GAMANL, A COMPUTER PROGRAM APPLYING
FOURIER TRANSFORMS TO THE ANALYSIS OF
GAMMA SPECTRAL DATA

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To The Analysis of Gamma Spectral Data

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GAMANL, A COMPUTER PROGRAM APPLYING FOURIER TRANSFORMS TO THE ANALYSIS OF GAMMA SPECTRAL DATA

by

T. Harper, T. Inouye*, and N. C. Rasmussen

Abstract

GAMANL, a computer code for automatically identifying the peaks in a complex spectra and determining their centers and areas, is described. The principal feature of the method is a data smoothing technique employing Fourier transforms. The smoothing eliminates most of the random fluctuations without effecting the spectral resolution and makes identification of maxima using a zero slope criterion possible. Using the same Fourier transform with different constants it is possible with a second transformation to improve the spectral resolution. The computer program has been written in FORTRAN IV for the M.I.T. IBM 360 model 65 computer and also for the Toshiba Electric Company G.E. 635 computer. The complete analysis of a 4096 channel spectrum containing one hundred twenty peaks requires about 75 seconds of computation time.

*Work done while on leave from Tokyo Shibaura (TOSHIBA) Electric Company, Ltd., Japan.
# TABLE OF CONTENTS

Abstract 2  
Figure Captions 4  

1. Introduction 6  

2. Theory 7  
   2.1 Data Smoothing 7  
   2.2 Background Subtraction 8  
   2.3 Resolution Improvement 9  
   2.4 Peak Selection and Intensity Determination 10  

3. Application of Method 12  
   3.1 Choice of Smoothing Filter Function 12  
   3.2 Choice of Resolution Improvement Filter Function 16  
   3.3 Transform Algorithm 23  

4. GAMANL - Description 24  

5. Conclusion 28  

Appendix A GAMANL List in FOURTRAN IV 29  
Appendix B List of GAMANL Input 74  
Appendix C Output From GAMANL, PKANAL Subroutine 80  
Appendix D Correction for System Nonlinearity 83  
Appendix E Background Calculation 84  
Appendix F Intensity Calculation 85  

References 86
Figure Captions

Figure 1 The absolute value of the Fourier transforms for two different 4096 channel γ-ray spectra. The energy width of a channel was changed as indicated. The solid lines indicate the approximate shape of the two components of $|F(\omega)|$.

Figure 2 The smoothing filter function $P(\omega)$ showing the shape for 3 different cutoffs used for the runs plotted in Fig. 3. A Gaussian shape with a $\sigma$ of $128 \times (\frac{2\pi}{4096})$ radian/channel is used to reduce function from unity to zero.

Figure 3 The effects of the three different filter functions of Fig. 2 on a doublet taken from the 0.971 keV/channel data. Curve (a) is the original data, curves (b, c and d) result when filter functions (b, c, d) are used. The four curves are arbitrarily displaced by $10^3$ counts for clarity of presentation.

Figure 4 The Fourier transform of a single peak and an unresolved doublet from the 0.724-keV/channel spectrum.

Figure 5 The upper curve $|G(\omega)|$ is the absolute value of Fourier transform of the smoothed background subtracted data of the 0.724-keV/channel spectrum. The lower curve $W(\omega)$ is the resolution improvement filter function used to produce Fig. 8. $1/H(\omega)$ is the inverse of the transform of a single spectral peak.

Figure 6 The observed data of an unresolved doublet from a
Figure Captions (Continued)

4096 channel spectrum having a 0.724-keV channel width.

Figure 7 The doublet of Fig. 6 following smoothing and background subtraction.

Figure 8 The unresolved doublet of Fig. 6 showing the effect of the Fourier transformation using the filter function $W(\omega)$ shown in Fig. 5. The small peaks on either side are spurious peaks introduced by the transformation process.

Figure 9 GAMANL Flow Diagram
1. Introduction

This paper describes a computer code employing Fourier transforms for analyzing complex \(\gamma\)-ray spectra such as those obtained with a Ge(Li) detector, multi-channel analyzer system. The code was originally developed to analyze the capture \(\gamma\)-ray spectra obtained with the M.I.T. triple coincidence spectrometer (1), but has since been used successfully on a variety of other spectral data. The object of the program is to automatically locate all the spectral peaks and determine their centers and areas. This problem has existed for a long time in spectroscopy and a number of methods for doing all or part of these operations have been proposed (2,3). Most of them were developed for NaI spectra where the total number of peaks was small and the peaks were identified by hand. In a Ge(Li) spectra there are often more than a hundred peaks so it becomes important to have a fast method for automatically identifying each peak. One method for doing this described by Mariscotti (4) uses a second difference to locate the peak. Our experience with second differences indicated that they tended to obscure weak peaks. Mariscotti has handled this problem by doing a multipoint smoothing of the second difference. In the approach described below we have chosen to smooth the original data by a Fourier transform method. Although the Fourier method was found to be a quick accurate way to locate the peaks, we had no runs on similar data using the Mariscotti code which would give a meaningful comparison of the two methods.

Section 2 of this paper describes the theory underlying the Fourier transform method. Section 3 indicates how the theory is applied to the actual data and shows typical results. Section 4 describes the computer code GAMANL. The appendices give the program list, input and partial output.
2. **Theory**

The method described here is an improved version of one we described earlier (5). It can be divided into four steps: 1) data smoothing, 2) background subtraction, 3) resolution improvement, and 4) energy and intensity determination of the peaks.

2.1 **Data Smoothing**

The smoothing of the observed data is accomplished by a Fourier analysis technique similar to that often used to separate the signal from the noise in communication theory. In communication theory a function of time is transformed into frequency space, multiplied by an appropriate filter function and then transformed back into time space. In the present case the original data is a function of energy or more exactly a function of channel number so the transformation is into inverse channel number space. By analogy we shall call this "energy frequency space", and use the symbol \( \omega \) which has units of radians/channel for the variable.

To describe the method mathematically, let the observed data \( f(E) \) be represented as the sum of two components

\[
f(E) = s(E) + n(E)
\]  

(1)

where \( s(E) \) is the true spectral information and \( n(E) \) is the noise which in this case is due principally to random fluctuations in the number of counts in a channel. The Fourier transform of \( f(E) \) denoted \( F(\omega) \) can be written in the usual notation as

\[
F(\omega) = \int_{-\infty}^{\infty} f(E) e^{-i\omega E} dE
\]  

(2)
or

\[ F(\omega) = S(\omega) + N(\omega) \]  

(3)

where \( S(\omega) \) and \( N(\omega) \) stand for the Fourier transforms of the components of \( f(E) \).

The success of the method depends upon \( S(\omega) \) and \( N(\omega) \) being different functions so that a filter function can be chosen which will eliminate at least part of \( N(\omega) \) without seriously affecting \( S(\omega) \). Fortunately this is true in most spectra since the spectral peaks are spread over a number of channels and so \( S(\omega) \) is made up principally of low frequencies. The noise on the other hand is channel to channel fluctuations and so \( N(\omega) \) contains many higher frequencies. Thus there will be a significant difference in \( N(\omega) \) and \( S(\omega) \) for cases when the spectral peaks are several or more channels wide and the method will be applicable.

Let us define the inverse transform

\[ s(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) P(\omega) e^{i\omega E} d\omega \]  

(4)

where \( P(\omega) \) is the filter function and \( s(E) \) will be a smoothed version of the original spectrum. The method of choosing \( P(\omega) \) is discussed later. For simplicity we have expressed all the transforms in their integral form; however, when the technique is applied to discrete data the transformations must be used in their discrete form.

### 2.2 Background Subtraction

In most cases the spectral peak sits on a background which must be subtracted in order to accurately determine the peak area. This background is the result of a number of processes in the source and in the detector and it often can not be expressed accurately
analytically. We have found that to a good approximation
the background can be represented as a slowly varying func-
tion which connects all the minima in the smoothed data
$s(E)$. Care must be exercised in applying this definition,
however, since the minima which occur in the case of par-
tially resolved peaks must be excluded. This is accomplished
by setting a maximum value for the slope of the background.
When the slope connecting two successive minima exceeds this
maximum value the minima is ignored and the background line
is connected to the next minima which will give an accept-
able slope. The smoothed background subtracted data is
designated $g(E)$.

2.3 Resolution Improvement

In complicated spectra such as those from $(n,\gamma)$
reactions there are a number of cases where lines are
only partially resolved. In order to determine the peak
centers accurately, it would be helpful to have a higher
energy resolution. Because of our knowledge of the res-
ponse of the detector to a monoenergetic $\gamma$ ray the math-
ematical limit of resolution is somewhat better than the
apparent limit usually expressed as the FWHM (full width
of half maximum) of a peak. The detailed theory under-
lying this method has already been described in the liter-
ature by Inouye (6) where it was applied to NaI spectra.
Here we briefly restate the results and show their appli-
cability to Ge(Li) spectra as well. To understand the
method let us consider Eq. 5.

$$g(E) = \int_{-\infty}^{\infty} h(E-E') \ j(E') \ dE'$$

where $g(E)$ is the smoothed background subtracted data
which can be expressed analytically as the integral
where $h(E-E')$ is the response function of the detector
and $j(E')$ is the incident spectra which in this case may
be considered to be a series of δ functions in energy as expressed in Eq. 6.

\[ J(E') = \sum_{i} A_{i} \delta(E' - E_{i}) \]  

(6)

Since Eq. 5 is a convolution integral, its transform can be expressed as

\[ G(\omega) = H(\omega) J(\omega) \]  

(7)

Now since we can experimentally determine \( g(E) \) and \( h(E' - E) \) we can calculate \( G(\omega) \) and \( H(\omega) \) and can therefore determine \( J(E) \), the incident spectrum as shown by Eq. 8.

\[ J(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)/H(\omega) e^{i\omega E} d\omega \]  

(8)

\[ = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega) W(\omega) e^{i\omega E} d\omega \]

where \( W(\omega) = \frac{1}{H(\omega)} \) is the resolution improvement filter function. The problem in practice is that \( g(E) \) has some noise in it since the smoothing processes eliminate only part of noise \( n(E) \) and the background subtraction also introduces some error. Thus there is no function \( W(\omega) \) which will exactly reproduce the input δ functions. Nevertheless, as will be evident in the next section, it is possible to obtain a significant increase in the apparent resolution using this procedure. The principal thing which limits this procedure is the statistical accuracy of the original data.

\[ \Rightarrow \]

2.4 Peak Selection and Intensity Determination

The peak selection is accomplished by identifying each maximum in the smoothed background subtracted data \( g(E) \). The peak center is obtained by finding the point of
zero slope of a 2nd order fit to the top of the peak. The accuracy of this procedure was checked by comparing the results for a number of peaks to those obtained by finding the centroid of a Gaussian which had been fit to the peak by a least squares method. The results agreed within ± 0.1 channels on peaks with a \( \sigma = 1.5 \) channels. In terms of energy this was an accuracy of about ± 0.2 keV and was considerably better than the overall reproducibility of about 0.7 keV of typical runs. However, where greater accuracy is required more sophisticated peak fitting methods (e.g., Ref. (3)) can be used. The peak center in channel number is converted to energy using calibration lines of known energy and a correction is made for the small nonlinearities of the system.

To determine the intensity of a \( \gamma \) ray it is necessary to know the peak area and both the intrinsic and geometric efficiency of the system. In addition, in the capture \( \gamma \)-ray work it was desired to convert this intensity into the number of \( \gamma \) rays per 100 captures. The number of captures was calculated by the code using a measured incident flux and the known cross section.

The area under a spectral peak was determined by two different methods. The first method simply added up all the counts between successive zeros in the smoothed background subtracted data. As noted earlier, cases of doublets and triplets were identified and treated separately. In a majority of the cases this method worked very well. However, occasionally a peak will have a small bump in its tail that is not picked up by the doublet identification method. When this happens in small peaks it can lead to a large error in peak area. To check this a second method of peak area determination developed by Hamawi (7) was added to the program.

The second method takes advantage of the fact that we know that spectral peaks are very nearly true Gaussians, and further, from a careful study of strong isolated peaks in the spectrum, the standard deviation as a function of energy can be determined. The peak area is then determined by
finding the peak center as before. Using the height of the peak and its standard deviation, the area is calculated.

3. **Application of Method**

3.1 **Choice of Smoothing Filter Function**

To determine the proper smoothing filter function it is useful to plot $|F(\omega)|$ vs. $\omega$. Such a plot for two typical 4096 channel spectra are shown in Fig. 1. The actual transformation used gives one $\omega$ point for each energy point. For clarity of presentation we have actually plotted only every fiftieth point in $\omega$ space. The x's represent a run where the gain was adjusted to produce a channel width of 0.971 keV. The circles represent a lower gain which gave a 2.063-keV channel spacing. The approximate shape of the components of $F(\omega)$ are shown as the solid lines. As expected in the 0.971-keV run where the peaks contain more channels the signal component $S(\omega)$ contains less high frequencies. The filter function must be of a form that passes frequencies below the break in the curve but eliminates those frequencies above the break where the noise component $N(\omega)$ dominates. A filter function shape that was found to work well is shown in Fig. 2. The three different curves represent functions with different cutoffs. A Gaussian shape used to reduce the curve from unity to zero has $\sigma = 128$. It is important that the filter function be a smoothly varying function in order that oscillations not be introduced in the inverse transformation. To illustrate the effect of changing the cutoff frequency that data used to obtain the 0.971 keV/channel curve of Fig. 1 was processed using the three different filter functions shown in Fig. 2. A portion of the 4096 channel spectrum showing the effect of each of these filter functions on a doublet is shown in Fig. 3. The cutoff that begins at $412 \left(\frac{2\pi}{4096}\right)$ rad/channel is the one predicted from Fig. 1 and it produces considerable smoothing action without decreasing the peak to valley ratio in the doublet. For clarity the curves were arbitrarily shifted by 1000 counts/
Figure 1
SMOOTHING FILTER FUNCTIONS

$\omega$ in units of $\frac{2\pi}{4096} = 0.001534$ radians

Figure 2
Figure 3

CURVES DISPLACED VERTICALLY BY $10^3$ COUNTS
channel. Careful analysis also revealed that the peak centers were not shifted by the smoothing process. In addition the smoothing action is rather insensitive to both the location of the cutoff and $\sigma$ of the Gaussian. Variations of 10 to 15% in either of these quantities gave appreciably the same results. Thus the same filter function can be used on all runs of approximately the same gain. As expected the function with the higher cutoff does not produce as much smoothing and the very low cutoff produces so much smoothing that considerable spectral information is lost.

3.2 Choice of Resolution Improvement Filter Function

According to the theory discussed above $W(\omega) = 1/H(\omega)$ where $H(\omega)$ is the transform of the response of the system to a unit $\delta$ function input. The $H(\omega)$ can be determined by carefully analyzing the response of the system to a single $\gamma$ ray. Figure 4 shows the transformation for a large single peak and also for an unresolved doublet. The case of the unresolved doublet will be discussed later. The function $1/H(\omega)$ is obtained using the normalized $A \cdot H(\omega)$. In Figure 5 the normalized function $1/H(\omega)$ is plotted for the singlet shown in Fig. 4. The function $|G(\omega)|$ is the transform of the smoothed data for the entire spectrum from which the single line was taken. Its cutoff is different from the previous examples because the gain for this run was set to give 0.724 keV/channel.

Although the theory predicts that $1/H(\omega)$ is the best filter function to use, in practice this is not the case because of the noise. As can be seen the function $1/H(\omega)$ increases without limit as the frequency increases. This would create no problem in the absence of noise since the signal tends toward zero equally rapidly but when the noise is multiplied by this very large value it produces many artificial peaks when the inverse transform is carried out. To eliminate this problem we have found that it is necessary
Figure 4

\[
\omega \text{ IN UNITS OF } \frac{2\pi}{1024} = 0.006136 \text{ RADIANS/CH. NO.}
\]
Figure 5
that $1/H(\omega)$ return to zero at frequencies above the cutoff in $G(\omega)$. By trial and error it has been found that a Gaussian plus a constant is a very satisfactory function for accomplishing the desired result. This function has four adjustable parameters: the center, amplitude, standard deviation of the Gaussian and the constant, all of which must be optimized for the data being analyzed. Once this is done for runs of a given gain it works equally well for subsequent runs at approximately the same gain.

In order to demonstrate the method the doublet of Fig. 3 was recorded under conditions which produced a much worse energy resolution in the system. The original data from this run in the region of the doublet are shown in Fig. 6. Figure 7 shows the results of smoothing and background subtraction as described above. The curve marked $|G(\omega)|$ in Fig. 5 is the transform of the smoothed background subtracted data. This was multiplied by the function $W(\omega)$ and the inverse transformation produced the doublet shown in Fig. 8.

Note that although a dramatic increase in resolution is possible the process introduces small fictitious peaks on either side of the doublet. The result is that the technique is fine for examining a specific doublet to determine its components but it cannot be applied in this drastic manner to the entire spectrum without introducing a number of small spurious peaks which will interfere with the identification of real, small peaks. In addition the area under a peak is sometimes changed by a spurious peak from a nearby true peak. In practice, therefore, all peaks are identified and their areas, centers and widths determined prior to the second transformation. Then those peaks with widths greater than expected are examined by the above process to locate the position of their components. The amplitude of the components is then determined by adjusting them to best fit the unresolved doublet in the smoothed data.

