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PEAKFIND: A FORTRAN PROGRAM
FOR LOCATING AND FITTING PEAKS IN
SEMICONDUCTOR DETECTOR SPECTRA

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Date Transmitted: June 1975

PREPARED FOR THE U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
UNDER CONTRACT W-7405-eng-82

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ABSTRACT

A FORTRAN program is described which locates peaks in semiconductor detector spectra and then fits a skewed-Gaussian line shape to certain of these peaks to determine centroids, areas, and peak shape parameters. The user may adjust the strictness of criteria used in the peak location procedure to permit the identification of virtually anything that might possibly be a peak, or he may specify that only well-defined peaks are to be found. An estimate is made of the centroid, energy, and intensity (corrected for the energy dependence of the detector efficiency) for each peak found. Fitting is then performed only where the estimated peak intensity exceeds a lower limit specified by the user. Alternatively, the user may specify which specific peaks he wishes to have fitted. The nonlinear least-squares fitting method is a modification of the procedure used in the companion program SKEWGAUS. PEAKFIND normally requires the user to supply only four input data cards for the analysis of a whole multichannel analyzer spectrum, and if default options are chosen for most parameters these cards will be largely blank.

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I. INTRODUCTION

PEAKFIND is a FORTRAN program used for finding and fitting peaks in multichannel analyzer (MCA) spectra obtained with semiconductor detectors. It first locates the peaks that are present in a spectrum and estimates their centroids and areas. It then fits an analytic function to the channels in the vicinity of certain of these peaks to determine (among other things) accurate centroids and areas. These centroids and areas may then be used by another program to determine transition energies and intensities.

The peak finding procedure is based on the method of Mariscotti.¹ It employs an examination of the smoothed second difference between adjacent channels in the MCA spectrum to locate the peaks. The criteria for identifying a peak have deliberately been made very loose, so that the program can be instructed to find virtually everything that might possibly be a peak (except where adjacent peaks are not resolved from each other). The user may adjust both the amount of smoothing and the tightness of the main peak identification criterion if he wishes to change the balance between the probability of missing real peaks on one hand, and of finding statistical fluctuations that are not real peaks on the other hand. The design of PEAKFIND is based on the assumption that the user will consider the missing of real peaks to be a far more serious problem than the finding of spurious peaks. Since any spurious peaks found by the program will usually be very weak, the user may discriminate against them by specifying that only the more intense peaks are to be fitted. This allows the computer to avoid the wasting of time in attempting to fit statistical fluctuations or other spurious features, while at the same time the user is still alerted to the existence of features which might perhaps be real peaks. On a subsequent

execution of the program with the same MCA spectrum the user may specify which specific peaks he wishes to have fitted. This makes it possible to fit the weaker real peaks in the spectrum without wasting time refitting the stronger peaks.

The fitting procedure is very similar to that used in program SKEWGAUS.² The fitting function is a Gaussian to which an exponential tail has been smoothly joined on the lower side. There are up to four variable parameters per peak: the height, the centroid, the full width at half maximum (FWHM), and a parameter (τ) which is the distance from the centroid to the junction point between the Gaussian and exponential functions. The latter two parameters may or may not be variable, depending on the intensity of the peak. If the separation between adjacent peaks is sufficiently small, they will be fit together as (part of) a multiplet. Multiplets with as many as nine component peaks can be handled. The background under the peaks is assumed to be linear.

Of course, no program is likely to recognize the separate existence of peaks which are totally unresolved from each other. For such cases it is necessary to use a different program (such as SKEWGAUS) which permits the user to provide input data for each fit to be performed -- in contrast to PEAKFIND, for which the user supplies input data only for the whole spectrum. SKEWGAUS may also prove useful where options are needed which cannot readily be provided in PEAKFIND. These options include the availability of three additional shape parameters per peak, the ability to constrain parameters of different peaks to maintain a fixed ratio during the fitting procedure, the use of a quadratic background, the opportunity to specify which channels are to be fit and to include gaps in the fitting

region, and other features. The greater flexibility of SKEWGAUS is achieved, however, at some cost in convenience: The user must determine for himself approximately where the peaks are located, and must supply some input data for each peak to be fit; PEAKFIND, on the other hand, requires the user to supply only four simple input data cards for the whole spectrum (which will be largely blank if the user has selected default input options), and the computer does the rest.

The author has found from experience that, for relatively simple spectra where no unresolved multiplets are present, PEAKFIND is usually adequate to perform all the fitting that is necessary. Where there are unresolved multiplets, or where more precise fitting is required, it is still very helpful to perform preliminary analysis with PEAKFIND and to leave only the 'problem' fits to SKEWGAUS.

PEAKFIND can handle MCA spectra with as many as 8192 channels. The maximum number of peaks that can be handled at one time is 250. Any number of MCA spectra may be analyzed in one execution of the program. In addition, it is possible to analyze one MCA spectrum several times, using different parameters or examining different parts of the spectrum each time.

The load module for PEAKFIND, when compiled with the H level FORTRAN compiler, is about 156 kilobytes long (39 K words) when no overlays are used. A simple overlay structure may be used to permit execution in a 128 kilobyte region of core storage.

The execution speed of PEAKFIND may be illustrated by the following example: A typical recent execution on the IBM 360/65 system at Iowa State University found 139 peaks in an 8192 channel MCA spectrum; performed 13 fits with an average of more than 50 channels in each fit, involving a

total of 29 peaks with 84 variable parameters, and requiring a total of 97 iterations; all in 24.3 seconds of CPU time (exclusive of the plot step).

II. PEAK FINDING PROCEDURE

The method used in PEAKFIND for locating peaks is a modification of the method of Mariscotti.¹ (Ref. 1 will henceforth be referred to as MAM.)

Let us assume temporarily that the MCA spectrum is a continuous curve, rather than a series of discrete points. The peaks that we wish to locate rise above a background that we shall assume is approximately linear in the vicinity of a peak. This background may be eliminated by taking the second derivative of the curve. The shape of the second derivative in the vicinity of the peak will depend, of course, on the shape of the peak itself; but for any reasonable peak shape, we may assume that the second derivative will be rather strongly negative near the highest point of the peak, becoming positive on either side of the peak and going to zero a short distance away from the peak. A fluctuation of this sort in the second derivative could be taken as the indication of the existence of a peak.

In reality, of course, the spectrum consists of discrete points rather than a continuous curve. This suggests the examination of the second difference of the MCA data channels. If there were no statistical fluctuations in the data, the statements of the previous paragraph would continue to be valid, with the phrase "second difference" replacing "second derivative." In fact, however, the statistical fluctuations in the second difference are quite significant. To illustrate, let us call the number of counts in the i th channel N_i , and let us assume that the statistical uncertainty in this

number is $\sqrt{N_i}$. The second difference is given by

$$S_i = N_{i+1} - 2 N_i + N_{i-1} \quad (1)$$

The statistical uncertainty in S_i is given by

$$F_i = \sqrt{N_{i+1} + 4 N_i + N_{i-1}} \quad (2)$$

Now suppose that we have a peak whose shape is a perfect Gaussian function with a height of 100 counts and a FWHM of 5 channels, rising above a flat background with an average height of 100 counts per channel. Such a peak would be easily recognizable, standing well above the statistical fluctuations in the background. But the value of S_i at the centroid of the peak (where the magnitude of S_i is greatest) would be -21 counts, while the uncertainty in this value would, from (2), be more than 34 counts. Thus, the peak might easily be overlooked in a search of S_i versus channel number. It follows that some procedure for smoothing the statistical fluctuations is essential if the second difference approach is to be used.

The simplest smoothing technique is to perform an unweighted average of the counts in a group of w adjacent channels centered about a given channel.

If this "smoothing window" w is an odd integer, we may set $w = 2m + 1$ and

$$\text{write } S_j^1 = \sum_{j=i-m}^{i+m} S_j^0 \quad (3)$$

where S_j^0 is given by (1). (A weighted average would involve dividing the right side of (3) by w , but it is not necessary to perform this calculation.)

Further smoothing is accomplished by repeating the application of (3), so that the relationship between successive smoothings of the data is

$$S_i^{n+1} = \sum_{j=i-m}^{i+m} S_j^n \quad (4)$$

where the superscript of S refers to the number of times the smoothing operation has been performed. MAM gives an extensive treatment of the determination of optimum values for the smoothing window, w , and the number of smoothings, z . The conclusion is drawn that 5 smoothings with w equal to the odd integer closest to $0.6 \times \text{FWHM}$ provides the best compromise between the objectives of being able to recognize small isolated peaks on a large background, and being able to recognize both members of closely-spaced doublets.

The experience of the author has indicated that the amount of smoothing is highly important to the success of the program when one is dealing with complicated spectra. Too much smoothing can cause both members of closely-spaced doublets to be missed, while too little smoothing can cause fairly prominent single peaks to be missed if the statistical fluctuations are great enough. Because of this, the restriction of w to odd integers has been found to be undesirable. An even value for w does not readily lend itself for use with equation (3) because of the fact that the values of j cannot be symmetrically placed about i . However, this problem can be overcome if the number of smoothings is even. One can easily show that the recursion formula for the result of two successive smoothings can be written as

$$S^{n+2}_i = w S^n_i + \sum_{j=1}^{w-1} (w-j) (S^n_{i-j} + S^n_{i+j}) \quad (5)$$

This expression is equally valid if w is even or odd. PEAKFIND performs its smoothing by applying (5) twice to the second difference, producing the effect of four smoothings. The default value for w is the integer (odd or even) closest to $0.6 \times \text{FWHM}$. The user may, if he wishes, override the default value for w merely by supplying his own value as part of the input data.

It is necessary to calculate the statistical uncertainty in S_i (we henceforth drop the superscript on S since the number of smoothings is assumed to be 4). Where the number of counts in nearby channels is approximately equal to N_i , this statistical uncertainty is easily shown to be

$$F_i = \sqrt{\varphi N_i} \quad (6)$$

where φ is a constant whose value depends on w and the number of smoothings. MAM has a tabulation of φ for odd values of w with z from 1 through 5. For $z=4$ as used in PEAKFIND, the values of φ are 6, 28, 82, 184, 350, 596..... for $w = 1, 2, 3, 4, 5, 6$, respectively.

In the vicinity of a peak, it is to be expected that S will have a form similar to that shown in Fig. 1. Here, i_1 and i_2 are the first and last channels in which S_i is greater than its statistical uncertainty F_i ; i_3 and i_5 are the first and last channels in which S_i is negative; and i_4 is the channel in which S_i has its maximum negative value. MAM contains a detailed theoretical investigation of the relationships to be expected among these channels under the assumption of a Gaussian peak shape. This investigation leads to the assignment of four conditions for the identification of a peak, based on (a) the magnitude of S_i at i_4 , (b) the width of the region between i_3 and i_5 , (c) the separation of channels i_2 and i_3 , and (d) the width of the region between i_1 and i_2 . These rather stringent conditions were established in MAM to prevent the mistaken identification of Compton edges, statistical fluctuations, or other spurious features as peaks.

The author's experience with the conditions of MAM have led him to the conclusion that they are far too restrictive for the purposes for which PEAKFIND is intended, in that they cause too many real peaks to be

Fig. 1. The shape of the smoothed second derivative in the vicinity of a Gaussian peak. The dashed line indicates the statistical uncertainty in the second derivative.

missed (especially in complicated spectra). Condition (d) frequently causes the upper component of a partially resolved doublet to be missed, and the lower component may be missed as well if it is smaller than the upper component, due to condition (b). Condition (d) can also prevent the identification of moderately weak peaks that happen to have large statistical fluctuations.

In an attempt to correct these problems, an entirely different set of conditions for recognizing peaks was adopted in PEAKFIND. These conditions were determined from experience rather than from theoretical considerations. It was found that any test on the region from i_1 to i_3 in Fig. 1 tends to cause real peaks to be missed, especially in partially resolved multiplets. Therefore, it was decided to test only on the region from i_3 to i_5 . The following conditions were established:

1. The region from i_3 to i_5 must be at least $w+1$ channels wide and not greater than $3 \times \text{FWHM}$ channels wide.
 2. The sum of the values of S_i between i_3 and i_5 inclusive must be great enough to satisfy inequality (7) where C (the peak limit parameter) is a constant whose default value is 2.0.
- $$\sum_{i=i_3}^{i_5} S_i > C \times w \times F_{i_3} \quad (7)$$

The first condition tends to prevent the mistaken identification of either narrow statistical fluctuations or broad features such as Compton edges and backscatter peaks. The second condition effectively determines the smallest peak that can be found by the program. It seems more reasonable, from statistical considerations, to base this condition on the total area of the negative region of S_i rather than on the height, as is done in MAM.

These conditions are sufficiently loose that PEAKFIND will occasionally find spurious features that are not real peaks. This generally presents no

problem since the spurious peaks may easily be rejected before fitting is performed, as described in the following section. However, the user may, if he wishes, reduce the tendency to find such spurious peaks by increasing the value of C in condition 2, but at some cost in the likelihood of missing real peaks that he is interested in.

Fig. 2 shows a portion of a typical gamma-ray spectrum of the sort with which PEAKFIND is commonly used, indicating the peaks that were found when the default options for w and C were chosen. The peak width is about 4.6 channels here, so the default value for w is 3 channels. The default value for C is always 2.0. The vertical scale in this figure is proportional to the square root of the number of counts. On such a plot the statistical error bars are approximately constant in length, and it is these error bars that are plotted in Fig. 2.

It will be noted that peak 7 in the figure is actually a Compton edge, and the existence of peaks 10 and 12 is open to question. All the other peaks, however, are almost certainly real. If the peak limit parameter C is raised to 3.0, the program does not find peaks 7, 10, and 12, but it does find all the other nineteen peaks. On the other hand, it may be observed that the program has failed to recognize that peak 6 is an unresolved doublet, that there is a weak component on the upper side of peak 9, and that there is an additional component below peak 14 and one above peak 15. Nothing can be done in PEAKFIND with peaks 6 and 9, but the additional components next to peaks 14 and 15 are found if the window width w is lowered to 2 while C is kept at its default value of 2.0. This combination of parameters also finds peak 12 to be a doublet, and finds two additional peaks (at channels 1157 and 1216) which are probably not real. However, the Compton edge near channel 970 is not mistaken for a peak when the combination $w = 3$, $C = 2.0$ is used.

Fig. 2. Typical gamma-ray spectrum showing peaks identified by PEAKFIND when default options were used. Vertical scale is proportional to the square root of the number of counts.

This example should serve to illustrate the effectiveness of PEAKFIND in locating peaks, and also the ways that the program parameters may be adjusted to suit the user's requirements. This is an example taken from actual practice -- the spectrum of which Fig. 2 is a part was analyzed during a study of the decay properties of 64-second ^{140}Cs .³

After a peak has been found, an estimate is made of its centroid and area from the smoothed second difference. The centroid of S_i in the region between i_3 and i_5 is used as the estimate of the peak centroid. This estimate usually proves to be quite accurate, rarely being in error by more than a few tenths of a channel for reasonably well resolved peaks. The centroid is converted into a peak energy using a linear calibration of channel number versus energy, supplied by the user.

