) =',
+ 1 'E11.4,/' S(3) =',E10.3,/' S(4) =',E10.3,/'
+ 2 ' S(5) =',F6.3,/' )
0047      CALL EXIT
0048      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE RDSK
C
C      THIS IS A ROUTINE FOR READING UNFORMATTED DIRECT ACCESS FILES
C      CONTAINING 64 FLOATING POINT VALUES PER RECORD.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE RDSK (NST,NDP,FNAM,ARRAY)
C
0002      DIMENSION BUF(64),FNAM(3),ARRAY(2)
C
0003      I = 1
0004      NDEV = 3
0005      CALL ASSIGN (NDEV,FNAM)
0006      DEFINE FILE NDEV (64,128,U,NREC)
0007      NREC = (NST - 1) / 64
0008      N1 = NST - 64 * NREC
0009      NREC = NREC + 1
0010 10      READ (NDEV,NREC) (BUF(L), L = 1,64)
0011 15      ARRAY(I) = BUF(N1)
0012          N1 = N1 + 1
0013          I = I + 1
0014          IF (I .GT. NDP) GO TO 30
0016          IF (N1 - 64) 15,15,20
0017 20      N1 = 1
0018          GO TO 10
0019 30      CALL CLOSE (NDEV)
0020          RETURN
0021      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      LOGICAL FUNCTION YESNO
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
0001      LOGICAL FUNCTION YESNO*1 (IANS)
0002      LOGICAL*1 IST(6),ISTR(4)
C
0003      5      CALL GETSTR(5,IST,3,ERR)
0004      IF(ERR.EQ.,TRUE.)GO TO 10
0006      CALL SUBSTR(IST,ISTR,1,1)
0007      CALL SCOMP('Y',ISTR,IVAL)
0008      IF(IVAL.EQ.0)GO TO 20
0010      CALL SCOMP('N',ISTR,IVAL)
0011      IF(IVAL.EQ.0)GO TO 30
0013      10     TYPE 100
0014      100    FORMAT(' PLEASE ANSWER Y OR N')
0015      GOTO 5
0016      20     YESNO = ,TRUE.
0017      RETURN
C
0018      30     YESNO = ,FALSE.
0019      RETURN
0020      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE MAXVAL
C
C
C      THIS ROUTINE RETURNS THE POSITION AND VALUE OF THE MAXIMUM VALUE
C      IN A GROUP OF DATA POINTS FROM NS TO NE INCLUSIVE.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE MAXVAL (NS,NE,JMAX,YMAX,Y)
0002      DIMENSION Y(2)
0003      YMAX = 0.0
0004      DO 2 I = NS,NE
0005      IF (Y(I) - YMAX) 2,2,4
0006      4      YMAX = Y(I)
0007      JMAX = I
0008      2      CONTINUE
0009      RETURN
0010      END

```

```

0001      SUBROUTINE MAXVAL (NS,NE,JMAX,YMAX,Y)
0002      DIMENSION Y(2)
0003      YMAX = 0.0
0004      DO 2 I = NS,NE
0005      IF (Y(I) - YMAX) 2,2,4
0006      4  YMAX = Y(I)
0007      JMAX = I
0008      2  CONTINUE
0009      RETURN
0010      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MINVAL
C
C      THIS ROUTINE RETURNS THE POSITION AND VALUE OF THE MINIMUM VALUE
C      IN A GROUP OF DATA POINTS FROM NS TO NE INCLUSIVE.
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE MINVAL (NS,NE,JMIN,YMIN,Y)
0002      DIMENSION Y(2)
0003      YMIN=1.0E3B
0004      DO 4 I=NS,NE
0005      IF (Y(I)-YMIN)2,4,4
0006 2      JMIN=I
0007      YMIN=Y(I)
0008 4      CONTINUE
0009      RETURN
0010      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      Subroutine NCNTS
C
C      This routine is similar to NCTS except it returns an average
C      background and an error associated with the total net count.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001 SUBROUTINE NCNTS (N1,N2,M1,M2,ND,S1,S2,ER,AVEBG,Y1,Y2)
0002 DIMENSION Y1(2),Y2(2)
C
0003 CHANS = M1 - N2 + 1
0004 XPTS = M2 + N2 - M1 - N1 + 1
0005 CALL NCTS (N1,N2,M1,M2,ND,S1,S2,AV1,AV2,Y1,Y2)
0006 AVEBG = 0.5 * (AV1 + AV2)
0007 IF (S2.LT.0.0)S2 = 0.0
0009 ER = SQRT (S2 + AVEBG * CHANS * (1. + CHANS / XPTS))
0010 RETURN
0011 END
```