It has been found that if the function $W(\omega)$ is not properly chosen it can shift the position of the components
Figure 6

OBSERVED DATA

CHANNEL NUMBER

COUNTS/CHANNEL x 10^3
Figure 7

SMOOTHED DATA

COUNTS/CHANNEL x 10^3

CHANNEL NUMBER

3140 3150 3160 3170 3180 3190 3200 3210 3220 3230 3240 3250 3260
Figure 8

RESOLUTION IMPROVED DATA

COUNTS / CHANNEL $\times 10^3$

CHANNEL NUMBER

Figure 8
by as much as 1 to 2 channels in data of the type shown here. It is necessary, therefore, to test the function prior to using it. The check that has been used consists of locating the peak centers of the single isolated peaks of the spectrum as described earlier and then performing the transformation using the proposed $W(\omega)$. If there is no resulting shift in the centers of single isolated peaks then the function is assumed to be satisfactory.

It is not always possible to know if the peak is an unresolved doublet. It is possible to check this, however, by looking at the transform of the peak in question. The transform of the unresolved doublet of Fig. 7 is shown in Fig. 4 where it is compared to a singlet peak from the same spectrum. The very noticeable minimum characteristic of doublets is explained by Inouye in Ref. 6.

3.3 Transform Algorithm

A computer code, GAMANL, has been developed for carrying out the gamma spectra analysis discussed above and is described in Section 4. One of the problems encountered with the use of the Fourier Transform equations in their usual form is that $N^2$ computation operations are required where $N$ is the number of points in energy space, i.e. the number of channels in the spectrum. This means that for $N = 4096$ the computing time becomes quite long, being on the order of $1/2$ hour. Two methods have been used to greatly reduce this computation time. The first method used was to section the data into $n$ smaller segments and to take the transform of each segment separately. This results in $n \left( \frac{N}{n} \right)^2$ operations and reduces the computation time by a factor of $\frac{1}{n^2}$. For a section length of 16 channels flanked by 10 and 11 channels on each side to correct for end effects, the sectioning method for $N = 4096$ channels required $256 \left( \frac{37}{4096} \right)^2$ operations or time reduction of a factor of $\frac{256 \left( \frac{37}{4096} \right)^2}{\left( \frac{1}{210} \right)^2} \approx \frac{1}{210}$ as compared to the direct method.
The second method used the Fast Fourier Transform (FFT) as developed by Cooley and Tukey (8). The time required by the FFT to transform $N$ energy points is $N(\log_2 N)$, which reduces the computation time by a factor of $\log_2 N/N$ as compared with the usual transformation. Thus for a 4096 channel spectra the time used by the FFT is $\log_2 4096/4096 = 1/256$ of the direct transform. In addition it gives a complete set of Fourier coefficients in $\omega$ space useful in the filter function determination. The sectioning does not give these coefficients in as convenient a form.

4. **GAMANL - Description**

The block diagram of GAMANL is given in Fig. 9. The program described here uses the FFT method of carrying out the transformation. The data for calculating the linearity of the multichannel analyzer system is read in first and calculated using subroutine LINEAR. A description of this subroutine is given in Appendix D. These correction factors are stored in the CNTR and CORR array. They are used later in determining the energy of a gamma peak.

The Smoothing and Improved Resolution parameters are then read in along with the efficiency data, run parameters and the gamma spectra input data. The spectra data is printed out and the smoothing filter function (determined by the input parameters) is calculated.

The data is smoothed by the use of the CTFFT subroutine. The Fast Fourier Transform is carried out by FOURT, a subroutine supplied by the MIT Computation Center and written by N. Brenner (9). Subroutine CTFFT performs the actual filtering of the data in which FOURT is used twice, once for the direct transform and again for the inverse transform after the data has been multiplied by the smoothing filter function. The magnitude of the Fourier coefficients in $\omega$ space are also printed out in CTFFT.
Upon return to the MAIN program the smoothed data is printed out and the background calculation and subtraction are carried out in subroutine BAKSUB, described in Appendix E.

Returning to the MAIN program the background and the smoothed, background-subtracted data are printed out. If no improved resolution is performed the program skips to the printing out of the background for every 10\textsuperscript{th} point. This is done so as to be able to use the array storing the background, TBL, for other purposes such as storing the peak parameters in PKANAL.

If improved resolution is carried out, the improved resolution filter function is calculated using the input parameters. The Fourier Transform of the smoothed, background-subtracted data is calculated using CTFFT and FOURT. The magnitudes of the Fourier Coefficients are printed out. The data in \( \omega \) space is filtered using the improved resolution filter function. The inverse Fourier Transform is carried out by FOURT and CTFFT. Returning to the MAIN program the improved resolution, background-subtracted, smoothed data is printed out along with the background for every 10\textsuperscript{th} point.

The energy calibration data for two peaks is read in; if the analysis is to be stopped the program transfers to the end of MAIN and stops. If the analysis is to continue subroutine PKALIB is called and the peak center, height and variance of the two energy calibration peaks are calculated. The linearity correction factors as calculated in LINEAR are used in subroutine ADJUST to calculate the corrected peak centers for the calibration lines. From the two calibration peaks the linear relation between channel number (corrected for linearity) and energy is determined.

The calculated calibration data and other data parameters are printed out and subroutine PKLOC is called. PKLOC locates and numbers the peaks using a first difference calculation; and prints out the number of peaks in the
Subroutine PKANAL performs the analysis of the spectral peaks. It is broken into two main parts. The first of which is the determination of a second order equation to determine the full width at half-maximum, FWHM, as a function of energy (channel number). A least squares fit is used using only the strong peaks of the spectra. From the equation so determined the FWHM of any peak can be calculated. It is this FWHM that is used in the Gaussian area calculation. The second part analyzes each peak in order of increasing energy. The data from PKLOC are used to determine if the particular peak considered is in singlet, doublet, triplet, or higher multiplet form. Each case is considered separately, while in the higher multiplet case the three strongest peaks are identified and then considered as a triplet case. Certain criteria are applied to the peak being considered, namely that it must have an area error less than a specified maximum value as determined from the input data. If it satisfies this criteria then the peak number, energy, center (channel number), height in counts, height to background ratio, area by summation method, area by Gaussian method, intensity, percent error in area by Gaussian method, FWHM measured, FWHM calculated by second order equation, width at base and multiplet order of peak are calculated and printed out.

The energy and peak center calculation use the linearity correction factors from LINEAR with the calculation being done in subroutine ADJUST. The intensity calculation uses the efficiency versus energy data, flux, cross section, time, and geometry corrections, and is performed by subroutine INTSTY, described in Appendix F.

After completing PKANAL the program returns to MAIN and reads a dummy variable MO. If there is more data, the program returns and reads the new data. If there is no more data the program is ended.

Compilation of the entire program required 50 seconds.
on the MIT System 360/65 computer. Execution of a 4096 channel data deck containing approximately 120 peaks with the improved resolution section being used, and thus requiring four transforms of 4096 channels took 74.8 seconds using the compiled machine deck. The final tabular output of PKANAL of this run is shown in Appendix C. An input list to GAMANL is given in Appendix B. The program list of GAMANL in FORTRAN IV is given in Appendix A.

5. Conclusion

The above program has been used at both M.I.T. and the Central Research Laboratory of Toshiba Electric Company on a wide variety of γ-ray spectra (10). In all these applications it has been found to be a fast, accurate method for automatically locating peaks and determining their centers and areas. As noted the smoothing allows the use of approximate methods for determining peak centers and the background function without serious loss of accuracy. In some very precise applications it may be desirable to use more exact methods for this but for the spectra studied the accuracy of the approximate methods was acceptable. The program is available in FORTRAN IV.
APPENDIX A

List of GAMANL, gamma analysis program, by subroutine. Subroutine FOURT was supplied by the M.I.T. Computation Center.
DATA ANALYSIS USING ORIGINAL DATA

COMPLEX DATA

COMMA DATA(4096), TBL(4096), TEK(4096), WT(4096), DTS(4096), CNTR(200)

1, CORR(200), EFFCY(100)

COMMNC IPUNCH, JREAD, JPRINT, JPUNCH

JREAD = 5
JPRINT = 6
JPUNCH = 7

LINEARITY CALCULATION

READ (JREAD, 200) LR, NOCHAN, N2, N3, XN, LIN

FORMAT (415, F5.0, 15)

C RUN NUMBER
C NOCHAN NUMBER OF CHANNELS IN THE LINEARITY RUN, NOCHAN LEQ 4095.
C N2 LOW CHANNEL PEAK NUMBER USED IN LINEARITY CALC.
C N3 HIGH CHANNEL PEAK NUMBER USED IN LINEARITY CALC.
C XN BACKGROUND SUBTRACTION LIMIT USED FOR LINEARITY CALC.
C IF LIN LEQ ZERO USES PREVIOUSLY CALC. LINEARITY DATA.

IF (LIN) 131, 131, 101

CONTINUE

CALL LINEAR (LRN2, N3, XN, NCH) GO TO 2002

WRITE (JPRINT, 152)

FORMAT (1, 14X, CTNTR ARRAY*, 5X, CCRR ARRAY*)

DO 132 M = 1, NOCHAN

READ (JREAD, 133) CTNTR(M), CCRR(M)

FORMAT (19X, F7.2, 9X, F7.2)

WRITE (JPRINT, 151) M, CTNTR(M), CCRR(M)

CONTINUE

FORMAT ('1, 4X, 15, 9X, F7.2, 5X, F7.2)

CONTINUE

CONTINUE

WT ARRAY DATA READ IN.

READ (JREAD, 1012) SIG1, MWTL01, WTC1, WTFL, SIG2, MWTL02, WTC2, WTFL

FORMAT (F5.0, 15, 2F5.2, F5.0, 15, 2F5.2)

SIG1 IS USED AS THE SIGMA IN WT FOR SMOOTHING
MWT01 IS USED AS THE CHANNEL NC AT WHICH THE SMOOTHING BEGINS
SIG2 IS THE SIGMA USED FOR WT IN IMP RES. CASE
MWT02 IS THE CHANNEL NC AGLTE WHICH THE IMP RES TAKES EFFECT.
MWT02 SHOULD BE LARGER THAN 3*SIG2 TO KEEP J1 FROM BEING LEQ 0.

IF MWTL02 IS LEQ 0 NO IMP RES IS DEEP.
DATE = 6-8222 11/31/52

C WTC1 AND WFT1 ARE CONSTANTS USEC IN WT SMOOTHING.
C WTC2 AND WFT2 ARE CONSTANTS USED IN WT IMPROVED RESOLUTION
0028 CONTINUE
0029 READ (JREAD,121) J2,FIREENG,DELENG
0030 121 FORMAT(15,2F5.0)
C J2 NUMBER OF POINTS IN THE EFFCY ARRAY
C FIRENG IS THE FIRST ENERGY (KEV) VALUE USED IN EFFICIENCY CALC.
C DELE IS THE ENERGY (KEV) DIFFERENCE BETWEEN EFFICIENCY POINTS.
C EFFCY EFFICIENCY DATA ARRAY.
0031 READ (JREAD,120) (EFFCY(I),I=1,J2)
0032 120 FORMAT (7E10.3)
C DATA READ IN
0033 CONTINUE
0034 READ (JREAD,1001) NUMRUN,NOCHAN,IMAX,DCR,ECR,BGER,IPUNCH,ERTM,
1 SANGLE,FLUX
0035 1001 FORMAT (3I5,F5.0,2F5.1,I5,F5.2,2E1C.4)
C NUMRUN THE DATA RUN NUMBER.
C NOCHAN NUMBER OF CHANNELS IN THE DATA RUN.
C IMAX CHANNEL NUMBER SLOPE CRITERION, CHANNELS LEQ IMAX ARE NOT
C ANALYZED.
C DCR SLOPE CRITERION USED FOR BACKGROUND CALCULATION.
C ECR ERROR CRITERION USED IN SUBROUTINE PKANAL.
C BGER THE CORRECTION FACTOR USED IN PKLOC TO LOCATE THE PEAKS.
C IPUNCH LESS THAN ZERO PUNCHES CUT PEAK ANALYSIS DATA
C IPUNCH EQUAL ZERO IMPLIES NO PUNCHED OUTPUT.
C IPUNCH EQUAL 1 PUNCHES OUT THE SMOOTHED DATA
C IPUNCH EQUAL 2 PUNCHES OUT THE SMOOTHED, BACKGROUND SUBTRACTED DATA
C IPUNCH EQUAL 3 PUNCHES OUT THE IMPROVED RESOLUTION DATA.
C ERTM IS THE ERROR TERM CORRECTION FACTOR DUE TO SMOOTHING. 1.69
C SANGLE IS THE SOLID ANGLE CORRECTION TERM
C FLUXT IS THE NUMBER OF CAPTURES/100 IN THE SAMPLE.
0036 READ (JREAD,100) (TBK(I),I=1,NOCHAN)
0037 C TBK IS THE DATA ARRAY
C NUM = NOCHAN + 1
C NUM SHOULD BE A POWER OF TWO FCR FASTEST RESULTS.
0038 TBK(NUM) = 0.0
0039 SUMOR = 0.0
0040 DO 1520 I = IMAX,NOCHAN
C SUMOR IS THE SUM OF NOCHAN-IMAX ORIGINAL DATA POINTS.
0041 1520 SUMOR = SUMOR + TBK(I)
0042 WRITE (JPRINT,1014) NUMRUN
0043 1014 FORMAT (1H1,4X,25H ORIGINAL DATA OF RUN NO ,I5)
0044 C LK = NOCHAN/10
0045 DO 1501 J = 1,LK
0046 1501 JU = J+10
0047 JL = JU - 9
C JU IS THE CHANNEL NUMBER FCR EVERY TENTH POINT
DATE = 68222 11/31/52

C START CF SMOOTHING OF TBK
C CALCULATION OF THE WEIGHTING ARRAY WT.

DO 134 I=1,NUM
134 WT(I) = WTC1 + WTF1
SIGSQ = SIG1*SIG1
NUP = NUM/2
DO 135 I=MWTLO1,NUP
WTPO = (FLOAT(I) - MWTLC1) * FLCAT(I - MWTLO1))/SIGSQ
WT(I) = WTC1 + WTF1 * EXP(-WTPO/2.C)
J = NUM - I

C SUBROUTINE CTFFT PERFORMS THE COOLEY-TUKEY FAST FOURIER TRANSFORM
CTFFT calculates the Fourier transform, filters the transformed data with WT and performs the inverse transform. The input array TBK is replaced by the filtered data at output.

CALL CTFFT (DATA, TBK, WT, NUP, JPRINT)

DO 1503 J = 1,LK
JU = J*10
CC76 WRITE (JPRINT,1504) (TEK(I),I=JL,JL),JU
1504 FORMAT(2X,10(F9.2,2X),16)
CC77 CONTINUE
C SUMSM = 0.0
DO 157 I=IMAX,NOCHAN
157 SUMSM = SUMSM + TBK(I)
C BACKGROUNd SUBTRACTION
CALL BAKSUB (NOCHAN, I, MAX, NCH)
C SUBROUTINE BAKSUB PERFORMS THE BACKGROUND SUBTRACTION ON ARRAY TBK. THE ORIGINAL TBK ARRAY IS REPLACED BY THE BACKGROUND
C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC82 LLO = 1

CC83 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC84 LLO = 1

CC85 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC86 LLO = 1

CC87 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC88 LLO = 1

CC89 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC90 LLO = 1

CC91 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC92 LLO = 1

CC93 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC94 LLO = 1

CC95 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC96 LLO = 1

CC97 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC98 LLO = 1

CC99 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC100 LLO = 1

CC101 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC102 LLO = 1

CC103 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC104 LLO = 1

CC105 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC106 LLO = 1

CC107 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC108 LLO = 1

CC109 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC110 LLO = 1

CC111 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC

CC112 LLO = 1

CC113 C SUBTRACTED ARRAY.

C SUBTRACTED BACKGROUND USES TBL ARRAY TO STORE THE BACKGROUND.

WRITE (JPRINT,154) NUMRUN

154 FORMAT (*1*,15,15)

C CALCULATED BACKGROUND CF RUN NO.