The peak area is assumed to be proportional to the area of the negative region of S_i . The latter area is divided by an approximate value for the efficiency of the detector, and then normalized using a value of 100 for the intensity of the strongest peak found. The detector efficiency is assumed to be represented by a straight line on a full logarithmic plot of efficiency versus energy, except at low energies where the straight line smoothly joins a concave-downward parabola. The efficiency curve is determined by only two parameters that may be supplied by the user -- the slope of the line giving $\log_{10}$ (efficiency) versus $\log_{10}$ (energy), and the energy at which the efficiency curve is a maximum. The default values supplied by the program for these parameters are 1.0 for the slope and 0.1 MeV for the energy of maximum efficiency. These are reasonable values for a moderate-sized coaxial Ge(Li) detector.

The intensity estimates obtained in this fashion are not, of course, expected to be extremely accurate. They are merely intended to aid the user in identifying the individual peaks and to provide a basis for deciding whether a peak is intense enough to be fitted. Experience has shown that the estimates are generally well within a factor of two of the correct values for reasonably well-defined peaks.

In the foregoing section, the FWHM has been treated as if it were constant throughout the whole spectrum. In fact, however, the peak widths usually increase with increasing energy. It is not feasible to permit FWHM to vary in the peak finding procedure. On the other hand, there is no problem in taking into account the variation of FWHM with peak energy when the fitting is performed. This is accomplished by permitting the user to supply, as part of his input data, the intercept and slope of a straight line giving FWHM as a function of energy. While the peak search is being performed, a unique value of FWHM is used by the program -- the value appropriate for a peak precisely at the center of the region being searched. After the peaks are found, each is assigned the FWHM value appropriate for its energy.

III. TO FIT OR NOT TO FIT

Before performing a fit to a peak, it is necessary to establish whether the peak is sufficiently well separated from nearby peaks to allow it to be fitted singly, or whether it must be included with other peaks as part of a multiplet. This decision is based on the FWHM of the peak, as obtained from the straight line supplied by the user giving FWHM as a function of energy. If the separation between two adjacent peaks is less than some constant times FWHM (the default value of this constant being 4.0), they

will be fitted together as (part of) a multiplet. Up to nine peaks may be included in one multiplet. The fitting region will extend below the centroid of the lowest peak a number of channels equal to a constant (default value, 3.0) times the FWHM of the lowest peak, and above the centroid of the highest peak a distance equal to another constant (default value, 2.5) times the FWHM of the highest peak.

It is to be expected that the user will not normally wish to fit all the peaks that have been found. Since the existence of many of the weaker peaks is often questionable, one may wish to specify that only the more intense peaks are to be fitted. Since each peak has been given an intensity estimate, it is possible to specify that only those peaks whose intensity exceeds some cutoff value shall be fitted. The default value for this cutoff is 2.0 (relative to 100 for the most intense peak), but this default value is often overridden in practice. In a multiplet fit, fitting will be performed if any component peak has an intensity exceeding the cutoff value.

A second intensity cutoff value is provided to make it possible to determine those peaks for which the FWHM is to be considered a variable fitting parameter. Since the shapes of the weak peaks are often poorly defined, it is desirable to fix FWHM for these peaks to the straight line values determined from the input supplied by the user. For the stronger peaks whose intensity exceeds the FWHM cutoff, the straight line values of FWHM will be treated only as initial estimates; the "best" values will be determined by the fit. The default value for the FWHM intensity cutoff is 5.0. If the user overrides this default by specifying a value greater than 100, then (since no peak has an intensity greater than 100) all peaks will have fixed FWHM's.

The peak shape parameter τ is treated in a manner similar to FWHM. The user supplies the slope and intercept of a line giving τ as a function of energy (or accepts default values, as described in the following section). A value of τ is assigned to each peak from the straight line. This value is considered to be fixed for any peak whose intensity is less than the τ cutoff, and is treated as an initial fitting estimate for a more intense peak. The default value for the τ cutoff is 10. By overriding with a value greater than 100, the user may fix the τ 's of all peaks.

Before any fitting is attempted, the program provides printed output giving a list of the peaks found with their estimated energies and intensities, as illustrated in the upper part of Fig. 3. Starred peaks are those whose intensities exceed the fit cutoff value. Next, output is provided to indicate how these peaks are grouped into multiplet fits, as illustrated in the lower part of Fig. 3. This list includes the number of peaks in each multiplet, the energy of the first peak of the multiplet, the first and last channels in the fitting region, the initial estimates of FWHM and τ for the first peak, and the centroids of all peaks in the multiplet. The output illustrated in Fig. 3 was obtained from an analysis of the spectrum of Fig. 2, using default values for all parameters except the energy calibration and FWHM.

At this point, the user has three options on how to proceed. The options are determined by the value of the index IFIT.

IFIT = 0: No fitting will be attempted. The user wishes to examine the output already provided before proceeding further.

IFIT = 1: Fitting will be attempted for all multiplets in which at least one component peak has an intensity greater than the fit cutoff value.

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PEAKFIND SEARCH BETWEEN CHANNELS 845 AND 1270 SMOOTHING WINDOW = 3 PEAK LIMIT PARAMETER = 2.0

CUTOFFS: FIT. 2.0 FITDEL = 3.0 ENERGY = -0.51 KEV + 0.736900 KEV PER CHANNEL TAIL = 0.0 + 0.0 PER MEV
 FWHM. 5.0 FITADV = 2.5 FWHM = 3.000 + 1.000 PER MEV SKULO = 0.0 + 0.0 PER MEV
 TAU. 10.0 SEP = 4.0 TAU = 2.450 + 0.0 PER MEV SKULI = 0.0 + 0.0 PER MEV

PEAK NUMBER	CHANNEL	ENERGY	INTENSITY	TO BE FIT
1	852.77	821.00	0.455	
2	860.78	827.80	1.273	
3	881.68	843.80	0.643	
4	894.89	858.94	0.782	
5	921.02	872.19	11.837	*
6	952.33	895.26	4.696	*
7	967.13	906.17	0.262	
8	996.34	927.69	0.592	
9	1007.88	936.19	4.566	*
10	1023.37	947.61	0.156	
11	1040.27	960.07	0.670	
12	1053.26	969.64	0.134	
13	1078.91	988.84	0.222	
14	1092.92	998.86	0.681	
15	1101.68	1005.32	0.821	
16	1122.53	1026.68	2.593	*
17	1136.39	1036.89	1.055	
18	1179.38	1082.87	0.391	
19	1194.52	1072.73	0.018	
20	1204.97	1081.43	0.741	
21	1241.57	1006.40	100.000	*
22	1255.89	1018.05	1.986	

SUMMARY OF PARAMETERS FOR FITS

FIT NO.	HPX	ENERGY	FIRST CHAN	LAST CHAN	FWHM	TAU	CENTROIDS
1	2	421.9	845	872	4.52	2.45	852.77 860.78
2	2	643.2	868	906	4.54	2.45	881.68 894.89
3	1	672.2	907	932	4.87	2.45	921.02
4	2	695.3	938	978	4.60	2.45	952.33 967.13
5	5	727.7	982	1064	4.63	2.45	996.34 1007.88 1023.37 1040.27 1053.26
6	3	788.5	1064	1113	4.64	2.45	1078.91 1092.92 1101.68
7	2	820.7	1108	1148	4.72	2.45	1122.53 1136.39
8	3	862.6	1165	1216	4.76	2.45	1179.38 1194.52 1204.97
9	2	908.4	1227	1267	4.81	2.45	1241.57 1255.89

NUMBER OF FITS IS 9

Fig. 3. Preliminary output provided by PEAKFIND for the spectrum of Fig. 2, indicating the peaks found and the grouping of these peaks into multiplets.

IFIT = 2: Fitting will be attempted for those specific multiplets designated by the user. Multiplets are identified by the fit number as given in the first column of the lower part of Fig. 3.

The last option is useful primarily for fitting selected weaker peaks in a spectrum whose stronger peaks have already been fitted on previous executions of PEAKFIND with IFIT = 1. Obviously, the user cannot know the numbers of the multiplets he wishes to fit unless he has previously obtained a listing similar to that shown in Fig. 3. Furthermore, it is necessary that most of the input parameters remain unchanged between executions in order to guarantee that exactly the same peaks will be found and that they will be grouped into multiplets in exactly the same way. However, those parameters that do not affect the finding or grouping of peaks (notably the cutoff and τ parameters) may safely be changed without affecting the multiplet identification.

IV. PEAK FITTING PROCEDURE

The peak fitting procedure is very similar to that used in program SKEWGAUS, and the reader is directed to Ref. 2 for complete details. Only a brief summary is given here.

The fitting function is a Gaussian to which a simple exponential function has been smoothly joined on its lower side. The four variable parameters are the peak height h , the centroid x_0 , the FWHM of the Gaussian, and the distance τ (in channels) from the centroid to the junction point. These parameters are illustrated in Fig. 4. The height and centroid are always treated as variable fitting parameters, but FWHM and τ are variable only for those peaks whose intensity estimates exceed the corresponding cutoff values, as explained in the previous section.

Fig. 4. Function used for peak fitting.

The fitting function used in SKEWGAUS includes three additional variable parameters which permit a wider variety of peak shapes to be fit. These additional parameters are the tail parameter (t in Fig. 4), which permits the fitting function to approach a constant value other than zero on its lower side; the lower skewness parameter, which permits some additional skewing of the lower side of the peak; and the upper skewness parameter, which provides for skewing on the upper side of the peak. These three are not available as variable parameters in PEAKFIND; however, provision has been made for the user to supply fixed values for these parameters for each peak. This is accomplished, as with FWHM and τ , by supplying the intercept and slope of a straight line giving the value of each parameter as a function of peak energy.

The background in PEAKFIND fits is a straight line given by the expression

$$f_B = A + B (x - x_1) \quad (8)$$

where x is channel number and x_1 is the number of the first channel in the fitting region. The use of a more complicated function allowing for curvature in the background has been found from experience to be undesirable, causing more problems than it solves. If a curved background is clearly called for, SKEWGAUS should be used.

Fitting is accomplished by the standard nonlinear least-squares (NLLS) method. The quantity

$$Q = \sum_i w_i (N_i - f_i)^2 \quad (9)$$

is minimized by an iterative process. Here, N_i is the number of counts in the i th channel, f_i is the fitting function evaluated at the i th channel, and w_i is a weight associated with the error in N_i . The weight w_i is given by

the following expression:

$$w_i = 1/[N_i(1 - c + d^2 N_i) + c N_m] \quad (10)$$

Here, d is the r.m.s. deviation in channel width of the analogue-to-digital convertor of the MCA (i.e., the differential nonlinearity), N_m is the maximum number of counts among the channels included in the fit. The constant c is included for the purpose of reducing somewhat the very large weight that would otherwise be given to channels with a small number of counts, where N_i is very small compared with N_m . The values of c and d built into the program are 0.02 and 0.005, respectively, but they may easily be changed if desired. Setting c and d both equal to zero will give standard statistical weighting.

Q is minimized by solving the set of nonlinear equations

$$\partial Q / \partial \alpha_j = 0 \quad (11)$$

where α_j represents the j th free parameter in the fitting function. Since equations (11) are not solvable analytically, an iterative procedure is used to get an approximate solution. Initial estimates are supplied for the values of the free parameters, and equations (11) are expanded in powers of small quantities. The nonlinear terms in the expansion are dropped, and the resulting linear equations are solved by the method of matrix inversion. The solution is a set of new (and hopefully better) values for the α_j , which are then used as estimates in the next iteration.

The iterative procedure continues until one of the following conditions occurs:

- (1) All parameters no longer change significantly on successive iterations (normal convergence). A "significant" change is defined to be a fractional change of 10^{-3} in h , 10^{-5} in x_0 , 10^{-3} in FWHM, 5×10^{-3} in τ , 10^{-4} in A , and 10^{-4} in the quantity $(B + 1000)$.

(2) Q increases on successive iterations, or fails to decrease fractionally by more than 10^{-4} . The test for this condition is not applied until the twentieth iteration since Q frequently increases on early iterations but subsequently decreases.

(3) The coefficient matrix is singular, so the equations resulting from the linearization of (11) cannot be solved. This usually means that some variable parameter is totally undefined.

(4) Thirty iterations have taken place and none of the above conditions has occurred.

After convergence has been achieved, or the iterative procedure has been stopped without convergence because of conditions (3) or (4), the final value of Q is divided by the number of degrees of freedom (the number of channels in the fit minus the number of variable parameters) to determine the variance of the fit. If only statistical fluctuations affected the quality of the fit, one could distinguish a good fit from a poor one by the requirement that the variance be close to 1.0 for a good fit. In fact, however, there are many non-statistical effects that must be considered, the most important being the fact that the fitting function is an arbitrarily chosen representation of the peak shape. Where the number of counts in a peak is large (say, on the order of 10^6), the statistical uncertainties in the data points are small enough to expose the small differences between the fitting function and the actual line shape, with the result that the variance may be significantly greater than 1.0 for a fit that is completely acceptable. On the other hand, a fit to a small multiplet rising above a large background may yield a variance close to 1.0 even if some major error has occurred, such

as the failure to find all of the components of the multiplet. It follows, then, that the variance alone cannot be relied upon blindly in determining whether a fit is acceptable. Examination of a plot of the fit is strongly recommended.

The uncertainty in the final value of each variable parameter is determined by taking the square root of the product of the appropriate diagonal element of the inverted coefficient matrix times the variance. These uncertainties must be interpreted with some care since they are based on statistical considerations only and do not take into account such non-statistical factors as the imperfect representation of the actual peak shape by the fitting function. Further discussion of the parameter uncertainties (as well as all the other topics covered in this section) may be found in Ref. 2.

The NLLS method of fitting requires that initial estimates be provided for all variable parameters. The background parameters A and B are initialized as, respectively, the number of counts in the first channel of the fitting region and the slope of a line drawn between the first and last channels of the region. The centroid estimates are provided when the peaks are found, as discussed above. The height of a peak is estimated to be the contents of the centroid channel minus the background contribution to that channel. FWHM and τ , as has been mentioned, are given estimates based on the assumption that these parameters vary linearly with energy. In practice, one simply estimates visually the FWHM for a few of the stronger peaks in the spectrum and fits these values to a straight line. The slope and intercept of this line must be supplied as part of the input data. It is not so easy to estimate τ visually, so the user may let the program

itself determine the initial estimates for τ . Since τ usually varies quite slowly with energy, the default initial estimate is the same for peaks of all energy, being equal to one-half the FWHM for a 1 MeV peak. After the stronger peaks in a spectrum have been analyzed, the user may wish to use the fitted values of FWHM and τ for these peaks to determine the best straight lines giving FWHM and τ as functions of energy. These straight lines may be used in fitting the weaker peaks. Experience has shown that the assumption of a linear variation of FWHM and τ with energy is generally quite satisfactory.

V. PROGRAM OUTPUT

A. Printed output

The preliminary output listing provided after the peaks have been found was discussed above and illustrated in Fig. 3.