```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      Subroutine NCTS
C
C      This routine return the net channel counts in a peak, the sum of
C      the net counts, the average background levels in front and back
C      of a peak group, and the number of data points in the net count
C      array.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE NCTS (N1,N2,M1,M2,ND,S1,S2,AV1,AV2,Y1,Y2)
0002      DIMENSION Y1(2),Y2(2)
0003      CALL AVE (N1,N2,S1,AV1,Y1)
0004      CALL AVE (M1,M2,S2,AV2,Y1)
0005      S1 = S1 + S2
0006      K = N2 + 1
0007      KK = M1 - 1
0008      CALL AVE (K,KK,S2,DUM,Y1)
0009      DBG = AV2 - AV1
0010      L = 0
0011      YS = 0.0
0012      XS = 0.0
0013      YSS = 0.0
0014      ITER = 0
0015      CHANS = KK - K + 1
0016      S2 = S2 - AV2 * CHANS
0017      IF (DBG) 1,4,4
0018 1      DO 2 I = K,KK
0019      YS = YS + Y1(I) - AV2
0020      BG = AV1 + DBG * YS / S2
0021      IF (ITER) 9,9,7
0022 7      YSS = YSS + Y1(I) - BG
0023      BG = AV1 + DBG * YSS / S3
0024 9      CNET = Y1(I) - BG
0025      IF (ITER) 2,2,11
0026 11     L = L + 1
0027      Y2(L) = CNET
0028 2      XS = XS + CNET
0029      IF (ITER) 5,5,8
0030 5      S3 = XS
0031      XS = 0.0
0032      YS = 0.0
0033      ITER = 1
0034      GO TO 1
0035 4      XK = KK - K + 1
0036      YS = AV1
0037      DBG = DBG / XK
0038      DO 6 I = K,KK
0039      L = L + 1
0040      YS = YS + DBG
0041      CNET = Y1(I) - YS
0042      Y2(L) = CNET
0043 6      XS = XS + CNET
0044 8      S2 = XS
0045      ND = L
0046      RETURN
0047      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE AVE
C
C      THIS ROUTINE DETERMINES THE AVERAGE COUNT OF A GROUP OF DATA
C      VALUES FROM NS TO NE INCLUSIVE. IT ALSO RETURNS THE SUM.
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE AVE (NS,NE,SUM,AV,Y)
0002      DIMENSION Y(2)
0003      SUM = 0.0
0004      SM = NE - NS + 1
0005      DO 2 I = NS,NE
0006      2   SUM = SUM + Y(I)
0007      AV = SUM / SM
0008      RETURN
0009      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE BKGRD
C
C
C      THIS SUBROUTINE CALCULATES THE BACKGROUND DISTRIBUTION
C      FOR THE GIVEN REGION
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE BKGRD(NS,NE,AVBG1,AVBG2,SLP1,SLP2,SUM,L,Y,YNET)
0002      DIMENSION Y(2),YNET(2)
0003      XPTS = NE - NS
0004      DBG = (AVBG2 - AVBG1) - 0.5 * (SLP1 + SLP2) * XPTS
0005      XPTS = XPTS - 1.0
0006      NS = NS + 1
0007      NE = NE - 1
0008      BG2 = AVBG2
0009      SM = 0.0
0010      DO 2 I = NS,NE
0011 2      SM = SM + Y(I)
0012      SM = SM - BG2 * XPTS
0013      XS = 0.0
0014      YS = 0.0
0015      FDY = 0.0
0016      L = 0
0017      XBG = AVBG1
0018      DSLP = SLP2 - SLP1
0019      S1 = SLP1
0020      DO 10 I = NS,NE
0021      L = L + 1
0022      DY = Y(I) - BG2
0023      HDY = 0.5 * DY
0024      YS = YS + HDY + FDY
0025      RT1 = YS/SM
0026      XBG = XBG + DBG * DY / SM + S1 + RT1 * DSLP
0027      FDY = HDY
0028      YNET(L) = Y(I) - XBG
0029 10      XS = XS + YNET(L)
0030      SUM = XS
0031      RETURN
0032      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE GFIT
C
C
C      THIS ROUTINE PERFORMS A GAUSSIAN FIT TO 5, 7, OR 9 POINTS
C      SURROUNDING THE L TH CHANNEL AND RETURNS THE EXACT PEAK POSITION
C      AND THE PEAK HEIGHT.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE GFIT (L,PKPOS,PKHT,NC,ALFA,EXP1,EXP2,Y)
0002      DIMENSION Y(2)
0003      SY = 0.0
0004      SXY = 0.0
0005      SXXY = 0.0
0006      LX = - NC / 2
0007      Y1 = Y(L+1)
0008      Y2 = Y(L-1)
0009      TPOS = .5 * (Y2-Y1) / (Y1 - 2. * Y(L) + Y2)
0010      Y0 = Y(L)
0011      DO 2 I = 1,NC
0012      K = L + LX
0013      XL = LX
0014      DLX = XL - TPOS
0015      Y1 = Y(K)
0016      IF (DLX) 1,7,7
0017      1 Y1 =Y1-Y0 * EXP1* EXP(EXP2 * DLX) * (1. -EXP(.4*ALFA*DLX*DLX))
0018      7 IF (Y1) 5,5,3
0019      5 Y1 = 1.0
0020      3 YLOG = ALOG (Y1)