C LEVEL 1, MCC
IF (WWTLC2) 142,142,143
0126 CONTINUE
C CALCULATION OF WT FOR IMPROVED RESOLUTION CASE.
C SIGSG = SIG2*SIG2
C MSIG = SIG2
C NUP = WWTLC2 + 3 * MSIG
C DO 130 I = 1,NUM
C WTP0 = FLOAT(I-WWTLO2)*FLCAT(I-WWTLC2)/SIGSQ
C WT(I) = WTLC2 + WTP2 + EXP(-WTF2/2.0)
C WT(J1) = WT(I)
C J4 = NLM - WWTLO2 + I - WWTLC2
C WT(J4) = WT(I)
C J3 = NLM - I
C WT(J3) = WT(I)
C CONTINUE
C CALL CTFFT (DATA,TBK,HT,NUP,JPRINT)
C C NEGLICTING ALL CHANNELS WITH CCATS LEQ 2.C.0.
C DO 130 I = 1,NUM
C IF (TBL(I)) 162,162,163
C CONTINUE
C TBL(I) = 0.0
C CONTINUE
C TBL(I) = 0.0
C IF (CUM) 139,139,138
C CONTINUE
C WRITE (JPRINT,140)
C FORMATTED DATA CP RUN NC *.15)
C WRITE (JPRINT,150) SIG2,WWTLC2,WTLC2,WT2
C 150 FORMAT ('*',*,*,*,*)
C 150 WRITE (JPRINT,1507) (TEK(I),I=JL,JA)
C CONTINUE
C JA = JU + 1
C WRITE (JPRINT,1502) (TEK(I),I=JA,JCHAN)
C IF (IPLNCH-3) 142,144,142
C 144 WRITE (JPRINT,100) (TBK(I),I=1,JCHAN)
CONTINUE

WRITE (JPRINT,159) (*1,*,BACKGROUND DATA FOR EVERY TENTH POINT *)

J10 = NCCHAN/10
DO 160 I =1,J10
K = 10 * I - 9
160 TBL(I) = TBL(K)
WRITE (JPRINT,161) (TBL(I),I=1,J10)
FORMAT (('1',10(F9.2,2X)))
CALIBRATION OF DATA USING TWO ENERGY STANDARDS.
READ (JREAD,1002) EGAM1,IP1,EGAM2,IP2,FPS,ERFW
EGAM1 IS THE ENERGY (KEV) OF THE FIRST CALIB. PEAK.
EGAM2 IS THE ENERGY (KEV) OF THE SECOND CALIB. PEAK.
IP1 IS THE PEAK CENTER OF THE FIRST PEAK.
IP2 IS THE PEAK CENTER OF THE SECOND PEAK.
FPS IS THE FIRST PEAK SIGMA USED IN PKEANL TO FIT THE FWHM.
ERFW IS THE RANGE THE FWHM IS ALLOWED TO DEVIATE FROM FPS.
FPS AND ERFW ARE GIVEN IN KEV.
IF ( EGAM1) .GT.146, CONTINUE
145 CONTINUE
CALL PKALIB (NCCHAN,EGAM1,IP1,EGAM2,IP2,SLP,WID1,WID2,
1 TPCL,TPC2)
SUBROUTINE PKALIB CALCULATES THE FWHM, TRUE PEAK CENTERS OF THE
CALIBRATION PEAKS, AND SLP TO CONVERT FROM CHANNEL NO. TO ENERGY.
PKALIB USES ADJUST TO CORRECT FOR THE NONLINEARITY OF THE SYSTEM.
WRITE (JPRINT,122) NUMRUN, NCCHAN
122 FORMAT (1H1,4X,9H RUN NC =,15,5X,22H NUMBER OF CHANNELS =,15)
WRITE (JPRINT,123) IMAX
123 FORMAT (5X,41H CHANNEL NUMBER SLPE CRITERION (IMAX) =,15)
WRITE (JPRINT,126) ECR
126 FORMAT ('1,4X,5H CRITERIA FOR PEAK ANALYSIS (PER-CENT) ',
1 F5.1)
WRITE (JPRINT,125) OCR
125 FORMAT (5X,51H CRITERIA FOR BACKGROUND IN UNITS OF SQRT OF,
14H BACKGROUND =, F6.2)
WRITE (JPRINT,120) BER
120 FORMAT (5X,65H CRITERIA FOR BACKGROUND IN UNITS OF SQRT OF BACKG
14HNU (EGER) =, F5.1)
WRITE (JPRINT,158) ERTW
158 FORMAT ('1,4X,5H CRITERIA FOR LINEARITY RLN NUMBER,5X,5H N2 =,15,5X,
15H N3 =,15,5X,5H XN =,F5.3)
WRITE (JPRINT,1019) FPS,ERFW
35
C192 1019 FORMAT ("*", 4X, "FIRST PEAK FWHM (KEV) FPS = ", F7.2, 5X, 
1 " FWHM VARIATION (KEV) ERFW = ", F7.2) 
WRITE (JPRINT,130) SLP 
C193 130 FORMAT ("*", 4X, "ENERGY PER CH. AC (KEV) = ", F6.3) 
C195 WRITE (JPRINT,128) EGAM1,IP1,TPC1,WID1 
C196 128 FORMAT ("*", 4X, "ENERGY-1 = ", F6.1, 4X, "CHANNEL NO = ", I6, 
1 4X, " TRUE PEAK CENTER = ", F6.1, 4X, "WIDTH (KEV) = ", F6.2) 
C197 WRITE (JPRINT,129) EGAM2,IP2,TPC2,WID2 
C198 129 FORMAT ("*", 4X, "ENERGY-2 = ", F6.1, 4X, "CHANNEL NO = ", I6, 
1 4X, " TRUE PEAK CENTER = ", F6.1, 4X, "WIDTH (KEV) = ", F6.2) 
C199 WRITE (JPRINT,149) SANCLEFLUX 
C200 149 FORMAT ("*", 4X, "SCLID ANGLE RADIANS = ", E10.4, 2X, "FLUX = ", 
1 E10.4) 
C201 WRITE (JPRINT,147) FIRENCE,CELEAC 
C202 147 FORMAT ("*", 4X, "EFFICIENCY DATA INITIAL ENERGY (KEV) = ", F5.0, 
1 2X, " DELTA ENERGY (KEV) = ", F5.0) 
C203 WRITE (JPRINT,148) (EFFCY(I),I=1,J2) 
C204 148 FORMAT ("*", 4X, 10(E10.3)) 
C
LOCATATION AND NUMBERING OF THE PEAKS 
SUBROUTINE PKLOC (NOCHAN,NI,IPAX,BCER) 
USING A FIRST DIFFERENCE CALCULATION IN THE CTS ARRAY. 
NI NUMBER OF THE PEAK. 

ANALYSIS OF THE GAMMA PEAKS 
SUBROUTINE PKANAL (NI,SLP,ECR,TPC1,EGAM1,WID1,FPS,ERFW,ERTM, 
1 FIRENCE,CELENG,SANGLE,FLUX1) 
SUBROUTINE PKANAL ANALYZES THE THE GAMMA PEAKS FOR AREA AND WIDTH 
FROM SINGLTS TO TRIPLETS. 

CONTINUE 
READ (JREAD,1008) MO 
1008 FORMAT (15) 
MO=1 PROGRAM LOOPS TO 2001,MO=2 PROGRAM LOOPS TO 2002, ETC. 
MO.LEC.0 CR MO.GTR.4 ENDS PROGRAM BY GOING TO 2010 
CONTINUE 
CALL EXIT 
END
SUBROUTINE LINEAR (LRN2, N3, XN, NCHAN)
C      SUBROUTINE LINEAR CALCULATES THE LINEARITY CORRECTION FACTOR
C      USING THE LINEARITY DATA GIVEN IN ARRAY TBL.
C      THE CORRECTION FACTOR, CORR, IS IN THE FORM OF AN ARRAY OF
C      DIMENSION L (L LEQ 200) CF THE L LINEARITY PEAKS CHARACTERIZING
C      THE DATA OF TBL.
C      THE ADJUST SUBROUTINE USES THE CORR FACTOR FOR ITS INTERPOLATION
C      TO CORRECT FOR LINEARITY.
C      XN IS THE LIMIT OF THE LINEARITY BACKGROUND. ONLY TRUE
C      CALIBRATION PEAKS ARE GT THAN XN.
C      TBL IS THE LINEARITY DATA.
C      N2 IS THE CHANNEL PEAK NO. CF THE LOW REFERENCE PEAK
C      N3 IS THE CHANNEL PEAK NO. CF THE HIGH REFERENCE PEAK.
C      CNTR(L) IS THE PEAK CENTER AS CALC BY WEIGHTING THE FIRST MOMENT
C      OF THE PEAK TO THE INTEGRAL UNDER THE PEAK.
C      CORR(L) IS THE LINEARITY CORRECTION FACTOR FOR THE L-TH PEAK.
C      SUM IS THE PEAK INTEGRAL.
C      XMOM IS THE FIRST MOMENT CF THE PEAK.
C      SLOPE IS THE LINEAR SLOPE BETWEEN THE N2 AND N3 PEAKS.
C
C      COMMON DATA
C      COMMON DATA (4096), TBL (4096), TBK (4096), WT (4096), DTS (4096), CNTR (200)
C      COMMON IPUNCH, JREAD, JPRINT, JPUNCH
C
0002 COMMON JNOCHAN, LNOCHAN, JNOCHAN, LNOCHAN, JNOCHAN, LNOCHAN
0003 COMMON I = 0, L = 0, I = 0
0004 I = I + 1
0005 IF (I = NOCHAN) GOTO 31
0006 J = J + 1
0007 IF (TBL(I) = XN) GOTO 3
0008 SUM = 0.
0009 XMOM = 0.
0010 DO 6 K2 = 1, J
0011 SUM = SUM + TBL(K1)
0012 XMOM = XMOM + FLOAT(K2) * TBL(K1)
0013 CONTINUE
0014 CONTINUE
0015 CONTINUE
0016 CNTR(L) = XMOM/SUM + FLOAT(I) - 1.0
0017 CONTINUE
0018 IF (L = NOCHAN) GOTO 3
0019 SLOPE = CNTR(N3) - CNTR(N2) / FLOAT(N3 - N2)
FORTRAN IV G LEVEL 1, MOD 2  LINEAR  DATE = 68214  20/05/11

0030       WRITE (JPRINT,9) LR,N2,N3,XN
0031       9 FORMAT ('1*,' LINEARITY RUN NUMBER ',I5,' N2 = ',I5,' N3 = ',
0032               1 I5,* XN = ',F5.0)
0033       WRITE (JPRINT,10)
0034       10 FORMAT ('0*14X,* CNTR ARRAY       CORR ARRAY *')
0035       DO 8 M=1,L
0036       CORR(M)=(CNTR(N2)+FLOAT (M-N2)*SLOPE)-CNTR(M)
0037       WRITE (JPRINT,11) M,CNTR(M),CORR(M)
0038       WRITE (JPUNCH,11) M,CNTR(M),CORR(M)
0039       11 FORMAT (' ',4X,I5,9X,F7.2,9X,F7.2)
0040       8 CONTINUE
0041       RETURN
0042       END
SUBROUTINE CTFFT (DATA,TBK,WT,NUM,JPRINT)

CTFFT TRANSFORMS THE ARRAY TBK, WEIGHTS IT WITH WT, AND PER-
FORMS THE INVERSE TRANSFORMATION.

DATA IS A COMPLEX ARRAY USED IN SUBROUTINE FOURT.

SUBROUTINE FOURT DOES THE ACTUAL FFT CALCULATION.

NUM SHOULD BE A POWER OF TWO FOR FASTEST RESULTS.

DO 1 I = 1,NUM
0005 DATA(I) = CMPLX(TBK(I),0.0)
0006 1 CONTINUE

C FAST FOURIER TRANSFORM Callable.

CALL FOURT (DATA,NUM,1,+1,+1,0)

C

DO 2 I = 1,NUM
0008 AR = REAL(DATA(I))
0009 AI = AIMAG(DATA(I))
0010 TBK(I) = SQRT(AR*AR + AI*AI)
0011 C TBK IS USED TO STORE THE MAGNITUDE OF EACH TRANSFORMED POINT.
0012 2 CONTINUE

W = 6.2831873/REAL(NUM)

NUM2 = NUM/2 + 2

WRITE (JPRINT,3) W

3 FORMAT (1H1,26H DELTA OMEGA IN RADIANS = ,F10.6)

WRITE (JPRINT,4)

4 FORMAT (1H1,19H TRANSFORM INTEGRAL)

WRITE (JPRINT,5) (TBK(I),I=1,NUM2)

5 FORMAT (1H1,10E11.4)

FILTERING THE TRANSFORMED DATA WITH WT(I).

DO 8 I = 1,NUM

SMOOTHING

DATA(I) = WT(I) * DATA(I)

8 CONTINUE

C INVERSE FOURIER TRANSFORM

CALL FOURT(DATA,NUM,1,-1,+1,0)

C

DO 10 I = 1,NUM

AR = REAL(DATA(I))

AI = AIMAG(DATA(I))

TBK(I) = SQRT(AR*AR + AI*AI)/REAL(NUM)

DIVIDING BY NUM IS TO CORRECTLY NORMALIZE THE OUTPUT DATA.

10 CONTINUE

RETURN

END
SUBROUTINE BAKSUB (NOCHAN,IMAX,DCR)

C SUBROUTINE BACKSUB
C PERFORMS THE BACKGROUND SUBTRACTION ON ARRAY C
C TBK. THE ORIGINAL TBK ARRAY IS REPLACED BY THE BACKGROUND C SUBTRACTED ARRAY.

COMPLEX DATA
COMMON DATA(4096),TBL(4096),TBK(4096),WT(4096),DTS(4096),CNTR(200)
1,CORR(200),EFFC(100)
COMMON IPUNCH,JREAD,JPRINT,JPUNCH

WRITE (JPRINT,498)
498 FORMAT(IH1,35X,37H CHosen MINIMA AND SLOPE BETWEEN THEM)
WRITE (JPRINT,499)
499 FORMAT(20X,29H NO. L CH. LEFT MIN , 131H RIGHT MIN SLOPE BASE)

JJ = NOCHAN - 1
DO 302 I = 1,JJ
302 DTS(I)=TBK(I+1)-TBK(I)
IMAX LOWER LIMIT ON SLOPE CRITERION.
LA = IMAX + 1
I = IMAX + 2
IMIN = 0
IX = 0
ILOOP = 0

XM NEGATIVE, DB POSITIVE DETERMINES A PEAK.
333 XM=DTS(I)*DTS(I-1)
DB=DTS(I)-DTS(I-1)
IF (XM) 305,305,303
305 IF (DB) 303,303,304
304 CONTINUE

GRADIENT CALCULATION FOR BACKGROUND UNDER THE PEAK.
310 GRAD=(TBK(I)-TBK(LA))/FLOAT (I-LA)

THE FIRST FOUR ELEMENTS OF THE TBL ARRAY ARE USED TEMPORARILY
C TO STORE THE SLOPES AND THE MINIMA OF TWO ADJACENT PEAKS

TBL(IX) = GRAD
TBL(IX+2) = FLOAT (I)
IF(IX-2) 303,564,564
CONTINUE
GRAD1 = TBL(1)
GRAD2 = TBL(2)
M1 IS THE RHS MINIMUM OF THE PEAK UNDER CONSIDERATION
AND M2 THE NEXT HIGHER MINIMUM
M1 = TBL(3)
M2 = TBL(4)
TB1 = TBK(LA) + GRAD1*FLOAT(M2-LA)
TB1 IS THE VALUE TBK(M2) WOULD HAVE IF THE ANGLE BETWEEN THE
TWO SLOPES WERE ZERO.
TB2 = TBK(M2)
TB12 = (TB1+TB2)/2.0
IF(TB12) 663,663,664
663 CRIT = DCR*FLOAT(M2-M1)
GO TO 665
664 CRIT = DCR*FLOAT(M2-M1)*SQRT(TB12)
665 CONTINUE
DCR IS READ IN AS DATA
IF(TB1-TB2) 565,565,666
666 IF(TB1-TB2-CRIT) 565,565,566
566 ILOOP = ILOOP + 1
667 I = M1
668 IX = 0
669 GO TO 303
665 ILOOP = 0
669 IX = 0
670 I = M1
THREE-POINT AVERAGING OF THE MINIMA
FROM HERE TO STATEMENT 533 THE PROGRAM AVERAGES THE MINIMA
BY WEIGHING THEM EQUALLY WITH THE ORIGINAL COUNTS IN THE TWO
CHANNELS CLOSEST TO THE MINIMUM (ONE ON EACH SIDE)
LL=I
LOOP = 0
IF THE AVERAGING PROCESS IS REPEATED MORE THAN 15 TIMES
FOR ANY ONE GIVEN MINIMUM THE AVERAGING PROCESS IS IGNORED
507 LOOP = LOOP + 1
508 IF(ILoop - 16) 525,510,510
525 CONTINUE
TB = (TBK(LL-1)+TBK(LL)+TBK(LL+1))/3.0
NEW MINIMA ARE SOUGHT
IF(TB-TBK(LL-2)) 603,603,602
602 IF(TB-TBK(LL-1)) 603,603,502
603 IF(TB-TBK(LL+2)) 503,503,604
604 IF(TB-TBK(LL+1)) 503,503,504
502 LL = LL-1
IF THE PROGRAM RETURNS TO THE ORIGINAL MINIMUM THE AVERAGING
C PROCESS IS STOPPED.
0062 IF(LL-I) 523,503,523
0063 523 CONTINUE
0064 IF(LL - LA) 303,303,507
0065 504 LL = LL + 1
0066 IF(LL-I) 524,503,524
0067 524 CONTINUE
0068 IF(LL-I-6) 507,510,510
C IF NO NEW MINIMUM IS FOUND WITHIN 6 CHANNELS ABOVE THE ORIGINAL
C MINIMUM THE AVERAGING PROCESS IS IGNORED
0069 510 LL = I
0070 GO TO 533
0071 503 CONTINUE
0072 TBK(LL) = (TBK(LL-I)+TBK(LL)+TBK(LL+1))/3.0
C C LA IS LOWER CHAN NO LIMIT FOR LINEAR BACKGROUND FIT.
C LL IS UPPER CHAN NO LIMIT FOR LINEAR BACKGROUND FIT.
0073 533 LB=LA+1
0074 LX=LL-1
C LBASE IS THE NUMBER OF CHANNELS OCCUPIED BY THE PEAK (FIRST CH=0)
0075 LBASE = LL - LA
C QSLOP IS THE SLOPE BETWEEN THE TWO MINIMA OF A PEAK
0076 C TBL IS A DUMMY ARRAY USED FOR CALCULATING THE BACKGROUND.
0077 TBL(LA)=TBK(LA)
0078 IF (LBASE - 8) 550,551,551
0079 551 CONTINUE
0080 IMIN = IMIN + 1
0081 WRITE (JPRINT,500) IMIN,LA,TBK(LA),TBK(LL),QSLOP,LBASE
0082 500 FORMAT(20X,17,3X,16,3XF9.2,3XF9.2,3XF9.3,3X,15)
0083 550 CONTINUE
C BACKGROUND - LINEAR FIT.
0084 DO 306 IK=LB,LX
0085 306 TBL(IK)=(TBK(LA)*FLOAT (LL-IK)+TBK(LL)*FLOAT (IK-LA))/FLOAT (LL-LA)
0086 LA=LL
0087 IF(I-LL) 520,303,303
0088 520 I = LL
0089 503 IF (I-JJ) 334,335,335
0090 334 I=I+1
0091 GO TO 333
0092 335 TBL(LA)=TBK(LA)
0093 LB=LA+1
0094 LX = JJ
0095 LL = NOCHAN
0096 DO 307 IK=LB,LX
0097 307 TBL(IK)=(TBK(LA)*FLOAT (LL-IK)+TBK(LL)*FLOAT (IK-LA))/FLOAT (LL-LA)
0098 TBL(NOCHAN) = TBK(NOCHAN)
0099 DO 404 I = 1, IMAX
0100 TBL(I) = TBK(I)
0101 TBK(I) = 0.0
0102 DTS(I) = 0.0
0103 IF (TBL(I)) 405, 404, 404
0104 405 TBL(I) = 0.0
0105 404 CONTINUE
0106 DO 401 I = IMAX, NOCHAN
0107 TBK(I) = TBK(I) - TBL(I)
0108 DTS(I-1) = TBK(I) - TBK(I-1)
   C CORRECTION FOR NEGATIVE VALUES.
0109 IF (TBL(I)) 406, 407, 407
0110 406 TBL(I) = 0.0
0111 407 CONTINUE
0112 IF(TBK(I)) 403, 403, 401
0113 403 TBK(I) = 0.0
0114 401 CONTINUE
0115 RETURN
0116 END
SUBROUTINE PKALIB (NOCHAN, EGAM1, IP1, EGAM2, IP2, SLP, WID1, WID2, 
1 TPC1, TPC2)