A listing of the values of all variable parameters after each iteration of each fit may optionally be provided. A typical listing for one fit is shown in Fig. 5. This fit consists of peaks 21 and 22 of Fig. 2. The parameter values listed under iteration 0 are the initial estimates. The parameters are numbered as follows:

- 1, height of first peak;
- 2, centroid of first peak;
- 3, FWHM of first peak;
- 4, τ of first peak;
- 5, height of second peak;
- 6, centroid of second peak.

In this example, the intensity estimate for the second peak was sufficiently small that its FWHM and τ (parameters 7 and 8) were not variable and hence

```

FIT NO. 9          CHANNELS 1227 THROUGH 1267      PEAKS 21 THROUGH 22

PARAMETERS FOR PEAK(1):  ENERGY = 000.4 KEV  FWHM = 4.608  TAU = 2.450  TAIL = 0.0  SKJLO = 9.0  SKUMI = 0.0

VALUES OF FREE PARAMETERS AFTER EACH ITERATION

      ITERATION
PARAM  0      1      2      3
1  1.27003E 05  1.32540E 05  1.33700E 05  1.33329E 05
2  1.24157E 03  1.24150E 03  1.24154E 03  1.24154E 03
3  4.40040E 00  4.40530E 00  4.41300E 00  4.41470E 00
4  2.45000E 00  1.81071E 00  1.81416E 00  1.81960E 00
5  2.44861E 03  2.70347E 03  2.80134E 03  2.80134E 03
6  1.25000E 03  1.25074E 03  1.25570E 03  1.25574E 03
7  2.11750E 04  2.80814E 04  2.19374E 04  2.19379E 04
10  0.43310E 02  0.81810E 02  0.31450E 02  0.31943E 02
0  1.03010E 03  3.04320E 02  2.09180E 02  2.09130E 02

CONVERGED IN 3 ITERATIONS

VARIANCE = 7.85      Q = 2.05913E 02      VARIANCE/SUM OF WEIGHTS = 8.4631E 03

```

Fig. 5. Typical output for one fit, which includes peaks 21 and 22 of Figs. 2 and 3.

are not listed. If there were a third peak, its parameters would be numbered 9 through 12, and so on. The next-to-last parameter (number 9 in this example) is always the background height A. The last free parameter is the background slope B plus 1000.

In the example of Fig. 5, convergence is achieved very quickly because the initial estimates are reasonably close to the correct values and the peaks are very well defined. In other cases convergence is not always so rapid.

After all fits have been performed on one MCA spectrum, a summary output of the essential results of the fits is provided. A typical summary output is shown in Fig. 6. The first few columns are the fit number, the number of peaks in the fit, the number of free parameters, the number of channels in the fit, the variance of the fit, and the reason for convergence or non-convergence. The final values of all parameters for the individual peaks follow. An error of 0.0 indicates that the parameter was not variable. The areas are obtained by numerically integrating the fitting function over all the channels included in the fit. The error in the area is a combination of the error in the height and the error in FWHM. Further details concerning areas may be found in Ref. 2.

This summary output is provided in the same job step as the rest of the program, rather than in a separate job step or a separate job, as is the case for the SKEWGAUS summary output.

B. Punched-card output

Two types of punched-card output may be provided by PEAKFIND. The first type is suitable for input to program SKEWGAUS, and is intended for situations where the fitting done by PEAKFIND is not adequate. One card is

CS 140 RUN 140-10 615-985 KEV

PEAKFIND SEARCH BETWEEN CHANNELS 845 AND 1270 SMOOTHING WINDOW = 3 PEAK LIMIT PARAMETER = 2.0

CUTOFFS: FIT. 2.0 FITDEL = 3.0 ENERGY = -0.51 KEV + 0.736900 KEV PER CHANNEL TAIL = 0.0 + 0.0 PER MEV
 FWHM. 5.0 FITABV = 2.5 FWHM = 3.900 + 1.000 PER MEV SKULO = 0.0 + 0.0 PER MEV
 TAU. 10.0 SEP = 4.0 TAU = 2.450 + 0.0 PER MEV SKUMI = 0.0 + 0.0 PER MEV

SUMMARY OF FITTING RESULTS

FIT	NPKS	NFREE	NPTS	VAR ENERGY	ICNV	MIT HEIGHT & ERROR	CENTROID & ERROR	FWHM & ERROR	TAU & ERROR	AREA & ERROR	% ERROR
3	1	0	26	1.54 672.2	5	5 20100.7 301.3	920.985 0.029	4.440 0.074	1.749 0.103	1.311E 05 2.692E 03	2.1
4	2	0	41	7.21 695.2 701.8	3	27 8243.6 424.1 690.7 344.7	952.265 0.124 961.245 1.034	4.506 0.0 4.506 0.0	2.450 0.0 2.450 0.0	4.194E 04 2.168E 03 4.543E 03 1.860E 03	5.1 40.9
5	5	12	63	2.48 728.3 736.1 747.4 759.9 773.0	2	20 2015.6 204.0 9567.9 220.6 192.5 180.0 829.4 186.5 563.2 199.6	997.202 3.282 1007.814 0.088 1023.091 0.000000 1040.089 0.574 1057.889 0.803	4.628 0.0 4.636 0.0 4.649 0.0 4.660 0.0 4.670 0.0	2.450 0.0 2.450 0.0 2.450 0.0 2.450 0.0 2.450 0.0	1.034E 04 1.046E 03 4.931E 04 1.133E 03 9.919E 02 9.278E 02 4.287E 03 9.638E 02 3.021E 03 1.034E 03	10.1 2.3 93.3 22.8 34.2
7	2	0	41	3.60 820.7 830.9	5	3 3393.4 224.9 1898.1 221.3	1122.513 0.165 1136.627 0.284	4.731 0.0 4.731 0.0	2.450 0.0 2.450 0.0	1.780E 04 1.179E 03 9.981E 03 1.163E 03	6.6 11.7
9	2	0	41	7.65 906.4 918.8	5	3 133320.3 1421.9 2651.4 341.1	1241.542 0.023 1255.745 0.292	4.415 0.047 4.619 0.0	1.620 0.063 2.450 0.0	6.836E 05 1.026E 04 1.831E 04 1.632E 03	1.8 12.0

EXPLANATION OF ICNV: 2 - 0 INCREASED ON LAST ITERATION
 3 - 0 DECREASED BY LESS THAN EPS0
 4 - ERROR MATRIX WAS SINGULAR
 5 - CONVERGED NORMALLY
 6 - DID NOT CONVERGE IN MAXIT ITERATIONS

Fig. 6. Summary output for fits performed as indicated in Fig. 3.

provided for every fit in the "Summary of Parameters for Fits" (Fig. 3), appropriate for use as data control card D of SKEWGAUS. These cards have the fit number punched in columns 78-80 for identification purposes. In addition, one card is punched for every peak found, in a manner appropriate for use as data control card E of SKEWGAUS.

The second type of punched-card output is intended for use where the results of the PEAKFIND fits are satisfactory, and are to be used to determine accurate energy and intensity values, including corrections for system nonlinearities, detector efficiency variation, and the like. This processing is done by a program called DRUDGE. PEAKFIND will optionally provide punched cards that may be used as input for DRUDGE. There will be one card for each peak that has been fitted, containing the following information: the centroid, the error in the centroid, the area, the height, the error in the height, FWHM, the error in FWHM, τ , and the error in τ . The first five quantities are punched in 10-column fields, the last four quantities in 5-column fields.

Note that these cards for DRUDGE are punched only for those peaks that were actually fitted, while the cards for SKEWGAUS are provided for all peaks found, whether or not any fitting was performed.

C. Graphical output

A graph of the results of a fit is an indispensable aid in determining the quality of the fit. Typical plots are shown in Figs. 7 and 8. It may be observed that the fit in Fig. 8 appears to be quite good, in spite of the fact that the variance of this fit is 7.85, which would normally be taken to indicate a very poor fit. This is a common situation where the height of the peak is in excess of 10^5 counts, as is the case here.

Fig. 7. Graphical output for fit 3 of Fig. 6 (peak 5 of Figs. 2 and 3).

Fig. 8. Graphical output for fit 9 of Fig. 6 (peaks 21 and 22 of Figs. 2 and 3). Output from this fit is also shown in Fig. 5.

The plots are drawn with a constant number of channels per inch (default value, 10). The channels plotted include five additional channels on either side of the fitting region that were not included in the fit. The fitting function is drawn as a smooth curve through only those channels that were actually included in the fit. The vertical scale is the square root of the number of counts. The plotting symbol is normally a vertical line whose length indicates the statistical uncertainty in the number of counts -- an error bar, in effect. If the number of counts is sufficiently large, the size of the error bar becomes too short for convenience. In this event, a triangle (whose size has no significance) is used as the plotting symbol.

The graphs are plotted by a Cal-Comp plotter. Most of the work of plotting is done by a set of routines designed locally by D. G. Scranton and known as SIMPLOTTER.⁴

It must be admitted that not all PEAKFIND fits are as successful as those graphed in Figs. 7 and 8. Because of the unresolved doublets in the spectrum of Fig. 2, it was necessary, when these data were analyzed during the study of the ^{140}Cs decay scheme,³ to resort to SKEWGAUS in order to get acceptable fits for a number of the multiplets.

VI. PROGRAM INPUT

A. MCA data

The MCA data may be in several forms -- on cards, magnetic tape, or magnetic disk -- that are appropriate for the MCA's with which this program is generally used. One subprogram, named INPUT, performs the sole function of reading these data. This subprogram is nearly identical with the subprogram of the same name in SKEWGAUS, which is described in detail in Ref. 2. The

only essential difference is that in PEAKFIND an additional option is provided which permits the reading of the MCA data to be bypassed, so that a given spectrum may be analyzed more than once.

It is assumed that the initial channel of the MCA spectrum being read is channel 0, not channel 1 (except for data on cards, for which the user may specify the initial channel number).

B. Data control cards

The input data deck consists basically of four cards for each MCA spectrum. These cards are designated by the letters A through D. If the option of fitting specified multiplets (IFIT=2) has been chosen, there will be one or more additional cards, of type E.

Card A specifies the form of the MCA data. The format of this card is given in Table I. It is identical to card A of SKEWGAUS, except that an additional option has been provided for variable IREAD.

Card B is a title card on which may appear any 80 characters. These will be printed as the heading of the printed output. In addition, the contents of columns 1-20 of this card will be the first line of the title on each graph.

Card C contains the options for finding and fitting peaks. The format for this card is given in Table II.

Card D contains the energy-dependent quantities. The format for this card is given in Table III.

Card(s) E appears only if IFIT is equal to 2 on card C. A letter T (for "true") will be punched in each column for which the correspondingly numbered multiplet is to be fitted. The numbering of the multiplet fits is given in the first column of the "Summary of Parameters for Fits" (as illustrated in the bottom of Fig. 3). If the number of multiplets is 80

or less, there will be only one card E. If the number of multiplet fits is between 81 and 160, there will be two cards E, and so on. The user would specify the fitting of multiplet 81 by punching a T in column 1 of the second card E.

After the program has finished with an MCA spectrum it returns to the beginning and reads card A for the next MCA spectrum. Any number of spectra can be handled in a single execution of PEAKFIND. A blank card at the end of the input deck will terminate execution properly. (This blank card is interpreted by the program as card A with IREAD=0.)

The data control cards used to analyze the spectrum of Fig. 2 and to produce the output illustrated in Figs. 3, 5, 6, 7 and 8 are shown in Fig. 9. Default values were accepted for most parameters, as may usually be done in practice.

Fig. 9. Typical data deck, showing the control cards which produced the output shown in Figs. 3, 5, 6, 7, and 8.

Table I. Format of data control card A. In this and the following tables, variable names in parentheses have standard default values and hence do not normally need to be supplied by the user.

Column	Format	Name	Interpretation
1	I1	IREAD	Designates source and format of MCA data. 1 - cards; 8F7.0 2 - cards; 10F7.0 3 - tape written by GEOS 4K analyzer; 3I6, 256F6.0 4 - tape written by TMC 4K analyzer; I6, 256F6.0 5 - tape written by TMC 16K analyzer; I6, 1024F6.0 6 - disk 7 - no data will be read; processing will continue on data previously read. A zero or blank will terminate execution.
3-10	A8	IDEN	Identification word for data on disk. Not required for data on tape or cards.
11-15 16-20 21-25 26-30	4I5	(LOCATN) array	Data on cards: LOCATN (1) and LOCATN (2) are the first and last channel numbers of the MCA channels to be read in. These data cards should follow immediately after card A. Data on disk: Not required unless data set is to be read by position rather than by identification word. If LOCATN (1) $\neq$ 0, array gives location(s) on disk of the data set to be read. Must also have NTHOUS $\neq$ 0 in this case.
31-35	I5	(NTHOUS)	Required only if data set on disk is to be located by position rather than by identification word. Gives length of data set in K (units of 1024 words).
36-80	--	--	Not referenced by program. May be used to identify data control deck if desired.

Table II. Format of data control card C.

Column	Format	Name	Interpretation
1-2	I2	IFIT	0 - No fitting will be performed. 1 - Multiplets having at least one peak with intensity greater than FITCTF will be fitted. 2 - Multiplets designated on card(s) E will be fitted.
3-4	I2	IPRINT	0 - Preliminary and summary printed output only are provided. 1 - Complete printed output is provided, including listing similar to Fig. 5 for each multiplet.
5-6	I2	IPUNCH	0 - No punched card output. 1 - Punched cards for input to SKEWGAUS are provided. 2 - Punched cards for input to DRUDGE are provided. 3 - Punched cards for both SKEWGAUS and DRUDGE are provided.
7-8	I2	IGRAPH	0 - No graphical output. 1 - One graph is plotted for each fit.
9-10	I2	(NWINDO)	Smoothing window w in equation (5). Default, $0.6 \times \text{FWHM}$ for a peak midway between channels NFIRST and NLAST
11-15	I5	(NFIRST)	First and last channel numbers of region to be searched for peaks. Default for NFIRST is 0. Default for NLAST is last channel of MCA spectrum.
16-20	I5	(NLAST)	
21-25	F5.0	(FITCTF)	If IFIT=1, fitting will be attempted for peaks with intensity greater than FITCTF. Default, 2.0.
26-30	F5.0	(FWCTF)	When fitting, FWHM will be treated as a variable parameter for peaks with intensity greater than FWCTF. Default, 5.0.
31-35	F5.0	(TAUCTF)	When fitting, τ will be treated as a variable parameter for peaks with intensity greater than TAUCTF. Default, 10.0.
36-40	F5.0	(PKLMT)	Peak limit parameter C in equation (7). Establishes smallest fluctuation recognizable as a peak. Default, 2.0.

Table II (continued)

Column	Format	Name	Interpretation
41-45 46-50	F5.0 F5.0	(FITBEL) (FITABV)	Fitting region extends from FITBEL * FWHM channels below centroid of first peak to FITABV * FWHM channels above centroid of last peak in multiplet. Defaults, 3.0 and 2.5, respectively.
51-55	F5.0	(SEP)	Peaks will be fitted together as (part of) a multiplet if the separation between their centroids is less than SEP * FWHM. Default, 4.0.
56-60	F5.0	(XSF)	Number of channels per inch on plots. Default, 10.0. Note F format!