0021      YX = XL * YLOG
0022      SXY = SXY + YX
0023      SY = SY + YLOG
0024      SXXY = SXXY + XL * YX
0025      LX = LX + 1
0026      2 CONTINUE
0027      PKP = L
0028      IF (NC - 7) 4,6,8
0029      4 PKPOS = SXY / (2.8571 * SY - 1.4286 * SXXY)
0030      PKHT = 0.4857 * SY - 0.14286 * SXXY + .05 * SXY * PKPOS
0031      GO TO 10
0032      6 PKPOS = SXY / (2.6666 * SY - 0.6666 * SXXY)
0033      PKHT = 0.3333 * SY - 0.04762 * SXXY + .017857 * SXY * PKPOS
0034      GO TO 10
0035      8 PKPOS = SXY / (2.597 * SY - 0.3896 * SXXY)
0036      PKHT = 0.2554 * SY - 0.021645 * SXXY + .0083333 * SXY * PKPOS
0037      10 PKHT = EXP (PKHT)
0038      PKPOS = PKPOS + PKP
0039      RETURN
0040      END

```

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CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE BWF
C
C      THIS SUBROUTINE CALCULATES THE LORENTZIAN BROADENED
C      DISTRIBUTION FOR X-RAYS. THE VALUES GIVEN FOR THE CA AND CB
C      ARRAYS ARE HEAVY ELEMENTS. THE VALUES GIVEN AT THE RIGHT SHOULD
C      BE ENTERED IN THE ARRAYS FOR LIGHT ELEMENTS.
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE BWF (X)
0002      DIMENSION CA(5),CB(6)
C
0003      HEAVY ELEMENTS                                LIGHT ELEMENTS
0004      CA(1) = .729281                                !.681634
0005      CA(2) = .0344557                              !.323828
0006      CA(3) = .127639                                !.138754
0007      CA(4) = -.0325239                             !-.0360606
0008      CA(5) = .00642257                             !.00687045
0009      CB(1) = .933301                                !1.09498
0010      CB(2) = -4.45603                               !-4.6894
0011      CB(3) = 1.16191                                !1.18068
0012      CB(4) = -.141124                              !.0241993
0013      CB(5) = -.0352464                              !.0952378
0014      CB(6) = .00744387                             !.0159129
0015      IF (X - 2.2) 2*10,10                          !REPLACE 2.2 WITH 2.3 FOR LIGHT Z
0016      2      XX = X * X
0017      SUM = 0.0
0018      DO 4 I = 1,5
0019      AX = AX * XX
0020      4      SUM = SUM + CA(I) * AX
0021      X = SUM * EXP (-XX)
0022      GO TO 20
0023      10      XLOG = ALOG (X)
0024      SUM = CB(1)
0025      DO 12 I = 2,6
0026      12      SUM = SUM + CB(I) * XLOG ** (I-1)
0027      X = EXP (SUM)
0028      20      RETURN
0029      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MLR
C
C      THIS IS THE FIRST PART OF A LEAST-SQUARES PROGRAM WHICH WAS
C      ADAPTED FROM THE "MLR" PROGRAM WRITTEN BY R. E. VON HOLDT,LLL.
C      THE SEQUEL IS MLRA OR MLRS.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE MLR (LB,M,N,Y,X,B,R,W,V,NFLG)
0002      DIMENSION Y(2),B(2),R(2),X(2),W(2),V(2)
0003      IB = LB
0004      DO 70 I = 1,N
0005          T = 0.
0006          IK = (I-1) * IB
0007          DO 20 K = I,M
0008              LL = IK + K
0009              T = T + B(LL) * B(LL)
0010 20      CONTINUE
0011          IF (T) 30,29,30
0012 29      NFLG = 2
0013          GO TO 75
0014 30      ST = SQRT (T)
0015          LL = IK + I
0016          W(I) = ST
0017          IF (B(LL)) 31,32,32
0018 31          W(I) = -ST
0019 32          B(LL) = B(LL) + W(I)
0020          V(I) = -B(LL) * W(I)
0021          IF (I-N) 35,75,35
0022 35      IP = I + 1
0023          IF(IP.GT.N)GO TO 70
0025          DO 60 J = IP,N
0026              T = 0.
0027              JK = (J-1) * IB
0028              DO 40 K = I,M
0029                  LL = IK + K
0030                  LLL = JK + K
0031 40          T = T + B(LL) * B(LLL)
0032          T = T / V(I)
0033          DO 50 L = I,M
0034              LL = JK + L
0035              LLL = IK + L
0036 50          B(LL) = B(LL) + T * B(LLL)
0037 60      CONTINUE
0038 70      CONTINUE
0039 75      CONTINUE
0040      RETURN
0041      END