C PKALIB USES ADJUST TO CORRECT FOR THE NONLINEARITY OF THE SYSTEM.
C CALIBRATION PEAKS, ANS SLP TO CONVNET FROM CHANNEL NO. TO ENERGY.
C SUBROUTINE PKALIB CALCULATES THE FWHM, TRUE PEAK CENTERS OF THE 
COMPLEX DATA

COMMON DATA(4096), TBL(4096), TBK(4096), WT(4096), DTS(4096), CNTR(200) 
1, CORR(200), EFFCY(100)

COMMON IPUNCH, JREAD, JPRINT, JPUNCH
JJ = NOCHAN - 1
DO 622 I = 1, JJ
DTS(I) = TBK(I+1) - TBK(I)
CONTINUE
DTS(NOCHAN) = 0.0
JP = 0
IP = IP1 - 3

SM = DTS(IP)*DTS(IP-1)
DP = DTS(IP)-DTS(IP-1)
IF (SM) 615, 615, 613
IF (DP) 617, 613, 613
IP = IP+1
GO TO 631

C PCNR IS PEAK CENTER.
617 PCNR = IP + DTS(IP)/(DTS(IP-1)-DTS(IP)) + 0.5
C GX IS A SECOND ORDER INTERPOLATION FIT.
619 GX = 0.5*(TBK(IP) + (PCNR-FLOAT(IP))*(DTS(IP)) + 0.5 * 
1*(PCNR-FLOAT(IP))*(PCNR-FLOAT(IP+1))*(DTS(IP)-DTS(IP-1)))

C SUBROUTINE ADJUST CALCULATES THE TRUE PEAK CENTER, TPC, USING 
DATA FROM THE LINEARITY SUBROUTINE.
CALL ADJUST (CNTR, CRR, PCNR, TPC)

C TPC1 TRUE PEAK CENTER FOR THE LOW ENERGY STANDARD.
620 TPC1 = TPC

C GX1 HALF MAXIMUM OF LOW ENERGY STANDARD.
622 GX1 = GX
JP = JP+1
IP = IP2 - 3
GO TO 631

C TPC2 TRUE PEAK CENTER FOR THE HIGH ENERGY STANDARD.
621 TPC2 = TPC

C GX2 HALF MAXIMUM OF HIGH ENERGY STANDARD.
628 GX2 = GX
C SLP SLOPE USED TO CONVNET CHANNEL NUMBER TO ENERGY.
629 SLP = (EGAM2-EGAM1)/(TPC2-TPC1)
JP1 = 0
GO TO 631

C SLP SLOPE USED TO CONVNET CHANNEL NUMBER TO ENERGY.
629 SLP = (EGAM2-EGAM1)/(TPC2-TPC1)
JP1 = 0
GO TO 631

C SLP SLOPE USED TO CONVNET CHANNEL NUMBER TO ENERGY.
629 SLP = (EGAM2-EGAM1)/(TPC2-TPC1)
JP1 = 0
GO TO 631
IF (TBK(J)-GX) 670,670,671
J=J-1
GO TO 672

PHL = CHANNEL NUMBER OF LOW ENERGY SIDE FOR FWHM CALCULATION.
PHL=FLOAT (J)*((GX-TBK(J))/(TBK(J+1)-TBK(J))
J=NP
682 IF (TBK(J)-GX) 680,680,681
681 J=J+1
GO TO 682

FWHM = FULL WIDTH AT HALF MAXIMUM.
FWHM=FLOAT (J)-(GX-TBK(J))/(TBK(J-1)-TBK(J))-PHL
WIDD = FWHM * SLP
WIDD IS FWHM IN KEV
IF (JP1) 686,686,687
JP1 = 0 AT BEGINNING.
WID1 = WIDD
WID1 IS FWHM (KEV) OF FIRST CALIB PEAK.
THE VARIANCE OF THE PEAK CAN BE OBTAINED FROM THE FWHM.
686 WID1 = WIDD

WID2 = WIDD
WID2 IS FWHM (KEV) OF SECOND CALIB PEAK.
RETURN
SUBROUTINE ADJUST (CNTR, CCRR, PCNR, TPC)

REAL CNTR(200), CCRR(200)

C SUBROUTINE ADJUST FINDS THE TRUE PEAK CENTER, TPC, BY CORRECTING
C THE DATA PEAK CENTER, PCAR, BY GX.
C GX IS DETERMINED BY A SECOND ORDER INTERPOLATION USING CNTR, THE
C CALCULATED PEAK CENTER, AND CORR, THE LINEARITY CORRECTION FACTOR
C FROM THE LINEARITY SUBROUTINE.
C A CALL TO LINEAR MUST PRECEDE A CALL TO ADJUST.

IOTA = 1
11 IF (CNTR(IOTA) - PCNR) 10, 10, 20
10 IOTA = IOTA + 1
20 GO TO 11

G1 = CORR(IOTA - 1)
G2 = CORR(IOTA)
G3 = CORR(IOTA + 1)
C1 = CNTR(IOTA - 1)
C2 = CNTR(IOTA)
C3 = CNTR(IOTA + 1)

CX = PCNR
D12 = (G2 - G1) / (C2 - C1)
D23 = (G3 - G2) / (C3 - C2)
D123 = (D23 - D12) / (C3 - C1)
GX = G1 + (CX - C1) * D12 + ((CX - C1) * (CX - C2) * D123)

TPC = PCAR + GX
RETURN
END
SUBROUTINE PKLOC (NOCHAN, NI, IMAX, BER)
C SUBROUTINE PKLOC LOCATES AND NUMBERS THE PEAKS OF THE TBK ARRAY
C USING A FIRST DIFFERENCE CALCULATION IN THE DTS ARRAY.
C NI NUMBER OF THE PEAK.
C COMPLEX DATA
COMMON DATA(4096), TBL(4096), TBK(4096), WT(4096), DTS(4096), CNTR(200)
1, CORR(200), EFFCY(100)
COMMON IPUNCH, JREAD, JPRINT, JPRUNC
NN = 0
JJ = NCCHAN - 1
I = IMAX
C ZM LEQ ZERO, DS LT ZERO DETERMINES A PEAK MAXIMUM.
ZM = DTS(I)*DTS(I-1)
DS = DTS(I) - DTS(I-1)
IF (ZM) 715, 715, 713
715 CONTINUE
C PEAKS WITH COUNTS LEQ CTLIM AT THEIR MAXIMUM WON'T BE ANALYZED.
K = I/10 + 1
IF (TBL(K)) 719, 720, 720
719 CTLIM = 10.0
GO TO 721
720 CONTINUE
721 CONTINUE
CTLM = BER*SQR(TBL(K)) + 10.0
721 CONTINUE
IF (TBK(I) - CTLIM) 713, 713, 718
718 CONTINUE
NI = NI + 1
C NI NUMBER OF THE PEAK.
C THE TBL DATA IS DESTROYED AND PTS 1 TO 1000 ARE USED FOR THE
C BACKGROUND DATA ARRAY. PTS 1001 AND UP ARE USED FOR LOCATING THE
C GAMMA PEAKS BY CHANNEL NUMBER FOR PEAK MAXIMUM.
TBL(NI+1000) = I
C TBL(NI+1000) IS THE CHANNEL NUMBER OF THE PEAK
IF (NI - 595) 713, 713, 732
713 CONTINUE
I = I + 1
IF (I - JJ) 731, 731, 732
731 CONTINUE
DO 733 J = 1, 5
NU = NI + J + 1000
733 CONTINUE
C TBL(NU) DUMMY VARIABLE FOR Pkanal SUBROUTINE.
TBL(NU) = TBL(NI+1000) + 15.0
RETURN
END
SUBROUTINE INTSTY (SAREA, EGAM, FIRENG, DELENG, SANGLE, FLUXT, AIGAM)
C
FUNCTION FINDS THE EFFICIENCY OF THE SYSTEM AT THE GAMMA PEAK
C
DATA IN THE EFFCY ARRAY AS THE KNOWN POINTS.
C
SAREA TOTAL COUNTS PER GAMMA PEAK.
C
FIRENG IS THE FIRST ENERGY (KEV) VALUE USED IN EFFICIENCY CALC.
C
DELE IS THE ENERGY (KEV) DIFFERENCE BETWEEN EFFICIENCY POINTS.
C
SANGLE IS THE SOLID ANGLE CORRECTION TERM
C
FLUXT IS THE NUMBER OF CAPTURES/100 IN THE SAMPLE.
C
AIGAM IS THE PEAK AREA CORRECTED FOR EFFCY. SOLID ANGLE, AND FLUX.
C
COMMON DATA
COMMON DATA(4096), TBL(4096), T8K(4096), WT(4096), DTS(4096), CNTR(200)
1, CORR(200), EFFCY(100)
COMMON IPUNCH, JREAD, JPRINT, JPUNCH
IEGAM=2
8 XEGAM = DELENG*FLOAT(IEGAM-1) + FIRENG
   IF (XEGAM-EGAM) 26, 27, 27
26 IEGAM=IEGAM+1
   GO TO 8
27 E1 = XEGAM - DELENG
   E2=XEGAM
   E3 = XEGAM + DELENG
   G1=EFFCY(IEGAM-1)
   G2=EFFCY(IEGAM)
   G3=EFFCY(IEGAM+1)
   D12=(G2-G1)/(E2-E1)
   D23=(G3-G2)/(E3-E2)
   D123=(D23-D12)/(E3-E1)
   GX = (G1 + (EGAM-E1)*D12 + (EGAM-E2)*D123)
AIGAM = SAREA/(GX*SANGLE*FLUXT)
RETURN
END
SUBROUTINE PKANAL (N1, SLIP, ECR, TPC1, EGAM1, WID1, FPS, ERFW, ERTM, 
1, FIRENG, DELENG, SANGLE, FLUX1)

SUBROUTINE PKANAL

SUBROUTINE PKANAL ANALYZES THE GAMMA PEAKS FOR AREA, WIDTH,
HEIGHT, MINIMA, BASE WIDTH AND BASE SLOPE

COMMON DATA (4096), TBL (4056), TBK (4056), WT (4096), DTS (4096), CNTR (200)
1, COPR2001, EFFCY (100)

COMMON IPUNCH, JREAD, JPRINT, JPRINT

NUMPK = NI
WRITE (JPRINT, 900) NUMPK

FORMAT (5X, 19H NUMBER OF PEAKS =, I5)
WRITE (JPRINT, 1001)

FORMAT (1H0, 5X, 48H AREA (A) = SUM(COUNTS), AREA (B) = FITTED GAUSSIAN)

EVALUATION OF LEAST-SQUARE-FITTED EQUATION FOR FWHM
ONLY STRONG PEAKS (INCLUDING WELL RESOLVED MULTIPLETS) OF
REASONABLE FWHM ARE CONSIDERED — 3 IF-STATEMENTS DETERMINE THAT

PEAK PARAMETERS CALCULATED HERE ARE STORED IN THE TBL ARRAY
AND USED AGAIN LATER

WRITE (JPRINT, 1850)

FORMAT (1H1, 25X, 36H PEAKS USED IN COMPUTING LSF OF FWHM)
WRITE (JPRINT, 1851)

FORMAT (1H0, 94H NUMBER PEAK N., ENERGY KEV WIDTH KEV)
1

HEIGHT, WEIGHT, ARE/GAUSSIAN

WEIT = 0.0
WEQ = 0.0
WE1 = 0.0
WE2 = 0.0
E1 = 0.0
E2 = 0.0
E3 = 0.0
E4 = 0.0
AREA+ = 0.0
AREA- = 0.0

FPS EXPECTED FWHM (KEV) OF FIRST PEAK EITHER READ IN OR CALC.
IF (FPS) 3034, 3034, 3035

3034 FPS = WID1
C WID1 IS FWHM (KEV) OF FIRST PEAK. CALC. IN PKALIB.

CONTINUE

FC = 6.0
C FC SETS THE VALUE OF THE FIRST CONDITION ON THE PEAK HEIGHT

IX = 0
MM = 0
I = 1
THL (1601) = 0.0
C FIRST PEAK NOT CONSIDERED HERE (SEE STATEMENT 4109 FOR REASON).
LOOP FCR LSF OF FWHM ECN. END OF LOOP AT 1818

IF(I - NUMPK) 1817,1817,1818

CONTINUE

THE FOLLOWING STATEMENT IS TO BE USED LATER TO IDENTIFY THE
PEAKS WHOSE PARAMETERS HAVE BEEN CALCULATED IN EVALUATING THE
LSF FWHM
TBL(I.+1600) = 0.0

COMPARISON OF THE PEAK HEIGHT TO THE BACKGROUND
LI IS THE CHANNEL NUMBER OF THE HIGHEST POINT IN THE PEAK
L1 = TBL(I.+1000)

J = LI
K = J/10 + 1

ERROR TERM CRITERIA. ECR IS REAL IN
PEAKS MUST HAVE PREDICTED ERROR IN AREA LESS THAN ECR
ER IS PERCENT ERROR IN AREA. TPK(J) IS PKHT. TBL(K) IS BKGND.
ER = 100.0 * SQR(2.0 * (TPK(J) + 1.5 * TBL(K)))/(ECR*TPK(J))

IF (ER-ECR) 1807,1807,1807

CONTINUE

ASB = TBL(K) + 80.
THE TERM .08.0 SETS THE MINIMUM VALUE OF ACCEPTABLE PEAK HEIGHT
TO ABOUT 9.0*FC(MIN) = 27.

SQ = SQR (ASB)

FIRST CONDITION - PEAK HEIGHT FAIRLY LARGE
IF(TPK(J) - FC*SQ) 1800,1800,1801

CONTINUE

IF MORE THAN EIGHT CONSECUTIVE PEAKS DO NOT MEET THE ABOVE
REQUIREMENTS THEN FC IS REDUCED SO AS TO MAKE SURE THAT THERE ARE
NO LARGE ENERGY GAPS BETWEEN THE CHOSEN PEAKS. THE OTHER
CONDITIONS STILL APPLY, HOWEVER, THE ORIGINAL VALUE OF FC IS

RESTORED

IF(I-IX-8) 1835,1835,1836

IF(IFC-2.0) 1835,1835,1837

I = IX
FC = FC - 1.0

GU TO 1800

FC = 6.0
IX = I
IA AND IL ARE THE LEFT AND RIGHT END POINTS OF THE PEAK
J = LI

IF(TPK(J)) 1802,1802,1803

J = J - 1
GU TO 4801

IA = J
J = TBL(I.+1000) + 1.0

IF(TPK(J)) 1805,1805,1806
FROM HERE TO STATEMENT 4113 THE MULTIPLETS ARE IDENTIFIED.

IF THE PEAKS ARE WELL RESOLVED, THE WIDTHS ARE ACCEPTED FOR THE LEAST-SQUARES FIT. HOWEVER MULTIPLETS ARE NOT CONSIDERED IN THE EVALUATION OF THE CORRECTION FACTOR TERA (SEE 4861).

LO AND L2 ARE THE CENTERS OF THE TWO PEAKS NEXT TO THE ONE EXAMINED.

BAD IS USED TO MARK THE MULTIPLETS FOR LATER IDENTIFICATION.

THE SAID PEAK IS EXCLUDED FROM THE LSF.