Table III. Format of data control card D.

Column	Format	Name	Interpretation
1-10	F10.0	E0	Energy calibration is given by $E(\text{keV}) = E0(\text{keV}) + ECH(\text{keV/channel}) * (\text{channel number})$
11-20	F10.0	ECH	
21-25	F5.3	FWHMO	FWHM is given by $FWHM(\text{channels}) = FWHMO(\text{channels}) + FWMEV(\text{channels/MeV}) * E(\text{MeV})$
26-30	F5.3	(FWMEV)	
31-35	F5.3	(TAU0)	τ is given by $\tau(\text{channels}) = TAU0(\text{channels}) + TAUMEV(\text{channels/MeV}) * E(\text{MeV})$ Defaults: TAU0, $0.5 \times (FWHMO + FWMEV)$; TAUMEV, 0.
36-40	F5.3	(TAUMEV)	
41-45	6F5.3	(TAIL1)	Intercept and slope of straight lines giving tail, lower skewness, and upper skewness as functions of energy. These parameters are not variable parameters in PEAKFIND as they are in SKEWGAUS, but they may be assigned fixed values.
46-50		(TAILS)	
51-55		(SKUL01)	
56-60		(SKUL0S)	
61-65		(SKUH11)	
66-70		(SKUH1S)	
71-75	F5.3	(EFFS)	Slope of straight line giving $\log_{10}$ (detector efficiency) versus $\log_{10}$ (peak energy). Default, 1.0.
76-80	F5.3	(EFMAX)	Energy (in MeV) of maximum efficiency of detector. Default, 0.1.

ACKNOWLEDGMENTS

PEAKFIND began as a revision of program PALMUD II, written by Taff and Champion⁵ as a revision of the original program of Mariscotti.⁶ It gradually became clear that some rather drastic changes were desirable, and so the program was rewritten almost from scratch, with only a few vestiges of the original programs remaining. Many aspects of SKEWGAUS were incorporated into PEAKFIND, and various additional features have been added in the five years that the program has been in use. Many of the past and present members of the TRISTAN group have contributed helpful suggestions during this time. The peak fitting function, which is also used in SKEWGAUS, was devised by Fred Wohn. The matrix inversion subroutine DUMNV was supplied by the I.S.U. Computation Center staff.

REFERENCES

1. M. A. Mariscotti, Nucl. Instrum. Methods 50, 309 (1967).
2. W. C. Schick, Jr., USAEC Report No. IS-3460 (1974).
3. W. C. Schick, Jr. and W. L. Talbert, Jr., Phys. Rev. C 9, 2328 (1974).
4. D. G. Scranton and E. G. Manchester, USAEC Report No. IS-2305 (revised 1972).
5. L. M. Taff and P. M. Champion, USAEC Report No. IS-1986 (1968).
6. M. A. Mariscotti, USAEC Report No. BNL-10904 (1966).

APPENDIX A. PROGRAM DESCRIPTION

PEAKFIND consists of a MAIN program; eight subroutines named INPUT, PKFIND, OUT1, PKFIT, NLLS, FUNCT, DUMNV, and OUT2; and seven labeled COMMON areas named COM1, COM2, COM3, COM4, COM6, COM7, and COM8. Additional subprograms required are all in the standard FORTRAN library, except for the subroutines GRAPH and ORIGIN, which are part of the SIMPLOTTER package and are used only for producing the graphical output.

MAIN establishes the standard values for various parameters; reads cards B, C, and D; assigns default values; and calls the various subprograms.

INPUT reads card A and the MCA data. MAIN calls INPUT once for each spectrum to be analyzed.

PKFIND finds the peaks and estimates their centroids, areas, and intensities. MAIN calls PKFIND once for each spectrum to be analyzed.

OUT1 writes the preliminary output. It groups the peaks into multiplets, determines the channels to be included in each multiplet fit, and finds the initial estimates of FWHM and τ for each peak. MAIN calls OUT1 once for each spectrum to be analyzed.

PKFIT decides whether to perform each fit. It initializes the various arrays that are needed for fitting. After a fit has been performed, PKFIT saves the results for the summary output. MAIN calls PKFIT once for each spectrum to be analyzed.

NLLS does the nonlinear least-squares fitting. It also prints the intermediate output, if required (i.e., the values of the variable parameters after each iteration). This subroutine is very similar to a subroutine of the same name in SKEWGAUS. PKFIT calls NLLS once for each fit to be performed.

FUNCT evaluates the fitting function and its partial derivatives with respect to the variable parameters. NLLS calls FUNCT once for each channel in each iteration of each fit. This subprogram is a somewhat simplified version of the subroutine of the same name in SKEWGAUS, because of the smaller number of variable parameters (four per peak instead of seven). FUNCT is also called by OUT2 when the summary output is provided.

DUMNV is a standard double-precision matrix-inversion routine. NLLS calls DUMNV once for each iteration of each fit.

OUT2 provides the summary output and the graphs. MAIN calls OUT2 once for each spectrum to be analyzed.

At the end of analysis of a given spectrum the program cycles back to the beginning to read the first data card for the next spectrum. Any number of spectra may be analyzed in a single execution of the program.

An overall flow chart for PEAKFIND is given in Fig. 10. A flow chart for subroutine PKFIND is given in Fig. 11.

Fig. 10. Overall flow chart for PEAKFIND. The subprograms in which the various operations are performed are indicated in brackets on the right.

Fig. 11. Flow chart for subroutine PKFIND.

APPENDIX B. PROGRAM REQUIREMENTS AND LIMITATIONS

The maximum number of channels that may be included in an MCA spectrum is 8192. This number may be changed simply by changing the dimension of array DATA in common area COM1, and of array A in subroutine PKFIND. The value assigned to variable LENGTH at the beginning of MAIN should also be changed accordingly.

The maximum number of peaks that can be handled is 250. This number may be changed by changing the dimension of all arrays dimensioned to 250 in common areas COM2 and COM8. The value assigned to variable MAXPKS at the beginning of MAIN should be changed accordingly.

The maximum number of channels in a given fit is 200. This number may be changed by changing the dimension of all arrays dimensioned to 200 in COM6, and the dimension of array YCAL in OUT2. In addition, the dimension of array XC in OUT2 should be one greater than the maximum number of channels, and the dimension of arrays X and Y should be 10 greater (to allow for the plotting of five additional channels on each side of the fitting region). The value assigned to variable MXFTSZ at the beginning of MAIN should be changed accordingly.

The maximum number of peaks in a multiplet fit is 9. To change this number one must change the dimension of all arrays dimensioned to 9 in common area COM7 (and of array TERM, which must be one greater) and also of all arrays dimensioned to 38. This number is the maximum number of variable parameters, equal to four times the maximum number of peaks plus two. The dimension of arrays in NLLS dimensioned to 38 must similarly be changed. Array A (the coefficient matrix) must have a first dimension equal to twice the number of variable parameters, and array AA (equivalenced to A) must

be dimensioned to the square of the number of variable parameters. The third argument in the CALL DUMNV statement (card NLLS0770) must also be equal to the maximum number of variable parameters. The value assigned to MLTPLT at the beginning of MAIN is the maximum number of peaks per fit.

The maximum number of iterations permitted per fit is 30. This number may be changed by changing the value assigned to MAXIT at the beginning of MAIN. The assignment of most other standard and default values is also done in MAIN so that they may easily be changed if desired.

As we observed in the Introduction, the load module for PEAKFIND is about 156 kilobytes long when no overlays are used. An overlay tree that will permit execution in a 128 kilobyte region of core is generated by the following set of instructions to the linkage editor:

```
INSERT MAIN
      OVERLAY ONE
INSERT INPUT
      OVERLAY ONE
INSERT PKFIND
INSERT OUT1
      OVERLAY ONE
INSERT FUNCT
INSERT COM6
INSERT COM7
INSERT COM8
      OVERLAY TWO
INSERT PKFIT
INSERT NLLS
INSERT DUMNV
      OVERLAY TWO
INSERT OUT2
```

C	PROGRAM 'PEAKFIND'	MAIN0010
C		MAIN0020
C	MAIN PROGRAM	MAIN0030
C		MAIN0040
	CCMMCN /COM1/ LENGTH,NFIRST,NLAST,NWINDJ,DATA(8192)	MAIN0050
	CCMMCN /COM2/ MAXPKS,NPEAKS,POS(250),ENERGY(250),AREA(250),	MAIN0060
	1 FWHM(250),TAU(250),NPKS(250),FITLO(250),FITHI(250),NFITS	MAIN0070
	CCMMCN /COM3/ EO,ECH,FWHMO,FWMEV,TAJO,TAUMEV,SKULOI,SKULOS,	MAIN0080
	1 SKUHII,SKUHIS,TAILI,TAILS,NSKULO,NSKUHI,NLOI,NHI1,MAXIT,ITQ,	MAIN0090
	1 EPSQ,EFFS,EFMXLG,EFTERM,PKLMT,NRDR,NPRTR,NPNCH	MAIN0100
	COMMON /COM4/ IFIT,IPRINT,IPUNCH,IGRAPH,IFIX,MLTPLT,MXFTSZ,EPSHT,	MAIN0110
	1 EPSX0,EPSTAU,EPSTAU,EPSA,EPSTB,DIFLIN,CONST,SEP,FITABV,FITBEL,	MAIN0120
	1 FITCTF,FWCTF,TAUCTF,XSF	MAIN0130
C		MAIN0140
	DIMENSION LABEL(20)	MAIN0150
C		MAIN0160
	NRDR=5	MAIN0170
C	FILE NUMBER FOR CARD READER	MAIN0180
	NPRTR=6	MAIN0190
C	FILE NUMBER FOR LINE PRINTER	MAIN0200
	NPNCH=7	MAIN0210
C	FILE NUMBER FOR CARD PUNCH	MAIN0220
	LENGTH=8192	MAIN0230
C	MAXIMUM NO. OF CHANNELS IN MCA SPECTRUM	MAIN0240
	MAXPKS=250	MAIN0250
C	MAXIMUM NO. OF PEAKS THAT MAY BE HANDLED	MAIN0260
	MXFTSZ=200	MAIN0270
C	MAXIMUM NO. OF CHANNELS IN ANY ONE FIT	MAIN0280
	MLTPLT=9	MAIN0290
C	MAXIMUM NO. OF PEAKS IN ANY ONE FIT	MAIN0300
	MAXIT=30	MAIN0310
C	MAXIMUM NO. OF ITERATIONS PERMITTED PER FIT	MAIN0320
C		MAIN0330
	10 CALL INPUT(DATA,LENGTH,I2)	MAIN0340
C		MAIN0350

C	READ CARDS B, C, AND D	MAIN0360
C		MAIN0370
	READ (NRDR,100) LABEL	MAIN0380
100	FORMAT (20A4)	MAIN0390
	READ (NRDR,102) IFIT,IPRINT,IPUNCH,IGRAPH,NWINDO,NFIRST,NLAST,	MAIN0400
1	FITCTF,FWCTF,TAUCTF,PKLMT,FITBEL,FITABV,SEP,XSF	MAIN0410
102	FORMAT (5I2,2I5,10F5.0)	MAIN0420
	READ (NRDR,104) E0,ECH,FWHM0,FWMEV,TAU0,TAUMEV,TAILI,TAILS,	MAIN0430
1	SKULOI,SKULOS,SKUHII,SKUHIS,EFFS,EFMAX	MAIN0440
104	FORMAT (2F10.0,12F5.3)	MAIN0450
C		MAIN0460
C	ASSIGN DEFAULT VALUES	MAIN0470
C		MAIN0480
	IF (NLAST .EQ. 0 .OR. NLAST .GE. I2) NLAST=I2-1	MAIN0490
	IF (FITCTF .EQ. 0.) FITCTF=2.0	MAIN0500
C	MINIMUM INTENSITY FOR PEAK TO BE FIT	MAIN0510
	IF (FWCTF .EQ. 0.) FWCTF=5.0	MAIN0520
C	MINIMUM INTENSITY FOR FWHM TO BE VARIABLE	MAIN0530
	IF (TAUCTF .EQ. 0.) TAUCTF=10.0	MAIN0540
C	MINIMUM INTENSITY FOR TAU TO BE VARIABLE	MAIN0550
	IF (XSF .EQ. 0.) XSF=10.0	MAIN0560
C	NUMBER OF POINTS PER INCH ON PLOTS	MAIN0570
	IF (FITBEL .EQ. 0.) FITBEL=3.0	MAIN0580
	IF (FITABV .EQ. 0.) FITABV=2.5	MAIN0590
C	FIT REGION EXTENDS FROM (FITBEL*FWHM) CHANNELS	MAIN0600
C	BELOW FIRST PEAK TO (FITABV*FWHM) CHANNELS ABOVE	MAIN0610
C	LAST PEAK	MAIN0620
	IF (SEP .EQ. 0.) SEP=4.0	MAIN0630
C	MAXIMUM SEPARATION BETWEEN PEAKS IN A MULTIPLET	MAIN0640
C	FIT IS (SEP*FWHM)	MAIN0650
	IF (FKLMT .EQ. 0.) PKLMT=2.0	MAIN0660
C	PKLMT DETERMINES SMALLEST FLUCTUATION IN 2ND	MAIN0670
C	DERIVATIVE THAT WILL BE RECOGNIZED AS A PEAK	MAIN0680
	IF (ECH .EQ. 0.) ECH=0.5	MAIN0690
	IF (FWHM0 .EQ. 0.) FWHM0=6.0	MAIN0700

	IF (TAU0 .EQ. 0.) TAU0=(FWHM0+FWMEV)/2.0	MAIN0710
	IF (EFS .EQ. 0.) EFS=-1.0	MAIN0720
	EFS=-ABS(EFS)	MAIN0730
C	SLOPE OF EFFICIENCY CURVE ON FULL LOG PLOT	MAIN0740
	IF (EFMAX .LE. 0.) EFMAX=0.1	MAIN0750
C	ENERGY WHERE EFFICIENCY IS A MAXIMUM	MAIN0760
	EFMXLG=ALOG10(EFMAX)	MAIN0770
	EFTERM=EFMXLG+0.1505	MAIN0780
C		MAIN0790
C	THE FOLLOWING QUANTITIES ARE CONVERGENCE CRITERIA FOR	MAIN0800
C	VARIABLE PARAMETERS	MAIN0810
C		MAIN0820
	EPSHT=.001	MAIN0830
	EPSX0=.00001	MAIN0840
	EPSFW=.001	MAIN0850
	EPSTAU=.005	MAIN0860
	EPSA=.0001	MAIN0870
	EPSB=.0001	MAIN0880
	EPSQ=.0001	MAIN0890
C		MAIN0900
C	FOLLOWING PARAMETERS ARE USED FOR MISCELLANEOUS PURPOSES	MAIN0910
C		MAIN0920
	ITQ=20	MAIN0930
C	ITERATION ON WHICH Q TEST IS FIRST APPLIED	MAIN0940
	DIFLIN=.005	MAIN0950
C	DIFFERENTIAL NONLINEARITY OF MCA	MAIN0960
	CCNST=.02	MAIN0970
C	CONSTANT USED TO REDUCE STATISTICAL WEIGHT GIVEN TO	MAIN0980
C	CHANNELS WITH A SMALL NUMBER OF COUNTS	MAIN0990
	NSKULO=2	MAIN1000
C	EXPONENT IN LOWER SKEWNESS TERM	MAIN1010
	NLCI=NSKULO-1	MAIN1020
	NSKUI=5	MAIN1030
C	EXPONENT IN UPPER SKEWNESS TERM	MAIN1040
	NHI1=NSKUI-1	MAIN1050