```

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CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MLFA
C
C      THIS IS A SEQUEL TO THE MLP LEAST-SQUARES ROUTINE ADAPTED
C      FROM THE MLP PROGRAM WRITTEN BY R. H. VON HOLTZALL.
C      THIS SUBROUTINE REQUIRES LES% CORE BECAUSE THE "A" MATRIX
C      IS STORED AS A FILE ON THE SYSTEM DEVICE.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001  SUBROUTINE MLFA (LB,M,N,Y,X,B,R,W,V,NFLG)
0002  DIMENSION Y(2),A(240),B(2),R(2),X(2),W(2),V(2)
0003  IB = LB
0004  DO 80 I = 1,M
0005  80  R(I) = Y(I)
0006  DO 90 I = 1,N
0007  90  X(I) = 0.
0008  S = 0.
0009  DO 100 L = 1,M
0010  100 S = S + R(L) * R(L)
0011  YE = S
0012  DO 130 I = 1,N
0013  130  T = 0.
0014  LK = (I-1) * IB
0015  DO 110 K = I,M
0016  110  LL = LK + K
0017  T = T + B(LL) * R(K)
0018  T = T/V(I)
0019  DO 120 L = I,M
0020  120  LL = LK + L
0021  R(L) = R(L) + T * B(LL)
0022  130 CONTINUE
0023  IN = N
0024  R(IN) = R(IN)/W(IN)
0025  150 J = IN
0026  155 J = J - 1
0027  IF (J) 190,190,160
0028  160  LL = (IN-1) * IB + J
0029  R(J) = R(J) + R(IN) * B(LL)
0030  GO TO 155
0031  190  IN = IN - 1
0032  IF (IN) 200,200,140
0033  200  DO 210 I = 1,N
0034  210  SC = Y(I)
0035  SD = R(I)
0036  XD = SC - SD
0037  X(I) = XB
0038  DO 215 I = 1,M
0039  215  R(I) = Y(I)
C      READ SECTIONS OF "A" MATRIX FROM PREVIOUSLY STORED "AMTRY" FILES
C      STORED ON SYS
0040  CALL ASSIGN(1,'SYS:AMTRY.DAT',0,'OLD','CC')
0041  DO 220 J = 1,N
0042  220  READ (1) (A(I) , I = 1,IB)
0043  XD = Y(J)
0044  DO 230 I = 1,M
0045  230  R(I) = R(I) - A(I) * XD
0046  220 CONTINUE
0047  CALL CLOSE(1)
0048  KF = 0.
0049  DO 240 I = 1,M
0050  240  RE = RE + R(I) * R(I)
0051  IF (RE - S) 250,270,270
0052  250  S = RE
0053  GO TO 105