SECOND CONDITION - PART ONE

SECOND CONDITION - PART TWO

EVALUATION OF AREA UNDER THE PEAK

AREA = 0.0

DO 1814 K = IA, IL

AREA = AREA + TBK(K)

PCNR IS CALCULATED PEAK CENTER

PCTB = FLOAT(L1) + .5*CTS(L1) - DTS(L1) + .5

CALL ADJUST (CNTR, CCRR, PCNR, TPC)

EGAM = EGAM + SLP*TPC

EGAM = EGAM + SLP*TPC

Area = 0.5*PKHT

Ly = L1

PKHT = TBK(LY) + (PCNR-FLAT(LY)) + CTS(LY) - DTS(LY) - 1

EVALUATION OF THE EWBM

GX = 0.5*PKHT

J = L1
OC89 1842 IF(TBK(J) - GX) 1840, 1840, 1841
OC80 1841 J = J - 1
CC91 GO TO 1842
C PHL CHANNEL NUMBER LOW ENERGY SIDE
OC92 1840 PHL=FLCAT (J)+(GX-TBK(J))/(TBK(J+1)- TBK(J))
OC93 J=L1
CC94 1848 IF(TBK(J) - GX) 1845, 1845, 1846
OC95 1846 J = J + 1
OC96 GO TO 1848
CC97 1845 W=FLOAT (J)-(GX-TBK(J))/(TBK(J-1)-TBK(J))-PHL
C W FWHM IN CHANNEL NUMBERS.
C WIDTH FWHM IN ENERGY
CC98 WIDTH=W*SLP
C THIRD CONDITION - PEAK MUST HAVE AN ACCEPTABLE FWHM
OC99 AFS = ABS (WIDTH - FPS)
C ERFW IS THE ALLOWABLE DEVIATION CF THE FWHM (KEV).
OC100 IF (AFS - ERFW) 1812, 1812, 186C
OC101 1812 CONTINUE
C A NEW VALUE IS ASSIGNED TC FPS TC BE USED WITH THE NEXT PEAK
OC102 FPS = (FPS + WIDTH)/2.C
C EVALUATION OF THE WEIGHING FUNCTION USED IN THE LEAST-SQUARES FIT
C WEIT IS THE WEIGHING FUNCTION USED IN THE LSF. IT IS EQUAL
C TO THE SQUARE OF THE INVERSE OF THE STANDARD DEVIATION IN WIDTH
C NOTE THAT (S.D.(FWHM)/FWHM) = +CH- (S.D.(PKHT)/PKHT) AND THAT
C THE S.D. IN PKHT IS SQRT(PKHT+1.5*PACKCOND)/ERTM WHERE
C THE ERTM REPRESENTS THE REDUCTION IN THE STANDARD DEVIATION
C INTRODUCED BY THE SMOOTHING.
OC103 SDWID = WIDTH * ER/(141.4214)
OC104 WEIT = 1.0/(SDWID*SDWID)
C CALCULATIONS ON AREAS
OC105 TBL(1 +4201) = PKAN
OC106 TBL(I +1600) = EGM
OC107 TBL(I +2200) = GX
OC108 TBL(I +2800) = WIDTH
OC109 TBL(I +3400) = AREA
OC110 TBL(I +3750) = ER
C AREA = AREA/AREA
C AREA IS THE RATIO OF THE AREA UNDER THE PEAK TO THE AREA UNDER
C THE EQUIVALENT GAUSSIAN
C THE FOLLOWING STATEMENT EXCLUDES MULTIPLES IN THE AREA SUMS
OC111 IF(BAD) 4880, 4880, 4882
OC112 4880 CONTINUE
C ALSO EXCLUDED ARE SINGLES WHICH ARE MORE THAN 30 PERCENT OFF.
IF (ABS(ERA-1.0) - 0.30) \(48E1,4Pe1,4882\)

AREA = AREAM + AREA

CAREAM = AREAM + AREA

C THE RATIO (AREA/H/AREAM) WILL BE USED LATER TO EVALUATE CORRECTION

C FOR THE NON-GAUSSIAN FORM OF THE PEAKS

CAREAM = AREAM + AREA

WRITE (1813) MM, I, EGAM, WIDF, WITF, PKHT, ERA

FORMAT (1H, 4X, I5, 5X, I5, 5X, F10.2, 5X, F10.2, 5X, 1 F10.4)

C FOLLOWING COMPUTATIONS TO BE USED IN THE EVALUATION OF THE
C LEAST-SQUARE-FIT COEFFICIENTS (STATEMENT 1831)

EGM = EGAM/1000.

WID = WIDTH*WIDTH

WE0 = WE0 + WIT*WID

WE1 = WE1 + WIT*WID*EGM

WE2 = WE2 + WIT*WID*EGM**2

E1 = E1 + WIT*EGM

E2 = E2 + WIT*EGM**2

E3 = E3 + WIT*EGM**3

E4 = E4 + WIT*EGM**4

WE11 = WE11 + WIT * WIT

GO TO 1800

C END OF LOOP FOR FITTING HRFM.

C EVALUATION OF THE LSF COEFFICIENTS

1818 CONTINUE

C ALL THE PARAMETERS ARE DIVIDED BY 100.0 TO AVOID DEALING WITH
C VERY_LARGE_NUMBERS

1831 RM = WEIT/100.0

WE0 = WE0/100.0

WE1 = WE1/100.0

WE2 = WE2/100.0

E1 = E1/100.0

E2 = E2/100.0

E3 = E3/100.0

E4 = E4/100.0

DLT = RM*E2*E4 + 2.0*E1*E2*E3 - E2**3 - RM*E3**2 - E4*E1**2

AQ = (WE0*E2*E4 + WE2*E1*E3 + WE1*E2*E3 - WE2*E2**2

1 - WE0*E3**2 - WE1*E4)*/DLT

A1 = (WE1*RM*E4 + WE0*E2*E3 + WE2*E1*E2 - WE1*E2**2

1 - WE2*E3*RM - WE0*E1*E4)*/DLT

A2 = (WE2*RM*E2 + WE1*E1*E2 + WE0*E1*E3 - WE0*E2**2

1 - WE1*RM*E3 - WE2*E1*E2)*/DLT

C EVALUATION OF THE RMS_ERRCR IN FITTING THE DATA

QWAK = 0.0

1 = 0
C149 2903 I = I+1
C150 IF (I-NLMPK) 2901,2901,2902
C151 2901 IF (TBL(I+1600)) 2903,2903,2904
C152 2904 EGM = TBL(I+1600)
C153 WIDTH = TBL(I+2801)
C154 ER = TFL(I+3750)
C155 WEIT = 20000*Q/WIDTH
C156 EGM = EGM/1000.
C157 FWH2 = AO + A1*EGM + A2*EGM*ECM
C158 QWIK = WIDTH*WIDTH - FWH2
C159 QWAK = QWAK + WEIT*QWIK
C160 GO TO 2903
C161 2902 CONTINUE
C162 EMS = SQRT(QWAK/WEIT)
C163 WRITE (JPRINT,1820)
C164 1820 FORMAT(1H.,20X,37H EQUATION OF LEAST SQUARE FITTED FWHM)
C165 WRITE (JPRINT,1821) AO,A1,A2
C166 1821 FORMAT (1',10X,1' FWHM**2 = ',F5.3, '+ ',F9.3, ' *E(MEV)**2 '
C167 WRITE (JPRINT,1819) MM
C168 1819 FORMAT (1H0,10X,17H NUMBER OF PEAKS USED, 16)
C169 WRITE (JPRINT,2905) EMS
C170 2905 FORMAT (1H0, 10X, 17H RMS ERROR IN LSF, F10.4)
C171 WRITE (JPRINT,1822) TERA
C172 1822 FORMAT (1H0, 10X, 24H AREA/GAUSSIAN AREA) = , F10.4)
C173 PEAK ANALYSIS - PEAKS THAT HAVE ALREADY BEEN ANALYSED ABOVE
C174 HAVE THEIR PARAMETERS STORED IN THE TBL ARRAY
C175 ALL TYPES OF PEAKS ARE CALCULATED IN TWO DIFFERENT WAYS
C176 (A) AREA = SUM OF COUNTS IN ALL CHANNELS UNDER PEAK (AREA)
C177 (B) AREA = 1.0645*PEAK HEIGHT*FWHM*TERA WHERE THE TERM TERA
C178 IS A CORRECTION FACTOR FOR THE NON-GAUSSIAN FORM OF THE
C179 PEAKS AND FWHM IS THE LEAST-SQUARE-FITTED VALUE
C180 CORRESPONDING TO THE PEAK ENERGY (TAREA)
C181 WRITE (JPRINT,2081)
C182 2081 FORMAT (1H1, 47X, 16H PEAK ANALYSIS)
C183 WRITE (JPRINT,1003)
C184 1003 FORMAT (1H1,46H), ENERGY PK CNTR HEIGHT H TO BG ,
C185 16H AREA(A) AREA(B) INT(B) ERRDR(B) W(A) W(B) BASE ,
C186 26H TYPE)
C187 WRITE (JPRINT,1004)
C188 1004 FORMAT (1H1,46H), KEV CHAN NC COUNTS RATIO ,
C189 16H COUNTS COUNTS PERCENT KEV CHAN)
C190 IF (IPUNCH) 1237,1238,1238
C181 WRITE (J PUNCH,1236)
C182 1236 FORMAT(4X, 12H NO. ENERGY(KEV), 12H AREA(GAUS), 12H AREA(SLM))
C183 1238 CONTINUE
C184 N = 1
C185 I = C
C186 LOOP F C R PEAK ANALYSIS
C187 810 CONTINUE
C188 IF(I-NUMPK) 1856, 1856, 870
C189 THE ZERQ POINTS OF A PEAK ARE CALCULATED AGAIN FOR ALL PEAKS
C190 1856 J = TBL(I+1000) - 1.0
C191 801 IF (TBL(J), 802, 803
C192 803 J = J - 1
C193 804 IA = J
C194 IA IS ZERO POINT LOW ENERGY SIDE
C195 805 J = TBL(I)+1000 + 1.0
C196 806 J = J + 1
C197 GO TO 804
C198 IL = J
C199 IL IS ZERO POINT HIGH ENERGY Side
C200 L1 = TBL(I+1000)
C201 L2 = TBL(I+1001)
C202 L3 = TBL(I+1002)
C203 L4 = TBL(I+1003)
C204 XL12=FCLAT (L2-L1)
C205 XL23=FCLAT (L3-L2)
C206 C LOGIC TO DETERMINE IF THE PEAK DATA IS IN MULTIPLET FORM
C207 IF (IL-L2) 811, 811, 812
C208 812 IF (IL-L3) 813, 813, 814
C209 814 IF (IL-L4) 815, 815, 816
C210 C SINGLET PEAK CALCULATION
C211 811 CONTINUE
C212 C CONDITION TO DETERMINE IF PEAK HAS BEEN USED IN EVALUATING THE
C213 C LSF FWHM IN THE PREVIOUS PART OF THE PROGRAM
C214 IF (TBL(I+1600)) 1855, 1855, 1860
C215 C SINGLETS PEAKS WHOSE PARAMETERS HAVE BEEN STORED IN THE TBL ARRAY
C216 1860 EGAM = TBL(I + 1600)
C217 GX = TBL(I + 2200)
C218 WIDF = TBL(I + 2800)
C219 SAREA = TBL(I + 3400)
FORTAN IV G LEVEL 1, MCD 2
PKANAL

DATE = 68223 19/29/33

0214 PCNR = TBL(1) + 420)
0215 PKHT = 2.0*G
0216 EGM = EGM/1000.
0217 FWH = sqrt(AO + A1*EGM + A2*EGM*EGM)
0218 TAREA = 2.1289*TERA*FWF*G*/SLP
0219 CALL INTSTY (TAREA,EGAM,FIRED,DELENG,SANGLE,FLXT,ALGAM)
0220 ER = THE PERCENT ERROR INVOLVED IN THE AREA CALCULATION (TAREA)
0221 Z = THE NUMBER OF CHANNELS OCCUPIED BY THE PEAK
0222 K = L1/10 + 1
0223 HTOB = PKHT/(TBL(K) + 5.C)
0224 WRITE (1PRINT,1000) n,EGAM,PCNR,PKHT,HTOB,SAREA,TAREA,ALGAM,ER,
1000 FORMAT(15,5(3X,F10.2))
0225 IF (IPUNCH) 1239,1240,1240
0226 1239 CONTINUE
0227 WRITE (IPUNCH,1235) n,EGAM,ALGAM,ER,TAREA,SAREA
1235 FORMAT(15,5(3X,F10.2))
0228 1240 CONTINUE
0229 n = n + 1
0230 GO TO 10.
0231 GO TO 1
0234 DD BC7 K=IA,IL
0235 .BC7 AREA=AREA+TBK(K)
0236 SAREA = AREA
0237 ORT = CALCULATED PEAK CENTER.
0238 ORT = FLOAT (L1) + DTS(L1)/(DTS(L1-1)-DTS(L1)) + 0.5
0239 PCNR=ORT
0240 PKHT = TBK(LY) + (PCNR-FLCAT(LY)) * DTS(LY) +
1 0.5 * (PCNR-FLCAT(LY)) *(PCNR-FLCAT(LY+1))#DTS(LY)*DTS(LY-1))
0241 K = L1/10 + 1
0242 ER = 100.0 * SQRT(2.0*(PKHT+1.5*TBL(K)))/(ERTM*PKHT)
56
C243 IF (ER-ECR) 871,871,810
C244 CONTINUE
C SUBROUTINE ADJUST CORRECTS PCNR TO OBTAIN THE TRUE PEAK CENTER
C USING CNTR AND CCFR ECN THE LINEARITY SUBROUTINE.
C245 CALL ADJUST (CNTR,CCFR,PCNR,TPC)
C246 EGAM = EGAM1*SLP*(TPC-TPC1)
C247 EVALLATION OF LEAST-SQUARE-FITTED FWHM
C248 IF (TPC) FWHM**2 IS .LE. (FPS-ERFW)**2 THEN FWHM = FPS.
C249 THIS CONDITION PREVENTS A POSSIBLE SRC (NEG. NO.).
C250 FWHM = FPS
C251 DUM = AC + A1*EAM + A2*ECR*EAM
C252 DUMM = DUM - (FPS-ERFW)*(FPS-ERFW)
C253 IF (DUMM,GE,0.0) FWHM = SQRT(DUM)
C254 GX = 0.5*PKHT
C255 TAREA = 2.1289*TERA*FWF*CX/SLP
C256 EVALUATION OF ACTUAL FWHM.
C257 J = 11
C258 IF (TBK(J)-GX) 840,840,841
C259 841 J=J-1
C260 GO TO 842
C261 J=J+1
C262 GO TO 848
C263 W=FLCAT (J)-(GX-TBK(J))/TBK(J)+1-PHL
C264 WIDTH = FHWM IN ENERGY.
C265 WRITE (JPUNCH,1241) N,EGAM,AIGAM,ER,
C266 DATA OUTPUT
C267 WRITE (JPUNCH,125) N,EGAM,ECR,ER,
C268 N = N + 1
GO TO 810
C
DOUBLE PEAK CALCULATION
C
THE PROCEDURE USED HERE IS SIMILAR TO THE SINGLET PEAK CALC.
C
TWO GAUSSIAN CURVES ARE FITTED TO THE DATA.
C

813 AREA=C.

DO 827 K=IA,IL
C
AREA=AREA+TBK(K)
C
ORT1 IS THE CALCULATED CENTER OF THE FIRST PEAK.

ORT1 = FLOAT(L1) + DTS(L1)/(DTS(L1-1)-DTS(L1)) + 0.5
C
ORT2 IS THE CALCULATED CENTER OF THE SECOND PEAK.

ORT2 = FLOAT(L2) + DTS(L2)/(DTS(L2-1)-DTS(L2)) + 0.5
C
AN AVERAGE FWHM IS CALCULATED FOR THE MULTIPLET IN ALL CASES
C

PCNR = ICRT1 + ORT2)/2.0
C
CALL ADJUST (CNTR,CCRR,PCNR,TPC)

EGAM = EGAM1 + SLP*(TPC-TPC1)
EGM = EGAM/1000.
FPH = FPS

DUM = AO + A1*EGM + A2*EGM^2

DOMM = DUM - (FPS-ERFW)*(FPS-ERFW)
IF (DOMM^2+0.0) FWH = SQRT(DUM)

WIDF = FWH

VRNC = (FWH/(SLP*2.35478))**2
C

C=EXP (-((X122**2)/12.*VRNC))
C
L1 IS THE CHANNEL NUMBER OF THE MAXIMUM OF THE FIRST PEAK.
C
L2 IS THE CHANNEL NUMBER OF THE MAXIMUM OF THE SECOND PEAK.

AREA1=AREA*(TBK(L1)-TBK(L2))*C)/I(TBP(L1)+TBK
AREA2=AREA2*TBK(L2)-TBK(L1)*C)/((TPK(L1)+TBK
L_Y = L1

DGE = 1.0645*ERA*FWH/SLF

DENOM = 1.0- C**2

PCNR = ORT1
PKHT = TBK(LY) + (PCNR-FLCAT(LY))* DTS(LY) +
1 0.5 * (PCNR-FLCAT(LY))* (PCNR-FLCAT(LY+1))* (CTS(LY)-DTS(LY-1))

PKHT1 = PKHT
PKHT2 = PKHT

PKHT = TBK(LY) + (PCNR-FLCAT(LY)) * DTS(LY) +
1 0.5 * (PCNR-FLCAT(LY)) * (PCNR-FLCAT(LY+1)) * (CTS(LY)-DTS(LY-1))

PKHT2 = PKHT
C
FIRST PEAK DATA CALCULATIONS

PKHT = (PKHT1 - C*PKHT2)/DENOM
IF (PKHT.LE.0.0) GC_JD 892

K = L1/10 + 1
ER = 100.0 * SQRT(2.0*(PKHT+1.5*TBK(K)))/(ERTM*PKHT)
IF (ER-ERFW) 872,772,492

PCNR=ORT1

TAREA = CCOE*PKHT
0311  SAREA=AREA1
0312  IF (SAREA.LE.0.0) GO TO 852
0313       CALL ADJUST (CNTR,CCRR,PCNR,TPC)
0314       EGAM=EGAMI+SLP*(TPC-TPC1)
0315       CALL INTSTY (TAREA,EGAM,FIRENG,DELENG,SANGLE,FLUXT,AIGAM)
0316       Z = FLCAT (IL-IA)
0317       HTOB = PKHT/TBL(K)+5.0
0318       WRITE (JPRINT,1009) N,EGAM,PCNR,PKHT,HTOB,SAREA,TAREA,AIGAM,ER,
          1 WIDTH,FWHM,Z,C
0319          1008 FMTAT14,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F8.1,3X,F8.1,3X,F8.1,3X,F7.2,
          1 3X,F7.2,3X,F5.2,3X,F5.2,3X,F4.2,D+*F4.2
0320 0321 1243 CONTINUE
0322 0323 1244 CONTINUE
0324       N = N + 1
0325       E92 I = I+1
C SECOND PEAK DATA CALCULATION.
C PKHT = (PKHT2 - C*PKHT1)/CEACK
0326 0327       IF (PKHT.LE.0.0) GO TO 810
0328       K = L2/10 + 1
0329       ER = 100.0*SQRT(12.0*(PKHT+1.5*TBL(K)))/(ERTM*PKHT)
0330 0331 .E73 PCNR=QRT2
0332 0333       TAREA = CCDE*PKHT
0334 0335       SAREA=AREA2
0336 0337       IF (SAREA.LE.0.0) GO TO 81C
0338       CALL ADJUST (CNTR,CCRR,PCNR,TPC)
0339       EGAM=EGAMI+SLP*(TPC-TPC1)
0340       CALL INTSTY (TAREA,EGAM,FIRENG,DELENG,SANGLE,FLUXT,AIGAM)
0341 0342 1245 CONTINUE
0343 0344 1246 CONTINUE
0345       N = N + 1
0346       GO TO 810
C C TRIPLET PEAK CALCULATION
C THE PROCEDURE USED HERE IS SIMILAR TO THE SINGLET PEAK CALC.
C THREE GAUSSIAN CURVES ARE FITTED TO THE TRIPLET DATA.
C AN AVERAGE FWHM IS CALCULATED FOR THE TRIPLET CASE.
0347 0348 815 AREA=C.
0349 837 AREA=AREA+TBK(K).
DATE = 68223 19/29/33

ORT1 = FLAT (L1) + DTS(L1)/(CTS(L1-1)-DTS(L1)) + 0.5
ORT2 = FLAT (L2) + DTS(L2)/(CTS(L2-1)-DTS(L2)) + 0.5
ORT3 = FLAT (L3) + DTS(L3)/(CTS(L3-1)-DTS(L3)) + 0.5
PCNR = (ORT1 + ORT2 + ORT3)/3.