C		MAIN1060
C		MAIN1070
C	FIND PEAKS	MAIN1080
C		MAIN1090
C		MAIN1100
	CALL PKFIND	MAIN1110
C		MAIN1120
C		MAIN1130
C	WRITE RESULTS OF PKFIND	MAIN1140
C		MAIN1150
C		MAIN1160
	CALL OUT1(LABEL)	MAIN1170
	IF (IFIT .EQ. 0) GO TO 10	MAIN1180
C		MAIN1190
C		MAIN1200
C	FIT PEAKS	MAIN1210
C		MAIN1220
C		MAIN1230
	CALL FKFIT	MAIN1240
C		MAIN1250
C		MAIN1260
C	WRITE RESULTS OF PEAK FITTING	MAIN1270
C		MAIN1280
C		MAIN1290
	CALL OUT2(LABEL)	MAIN1300
	GO TO 1C	MAIN1310
	END	MAIN1320
	SUBROUTINE INPUT(DATA,LENGTH,12)	INPU0010
C		INPU0020
C	THIS IS A GENERAL SUBROUTINE FOR READING AN MCA SPECTRUM INTO	INPU0030
C	ARRAY 'DATA'. LENGTH IS THE SIZE OF THE ARRAY. 12 IS THE SIZE	INPU0040
C	OF THE SPECTRUM.	INPU0050
C		INPU0060
	DIMENSION DATA(LENGTH)	INPU0070
	REAL *8 IDEN, IDWORD(175)	INPU0080

DIMENSION LENGTH(175) ,LCCATN(4)	INPU0090
INTEGER*2 TEMP(2)	INPU0100
LOGICAL CHECK	INPU0110
EQUIVALENCE (LTEMP,TEMP(1))	INPU0120
C	INPU0130
C READ CARD A	INPU0140
C	INPU0150
READ (5,100,END=80) IREAD,IDEN,LOCATN,NTHOUS	INPU0160
100 FORMAT (I1,1X,A8,5I5)	INPU0170
IF (IREAD .LT. 1) STOP	INPU0180
MXTHOS=LENGTH/1024	INPU0190
IF(NTHOUS .GT. MXTHOS) NTHOUS=MXTHOS	INPU0200
IF (IREAD .GT. 2) GO TC 20	INPU0210
C	INPU0220
C READ CARDS	INPU0230
C	INPU0240
I1=LOCATN(1)+1	INPU0250
I2=LOCATN(2)+1	INPU0260
IF (I2 .GT. LENGTH) I2=LENGTH	INPU0270
IF (IREAD .EQ. 2) GO TC 12	INPU0280
READ (5,102) (DATA(I),I=I1,I2)	INPU0290
102 FCRMAT (8F7.0)	INPU0300
GO TO 14	INPU0310
12 READ (5,104) (DATA(I),I=I1,I2)	INPU0320
104 FCRMAT (10F7.0)	INPU0330
14 WRITE (6,106) I2	INPU0340
106 FCRMAT ('0 CARDS READ *** DATA SET LENGTH',I6)	INPU0350
RETURN	INPU0360
C	INPU0370
C READ TAPES	INPU0380
C	INPU0390
20 IF (IREAD .GT. 5) GO TC 60	INPU0400
LREC=256	INPU0410
IF (IREAD .EQ. 5) LREC=1024	INPU0420
I1=1	INPU0430

	I2=LREC	INFU0440
	IF (IREAD .EQ. 3) GO TO 30	INPU0450
C	TMC 4K OR 16K ANALYZER	INPU0460
	DO 26 J=1,17	INPU0470
	READ (8,122,END=28) ID,(DATA(I),I=I1,I2)	INPU0480
122	FCRMT (I6,8(128F6.0))	INPU0490
	I1=I1+LREC	INPU0500
26	I2=I2+LREC	INPU0510
28	I2=I2-LREC	INPU0520
	WRITE (6,124) ID,I2	INPU0530
124	FORMAT ('DATA SET',I7,' HAS BEEN READ FROM TAPE, LENGTH',I6)	INPU0540
	RETURN	INPU0550
C	GEOS 4K ANALYZER	INPU0560
30	DO 32 J=1,17	INPU0570
	READ (8,126,END=28) ID,ID1,ID2,(DATA(I),I=I1,I2)	INPU0580
126	FCRMT (3I6,128F6.0,128F6.0)	INPU0590
	I1=I1+LREC	INPU0600
32	I2=I2+LREC	INPU0610
	GO TO 23	INPU0620
C		INPU0630
C	READ DISK	INPU0640
C		INPU0650
60	IF (IREAD .GT. 6) RETURN	INPU0660
	DEFINE FILE 10(6000,525,U,IP)	INPU0670
	IF (LOCATN(1) .GT. 0) GO TO 66	INPU0680
C	LOCATE DATA SET	INPU0690
	K=1	INPU0700
	DO 64 J=1,5	INPU0710
	READ (10,J) (IDWORD(I),LNGTH(I),I=1,175)	INPU0720
	DO 62 I=1,175	INPU0730
	IF (IDWORD(I) .NE. IDEN) GO TO 62	INPU0740
	LOCATN(K)=I+175*(J-1)	INPU0750
	IF (LCCATN(K) .GE. 750) GO TO 66	INPU0760
	LTEMP=LNGTH(I)	INPU0770
	NTHOUS=LTEMP(2)	INPU0780

NTHIS=TEMP(1)*4	INPU0790
IF (NTHIS .GE. NTHOUS) GO TO 66	INPU0800
K=K+1	INPU0810
62 CONTINUE	INPU0820
64 CCNTINUE	INPU0830
WRITE (6,130) IDEN	INPU0840
130 FORMAT ('- *** ALL OF DATA SET NO. ',A8,' COULD NOT BE FOUND IN TA	INPU0850
BLE OF CONTENTS')	INPU0860
IF (LOCATN(1) .LE.0) STOP	INPU0870
NTHCLS=(K-1)*4	INPU0880
C READ DATA SET	INPU0890
66 JSTOP=2*NTHOUS	INPU0900
JJ=1	INPU0910
I1=1	INPU0920
I2=512	INPU0930
DO 74 K=1,4	INPU0940
IFCINT=8*LOCATN(K)+1	INPU0950
IF (IPOINT .LE. 8) GO TO 76	INPU0960
CC 72 J=1,8	INPU0970
READ (10,IPOINT) IDWORD(J),(DATA(I),I=I1,I2)	INPU0980
IF (IDWORD(J) .EQ. IDEN) GO TO 67	INPU0990
WRITE (6,132) IDEN,IDWORD(J),JJ	INPU1000
132 FORMAT ('- *** POSSIBLE ERROR -- YOU ASKED FOR DATA SET ',A8,	INPU1010
1 ' BUT IDENTIFICATION WORD ',A8,' APPEARS AT THE BEGINNING OF ',	INPU1020
2 'RECORD',I3)	INPU1030
67 IF (JJ .GE. JSTOP) GO TO 76	INPU1040
JJ=JJ+1	INPU1050
IF (I2 .GE. LENGTH) GO TO 76	INPU1060
I1=I1+512	INPU1070
I2=I2+512	INPU1080
IFCINT=IPOINT+1	INPU1090
72 CCNTINUE	INPU1100
74 CONTINUE	INPU1110
76 WRITE (6,134) IDEN,LOCATN	INPU1120
134 FORMAT ('0DATA SET ',A8,' HAS BEEN READ FROM LOCATIONS ',4I4)	INPU1130

RETURN	INPU1140
80 STOP	INPU1145
END	INPU1150
SUBROUTINE PKFIND	PKFD0010
C	PKFD0020
C PEAK FINDING PROCEDURE REFERENCE: M.A. MARISCOTTI, NUC.. INST.	PKFD0030
C AND METH.. VOL. 50 (1967), PAGES 309-320	PKFD0040
C	PKFD0050
COMMON /COM1/ LENGTH,NFIRST,NLAST,NWINDO,DATA(8192)	PKFD0060
COMMON /COM2/ MAXPKS,NPEAKS,POS(250),ENERGY(250),AREA(250),	PKFD0070
1 FWHM(250),TAU(250),NPKS(250),FITLO(250),FITHI(250),NFITS	PKFD0080
COMMON /COM3/ EQ,ECH,FWHM0,FWMEV,TAU0,TAUMEV,SKULOI,SKULOS,	PKFD0090
1 SKUHII,SKUHIS,TAILI,TAILS,NSKULO,NSKUHI,NLOI,NHII,MAXIT,ITQ,	PKFD0100
1 EPSQ,EFFS,EFXLG,EFTERM,PKLMT,NRDR,NPRTR,NPNCH	PKFD0110
DIMENSION A(8192),XN(15)	PKFD0120
REAL FCTR(15)/6., 28., 82., 184., 350., 596., 938., 1392., 1974.,	PKFD0130
1 2700., 3586., 4648., 5902., 7364., 9050. /,NOPEAK	PKFD0140
C	PKFD0150
C FIND SECOND DIFFERENCE	PKFD0160
C	PKFD0170
IMIN=NFIRST+1	PKFD0180
IMAX=NLAST+1	PKFD0190
I1=IMIN+1	PKFD0200
I2=IMAX-1	PKFD0210
DO 20 I=I1,I2	PKFD0220
20 A(I)=DATA(I+1)-2.0*DATA(I)+DATA(I-1)	PKFD0230
A(IMIN)=0.	PKFD0240
A(IMAX)=0.	PKFD0250
C	PKFD0260
C FIND NWINDO	PKFD0270
C	PKFD0280
CHMID=(NFIRST+NLAST)/2	PKFD0290
EMID=(EQ+ECH*CHMID)/1000.	PKFD0300
FWMID=FWHM0+FWMEV*EMID	PKFD0310
IF (NWINDO .EQ. 0) NWINDO=0.6*FWMID+0.5	PKFD0320

IF (NWINDO .LE. 15) GO TO 21	PKFD0330
WRITE (NPRTR,100) NWINDO	PKFD0340
100 FORMAT ('- *** ERROR--NWINDO IS',I3,' WHICH IS GREATER THAN 15')	PKFD0350
STOP	PKFD0360
21 N1=NWINDO-1	PKFD0370
WINDOW=NWINDO	PKFD0380
IF (N1 .LE. 0) GO TO 32	PKFD0390
DO 22 I=1,N1	PKFD0400
22 XN(I)=NWINDO-I	PKFD0410
C	PKFD0420
C SMOOTH SECOND DIFFERENCE 4 TIMES WITH AN NWINDO CHANNEL WINDOW	PKFD0430
C	PKFD0440
I1=IMIN+N1	PKFD0450
I2=IMAX-N1	PKFD0460
DO 30 I1=1,2	PKFD0470
DO 26 I=I1,I2	PKFD0480
SUM=WINDOW*A(I)	PKFD0490
DO 24 L=1,N1	PKFD0500
24 SUM=SUM+XN(L)*(A(I-L)+A(I+L))	PKFD0510
26 A(I-N1)=SUM	PKFD0520
DO 28 I=I1,I2	PKFD0530
I3=I1+I2-I	PKFD0540
28 A(I3)=A(I3-N1)	PKFD0550
C TAKE CARE OF ENDS	PKFD0560
DO 30 L=1,N1	PKFD0570
A(IMIN-1+L)=A(I1)	PKFD0580
A(IMAX+1-L)=A(I2)	PKFD0590
30 CONTINUE	PKFD0600
C	PKFD0610
C INITIALIZE PARAMETERS	PKFD0620
C	PKFD0630
32 N1MINUS=NWINDO+1	PKFD0640
N1PLUS=3.0*FWID	PKFD0650
NOPEAK=PKLMT*WINDOW	PKFD0660
FACTOR=FCR(NWINDO)	PKFD0670

F1=SQRT(ABS(FACTOR*DATA(IMIN)))/1000.	PKFD 0680
IF (DATA(I) .LT. 1.) F1=SQRT(FACTOR)/1000.	PKFD 0690
S1=A(IMIN)/1000.	PKFD 0700
I3=IMIN	PKFD 0710
I5=IMIN	PKFD 0720
II=IMIN+1	PKFD 0730
J=0	PKFD 0740
C J COUNTS PEAKS FOUND	PKFD 0750
C	PKFD 0760
C MAIN LOOP	PKFD 0770
C	PKFD 0780
DO 60 I=II,IMAX	PKFD 0790
F=SQRT(ABS(FACTOR*DATA(I)))/1000.	PKFD 0800
IF (DATA(I) .LT. 1.) F=SQRT(FACTOR)/1000.	PKFD 0810
S=A(I)/1000.	PKFD 0820
IF (S .GT. 0.) GO TO 42	PKFD 0830
IF (S1 .LE. 0.) GO TO 58	PKFD 0840
I3=I	PKFD 0850
FS=F1	PKFD 0860
GO TO 58	PKFD 0870
42 IF (S1 .GE. 0.) GO TO 58	PKFD 0880
I5=I-1	PKFD 0890
C	PKFD 0900
C CHECK SIZE OF REGION OF NEGATIVE SECOND DERIVATIVE	PKFD 0910
C	PKFD 0920
NWIDE=I5-I3+1	PKFD 0930
IF (NWIDE .LT. N1MNUS .OR. NWIDE .GT. N1PLUS) GO TO 58	PKFD 0940
C	PKFD 0950
C CHECK MAGNITUDE OF NEGATIVE SECOND DERIVATIVE	PKFD 0960
C	PKFD 0970
SUM=0.	PKFD 0980
DO 44 K=I3,I5	PKFD 0990
44 SUM=SUM+A(K)	PKFD 1000
SUM=-SUM/1000.	PKFD 1010
RATIO=SUM/FS	PKFD 1020