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```

0054 270  IF (RE - YE) 280,290,290
0055 280  NPLG = 3
0056 280  RETURN
0057     END

```



```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SUBROUTINE MLRE
C
C      THIS ROUTINE OBTAINS THE DIAGONAL MATRIX ELEMENTS FOLLOWING A
C      LEAST-SQUARES CALCULATION.  THESE CAN BE USED FOR ERROR
C      ANALYSIS.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
0001      SUBROUTINE MLRE(D,IA,NN,B,W)
0002      DIMENSION D(2),B(2),W(2)
0003      N = NN
0004      DO 6 I =1,N
0005      D(I) = -1. / W(I)
0006      IF(N-1)4,4,1
0007 1      JJ = I + 1
0008      IF(JJ.GT.N)GOTO 4
0010      DO 3 J =JJ,N
0011      S = 0.
0012      KJ = J -1
0013      DO 2 K =I,KJ
0014      LL = (J - 1) * IA + K
0015      S = S + D(K) * B(LL)
0016 2      CONTINUE
C
C
C
0017      D(J) = S * 1./W(J)
0018 3      CONTINUE
0019 4      S = 0
0020      DO 5 L =I,N
0021      S = S + D(L) **2
0022 5      CONTINUE
0023      D(I) = S
0024 6      CONTINUE
0025      RETURN
0026      END

```

```

C      GPM
0001  SUBROUTINE GPM (EPK,ELOG,GDOM,SURFC,DEPTH,SMU,VALUE,GAMAS,DCNST)
0002  DIMENSION DCNST(2)
0003  EXOVR = DCNST(12)
0004  DETHT = DCNST(13)
0005  RSQ = DCNST(14) * DCNST(14)
0006  XMU = -2.316 + 4.2 * EXP(-.478 * ELOG - 1.434)
0007  XMU = EXP (XMU)
0008  XM = 1.0 / XMU
0009  SEE = EXP (-DETHT * XMU)
0010  XM = XM * (1. - XMU * DETHT * SEE / (1. - SEE))
0011  GM = GDOM + XM
0012  GG = GM * GM
0013  ROSQ = -GG + .5 * RSQ / (1. - GM/SQRT (GG+ RSQ))
0014  ERSQ = ROSQ * (1.1 - XM / SQRT (DETHT))
0015  GGSQ = GG + ERSQ
0016  GLOST = 1.
0017  GCORR = 1.
0018  SQGCR = 1.
0019  SATN = 1.
0020  IF (SURFC) 21,31,21
0021  21 RR = SURFC / 3.1416
0022  GM2 = GM - DEPTH * (1. - EXP (-SMU))
0023  GG2 = GM2 * GM2
0024  RR = RR * (1.4 - .4 / GM2)
0025  GCORR = RR / (GG2 * ALOG ((GG2 + RR)/GG2))
0026  SQGCR = SQRT (GCORR)
0027  SMU = SMU * SQGCR
0028  UL = SMU * SMU
0029  TOLQA = 2. * DEPTH / GM
0030  ADD = 1.
0031  DFACT = 1.
0032  ASQ = GGSQ * GCORR
0033  TOTAL = (ASQ / (ASQ - DEPTH*DEPTH)) + .1 * SMU * (TOLQA **3)
0034  DO 25 I = 1,10
0035  XK = 2 * I
0036  DFACT = DFACT * XK * (XK + 1.)
0037  ADD = UL * ADD
0038  AD = ADD / DFACT
0039  IF (TOTAL - AD * 200.) 24,24,27
0040  24 TOTAL = TOTAL + AD
0041  25 CONTINUE
0042  27 TOTAL = TOTAL + AD
0043  ADD = SMU
0044  DFACT = 1.
0045  DO 28 I = 1,5
0046  XK = 2 * I - 1
0047  AD = TOLQA * ADD / ((XK + 2.) * DFACT)
0048  IF (TOTAL - AD * 200.) 29,29,30
0049  29 TOTAL = TOTAL + AD
0050  ADD = ADD * UL
0051  DFACT = DFACT * (XK + 1.) * (XK + 2.)
0052  28 CONTINUE
0053  30 TOTAL = TOTAL + AD
0054  SATN = EXP (-SMU)
0055  GLOST = TOTAL * SATN
0056  31 GM = GM - DEPTH * (1. - SATN)
0057  SGSQ = SQRT (GM * GM + ROSQ)
0058  SMU = DCNST(16) * (SGSQ - GM) / (SGSQ + GM)
0059  N = 1
0060  M = 4
0061  IF (EPK - EXOVR) 32,32,34
0062  32 N = 7
0063  M = 11
0064  34 EFLOG = DCNST(N)

```