CALL ADJUST (CNTR, CCRR, PCNR, TPC)
EGAM = EGAM1 + SLP*(TPC-TPC1)
EGM = EGAM/1000
FWS = FPS
DUM = AO + A1*EGM + A2*EGM*EGM
DUMM = DUM - (FPS-ERFW)*(FPS-ERFW)
IF (DUMM <= 0.0) FWS = SQRT(DUMM)
WIDTF = FWH
VRNC = [FWH/(SLP*2.35478)]**2
C = EXP (-(XL12**2)/(2.*VRNC))
D = EXP (-(XL23**2)/(2.*VRNC))

TBSM=TBK(L1)*(1.-D**2-C(1.-D))*TBK(L2)*(1.-C-D)*TBK(L3)*
(11.-C**2-D**2*(1.-C))

AREA1=AREA*(TBK(L1)*(1.0-D**2)-FKHT2*C)*PKHT3*C*D)/DENOM
AREA2=AREA*(1.0-PKHT1)*(1.0-D**2-TPK(L2)*C+TBK(L3)*C*D)/TBSM
AREA3=AREA*(TBK(L1)*C-TBK(L2)*C+TBK(L3)*(1.-C**2))/TBSM

TCOE = 1.0645*TERA*FWH/SLP

IF (PKHT<0.0) GO TO 846

PCNR = ORT1
PKHT = PKHT + (PCNR-FLAT(LY)) * CTS(LY) *
1.05 * (PCNR-FLAT(LY+1)) * (CTS(LY)-DTS(LY-1))

PKHT1 = PKHT*

LY = L1
PKHT = PKHT + (PCNR-FLAT(LY)) * CTS(LY) *
1.05 * (PCNR-FLAT(LY+1)) * (CTS(LY)-DTS(LY-1))

PKHT2 = PKHT*
LY = L2
PKHT = PKHT + (PCNR-FLAT(LY)) * CTS(LY) *
1.05 * (PCNR-FLAT(LY+1)) * (CTS(LY)-DTS(LY-1))

PKHT3 = PKHT*

C FIST FEM DATA CALCULATION
PKHT = (PKHT1*(1.0-D**2)-PKHT2*C)PKHT3*C*D)/DENOM
IF (PKHT.LT.0.0) GO TO 854
K = L1/10 + 1
ER = 100.0 * SQRT(2.0*(PKHT+1.5*TBK(K)))/(ERTM*PKHT)
IF (ER-ECR) 874,874,894

PCNR=ORT1
TAREA = TCOE*PKHT
SAREA=AREA1
IF (SAREA.LE.0.0) GO TO 854

CALL ADJUST (CNTR, CCRR, PCNR, TPC)
C393  EGAM = ECAM1 + SLP*(TPC-TPC1)
0394
0395  CALL INTSTY (TAREA, EGAM, FIREG, DELENG, SANGLE, FLUXT, AIGAM)
0396  Z = FLCAT (IL-IA)
0397  HTOB = PKHT/(TBL(K1) + 5.0).
0398  WRITE (JPRINT,1009) N,EGAM,PCNR,PKHT,HTOB,SAREA,TAREA,AIGAM,ER,
0399  1 WIDTH,FWH,Z,C,D
1009  FORMAT(14,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.1,3X,F7.2,
0400  3X,F7.2,3X,F7.2,3X,F5.2,3X,F5.2,3X,F5.2,2X,FA.C,'T',F4.2,1X,F4.2)
C400  IF (IPUNCH) 1247,1248,1248
C401  CONTINUE
C402  WRITE (JPUNCH,1235) N,EGAM,AIGAM,ER,TAREA,SAREA
C403  CONTINUE
C404  N = N + 1
C405  894  I = I + 1
C406  SECOND PEAK DATA CALCULATION.
C407  PKHT = (PKHT1*C + PKHT2 - PKHT3*D)/DENOM.
C408  IF (PKHT.LE.0.0) GO TO 855
C409  K = 12/10 + 1
C410  ER = 100.0 * SQRT(2.0*(PKHT+1.5*TBL(K))/ERTM*PKHT)
C411  IF (ER-ECR) 875,876,876
C412  875  PCNR=ORT2
C413  TAREA=TCOE*PKHT
C414  SAREA=AREA2
C415  IF (SAREA.LE.0.0) GO TO 855
C416  CALL ADJUST (CNTR,CCRR,PCNR,TPC)
C417  EGAM=ECAM1+SLP*(TPC-TPC1)
C418  CALL INTSTY (TAREA,EGAM,FIREG,DELENG,SANGLE,FLUXT,AIGAM)
C419  Z = FLCAT (IL-IA)
C420  HTOB = PKHT/(TBL(K) + 5.0)
C421  WRITE (JPRINT,1009) N,EGAM,PCNR,PKHT,HTCR,SAREA,TAREA,AIGAM,ER,
C422  1 WIDTH,FWH,Z,C,D
C423  IF (IPUNCH) 1249,1250,1250
C424  CONTINUE
C425  CONTINUE
C426  1250 N=N+1
C427  895 I = I + 1
C428  THIRD PEAK DATA CALCULATION.
C429  PKHT=(PKHT1*C*D-PKHT2*D+PKHT3*(1.0-C**2))/DENOM
C430  IF (PKHT.LE.0.0) GO TO 810
C431  K = 13/10 + 1
C432  ER = 100.0 * SQRT(2.0*(PKHT1+1.5*TBL(K))/ERTM*PKHT)
C433  IF (ER-ECR) 876,876,876
C434  876  PCNR=ORT3
C435  TAREA=TCOE*PKHT
C436  SAREA=AREA3
C437  IF (SAREA.LE.0.0) GO TO 810
C438  CALL ADJUST (CNTR,CCRR,PCNR,TPC)
C MULTIPLE PEAK ANALYSIS
C MULTIPLETS WHICH ARE SO LARELED BECAUSE OF TINY PEAKS AT THE
C WINGS OF STRONG ONES ARE ANALYSED AS TRIPLETS. THE THREE
C STRONGEST PEAKS IN THE MULTIPLETS ARE CHOSEN FOR THAT PURPOSE.
C THE SMOOCHED DATA SHOULD BE EXAMINED TO INSURE THIS.

0447 816 CONTINUE
0448 II = 3
0449 WT(1) = FLCAT(1)
0450 WT(2) = FLCAT(2)
0451 WT(3) = FLCAT(3)
0452 WT(4) = FLCAT(4)

C EVALUATION OF II, THE NUMBER OF PEAKS IN THE MULTIPLETS

0453 817 II = II + 1
0454 I3 = II + 1 + 1000
0455 WT(I3+1) = TBL(I3)
0456 L3 = TBL(I3)
0457 IF(I3-L3) 819,819,817

C ORDERING OF THE PEAKS IN TERMS OF DECREASING PEAK HEIGHT

0458 819 DO 3019 IE = 1,II
0459 LS = WT(I)
0460 WT(I+10) = TBL(5)
0461 3019 WT(I+20) = TBL(5)

C WT(I+20) ARE THE PEAK HEIGHTS IN ORDER THEY APPEAR.
C WT(I+10) ARE THE VALUES OF THE PEAK HEIGHTS ORDERED BY
C DECREASING VALUE.

0462 DO 3020 IP = 1,II
0463 DO 3020 IE = IP,II
0464 IF(WT(IP+10) = WT(I+10)) 3021,3020,3020
0465 3021 ROK = WT(I+10)
0466 WT(IP+10) = ROK
0467 WT(IP+10) = ROK

DO 3020 CONTINUE
0469 NR = 0
0470 DO 3025 NP=1,3
0471 DO 3026 NP=1,II
IF (WT(NP+10) - WT(NQ+20)) \( \leq \begin{array}{c} 3 \\leq 3 \end{array} \), \( \text{NR} = \text{NR} + 1 \)
\( \text{IV} = \text{I} + 999 + \text{NQ} \)
WT(NR) = TBL(IV)
GO TO 3025
3026 CONTINUE
3025 CONTINUE
L1 = WT(1)
L2 = WT(2)
L3 = WT(3)
XL12 = FLOAT(L2-L1)
XL23 = FLOAT(L3-L2)
WRITE (JPRINT,820)
820 FORMAT(1H,23X,27H NUMBER OF MULTIPLE PEAKS =,I5)
WRITE (JPRINT,3033)
3033 FORMAT(1H,49H THE 3 STRONGEST PEAKS ARE ANALYSED AS A TRIPLET.,
134H CHECK BACKGROUND SUBTRACTED DATA.)
L = I + II - 3
GO TO 615
C
CONTINUE
RETURN
END
THE COOLEY-TUKEY FAST FOURIER TRANSFORM IN USASI BASIC FORTRAN

TRANSFORM(J1,J2,...) = SUM(CDATA(I1,I2,...)*WI**(I1-1)*(J1-1))

WHERE I1 AND J1 RUN FROM 1 TO NN(I1) AND WI=EXP(ISIGN*2*PI*
SQR(-1)/NN(I1)), ETC. THERE IS NO LIMIT ON THE DIMENSIONALITY
NUMBER OF SUBSCRIPTS) OF THE DATA ARRAY. IF AN INVERSE
TRANSFORM (ISIGN=+1) IS PERFORMED UPON AN ARRAY OF TRANSFORMED
DATA, THE ORIGINAL DATA WILL REAPPEAR,
MULTIPLIED BY NN(I1)*NN(I2)*... THE ARRAY OF INPUT DATA MAY BE
REAL OR COMPLEX, AT THE PROGRAMMERS OPTION. WITH A SAVING OF
UP TO FORTY PER CENT IN RUNNING TIME FOR REAL OVER COMPLEX.
FOR FASTEST TRANSFORM OF REAL DATA, NN(I1) SHOULD BE EVEN.
THE TRANSFORM VALUES ARE ALWAYS COMPLEX, AND ARE RETURNED IN THE
ORIGINAL ARRAY OF DATA, REPLACING THE INPUT DATA. THE LENGTH
OF EACH DIMENSION OF THE DATA ARRAY MAY BE ANY INTEGER. THE
PROGRAM RUNS FASTER ON COMPOSITE INTEGERS THAN ON PRIMES, AND IS
PARTICULARLY FAST ON NUMBERS RICH IN FACTORS OF TWO.

TIMING IS IN FACT GIVEN BY THE FOLLOWING FORMULA. LET NTOT BE THE
TOTAL NUMBER OF POINTS (REAL OR COMPLEX) IN THE DATA ARRAY. THAT IS, NTOT=NN(I1)*NN(I2)*...
DECOMPOSE NTOT INTO ITS PRIME FACTORS, SUCH AS 2**K2 * 3**K3 * 5**K5 * ... LET SUM2 BE THE SUM OF ALL
THE FACTORS OF TWO IN NTOT, THAT IS, SUM2 = 2**K2. LET SUMF BE
THE SUM OF ALL OTHER FACTORS OF NTOT, THAT IS, SUMF = 3**K3+5**K5...
The time taken by a multidimensional transform on these NTOT data
is T = NTOT*(T1+2*T2+SUM2+T3*SUMF). ON THE CDC 3300 (FLOATING
POINT ADD TIME = SIX MICROSECONDS), T = 3000 + NTOT*(1600+40*SUM2+
175+SUMF) MICROSECONDS ON COMPLEX DATA.

IMPLEMENTATION OF THE DEFINITION BY SUMMATION WILL RUN IN A TIME
PROPORTIONAL TO NTOT*(NN(I1)+NN(I2)*...). FOR HIGHLY COMPOSITE NTOT,
THE SAVINGS OFFERED BY THIS PROGRAM CAN BE DRAMATIC. A ONE-DIMEN-
SIONAL ARRAY 4000 IN LENGTH WILL BE TRANSFORMED IN 4000*(5+2*2+2+2+2)+175*(5+5+5) = 14.5 SECONDS VERSUS ABOUT 4000*
4000*175 = 2800 SECONDS FOR THE STRAIGHTFORWARD TECHNIQUE.

THE CALLING SEQUENCE IS--
CALL FOURTC(DATA,NN,NDIM,ISIGN,IFORM,WORK)

DATA IS THE ARRAY USED TO HOLD THE REAL AND IMAGINARY PARTS
OF THE DATA ON INPUT AND THE TRANSFORMED VALUES ON OUTPUT. IT
IS A MULTIDIMENSIONAL FLOATING POINT ARRAY, WITH THE REAL AND
IMAGINARY PARTS OF A DATUM STORED IMMEDIATELY ADJACENT IN STORAGE
(SUCH AS FORTRAN IV PLACES THEM). THE EXTENT OF EACH DIMENSION
IS GIVEN IN THE INTEGER ARRAY NN, OF LENGTH NDIM. ISIGN IS -1
TO INDICATE A FORWARD TRANSFORM (EXPONENTIAL SIGN IS +) AND +1
FOR AN INVERSE TRANSFORM (SIGN IS +). IFORM IS +1 IF THE DATA AND
THE TRANSFORM VALUES ARE COMPLEX. IT IS 0 IF THE DATA ARE REAL
BUT THE TRANSFORM VALUES ARE COMPLEX. IF IT IS 0, THE IMAGINARY
PARTS OF THE DATA SHOULD BE SET TO ZERO. AS EXPLAINED ABOVE, THE
TRANSFORM VALUES ARE ALWAYS COMPLEX AND ARE STORED IN ARRAY DATA.
WORK IS AN ARRAY USED FOR WORKING STORAGE. IT IS NOT NECESSARY
IF ALL THE DIMENSIONS OF THE DATA ARE POWERS OF TWO. IN THIS CASE
IT MAY BE REPLACED BY 0 IN THE CALLING SEQUENCE. THUS, USE OF
POWERS OF TWO CAN FREE A GOOD DEAL OF STORAGE. IF ANY DIMENSION
IS NOT A POWER OF TWO, THIS ARRAY MUST BE SUPPLIED. IT IS A
FLOATING POINT, ONE DIMENSIONAL OF LENGTH EQUAL TO TWICE THE
LARGEST ARRAY DIMENSION (I.E., NN(I1) ) THAT IS NOT A POWER OF
TWO. THEREFORE, IN ONE DIMENSION FOR A NON POWER OF TWO,
WORK OCCUPIES AS MANY STORAGE LOCATIONS AS DATA. IF SUPPLIED,
WORK MUST NOT BE THE SAME ARRAY AS DATA. ALL SUBSCRIPTS OF ALL
ARRAYS BEGIN AT ONE.

THE FAST FOURIER ALGORITHM PLACES TWO RESTRICTIONS UPON THE
NATURE OF THE DATA BEYOND THE USUAL RESTRICTION THAT
THE DATA FORM ONE CYCLE OF A PERIODIC FUNCTION. THEY ARE--
1) THE NUMBER OF INPUT DATA AND THE NUMBER OF TRANSFORM VALUES
MUST BE THE SAME.
2) CONSIDERING THE DATA TO BE IN THE TIME DOMAIN,
THEY MUST BE EQUI-SPACED AT INTERVALS OF DT. FURTHER, THE TRANS-
FORM VALUES, CONSIDERED TO BE IN FREQUENCY SPACE, WILL BE EQUI-
SPACED FROM 0 TO 2*PI/(NN(I)-1)/(NN(I)*DT) AT INTERVALS OF
2*PI/(NN(I)*DT) FOR EACH DIMENSION OF LENGTH NN(I). OF COURSE,
DT NEED NOT BE THE SAME FOR EVERY DIMENSION.