IF (RATIO .LE. NOPEAK) GO TO 58	PKFD1030
C	PKFD1040
C HOORAY, WE HAVE A PEAK, COMPUTE POSITION AND AREA.	PKFD1050
C	PKFD1060
J=J+1	PKFD1070
TOT=0.	PKFD1080
DO 50 K=I3, I5	PKFD1090
CH=K-1	PKFD1100
50 TOT=TOT+A(K)*CH	PKFD1110
PCS(J)=-TOT/(1000.*SUM)	PKFD1120
AREA(J)=SUM*NWIDE	PKFD1130
IF (J .GE. MAXPKS) GO TO 80	PKFD1140
C	PKFD1150
C FINISH MAIN LOOP	PKFD1160
C	PKFD1170
58 S1=S	PKFD1180
F1=F	PKFD1190
60 CONTINUE	PKFD1200
C	PKFD1210
C NORMALIZE AREAS AND CORRECT FOR EFFICIENCY	PKFD1220
C	PKFD1230
80 NPEAKS=J	PKFD1240
AMAX=0.	PKFD1250
XOVER=EFTERM+0.1505	PKFD1260
DO 86 J=1, NPEAKS	PKFD1270
ENERGY(J)=A3 S(E0+ECH*POS(J))	PKFD1280
ELOG=ALOG10(ENERGY(J))-3.0	PKFD1290
IF (ELOG .LT. XOVER) GO TO 82	PKFD1300
EFF=EFFS*ELOG	PKFD1310
GO TO 84	PKFD1320
82 EFF=EFFS*(1.66096*(ELOG-EFMXLG)**2+EFTERM)	PKFD1330
84 AREA(J)=AREA(J)/(10.**EFF)	PKFD1340
IF (AREA(J) .LE. AMAX) GO TO 86	PKFD1350
AMAX=AREA(J)	PKFD1360
86 CONTINUE	PKFD1370

DO 88 J=1,NPEAKS	PKFD1380
88 AREA(J)=100.*AREA(J)/AMAX	PKFD1390
RETURN	PKFD1400
END	PKFD1410
SUBROUTINE OUT1(LABEL)	OUT10010
C	OUT10020
COMMON /COM1/ LENGTH,NFIRST,NLAST,NWINDO,DATA(8192)	OUT10030
CCOMMON /COM2/ MAXPKS,NPEAKS,POS(250),ENERGY(250),AREA(250),	OUT10040
1 FWHM(250),TAU(250),NPKS(250),FITLO(250),FITHI(250),NFITS	OUT10050
COMMON /COM3/ E0,ECH,FWHM0,FWMEV,TAU0,TAUMEV,SKULOI,SKULOS,	OUT10060
1 SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,SKUHI,	OUT10070
1 EPSQ,EFFS,EFMXLG,EFTERM,PKLMT,NRDR,NPRTR,NPNCH	OUT10080
COMMON /COM4/ IFIT,IPRINT,IPUNCH,IGRAPH,IFIX,MLTPLT,MXFSZ,EPST,	OUT10090
1 EPSX0,EPSFW,EPSTAU,EPSA,EPSB,DIFLIN,CONST,SEP,FITABV,FITBEL,	OUT10100
1 FITCTF,FWCTF,TAUCTF,XSF	OUT10110
DIMENSION LABEL(20)	OUT10120
INTEGER FITHI,FITLO	OUT10130
C	OUT10140
C PRINT OUT RESULTS OF PKFIND	OUT10150
C	OUT10160
WRITE (NPRTR,100) LABEL	OUT10170
100 FORMAT (1H1,25X,20A4/1H0)	OUT10180
WRITE (NPRTR,102) NFIRST,NLAST,NWINDO,PKLMT	OUT10190
102 FORMAT (' PEAKFIND SEARCH BETWEEN CHANNELS ',I4,' AND ',I4,	OUT10200
1 10X,'SMOOTHING WINDOW =',I3,10X,'PEAK LIMIT PARAMETER =',F5.1)	OUT10210
WRITE (NPRTR,104) FITCTF,FITBEL,E0,ECH,TAU0,TAUMEV	OUT10220
104 FORMAT ('CUTOFFS: FIT,',F7.1,7X,'FITBEL =',F4.1,7X,'ENERGY =',	OUT10230
1 F7.2,' KEV +',F9.6,' KEV PER CHANNEL',7X,'TAIL =',F6.3,' +',	OUT10240
1 F6.3,' PER MEV')	OUT10250
WRITE (NPRTR,106) FWCTF,FITABV,FWHM0,FWMEV,SKULOI,SKULOS	OUT10260
106 FORMAT (11X,'FWHM',F6.1,7X,'FITABV =',F4.1,9X,'FWHM =',F6.3,	OUT10270
1 ' +',F7.3,' PER MEV',19X,'SKULO =',F6.3,' +',F6.3,' PER MEV')	OUT10280
WRITE (NPRTR,108) TAUCTF,SEP,TAUC,TAUMEV,SKUHI,SKUHI	OUT10290
108 FORMAT (11X,'TAU',F7.1,10X,'SEP =',F4.1,10X,'TAU =',F6.3,' +',	OUT10300
1 F7.3,' PER MEV',19X,'SKUHI =',F6.3,' +',F6.3,' PER MEV'/1H-)	OUT10310

	WRITE (NPRTR,110)	OUT10320
110	FORMAT ('0 PEAK NUMBER CHANNEL ENERGY',9X,	OUT10330
	1 'INTENSITY TO BE FIT'/1H0)	OUT10340
	DO 12 J=1,NPEAKS	OUT10350
	IF (AREA(J) .GT. FITCTF) GO TO 10	OUT10360
	WRITE (NPRTR,112) J,POS(J),ENERGY(J),AREA(J)	OUT10370
112	FORMAT (12X,I3,10X,F7.2,10X,F7.2,10X,F7.3)	OUT10380
	GO TO 12	OUT10390
	10 WRITE (NPRTR,114) J,POS(J),ENERGY(J),AREA(J)	OUT10400
114	FORMAT (12X,I3,10X,F7.2,10X,F7.2,10X,F7.3,8X,1H*)	OUT10410
	12 CONTINUE	OUT10420
	IF (NPEAKS .LT. MAXPKS) GO TO 14	OUT10430
	WRITE (NPRTR,116) MAXPKS	OUT10440
116	FORMAT ('0NUMBER OF PEAKS FOUND EXCEEDS ',I3)	OUT10450
C		OUT10460
C	WRITE OUT PARAMETERS FOR FITS	OUT10470
C		OUT10480
	14 WRITE (NPRTR,120)	OUT10490
120	FORMAT ('1 SUMMARY OF PARAMETERS FOR FITS'/'-FIT NPKS	EOUT10500
	1ENERGY FIRST LAST FWHM TAU CENTROIDS'/' NO.',17X,	OUT10510
	1 'CHAN CHAN' /)	OUT10520
	DO 16 J=1,NPEAKS	OUT10530
	FWHM(J)=FWHMO+FWMEV*ENERGY(J)/1000.	OUT10540
	16 TAU(J)=TAUO+TAUMEV*ENERGY(J)/1000.	OUT10550
C		OUT10560
C	MAIN LOOP--J LABELS PEAKS, K COUNTS FITS	OUT10570
C		OUT10580
C	DETERMINE NUMBER OF PEAKS IN EACH FIT, ALSO 1ST AND LAST CHANNELS	OUT10590
C		OUT10600
	J=1	OUT10610
	K=1	OUT10620
20	J1=J+MLTPLT-1	OUT10630
	FITLO(K)=POS(J)-FITBEL*FWHM(J)	OUT10640
	IF (FITLO(K) .LT. NFIRST) FITLO(K)=NFIRST	OUT10650
	DO 22 JJ=J,J1	OUT10660

IF (JJ .EQ. NPEAKS) GO TO 24	OUT10670
IF ((POS(JJ+1)-POS(JJ)) .GT. SEP*FWHM(JJ)) GO TO 24	OUT10680
IF (POS(JJ+1)+FITABV*FWHM(JJ+1) .GE. FITLO(K)+MXFTSZ) GO TO 24	OUT10690
22 CCNTINUE	OUT10700
JJ=J+MLTPLT-1	OUT10710
24 NPKS(K)=JJ-J+1	OUT10720
FITHI(K)=POS(JJ)+FITABV*FWHM(JJ)	OUT10730
IF (FITHI(K) .GT. NLAST) FITHI(K)=NLAST	OUT10740
IF (FITHI(K)-FITLO(K) .GE. MXFTSZ) FITHI(K)=FITLO(K)+MXFTSZ-1	OUT10745
WRITE (NPRTR,122) K,NPKS(K),ENERGY(J),FITLO(K),FITHI(K),FWHM(J),	OUT10750
1 TAU(J),{POS(I),I=J,JJ}	OUT10760
122 FCRMAT (1X,I3,I5,F9.1,2I7,2F7.2,9F9.2)	OUT10770
C	OUT10780
C PUNCH CARDS IF IPUNCH=1 OR 3	OUT10790
C	OUT10800
IF (IPUNCH .EQ. 0 .OR. IPUNCH .EQ. 2) GO TO 28	OUT10810
WRITE (NPNCH,124) NPKS(K),ENERGY(J),FITLO(K),FITHI(K),K	OUT10820
124 FORMAT (12,' 1 1 ',F6.1,' KEV',10X,2I5,37X,I3)	OUT10830
DO 26 I=J,JJ	OUT10840
WRITE (NPNCH,126) POS(I)	OUT10850
126 FCRMAT ('11',18X,F10.2)	OUT10860
26 CCNTINUE	OUT10870
28 IF (JJ .GE. NPEAKS) GO TO 30	OUT10880
J=JJ+1	OUT10890
K=K+1	OUT10900
GO TO 20	OUT10910
C	OUT10920
30 NFITS=K	OUT10930
WRITE (NPRTR,130) NFITS	OUT10940
130 FORMAT (1H0/1H0,20X,'NUMBER OF FITS IS ',I3)	OUT10950
RETURN	OUT10960
END	OUT10970
SUBROUTINE PKFIT	PKFT0010
C	PKFT0020
COMMON /COM1 / LENGTH,NFIRST,NLAST,NWINDO,DATA(8192)	PKFT0030

COMMON /COM2/ MAXPKS,NPEAKS,POS(250),ENERGY(250),AREA(250),	PKFT0040
1 FWHM(250),TAU(250),NPKS(250),FITLO(250),FITHI(250),NFITS	PKFT0050
COMMON /COM3/ E0,ECH,FWHM0,FWMEV,TAU0,TAUMEV,SKULOI,SKULOS,	PKFT0060
1 SKUHII,SKUHI,TAIIL,TAILS,NSKULO,NSKUHI,NLOI,NHII,MAXIT,ITQ,	PKFT0070
1 EPSQ,EFFS,EFMXLG,EFTERM,PKLMT,NPDR,NPRTR,NPNCH	PKFT0080
COMMON /COM4/ IFIT,IPRINT,IPUNCH,IGRAPH,IFIX,MLTPLT,MXFTSZ,EPSHT,	PKFT0090
1 EPSX0,EPSTAU,EPSTAU,EPSTAU,EPSTAU,EPSTAU,EPSTAU,EPSTAU,EPSTAU,	PKFT0100
1 FITCTF,FWCTF,TAUCTF,XSF	PKFT0110
COMMON /COM6/ W(200),X(200),Y(200),NPTS,EPS(38),STDE(38),	PKFT0120
1 VAR,ICONV,ITRATN,SCAREA	PKFT0130
COMMON /COM7/ P(38),IHOLD(38),DERIV(38),TERM(10),ALPHA1(9),	PKFT0140
1 ALPHA2(9),BETA1(9),BETA2(9),BETA3(9),TAIL(9),SKULO(9),SKUHI(9),	PKFT0150
1 NPRMS,NP,NFREE,NJ,I OPT,XFIRST,BPRIME	PKFT0160
COMMON /COM8/ NFRSV(250),ICNVSV(250),ITRNSV(250),VARSV(250),	PKFT0170
1 HEIGHT(250),SDHT(250),SDX0(250),SDFW(250),SDTAU(250),ASV(250),	PKFT0180
1 BSV(250),LFIT(252)	PKFT0190
REAL MEV	PKFT0200
INTEGER FITHI,FITLO	PKFT0210
INTEGER*2 NFRSV,ICNVSV,ITRNSV	PKFT0220
LOGICAL*1 L=IT	PKFT0230
C	PKFT0240
C READ CARD(S) E	PKFT0250
C	PKFT0260
IF (IFIT .NE. 2) GO TO 6	PKFT0270
READ (NRDR,110) (LFIT(L),L=1,NFITS)	PKFT0280
110 FORMAT (80L1)	PKFT0290
C	PKFT0300
C MAIN LOOP--L LABELS FITS, J LABELS PEAKS, K LABELS PARAMETERS	PKFT0310
C	PKFT0320
6 JMAX=0	PKFT0330
DO 50 L=1,NFITS	PKFT0340
JMIN=JMAX+1	PKFT0350
JMAX=JMAX+NPKS(L)	PKFT0360
C	PKFT0370
C DECIDE WHETHER TO PERFORM FIT	PKFT0380

C	IF (IFIT .EQ. 2) GO TO 10	PKFT0390
	DO 8 J=JMIN,JMAX	PKFT0400
	IF (AREA(J) .LT. FITCTF) GO TO 8	PKFT0410
	LFIT(L)=.TRUE.	PKFT0420
	GO TO 12	PKFT0430
8	CONTINUE	PKFT0440
	LFIT(L)=.FALSE.	PKFT0450
	GO TO 50	PKFT0460
10	IF (.NOT. LFIT(L)) GO TO 50	PKFT0470
C		PKFT0480
C	INITIALIZE X(CHANNEL NUMBER) AND Y(COUNTS PER CHANNEL) ARRAYS	PKFT0490
C		PKFT0500
12	IMIN=FITLO(L)	PKFT0510
	IMAX=FITHI(L)	PKFT0520
	NPTS=IMAX-IMIN+1	PKFT0530
	X(1)=IMIN	PKFT0540
	XFIRST=X(1)	PKFT0550
	Y(1)=DATA(IMIN+1)	PKFT0560
	IF (Y(1) .LT. 1.0) Y(1)=0.5	PKFT0570
	YMAX=Y(1)	PKFT0580
	DO 14 I=2,NPTS	PKFT0590
	X(I)=X(I-1)+1.	PKFT0600
	Y(I)=DATA(IMIN+I)	PKFT0610
	IF (Y(I) .LT. 1.0) Y(I)=0.5	PKFT0620
	IF (Y(I) .LE. YMAX) GO TO 14	PKFT0630
	YMAX=Y(I)	PKFT0640
14	CONTINUE	PKFT0650
C		PKFT0660
C	INITIALIZE WEIGHT ARRAY	PKFT0670
C		PKFT0680
	C1=1.0-CONST	PKFT0690
	C2=CCNST*YMAX	PKFT0700
	D2=DIFLIN*DIFLIN	PKFT0710
	DO 16 I=1,NPTS	PKFT0720
		PKFT0730