```

0065      L = N+1
0066      DO 36 I = L,M
0067 36     EFLOG = EFLOG + DCNST(I) * ELOG ** (I-N)
0068      EFF = EXP (EFLOG)
0069      GAHAS = VALUE * GGSQ * GCORR / (EFF * GLOST)
0070      RD = .7 * DCNST(14)
0071      VALUE = (1. + RD / GG) * SQGCR
0072      RETURN
0073      END

```

```

C      CALMU
0001  SUBROUTINE CALMU (M,XMU,EPK,ELOG,LABZ,AMAS,KABZ,EDGE,COFMU)
0002  REAL*8 COFMU
0003  DIMENSION LABZ(2),AMAS(2),KABZ(2),EDGE(2),COFMU(8,20)
0004  XMU = 0.0
0005  DO 10 L = 1,M
0006  DO 2 K = 1,20
0007  IF (LABZ(L) - KABZ(K)) 2,4,2
0008  2  CONTINUE
0009  WRITE (6,120)
0010 120  FORMAT ('CANNOT MAKE LIBRARY MATCH WITH MATERIALS SPECIFIED')
0011  K = 1
0012  4  ABSMU = COFMU (1,K)
0013  DO 6 J = 2,8
0014  6  ABSMU = ABSMU + COFMU(J,K) * ELOG ** (J - 1)
0015  ABSMU = EXP (ABSMU)
0016  IF (EPK - EDGE(K)) 7,7,8
0017  7  XJUMP = .10266 + .006798 * SQRT (EDGE(K)) + .0006539 * EDGE(K)
0018  ABSMU = ABSMU * XJUMP
0019  8  XMU = XMU + ABSMU * AMAS(L)
0020 10  CONTINUE
0021  RETURN
0022  END

```

```

C      CALGPM
0001  SUBROUTINE CALGPM (EPK,VALUE)
0002  REAL*8 COFMU
0003  COMMON/PASS/ENJ(20),IST,IEND,NUMSJ,NUMEJ,GAINJ,ZEROJ,ST1J,
1  ST2J,STRJ(20),NENUM,ALPJ,TAMP,TSLP,TLAMP,TLSLP,BKGSLP(2),
2  CFILE(3),SSS,YES,BK1,NGAIN,IREGG,LISTFG,DFILE(3),
3  YSUM(20),QFT(100),SDDF(20),SUMR(20),EDGE(20),NSMBL(20),
4  COFMU(8,20),MTLZ(5),CMPOS(5),NABS(5),ABSRB(5),DCNST(16),
5  NF1,NF2,GEOM,SURFC,SHPWT,DEPTH
0004  DATA MTRL/'GE'/
0005  ELOG = ALOG (.001 * EPK)
0006  SMU = 0.0
0007  DEPTH = 0.5 * DEPTH
0008  IF (NF1) 14,14,13
0009 13  CALL CALMU (NF1,SMU,EPK,ELOG,MTLZ,CMPOS,NSMBL,EDGE,COFMU)
0010 14  CALL GPM (EPK,ELOG,GEOM,SURFC,DEPTH,SMU,VALUE,GAMAS,DCNST)
0011  IF (EPK - 500.) 9,9,10
C      CORRECT FOR GE "DEAD LAYER" ATTENUATION.
0012 9  CALL CALMU (1,XMU,EPK,ELOG,MTRL,SMU,NSMBL,EDGE,COFMU)
0013  GAMAS = GAMAS * EXP (XMU)
0014 10  IF (NF2) 15,18,15
0015 15  ATN = 0.0
0016  CALL CALMU (NF2,AMU,EPK,ELOG,NABS,ABSRB,NSMBL,EDGE,COFMU)
C      ADJUST ABSORBER ATTENUATION TO ACCOUNT FOR GAMMAS TRAVERSING
C      THE ABSORBER AT SKEWED ANGLES.
0017  AMU = AMU * VALUE
0018  IF (AMU - 6.9) 16,17,17
0019 16  ATN = EXP (AMU)
0020 17  GAMAS = GAMAS * ATN
0021 18  VALUE = GAMAS
0022  RETURN
0023  END

```