THERE ARE NO ERROR MESSAGES OR ERROR HALTS IN THIS PROGRAM. THE
PROGRAM RETURNS IMMEDIATELY IF NDIM OR ANY NN(I) IS LESS THAN ONE.
EXAMPLE 1. THREE-DIMENSIONAL FORWARD FOURIER TRANSFORM OF A
COMPLEX ARRAY DIMENSIONED 32 BY 25 BY 13 IN FORTRAN IV.
DIMENSION DATA(32,25,13),WORK(50),NN(3)
COMPLEX DATA
DATA NN/32,25,13/
DO 1 J=1,32
DO 1 K=1,13
1 DATA(I,J,K)=COMPLEX VALUE
CALL FOURT(DATA,NN,3,-1,1,WORK)

EXAMPLE 2. ONE-DIMENSIONAL FORWARD TRANSFORM OF A REAL ARRAY OF
LENGTH 64 IN FORTRAN II.
DIMENSION DATA(2,64)
DO 2 I=1,64
DATA(I)=REAL PART
2 DATA(I)=0.
CALL FOURT(DATA,64,1,-1,0,0)

FOR THE DIGIT REVERSAL WAS SUGGESTED BY RALPH ALTER (ALSO MIT LL).
THIS IS THE FASTEST AND MOST VERSATILE VERSION OF THE FFT KNOWN
TO THE AUTHOR. A PROGRAM CALLED FOUR2 IS AVAILABLE THAT ALSO
PERFORMS THE FAST FOURIER TRANSFORM AND IS WRITTEN IN USASI BASIC
FORTRAN. IT IS ABOUT ONE THIRD AS LONG AND RESTRICTS THE
DIMENSIONS OF THE INPUT ARRAY (WHICH MUST BE COMPLEX) TO BE POWERS
OF TWO. ANOTHER PROGRAM, CALLED FOUR1, IS ONE TENTH AS LONG AND
RUNS TWO THIRDS AS FAST ON A ONE-DIMENSIONAL COMPLEX ARRAY WHOSE
LENGTH IS A POWER OF TWO.

REFERENCE--
FAST FOURIER TRANSFORMS FOR FUN AND PROFIT, W. GENTLEMAN AND
G. SANDE, 1966 FALL JOINT COMPUTER CONFERENCE.

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**PROGRAM** BY NORMAN BRENNER FROM THE BASIC PROGRAM BY CHARLES RADER (BOTH OF MIT LINCOLN LABORATORY), MAY 1967. THE IDEA

SUBROUTINE FOURT(CAT, NN, NDIM, ISIGN, IFORM, WORK)

THE FAST FOURIER TRANSFORM IN USASI BASIC FORTRAN

DIMENSION CAT(1), NN(11), IFACT(32), WORK(1)

TWOPI = 6.283185307
RTHLF = 70710.67812
IF(NDIM-1)*920, 1, 1
I
DO 2 IDIM = 1, NDIM
LF(NDIM-IDIM)*920, 920, 2
2
NTOT = NTOT*NN(IDIM)

MAIN LOOP FOR EACH DIMENSION

NP1 = 2
DO 9 NTOT = 1, NDIM
NN = NN(IDIM)
NP2 = NP1*NN
LF(N-IDIM)*920, 5
C IS N A POWER OF TWO AND IF NOT, WHAT ARE ITS FACTORS

M = N
NTWO = NP1
IF = 1
IDIV = 2
10 IQUOT = M/IDIV
IREM = M- IDIV * IQUOT
IF(IQUOT-IDIV)*50, 11, 11
11 IF(IREM)*20, 12, 20
12 NTWO = NTWO+NTWO
IFACT = IF*IDIV
IF = IF+1
M = IQUOT
GO TO 10
20 IDIV = 3
INON2 = IF
30 IQUOT = M/IDIV
IREM = M- IDIV * IQUOT
IF(IQUOT-IDIV)*60, 31, 31
31 IF(IREM)*60, 32, 40
32 IFACT = IFACT*IDIV
IF = IF+1
M = IQUOT
GO TO 30
40 IDIV = IDIV+2
GO TO 30
50 INON2 = IF
IF(IREM)*60, 51, 60
51 NTWO = NTWO+NTWO
GO TO 70
60 IFACT = IF*M
70 NON2P = NP2/NTWO
C SEPARATE FOUR CASES--
1. COMPLEX TRANSFORM
   REAL TRANSFORM FOR THE 2ND, 3RD, ETC., DIMENSION. METHOD --
   TRANSFORM HALF THE DATA, SUPPLYING THE OTHER HALF BY CONJUGATE SYMMETRY.

2. REAL TRANSFORM FOR THE 2ND, 3RD, ETC., DIMENSION. METHOD --
   TRANSFORM HALF THE DATA, SUPPLYING THE OTHER HALF BY CONJUGATE SYMMETRY.

3. REAL TRANSFORM FOR THE 1ST DIMENSION, N ODD. METHOD --
   SET THE IMAGINARY PARTS TO ZERO.

4. REAL TRANSFORM FOR THE 1ST DIMENSION, N EVEN. METHOD --
   TRANSFORM A COMPLEX ARRAY OF LENGTH N/2 WHOSE REAL PARTS ARE THE EVEN NUMBERED REAL VALUES AND WHOSE IMAGINARY PARTS ARE THE ODD NUMBERED REAL VALUES, SEPARATE AND SUPPLY THE SECOND HALF BY CONJUGATE SYMMETRY.

ICASE = 1
IFMIN = 1
11RNG = NP1
IF(IDIM-4) 74, 100, 100
11RNG = NP0*(1+NPREV/21
IF(IDIM-1) 72, 72, 100
11RNG = NP1
IF(NTWO-NP1) 100, 100, 73
11RNG = NP1
IF(INOT=NTWO/2
N = N/2
NP2 = NP2/2
NTOT = NTOT/2
I = 1
DO 80 J = 1, NTOT
DATA(J) = DATA(I)
I = I + 2

SHUFFLE DATA BY BIT REVERSAL, SINCE N = 2**K, AS THE SHUFFLING CAN BE DONE BY SIMPLE INTERCHANGE, NO WORKING ARRAY IS NEEDED.

IF(NCPNP2 = 11101, 101, 200
NP2HF = NP2/2
J = 1
DO 150 I = 1, NP2, NP1
IF(J - 12) 121, 130, 130
I = I + 2
11MAX = 12 + NP1 - 2
DO 125 I = 12, I1MAX, 2
DO 125 J = 12, I1MAX, 2
JEM = J + 12
TEMPI = DATA(I + 1)
DATA(I + 1) = DATA(J + 12)
DATA(J + 12) = TEMPI
125 DATA(J + 1) = TEMPI
M = NP2HF
140 IF(J = M*150, 150, 141
141 J = J - M
M = M/2
IF(M-NP1) 150, 140, 140
150   J=J+M
GO TO 300
C
C   SHUFFLE DATA BY DIGIT REVERSAL FOR GENERAL N
C
200   NWORK=2*N
DO 270  I=1,NP1,2
DO 270  I=13,11*NTOT,NP2
J=13
DO 260  I=1,NWORK,2
IF(ICA9E=3)210,220,210
210   WORK(I)=DATA(J)
WORK(I+1)=DATA(J+1)
GO TO 240
220   WORK(I)=DATA(J)
WORK(I+1)=0.
240   IFP2=NP2
IF=IFMIN
250   IFP1=IFP2/IFACT(IF)
J=J+IFP1
IF(J-I3=IFP2)260,255,255
255   J=J-IFP2
IFP2=IFP1
IF(IFP2-NP1)260,260,250
260   CONTINUE
L2MAX=I3*NP2-NP1
L=1
DO 270  I=13,I2MAX,NP1
DATA(I2)=WORK(I)
DATA(I2+1)=WORK(I+1)
270   L=L+2
C
C   MAIN LOOP FOR FACTORS OF W
C   W=EXP(ISIGN*2*PI*SQRT(-1)*M/(4*MMAX)). CHKCK FOR W=ISIGN*SQRT(-1)
C   AND RBPET FOR W=W*(1+ISIGN*SQRT(-1))/SQRT(2).
C
300   IF(NTWO-NP1)600,600,305
305   NP1TW=NP1*NP1
IPAR=NTWO/NP1
310   IF(IPAR-2)350,330,320
320   IPAR=IPAR/4
GO TO 310
330   DO 340  I=1,1RNG,2
DO 340  K1=11,NTOT,NP1TW
K2=K1+NP1
TEMPR=DATA(K2)
TEMPI=DATA(K2+1)
DATA(K2)=DATA(K1)-TEMPR
DATA(K2+1)=DATA(K1)+TEMPI
340   DATA(K1)=DATA(K1+1)+TEMPI
350   MMAX=NP1
360   IF(MMAX-NTWO/2)370,600,600
370   LMAX=MAX0(NP1TW,MMAX/2)
DO 570  L=NP1,LMAX,NP1TW
N=L
68
IF(MMAX-NP1) 420, 420, 380
THETA = TWOPI/FLOAT(LI/FLOAT(4*MMAX))
IF(ISIGN) 400, 390, 390
THETA = -THETA
400 WR = COS(THETA)
WI = SIN(THETA)
410 W2R = WR*WR - WI*WI
W2I = 2.*WR*WI
W3R = W2R*WR - W2I*WI
W3I = W2R*WI + W2I*WR
420 DO 530 I = 1, I1RNG*2
KMIN = I1 + IPAR*M
IF(MMAX-NP1) 430, 430, 440
430 KMIN = I1
440 KDIF = IPAR*MMAX
450 KSTEP = 4*KDIF
IF(MSTEP = NTWO) 460, 460, 530
460 DO 520 K = K1, KMIN, NTOT, KSTEP
K2 = K1 + KDIF
K3 = K2 + KDIF
K4 = K3 + KDIF
IF(MMAX-NP1) 470, 470, 480
470 U1R = DATA(K1) + DATA(K2)
U1I = DATA(K1 + 1) + DATA(K2 + 1)
U2R = DATA(K3) + DATA(K41
U2I = DATA(K3 + 1) + DATA(K41 + 1)
U3R = DATA(K11) - DATA(K21
U3I = DATA(K1 + 1) - DATA(K2 + 1)
IF(ISIGN) 471, 472, 472
471 U4R = DATA(K3 + 1 + I) - DATA(K4 + 1)
U4I = DATA(K4) - DATA(K31
GO TO 510
472 U4R = DATA(K4 + 1) - DATA(K3 + 1)
U4I = DATA(K3) - DATA(K41
GO TO 510
480 T2R = W2R*DATA(K2) - W2I*DATA(K2 + 1)
T2I = W2R*DATA(K2 + 1) + W2I*DATA(K21
T3R = WR*DATA(K3) - WI*DATA(K3 + 1)
T3I = WR*DATA(K3 + 1) + WI*DATA(K3)
T4R = W3R*DATA(K4) - W3I*DATA(K4 + 1)
T4I = W3R*DATA(K4 + 1) + W3I*DATA(K41
U1R = DATA(K1) + T2R
U1I = DATA(K1 + 1) - T2I
U2R = T3R + T4R
U2I = T3I + T4I
U3R = DATA(K11) - T2R
U3I = DATA(K1 + 1) - T2I
IF(ISIGN) 490, 500, 500
490 U4R = T3I - T4I
U4I = T4R - T3R
GO TO 510
500 U4R = T4I - T3I
U4I = T3R - T4R
510 DATA(K1) = U1R + U2R
DATA(K1 + 1) = U1I + U2I
DATA(K2) = U3R + U4R
DATA(K2 + 1) = U3I + U4I
69
DATA(K3)=U1R-U2R
DATA(K3+1)=U1I-U2I
DATA(K4)=U3R-U4R
DATA(K4+1)=U3I-U4I

KMIN=4*(KMIN-1)+11
GO TO 450

CONTINUE
M=M+LMAX
IF(M-MMAX)540,540,570

IF(ISIGN)550,560,560
0 TEMPR=WR
WR=(WR+WI)*RTHLF
WI=(WI-TEMPR)*RTHLF
GO TO 410

560 TEMPR=WR
WR=(WR+WI)*RTHLF
WI=(TEMPR+WI)*RTHLF
GO TO 410

CONTINUE
IPAR=3-IPAR
MMAX=MMAX*M
GO TO 360

C MAIN LOOP FOR FACTORS NOT EQUAL TO TWO
C VREXP=EXP(ISIGN*2*PI*SQRT(-1)*(J1+J2-13-1)/IFP2)
C 0 IF(NON2P<1.17CC0,700,601
601 IFP1=NTWO
IF=INON2
610 IFP2=IFACT(IF)*IFP1
THETA=TWOP1/FLOAT(IFACT(IF))
IF(ISIGN)612,611,611

611 THETA=-THETA
612 WSTPR=COS(THETA)
WSTPI=SLN(THETA)
DO 650 J1=1,1,IFP1,1
THEM=-TWOP1/FLOAT(J1-1)/FLOAT(IFP2)
IF(ISIGN)614,613,613
613 THEM=-THEM
614 WMNR=COS(THEM)
WMNR=SLN(THEM)
I1MAX=J1+1RNG-2
DO 650 I1=J1,I1MAX,2
DO 650 I3=I1,NTOT,NP2
1=1
WR=WMNR
WI=WMNR
J2MAX=13*IFP2-IFP1
DO 640 J2=13,J2MAX,1
TWOWR=WR+WR
J3MAX=J2+NP2-IFP2
DO 630 J3=J2,J3MAX,IFP2
J=JMIN+IFP2-IFP1
3R=DATA(JJ)
SI=DATA(J+1)
OLDSR=0.
OLDSI=0.
J=J-1FP1
620
STMPR=SR
STMPI=SI
SR=TOWWR*SR-OLDSR*DATA(J)
SI=TOWWR*SI-OLDSI+DATA(J+1)
OLDSR=STMPR
OLDSI=STMPI
J=J-1FP1
IF(J-JMIN)621,621,620
1 WORK[I]=WR-SR-WI*SI-OLDSR*DATA(J)
WORK(I+1)=WI-SR*WR+SI-OLDSI+DATA(J+1)
630
I=I+2
WTEMP=WR*STPI
WR=WR*STPR-WI*STPI
640
WI=WI*STPR+WTEMP
I=1
DO 650 J2=I3,J2MAX,1FP1
J2MAX=J2+NP2-1FP2
DO 650 J3=J2,J3MAX,1FP2
DATA(J3)=WORK(I1)
DATA(J3+1)=WORK(I4)
50
I=I+2
IF=IF+1
IFPI1=IFP2
IF(IFP1-NP2)610,700,700
COMPLETE A REAL TRANSFORM IN THE 1ST DIMENSION, N EVEN, BY CON-
CUGATE SYMMETRIES.
C
700
GO TO (900,800,900,701,ICASE
701
NHALLF=N
N=N+N
THETA=TWOPI/FLOAT(N)
ICASE=701,702,702
702
THETA=-THETA
703
STPR=COS(THETA)
STPI=SIN(THETA)
WR=STPR
WI=STPI
LMIN=3
JMIN=2*NHALLF+1
GO TO 726
710
J=JMIN
DO 720 I=MIN,NTOT,1FP2
SUMR=(DATA(I)+DATA(I+J1))/2.
SUMI=(DATA(I+1)+DATA(I+J1+1))/2.
DIFR=(DATA(I)-DATA(J))/2.
DIFI=(DATA(I+1)+DATA(J+1))/2.
DIFI=(DATA(I+1)-DATA(J+1))/2.
TEMPR=WR*SUMI*WI*DIFR
TEMPI=WI*SUMR-TEMPR
DATA(I)=SUMR+TEMPR
DATA(I+1)=DIFI+TEMPI
DATA(J+1)=DIFI*TEMPI
71
APPENDIX B

List of GAMANL input. Table B.1 lists the cards in the order in which they appear in the data deck. The parameters are indicated and the formats used are shown below the parameters. Cards labeled (2)b and (7) represent a group of data cards giving the Linearity and Gamma Spectra Data, respectively. For a 4096 channel spectrum, 512 data cards are required to read in the Gamma Spectra Data.