16	W(I)=1.0/(Y(I)*(C1+D2*Y(I))+C2)	PKFT0740
C		PKFT0750
C	INITIALIZE PARAMETER, IHOLD, AND EPS ARRAYS	PKFT0760
C	DO BACKGROUND PARAMETERS FIRST	PKFT0770
C		PKFT0780
	NJ=NPKS(L)	PKFT0790
	NP=4*NJ	PKFT0800
	NPRMS=NP+2	PKFT0810
	P(NP+1)=Y(1)	PKFT0820
	BPRIME=(Y(NPTS)-Y(1))/(X(NPTS)-X(1))	PKFT0830
	P(NP+2)=BPRIME+1000.	PKFT0840
	IHOLD(NP+1)=1	PKFT0850
	IHOLD(NP+2)=1	PKFT0860
	EPS(NP+1)=EPSA	PKFT0870
	EPS(NP+2)=EPSB	PKFT0880
C	INITIALIZE PEAK PARAMETERS	PKFT0890
	K=1	PKFT0900
	DO 20 J=JMIN,JMAX	PKFT0910
C	P(K+1) = CENTROID	PKFT0920
	P(K+1)=POS(J)	PKFT0930
	IHOLD(K+1)=1	PKFT0940
	EPS(K+1)=EPSXC	PKFT0950
	IPOS=POS(J)+1.5	PKFT0960
C	P(K) = HEIGHT	PKFT0970
	P(K)=DATA(IPOS)-P(NP+1)-BPRIME*(P(K+1)-XFIRST)	PKFT0980
	IF (P(K) .LT. 1.0) P(K)=1.0	PKFT0990
	IHOLD(K)=1	PKFT1000
	EPS(K)=EPSHT	PKFT1010
C	P(K+2) = FWHM	PKFT1020
	P(K+2)=FWHM(J)	PKFT1030
	IHOLD(K+2)=1	PKFT1040
	IF (AREA(J) .LT. FWCTF) IHOLD(K+2)=0	PKFT1050
	EPS(K+2)=EPSFW	PKFT1060
C	P(K+3) = TAU	PKFT1070
	P(K+3)=TAU(J)	PKFT1080

	IHOLD(K+3)=1	PKFT1090
	IF (AREA(J) .LT. TAUCTF) IHOLD(K+3)=0	PKFT1100
	EPS(K+3)=EPSTAU	PKFT1110
20	K=K+4	PKFT1120
C		PKFT1130
C	INITIALIZE QUANTITIES NEEDED FOR FUNCTION EVALUATION	PKFT1140
C		PKFT1150
	K=1	PKFT1160
	DO 22 J=1,NJ	PKFT1170
	MEV=ENERGY(J+JMIN-1)/1000.	PKFT1180
	ALPHA1(J)=1.66511/P(K+2)	PKFT1190
	ALPHA2(J)=P(K+3)*ALPHA1(J)	PKFT1200
	TAIL(J)=TAILI+TAILS*MEV	PKFT1210
	SKULO(J)=SKULOI+SKULCS*MEV	PKFT1220
	SKUHI(J)=SKUHII+SKUHIS*MEV	PKFT1230
	BETA1(J)=P(K)*TAIL(J)	PKFT1240
	BETA2(J)=NSKULO*P(K)*SKULO(J)	PKFT1250
	BETA3(J)=NSKUHI*P(K)*SKUHI(J)	PKFT1260
22	K=K+4	PKFT1270
C		PKFT1280
C	DETERMINE NUMBER OF FREE PARAMETERS	PKFT1290
C		PKFT1300
	NFREE=0	PKFT1310
	DO 24 K=1,NPRMS	PKFT1320
	IF (IHOLD(K) .EQ. 1) NFREE=NFREE+1	PKFT1330
24	CONTINUE	PKFT1340
C		PKFT1350
C	PRINT HEADING FOR NLLS OUTPUT	PKFT1360
C		PKFT1370
	IF (IPRINT .EQ. 0) GO TO 26	PKFT1380
	WRITE (NPRTR,100) L,IMIN,IMAX,JMIN,JMAX	PKFT1390
100	FORMAT ('1',10X,'=IT NO.',I4,10X,'CHANNELS',I5,' THROUGH ',I5,	PKFT1400
	1 10X,'PEAKS', I5,' THROUGH ',I5)	PKFT1410
	WRITE (NPRTR,102) ENERGY(JMIN),P(3),P(4),TAIL(1),SKULO(1),SKUHI(1)	PKFT1420
102	FORMAT ('-PARAMETERS FOR PEAK(1): ENERGY =',F7.1,' KEV =WHM	PKFT1430

	1=' ,F7.3,4X,'TAU =' ,F7.3,4X,'TAIL =' ,F7.3,3X,'SKULO =' ,F7.3,3X,	PKFT1440
	1 'SKUHI =' ,F7.3/1H0)	PKFT1450
C		PKFT1460
C	PERFORM FIT	PKFT1470
C		PKFT1480
	26 CALL NLLS(IPRINT)	PKFT1490
C		PKFT1500
C	SAVE RESULTS OF FIT	PKFT1510
C		PKFT1520
	NFRSV(L)=NFREE	PKFT1530
	VARSV(L)=VAR	PKFT1540
	ICNVSV(L)=ICONV	PKFT1550
	ITRNSV(L)=ITRATN	PKFT1560
	ASV(L)=P(NP+1)	PKFT1570
	BSV(L)=BPRIME	PKFT1580
	K=1	PKFT1590
	DO 30 J=JMIN,JMAX	PKFT1600
	HEIGHT(J)=P(K)	PKFT1610
	PCS(J)=P(K+1)	PKFT1620
	FWM(J)=P(K+2)	PKFT1630
	TAU(J)=P(K+3)	PKFT1640
	SCHT(J)=STDE(K)	PKFT1650
	SDX0(J)=STDE(K+1)	PKFT1660
	SDFW(J)=STDE(K+2)	PKFT1670
	SDTAL(J)=STDE(K+3)	PKFT1680
	ENERGY(J)=E0+ECH*POS(J)	PKFT1690
	30 K=K+4	PKFT1700
C		PKFT1710
C	END OF MAIN LOOP	PKFT1720
C		PKFT1730
	50 CONTINUE	PKFT1740
	RETURN	PKFT1750
	END	PKFT1760
	SUBROUTINE NLLS(IPRINT)	NLLS0010
C		NLLS0020

CCMMCN /COM3/ E0,ECH,FWHM0,FWMEV,TAU0,TAUMEV,SKULOI,SKULOS,	NLLS0030
1 SKUHII,SKUHIS,TAILI,TAILS,NSKULC,NSKUHI,NLOI,NHI1,MAXIT,ITQ,	NLLS0040
1 EPSQ,EFFS,EFMXLG,EFTERM,PKLMT,NRDR,NPSTR,NPNCH	NLLS0050
CCMMCN /COM6/ W(200),X(200),Y(200),NPTS,EPS(39),STDE(38),	NLLS0060
1 VAR,ICONV,ITRATN,SCAREA	NLLS0070
CCMMCN /COM7/ P(39),IHOLD(39),DERIV(38),TERM(10),ALPHA1(9),	NLLS0080
1 ALPHA2(9),BETA1(9),BETA2(9),BETA3(9),TAIL(9),SKULO(9),SKUHI(9),	NLLS0090
1 NPRMS,NP,NFREE,NJ,IOPT,XFIRST,BPRIME	NLLS0100
C	NLLS0110
REAL*8 DET,AA(1444),A*4(76,39)	NLLS0120
EQUIVALENCE (AA(1),A(1))	NLLS0130
DIMENSION MPRNT(8),QPRNT(8),B(38),IND1(38),IND2(38),DELTAP(38),	NLLS0140
1 PPRNT(38,8)	NLLS0150
EQUIVALENCE (IND1(1),DELTAP(1))	NLLS0160
REAL MEV	NLLS0170
C	NLLS0180
C	NLLS0190
C	NLLS0200
ICCNV=1	NLLS0210
IOPT=1	NLLS0220
NNF=2*NFREE	NLLS0230
M=1	NLLS0240
ITRATN=C	NLLS0250
Q=1.E20	NLLS0260
MPRNT(1)=0	NLLS0270
L=0	NLLS0280
DO 8 K=1,NPRMS	NLLS0290
STDE(K)=0.	NLLS0300
IF (IHOLD(K) .NE. 1) GO TO 8	NLLS0310
L=L+1	NLLS0320
PPRNT(L,1)=P(K)	NLLS0330
8 CONTINUE	NLLS0340
C	NLLS0350
C	NLLS0360
C	NLLS0370
EVALUATE ERROR MATRIX	

10	ITRATN=ITRATN+1	NLLS0380
	IF (ITRATN .LE. MAXIT) GO TO 12	NLLS0390
	ICCNV=6	NLLS0400
	GO TO 50	NLLS0410
12	DO 14 K=1,NFREE	NLLS0420
	B(K)=0.	NLLS0430
	DO 14 L=1,NNF	NLLS0440
14	A(L,K)=0.	NLLS0450
	OLDQ=Q	NLLS0460
	Q=0.	NLLS0470
	DO 18 I=1,NPTS	NLLS0480
	CALL FUNCT(X(I),YC)	NLLS0490
	DIFF=Y(I)-YC	NLLS0500
	DO 16 K=1,NFREE	NLLS0510
	DW=W(I)*DERIV(K)	NLLS0520
	B(K)=B(K)+DW*DIFF	NLLS0530
	DO 16 L=K,NFREE	NLLS0540
16	A(2*L-1,K)=A(2*L-1,K)+DW*DERIV(L)	NLLS0550
18	Q=Q+W(I)*DIFF*DIFF	NLLS0560
	GFFNT(M)=Q	NLLS0570
	DO 20 K=2,NFREE	NLLS0580
	K1=K-1	NLLS0590
	DO 20 L=1,K1	NLLS0600
20	A(2*L-1,K)=A(2*K-1,L)	NLLS0610
C		NLLS0620
C	CHECK FOR Q CONVERGENCE. CHECK FOR FULL PRINT ARRAYS.	NLLS0630
C		NLLS0640
	IF (ITRATN .LT. ITQ) GO TO 24	NLLS0650
	IF (Q .LE. OLDQ) GO TO 22	NLLS0660
	ICCNV=2	NLLS0670
	GO TO 50	NLLS0680
22	IF ((OLDQ/Q-1.0) .GT. EPSQ) GO TO 24	NLLS0690
	ICONV=3	NLLS0700
	GO TO 50	NLLS0710
24	CONTINUE	NLLS0720

30	IF (M .EQ. 8) GO TO 50	NLLS0730
C		NLLS0740
C	INVERT MATFIX AND GET NEW PARAMETERS	NLLS0750
C		NLLS0760
32	CALL DUMNV(AA,NFREE,38,DET,IND1,IND2)	NLLS0770
	IF (DET .NE. 0.00) GO TO 34	NLLS0780
	ICONV=4	NLLS0790
	GO TO 50	NLLS0800
34	DO 36 K=1,NFREE	NLLS0810
	DELTAP(K)=0.	NLLS0820
	DO 36 L=1,NFREE	NLLS0830
36	DELTAP(K)=DELTAP(K)+A(2*L-1,K)*B(L)	NLLS0840
	ICONV=5	NLLS0850
	M=M+1	NLLS0860
	L=0	NLLS0870
	DO 38 K=1,NPRMS	NLLS0880
	IF (IHOLD(K) .NE. 1) GO TO 38	NLLS0890
	L=L+1	NLLS0900
	IF (MOD(K,4) .NE. 2) GO TO 37	NLLS0910
	IF (K .GT. NP) GO TO 37	NLLS0920
	IF (ABS(DELTAP(L)) .GT. .5) DELTAP(L)=SIGN(.5,DELTAP(L))	NLLS0930
C	THIS STATEMENT LIMITS CENTROID CHANGE TO .5 CHANNELS	NLLS0940
37	DP=DELTAP(L)/P(K)	NLLS0950
	IF (ABS(DP) .GT. EPS(K)) ICONV=1	NLLS0960
	IF (ABS(DP) .GT. 0.5) DP=SIGN(0.5,DP)	NLLS0970
C	THIS STATEMENT LIMITS ALL PARAMETER CHANGES TO	NLLS0980
C	0.5 TIMES PREVIOUS VALUE	NLLS0990
	P(K)=P(K)*(1.0+DP)	NLLS1000
	PPRNT(L,M)=P(K)	NLLS1010
38	CONTINUE	NLLS1020
	MPRNT(M)=ITRATN	NLLS1030
	K=1	NLLS1040
	DO 42 J=1,NJ	NLLS1050
	MEV=(E0+ECH*P(K+1))/1000.0	NLLS1060
	ALPHA1(J)=1.66511/P(K+2)	NLLS1070

ALPHA2(J)=P(K+3)*ALPHA1(J)	NLLS1080
TAIL(J)=TAILI+TAILS*MEV	NLLS1090
SKULO(J)=SKULOI+SKULOS*MEV	NLLS1100
SKUHI(J)=SKUHI I+SKUHIS*MEV	NLLS1110
BETA1(J)=P(K)*TAIL(J)	NLLS1120
BETA2(J)=NSKULO*P(K)*SKULO(J)	NLLS1130
BETA3(J)=NSKUHI*P(K)*SKUHI(J)	NLLS1140
42 K=K+4	NLLS1150
BPRIME=P(K+1)-1000.	NLLS1160
C	NLLS1170
C SAVE DIAGONAL ELEMENTS FOR ERRORS	NLLS1180
C	NLLS1190
L=0	NLLS1200
LL=-1	NLLS1210
DO 44 K=1,NPRMS	NLLS1220
IF (IHOLD(K) .NE. 1) GO TO 44	NLLS1230
L=L+1	NLLS1240
LL=LL+2	NLLS1250
STDE(K)=ABS(A(LL,L))	NLLS1260
44 CCNTINUE	NLLS1270
C	NLLS1280
C RETURN FOR NEXT ITERATION UNLESS ICONV=5	NLLS1290
C	NLLS1300
IF (ICONV .EQ. 1) GO TO 10	NLLS1310
C	NLLS1320
C PRINT OUT CONTENTS OF PRNT ARRAYS	NLLS1330
C	NLLS1340
50 IF (IPRINT .LE. 0) GO TO 58	NLLS1350
WRITE (NPRTR,100)	NLLS1360
100 FORMAT('VALUES OF FREE PARAMETERS AFTER EACH ITERATION'/1H0,	NLLS1370
1 26X,'ITERATION')	NLLS1380
WRITE (NPRTR,102) (MPRNT(L),L=1,M)	NLLS1390
102 FORMAT (' PARAM',I6,7I14)	NLLS1400
L=0	NLLS1410
DO 52 K=1,NPRMS	NLLS1420