Table B.2 explains each of the input parameters in greater detail, and Table B.3 shows a typical input deck.
TABLE B.1

(1) **Variable** 
**FORMAT** 
\[ \text{LRT, NOCHAN, (N3, N2, N1)} \text{LIN} \] 
\[ (4I5, F5.0, I5) \]

(2a) **for LIN.LE. zero** 
**Variable** 
Previously Calc. Linearity Correction data, CNTR and CORR arrays 
**FORMAT** 
\[ (19X, F7.2, 9X, F7.2) \]

(2b) **for LIN.GT. zero** 
**Variable** 
Linearity Data, TBL array 
**FORMAT** 
\[ ((7X, 7(F6.0, 1X))/(8 (F6.0, 1X))) \]

(3) **Variable** 
S1G1, MWTL01, WTC1, W1F, S1G2, MWTL02, WTC2, W1F 
**FORMAT** 
\[ (F5.0, I5, 2F5.2, F5.0, I5, 2F5.2) \]

(4) **Variable** 
J2, FIRENG, DELENG 
**FORMAT** 
\[ (I5, 2F5.0) \]

(5) **Variable** 
Efficiency Data Array, EFFCY. 
**FORMAT** 
\[ (7 (E10.3)) \]

(6) **Variable** 
NUMRUN, NOCHAN, IMAX, DCR, ECR, BGER, IPUNCH, ERTM, SANGLE, FLUXT 
**FORMAT** 
\[ (3I5, F5.0, 2F5.1, I5, F5.0, 2E10.4) \]

(7) **Variable** 
Gamma Spectra Data, TBK array 
**FORMAT** 
\[ ((7X, 7(F6.0, 1X))/(8 (F6.0, 1X))) \]

(8) **Variable** 
EGAM1, IP1, EGAM2, IP2, FPS, ERFW 
**FORMAT** 
\[ (4X, F6.1, 4X, I6, 4X, F6.1, 4X, I6, 3X, F7.2, 3X, F7.2) \]

(9) **Variable** 
MO 
**FORMAT** 
\[ (I5) \]
<table>
<thead>
<tr>
<th>Card</th>
<th>Variable</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>LR</td>
<td>Linearity run number</td>
</tr>
<tr>
<td></td>
<td>NOCHAN</td>
<td>Number of channels in linearity run, generally 4095</td>
</tr>
<tr>
<td></td>
<td>N2</td>
<td>First calibration peak for linearity data, if there are 100 peaks, N2 = 20</td>
</tr>
<tr>
<td></td>
<td>N3</td>
<td>Second calibration peak for linearity data, if there are 100 peaks, N3 = 80</td>
</tr>
<tr>
<td></td>
<td>XN</td>
<td>Background limit for linearity data, peaks must have counts greater than XN in order to be analysed</td>
</tr>
<tr>
<td></td>
<td>LIN</td>
<td>LIN.LEQ.0 uses previously calculated linearity data, in which case NOCHAN is the number of peaks being read in under FORMAT (19X, F7.2, 9X, F7.2) LIN.GTR.0 calculates linearity correction factors using subroutine LINEAR</td>
</tr>
<tr>
<td>(2a)</td>
<td>CNTR</td>
<td>CNTR(I) is channel number at which correction CORR(I) is to be applied to correct for system nonlinearity</td>
</tr>
<tr>
<td></td>
<td>CORR</td>
<td>Linearity Data Deck TBL(I), I=1, NOCHAN</td>
</tr>
<tr>
<td>(2b)</td>
<td>TBL</td>
<td>The width of the Gaussian used in the smoothing calculation. Typical value SlGl = 128</td>
</tr>
<tr>
<td>(3)</td>
<td>S1G1</td>
<td>Cutoff channel at which the smoothing weighting function begins to decrease from WTC1 + WTF1. MWTL01 = 512</td>
</tr>
<tr>
<td></td>
<td></td>
<td>The constant term in the smoothing function. WTC1 = 0.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>The varying term in the smoothing function. WTF1 = 1.00</td>
</tr>
<tr>
<td></td>
<td>MWTL02</td>
<td>Channel about which the imp. res. weighting function deviates from WTC2. MWTL02 = 412</td>
</tr>
<tr>
<td></td>
<td>S1G2</td>
<td>The width of the Gaussian used in the improved resolution calculation. Typical value S1G1 = 128.</td>
</tr>
<tr>
<td></td>
<td>WTC2</td>
<td>Constant term in imp. res. function. WTC2 = 0.90</td>
</tr>
<tr>
<td></td>
<td>WTF2</td>
<td>Varying term indicative of how much imp. res. is desired. WTF2 = 2.00</td>
</tr>
<tr>
<td>(4)</td>
<td>J2</td>
<td>Number of points in EFFCY, efficiency array. J2 = 19</td>
</tr>
<tr>
<td></td>
<td>FIRENG</td>
<td>First energy value of EFFCY data (in keV). FIRENG = 1000</td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Function</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>----------</td>
</tr>
<tr>
<td></td>
<td>DELENG</td>
<td>Difference in energy between EFFCY points (in keV)  ( \text{DELENG} = 500 )</td>
</tr>
<tr>
<td>(5)</td>
<td>EFFCY</td>
<td>Data represents efficiency data at equally spaced energy points. Obtained from experimental results</td>
</tr>
<tr>
<td>(6)</td>
<td>NUMRUN</td>
<td>Run Number of Data Spectra</td>
</tr>
<tr>
<td></td>
<td>NOCHAN</td>
<td>Number of Data Points ( 2^{N-1} )</td>
</tr>
<tr>
<td></td>
<td>IMAX</td>
<td>Channel Number at which analysis is to begin</td>
</tr>
<tr>
<td></td>
<td>DCR</td>
<td>Slope criterion used in BAKSUB to determine if multiplet peaks are present</td>
</tr>
<tr>
<td></td>
<td>ECR</td>
<td>Error criterion used in PKANAL, peaks with percent errors in area greater than ECR are not analysed</td>
</tr>
<tr>
<td></td>
<td>BGER</td>
<td>Background factor for peak height. Peaks with heights less than or equal to ( \text{BGER} \times \sqrt{\text{background}} + 10.0 ) are not analysed</td>
</tr>
<tr>
<td></td>
<td>IPUNCH</td>
<td>If ( &lt; 0 ) Peak analysis data from PKANAL is punched out. If ( = 0 ) no punched output If ( = 1 ) smoothed data punched out ( \checkmark ) If ( = 2 ) smoothed, background subtracted data punched out ( \checkmark ) If ( = 3 ) improved resolution data punched out</td>
</tr>
<tr>
<td></td>
<td>ERTM</td>
<td>Correction factor, used in error term calculation, due to smoothing</td>
</tr>
<tr>
<td></td>
<td>SANGLE</td>
<td>Solid angle factor used in INTSTY</td>
</tr>
<tr>
<td></td>
<td>FLUXT</td>
<td>Flux, cross-section, time, and misc. correction factor used in INTSTY</td>
</tr>
<tr>
<td>(7)</td>
<td>TBK</td>
<td>Data Deck ( \text{TBK}(I), I = 1, ) NOCHAN</td>
</tr>
<tr>
<td>(8)</td>
<td>EGAM1</td>
<td>Energy (in keV) of first calibration peak. ( \text{EGAM1} = 0 ) deletes the peak analysis</td>
</tr>
<tr>
<td></td>
<td>IP1</td>
<td>Peak center of first calibration peak. Program starts search for calibration peak at ( \text{IP1}-4 ) channels. Also need ( \text{TBK}(\text{IP1}) ) to be greater than the half-maximum of the calibration peak height</td>
</tr>
<tr>
<td></td>
<td>EGAM2</td>
<td>Energy (keV) of second calibration peak.</td>
</tr>
<tr>
<td></td>
<td>IP2</td>
<td>Peak center of second calibration peak.</td>
</tr>
<tr>
<td>Card</td>
<td>Variable</td>
<td>Function</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>----------</td>
</tr>
<tr>
<td>FPS</td>
<td>First peak FWHM (keV), used in PKANAL to fit the FWHM. FPS.LE. zero implies FPS = FWHM of first calibration peak.</td>
<td></td>
</tr>
<tr>
<td>ERFW</td>
<td>Allowable range for FWHM to vary from FPS.</td>
<td></td>
</tr>
<tr>
<td>MO</td>
<td>MO.LE.0 or MO.GT.4 ends the program</td>
<td></td>
</tr>
</tbody>
</table>
|      | \[ \begin{align*} 
|      | MO = 1 & \text{loops to 2001 to accept more data} \\
|      | MO = 2 & \text{loops to 2002 to accept more data} \\
|      | MO = 3 & \text{loops to 2003 to accept more data} \\
|      | MO = 4 & \text{loops to 2004 to accept more data} 
|      | \end{align*} \] |
### TABLE B.3

**C SAMPLE GAMANL INPUT DECK**

```
//G.SYSIN DD *
393 93 20 80 10 0
 1   132.26  -8.94
 2   173.35  -6.94
 3   214.07  -4.56
 4   255.44  -2.84
```

**C LINEARITY CORRECTION FACTORS FOR 93 PEAKS, AS PREVIOUSLY CALC.**

```
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>3956.23</td>
<td>2.47</td>
<td></td>
</tr>
<tr>
<td>91</td>
<td>3999.06</td>
<td>2.75</td>
<td></td>
</tr>
<tr>
<td>92</td>
<td>4041.72</td>
<td>3.17</td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>4084.49</td>
<td>3.50</td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>1024</td>
<td>0.00</td>
<td>1.00</td>
</tr>
<tr>
<td>128</td>
<td>896</td>
<td>1.00</td>
<td>0.40</td>
</tr>
<tr>
<td>19100</td>
<td>500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.100E-05</td>
<td>0.660E-04</td>
<td>0.220E-03</td>
<td>0.400E-03</td>
</tr>
<tr>
<td>0.970E-03</td>
<td>0.970E-03</td>
<td>0.960E-03</td>
<td>0.920E-03</td>
</tr>
<tr>
<td>0.850E-03</td>
<td>0.770E-03</td>
<td>0.690E-03</td>
<td></td>
</tr>
<tr>
<td>0.610E-03</td>
<td>0.530E-03</td>
<td>0.440E-03</td>
<td>0.330E-03</td>
</tr>
<tr>
<td>701</td>
<td>4095</td>
<td>150</td>
<td>0.5</td>
</tr>
<tr>
<td>20.0</td>
<td>2.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>1.69</td>
<td>0.576E-05</td>
<td>6.000E-11</td>
</tr>
</tbody>
</table>
```

**C GAMMA SPECTRA DATA DECK CHANNELS 1 TO 4095**

```
000017 000014 000019 000017 000015 000020 000022 000016 004071
000016 000021 000018 000027 000015 000017 000019 000006 004079
000022 000024 000020 000021 000014 000014 000022 000010 004087
000017 000011 000016 000015 000019 000021 000017 000015 004095
```

/*
APPENDIX C

Output from GAMANL, Pkanal subroutine, listing gamma spectral peaks and results. The data recorded was from an iron sample irradiation in the M.I.T. Triple-Coincidence \( \gamma \)-Spectrometer (1).
<table>
<thead>
<tr>
<th>Number</th>
<th>Peak No.</th>
<th>Energy KeV</th>
<th>Width KeV</th>
<th>Weight</th>
<th>PK Height</th>
<th>Area/Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1613.61</td>
<td>7.211</td>
<td>9.248</td>
<td>578.19</td>
<td>1.1088</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1725.10</td>
<td>7.222</td>
<td>21.574</td>
<td>926.10</td>
<td>1.2583</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>2129.56</td>
<td>5.428</td>
<td>2.265</td>
<td>192.62</td>
<td>0.9447</td>
</tr>
<tr>
<td>4</td>
<td>17</td>
<td>2470.19</td>
<td>5.925</td>
<td>2.378</td>
<td>212.77</td>
<td>0.9686</td>
</tr>
<tr>
<td>5</td>
<td>20</td>
<td>2682.34</td>
<td>7.360</td>
<td>2.021</td>
<td>256.13</td>
<td>0.9375</td>
</tr>
<tr>
<td>6</td>
<td>23</td>
<td>2721.50</td>
<td>7.419</td>
<td>12.280</td>
<td>736.24</td>
<td>1.0275</td>
</tr>
<tr>
<td>7</td>
<td>25</td>
<td>2835.21</td>
<td>7.161</td>
<td>4.763</td>
<td>406.33</td>
<td>1.0705</td>
</tr>
<tr>
<td>8</td>
<td>26</td>
<td>2873.74</td>
<td>7.018</td>
<td>1.725</td>
<td>225.05</td>
<td>1.1164</td>
</tr>
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**RUN NO = 701**
**NUMBER OF CHANNELS = 4095**
**CHANNEL NUMBER SLOPE CRITERION (IMAX) = 150**
**ERROR CRITERION FOR PEAK ANALYSIS (PER-CENT) 20.0**
**SLOPE CRITERION FOR BACKGROUND IN UNITS OF SQRT CF BACKGROUND = 0.30**
**PEAK LOCATION CRITERION IN UNITS OF SQRT CF BACKGROUND (BGER) = 2.0**
**ERROR TERM REDUCTION DUE TO SMOOTHING 1.69**
**LINEARITY RUN NUMBER 393**
**T2 = 20**
**N3 = 80 XN = 10.**
**FIRST PEAK FWHM (KEV) FFW = 7.20**
**FWHM VARIATION (KEV) ERFW = 3.00**
**ENERGY PER CH.NC (KEV) = 2.145**

**ENERGY-1 = 2223.3**
**CHANNEL NO = 563**
**TRUE PEAK CENTER = 562.6**
**WIDTH (KEV) = 7.06**

**ENERGY=2 = 7367.7**
**CHANNEL NO = 2563**
**TRUE PEAK CENTER = 2961.0**
**WIDTH (KEV) = 8.35**

**SOLID ANGLE RADIANS = 0.57600E-05**
**FLUX = 0.6000E 12**

**EFFICIENCY DATA INITIAL ENERGY (KEV) = 100.0 DELTA ENERGY (KEV) = 500.**

**0.100E-05 0.660E-04 0.220E-03 0.400E-03 0.580E-03 0.760E-03 0.890E-03 0.970E-03 0.970E-03 0.960E-03**

**0.920E-03 0.850E-03 0.770E-03 0.690E-03 0.610E-03 0.530E-03 0.440E-03 0.330E-03 0.220E-03**

**NUMBER OF PEAKS = 119**

**AREAT(A) = SOM(COUNTS), AREAT(B) = FITTED GAUSSIAN**
| NO. | ENERGY (keV) | PK CNTR CHAN NO. | CHAIN CHN NO. | HEIGHT | PK H TO BG | PK INT INTI | PK AREA(A) | INT AREA(A) | PK INT ERROR | PK INT ERROR | PEAK TYPE | PK INT CHAN | PK INT KEV | PK INT KEY | PK INT BASE |
|-----|--------------|------------------|----------------|--------|------------|-------------|-------------|-------------|-------------|-------------|-----------|-----------|-------------|------------|------------|-------------|
| 1   | 1575.2       | 244.1            | 477.6          | 0.499  | 1513.2     | 1813.0      | 6.96        | 1.65        | 67.9        | 67.2        | 7.13      | 7.13      | 7.13        | 7.13       | 7.13       |
| 2   | 1613.6       | 280.5            | 578.2          | 0.679  | 2294.1     | 2193.3      | 6.43        | 1.65        | 67.3        | 67.2        | 7.13      | 7.13      | 7.13        | 7.13       | 7.13       |
| 3   | 1810.6       | 370.9            | 161.4          | 0.223  | 405.8      | 611.7       | 1.12        | 18.24       | 5.49        | 7.12        | 5.12      | 5.12      | 5.12        | 5.12       | 5.12       |
| 4   | 2129.6       | 518.7            | 192.6          | 0.216  | 490.8      | 729.7       | 0.75        | 17.51       | 5.43        | 7.12        | 5.12      | 5.12      | 5.12        | 5.12       | 5.12       |

The 3 strongest peaks are analysed as a triplet. Check background subtracted data.
APPENDIX D

Correction for System Nonlinearity

In order to correct for the nonlinearity of the data collecting system (gamma detector, amplifier and multi-channel analyser) a method described by Heath, et al. (11) is used. A high precision dc voltage standard (0-10 volt output) with an absolute accuracy of 1 part in $10^4$ is used in conjunction with a mercury relay pulser to perform the linearity check. Test pulses are inserted into the 4096 channel analyser through the preamplifier with a uniform voltage spacing. The choice of spacing depends on the gain settings of the system.

Usually 100 equally spaced peaks are put into the analyser. Two peaks, one near the low energy end and the other near the high energy end of the spectrum, are assumed to have zero linearity correction factor and the remaining peaks are fitted linearly to those two standard peaks. The standard peaks chosen could be, for example, the twentieth and the eightieth peaks. The actual peak center at channel $C$ compared with the predicted peak center for linearity at the same channel gives the correction factor for the non-linearity of the system at channel $C$.

Subroutine LINEAR calculates these correction factors and stores them in array CORR, it also needs an array CNTR to store the peak center at which the correction factor applies.

Subroutine ADJUST performs the linearity correction to a given peak center, PCNR, by use of a second order interpolation using the CNTR and CORR arrays to determine the true peak center, TPC.

It is possible to bypass the linearity correction calculation by either deleting the subroutines from the program, which means rewriting parts of the program, or by reading in linearity correction factors which are all zero. This can be done by appropriately arranging the input deck, see Appendix B.
Subroutine BAKSUB performs the background calculation and subtraction on the spectra. Basically the program finds the peaks by using a first difference calculation and sets the background as a linear fit from minima to minima of the peak. However in the case of partially resolved peaks the minima must be excluded. To do this, a slope criteria is established which sets a maximum value for the slope of the background. When the angle between the slopes of the background of two adjacent peaks is greater than the slope criterion the pair will be considered as a multiplet. This procedure is repeated for up to a maximum of five peaks. The slope criteria is expressed as DCR in the input list and is multiplied by the difference in channel numbers between two minima and by the square root of the background at the upper minima.

To make the minima of a peak more representative of the true background, the counts in the two channels, one on each side of the minima, are added to the minima counts, and the average is taken. New minima are sought using this averaged value, and it is these new minima from which the linear background fit under the peak is calculated.

BAKSUB also prints out the lower channel number of each peak, the number of counts in the lower and upper channel numbers, the slope between the two minima of a peak, and the width of the peak in channels.
APPENDIX F

Intensity Calculation

Subroutine INTSTY calculates the intensity of a gamma ray at energy E after being given its area as calculated in PKANAL. There are several options open to the user in converting from the area in counts to some other quantity. Basically as INTSTY is written the area is divided by two constants, SANGLE and FLUXT, and also by a quantity GX which varies with the energy of the gamma peak being considered.

For thermal neutron capture gamma spectra, the number of gamma rays of energy E per 100 neutrons captured is the quantity of interest. Thus the factor SANGLE represents the solid angle geometry factor for the detector as well as any minor correction factors; FLUXT represents the total number of neutron captures in the sample divided by 100; and GX is the detector efficiency at energy E as obtained by second order energy interpolation of data in the EFFCY array.

The parameters SANGLE, FLUXT, and EFFCY are inputed to the program and are determined by previous calculations.
References


9. Program FOURT available from IBM Program Information Department, 40 Sawmill River Road, Hawthorn, New York 10532
10. N. C. Rasmussen, Y. Hukai, T. Inouye and V. J. Orphan
"Thermal Neutron Capture γ-Ray Spectra of the Elements", MITNE-85 (prepublication)