IF (IHOLD(K) .NE. 1) GO TO 52	NLLS1430
L=L+1	NLLS1440
WRITE (NPRTR,104) K,(PFRNT(L,MM),MM=1,M)	NLLS1450
104 FCRMAT (I3,1P8E14.5)	NLLS1460
52 CCNTINUE	NLLS1470
IF (ICONV .LT. 5) GO TO 56	NLLS1480
Q=0.	NLLS1490
IOPT=0	NLLS1500
DC 54 I=1,NPTS	NLLS1510
CALL FUNCT(X(I),YC)	NLLS1520
54 Q=Q+W(I)*(YC-Y(I))**2	NLLS1530
QFRNT(M)=Q	NLLS1540
56 WRITE (NPRTR,106) (QPRNT(L),L=1,M)	NLLS1550
106 FCRMAT ('O Q',1P8E14.5)	NLLS1560
58 M=0	NLLS1570
IF (ICONV .EQ. 1) GO TO 32	NLLS1580
IF (IFRINT .EQ. 0) GO TO 70	NLLS1590
GO TO (32,60,62,64,66,68),ICONV	NLLS1600
C	NLLS1610
C PRINT OUT CONVERGENCE MESSAGES	NLLS1620
C	NLLS1630
60 WRITE (NPRTR,110)	NLLS1640
110 FORMAT ('O ITERATION STOPPED BECAUSE Q INCREASED')	NLLS1650
L=0	NLLS1660
DC 61 K=1,NFREE	NLLS1670
IF (IHOLD(K) .NE. 1) GO TO 61	NLLS1680
L=L+1	NLLS1690
P(K)=P(K)-DELTAP(L)	NLLS1700
61 CCNTINUE	NLLS1710
Q=CLOG	NLLS1720
GO TO 70	NLLS1730
62 WRITE (NPRTR,112) EPSQ	NLLS1740
112 FCRMAT ('OQ DECREASED BY LESS THAN',1P8E1)	NLLS1750
GO TO 70	NLLS1760
64 WRITE (NPRTR,114) ITRATN	NLLS1770

114	FCRMT ('OMATRIX A IS SINGULAR ON ITERATION',I3)	NLLS1780
	GO TO 70	NLLS1790
66	WRITE (NPRTR,116) ITRATN	NLLS1800
116	FORMAT ('OCONVERGED IN',I3,' ITERATIONS')	NLLS1810
	GO TO 70	NLLS1820
68	WRITE (NPRTR,118) MAXIT	NLLS1830
118	FORMAT ('ODID NOT CONVERGE IN',I3,' ITERATIONS')	NLLS1840
C		NLLS1850
C	FIND VARIANCE AND ERRORS	NLLS1860
C		NLLS1870
70	VAR=Q/FLOAT(NPTS-NFREE)	NLLS1880
	SUMW=0.	NLLS1890
	DO 72 I=1,NPTS	NLLS1900
72	SUMW=SUMW+W(I)	NLLS1910
	VSW=VAR/SUMW	NLLS1920
	IF (IPRINT .EQ. 0) GO TO 74	NLLS1930
	WRITE (NPRTR,120) VAR,Q,VSW	NLLS1940
120	FCRMT ('O VARIANCE =',F6.2,6X,'Q =',1PE11.4,6X,' VARIANCE/SUM OF W	NLLS1950
	HEIGHTS =',E11.4)	NLLS1960
74	DO 76 K=1,NPRMS	NLLS1970
76	STDE(K)=SQRT(STDE(K)*VAR)	NLLS1980
	RETURN	NLLS1990
	END	NLLS2000
	SLBROUTINE FUNCT(X,Y)	FUNC0010
C		FUNC0020
	CCMMCN /COM3/ E0,ECH,FWHM0,FWMEV,TAJ0,TAUMEV,SKULOI,SKULJS,	FUNC0030
1	SKUHII,SKUHIS,TAI1,TAILS,NSKULO,NSKUHI,NLO1,NHI1,MAXIT,ITQ,	FUNC0040
1	EPSQ,EFFS,EFMXLG,EFTERM,PKLMT,NRDR,NPRTR,NPNCH	FUNC0050
	CCMMGN /COM7/ P(38),IHCLD(38),DERIV(38),TERM(10),ALPHA1(9),	FUNC0060
1	ALPHA2(9),BETA1(9),BETA2(9),BETA3(9),TAIL(9),SKULO(9),SKUHI(9),	FUNC0070
1	NPRMS,NP,NFREE,NJ,IOPT,XFIPST,BPRIME	FUNC0080
	INTEGER REGION	FUNC0090
C		FUNC0100
C	FIND BACKGROUND FIRST	FUNC0110
C		FUNC0120

	X1=X- XFIRST	FUNC0130
	TERM(NJ+1)=P(NP+1)+BPRIME*X1	FUNC0140
	Y=TERM(NJ+1)	FUNC0150
C		FUNC0160
C	MAIN LOOP	FUNC0170
C	IF IOPT=0, DERIVATIVES ARE NOT TO BE CALCULATED	FUNC0180
C		FUNC0190
	K=1	FUNC0200
	L=0	FUNC0210
	DC 50 J=1,NJ	FUNC0220
	Z=ALPHA1(J)*(X-P(K+1))	FUNC0230
	Z1=-Z-ALPHA2(J)	FUNC0240
	Z2=Z*Z	FUNC0250
	IF (Z1 .GT. 0.0) Z2=Z2-Z1*Z1	FUNC0260
	IF (Z2 .GT. 25.0) GO TC 8	FUNC0270
	ZETA=EXP(-Z2)	FUNC0280
	GC TO 10	FUNC0290
	8 ZETA=0.0	FUNC0300
C		FUNC0310
C	Z1 > 0 DEFINES REGION I	FUNC0320
C		FUNC0330
	10 IF (Z1 .LE. 0.0) GO TO 12	FUNC0340
	REGION=1	FUNC0350
	Z=Z1	FUNC0360
	GAMMA=Z**NLO1	FUNC0370
	DELTA=P(K)*ZETA*(1.0-TAIL(J)+SKULO(J)*GAMMA*Z)	FUNC0380
	TERM(J)=DELTA+BETA1(J)	FUNC0390
	Y=Y+TERM(J)	FUNC0400
	IF (IOPT .EQ. 0) GO TO 50	FUNC0410
	DELTA2=2.0*DELTA	FUNC0420
	ETA=ZETA*GAMMA*BETA2(J)	FUNC0430
	THETA=ALPHA2(J)	FUNC0440
	GO TO 20	FUNC0450
C		FUNC0460
C	Z < 0 AND Z1 < 0 DEFINE REGION II	FUNC0470

C		FUNC0480
	12 IF (Z .GT. 0.0) GO TO 14	FUNC0490
	REGION=2	FUNC0500
	GAMMA=0.0	FUNC0510
	DELTA=P(K)*ZETA*(1.0-TAIL(J))	FUNC0520
	TERM(J)=DELTA+BETA1(J)	FUNC0530
	Y=Y+TERM(J)	FUNC0540
	IF (IDPT .EQ. 0) GO TO 50	FUNC0550
	DELTA2=2.0*DELTA	FUNC0560
	ETA=0.0	FUNC0570
	THETA=Z	FUNC0580
	GO TO 20	FUNC0590
C		FUNC0600
C	Z > 0 DEFINES REGION III	FUNC0610
C		FUNC0620
	14 REGION=3	FUNC0630
	GAMMA=Z**NHI1	FUNC0640
	DELTA=P(K)*ZETA*(1.0+SKUHI(J)*GAMMA*Z)	FUNC0650
	TERM(J)=DELTA	FUNC0660
	Y=Y+TERM(J)	FUNC0670
	IF (IDPT .EQ. 0) GO TO 50	FUNC0680
	DELTA2=2.0*DELTA	FUNC0690
	ETA=ZETA*GAMMA*BETA3(J)	FUNC0700
	THETA=Z	FUNC0710
C		FUNC0720
C	CALCULATE DERIVATIVES	FUNC0730
C		FUNC0740
	20 IF (IHOLD(K) .EQ. 0) GO TO 24	FUNC0750
	DRV=TERM(J)/P(K)	FUNC0760
	L=L+1	FUNC0770
	DERIV(L)=DRV	FUNC0780
	24 IF (IHOLD(K+1) .EQ. 0) GO TO 28	FUNC0790
	DRV=(DELTA2*THETA-ETA)*ALPHA1(J)	FUNC0800
	IF (REGION .EQ. 1) DRV=-DRV	FUNC0810
	L=L+1	FUNC0820

DERIV(L)=DRV	FUNC0830
28 IF (IHOLD(K+2) .EQ. 0) GO TO 32	FUNC0840
DRV=(DELTA2*Z2-ETA*Z)/F(K+2)	FUNC0850
L=L+1	FUNC0860
DERIV(L)=DRV	FUNC0870
32 IF (IHOLD(K+3) .EQ. 0) GO TO 50	FUNC0880
DRV=0.	FUNC0890
IF (REGION .EQ. 1) DRV=-ALPHA1(J)*(ETA+DELTA2*Z)	FUNC0900
L=L+1	FUNC0910
DERIV(L)=DRV	FUNC0920
C	FUNC0930
50 K=K+4	FUNC0940
DERIV(L+1)=1.0	FUNC0950
DERIV(L+2)=X1	FUNC0960
RETURN	FUNC0970
END	FUNC0980
SUBROUTINE DUMNV(A,N,NN,D,L,M)	FUNC0990
C	FUNC1000
C PURPOSE	FUNC1010
C INVERT A MATRIX USING DOUBLE PRECISION ARITHMETIC.	FUNC1020
C	FUNC1030
C USAGE	FUNC1040
C CALL DUMNV(A,N,NN,D,L,M)	DUMV0010
C	DUMV0020
C DESCRIPTION OF PARAMETERS	DUMV0030
C A - DOUBLE PRECISION INPUT MATRIX, DESTROYED IN COMPUTATION	DUMV0040
C AND REPLACED BY THE RESULTANT INVERSE.	DUMV0050
C N - ORDER OF MATRIX A.	DUMV0060
C NN- FIRST DIMENSION OF THE A ARRAY.	DUMV0070
C D - RESULTANT DETERMINANT (DOUBLE PRECISION).	DUMV0080
C L - INTEGER WORK VECTOR OF LENGTH N.	DUMV0090
C M - INTEGER WORK VECTOR OF LENGTH N.	DUMV0100
C	DUMV0110
C METHOD	DUMV0120
C THE STANDARD GAUSS-JORDAN METHOD IS USED. THE DETERMINANT	DUMV0130

C	IS ALSO CALCULATED. A DETERMINANT OF ZERO INDICATES THAT	DUMV0140
C	THE MATRIX IS SINGULAR.	DUMV0150
C		DUMV0160
	DIMENSION A(1),L(1),M(1)	DUMV0170
	DCUBLE PRECISION A,D,BIGA,HOLD	DUMV0180
C		DUMV0190
C	SEARCH FOR LARGEST ELEMENT	DUMV0200
C		DUMV0210
	D=1.D0	DUMV0220
	NK=-NN	DUMV0230
	DO 80 K=1,N	DUMV0240
	NK=NK+NN	DUMV0250
	L(K)=K	DUMV0260
	M(K)=K	DUMV0270
	KK=NK+K	DUMV0280
	BIGA=A(KK)	DUMV0290
	DO 20 J=K,N	DUMV0300
	IZ=NN*(J-1)	DUMV0310
	DO 20 I=K,N	DUMV0320
	IJ=IZ+I	DUMV0330
	10 IF(DABS(BIGA)-DABS(A(IJ))) 15,20,20	DUMV0340
	15 BIGA=A(IJ)	DUMV0350
	L(K)=I	DUMV0360
	M(K)=J	DUMV0370
	20 CONTINUE	DUMV0380
C		DUMV0390
C	INTERCHANGE ROWS	DUMV0400
C		DUMV0410
	J=L(K)	DUMV0420
	IF(J-K) 35,35,25	DUMV0430
	25 KI=K-NN	DUMV0440
	DO 30 I=1,N	DUMV0450
	KI=KI+NN	DUMV0460
	HOLD=-A(KI)	DUMV0470
	J I=K I-K+J	DUMV0480

	A(KI)=A(JI)	DUMV0490
30	A(JI)=HOLD	DUMV0500
C		DUMV0510
C	INTERCHANGE COLUMNS	DUMV0520
C		DUMV0530
35	I=M(K)	DUMV0540
	IF(I-K) 45,45,38	DUMV0550
38	JF=NN*(I-1)	DUMV0560
	DO 40 J=1,N	DUMV0570
	JK=NK+J	DUMV0580
	JI=JP+J	DUMV0590
	HOLD=-A(JK)	DUMV0600
	A(JK)=A(JI)	DUMV0610
40	A(JI)=HOLD	DUMV0620
C		DUMV0630
C	DIVIDE COLUMN BY MINUS PIVOT (VALUE OF PIVOT ELEMENT IS	DUMV0640
C	CONTAINED IN BIGA)	DUMV0650
C		DUMV0660
45	IF(BIGA) 48,46,48	DUMV0670
46	D=0.D0	DUMV0680
	RETURN	DUMV0690
48	DO 55 I=1,N	DUMV0700
	IF(I-K) 50,55,50	DUMV0710
50	IK=NK+I	DUMV0720
	A(IK)=A(IK)/(-BIGA)	DUMV0730
55	CONTINUE	DUMV0740
C		DUMV0750
C	REDUCE MATRIX	DUMV0760
C		DUMV0770
	DO 65 I=1,N	DUMV0780
	IK=NK+I	DUMV0790
	HOLD=A(IK)	DUMV0800
	IJ=I-NN	DUMV0810
	DO 65 J=1,N	DUMV0820
	IJ=IJ+NN	DUMV0830

IF(I-K) 60,65,60	DUMV0840
60 IF(J-K) 62,65,62	DUMV0850
62 KJ=IJ-I+K	DUMV0860
A(IJ)=HOLD*A(KJ)+A(IJ)	DUMV0870
65 CONTINUE	DUMV0880
C	DUMV0890
C DIVIDE ROW BY PIVOT	DUMV0900
C	DUMV0910
KJ=K-NN	DUMV0920
DO 75 J=1,N	DUMV0930
KJ=KJ+NN	DUMV0940
IF(J-K) 70,75,70	DUMV0950
70 A(KJ)=A(KJ)/BIGA	DUMV0960
75 CONTINUE	DUMV0970
C	DUMV0980
C PRODUCT OF PIVOTS	DUMV0990
C	DUMV1000
D=D*BIGA	DUMV1010
C	DUMV1020
C REPLACE PIVOT BY RECIPROCAL	DUMV1030
C	DUMV1040
A(KK)=1.D0/BIGA	DUMV1050
80 CCNTINUE	DUMV1060
C	DUMV1070
C FINAL ROW AND COLUMN INTERCHANGE	DUMV1080
C	DUMV1090
K=N	DUMV1100
100 K=(K-1)	DUMV1110
IF(K) 150,150,105	DUMV1120
105 I=L(K)	DUMV1130
IF(I-K) 120,120,108	DUMV1140
108 JQ=NN*(K-1)	DUMV1150
JR=NN*(I-1)	DUMV1160
DO 110 J=1,N	DUMV1170
JK=JQ+J	DUMV1180

HOLD=A(JK)	DUMV1190
JI=JR+J	DUMV1200
A(JK)=-A(JI)	DUMV1210
110 A(JI) =HOLD	DUMV1220
120 J=M(K)	DUMV1230
IF(J-K) 100,100,125	DUMV1240
125 KI=K-NN	DUMV1250
DO 130 I=1,N	DUMV1260
KI=KI+NN	DUMV1270
HOLD=A(KI)	DUMV1280
JI=KI-K+J	DUMV1290
A(KI)=-A(JI)	DUMV1300
130 A(JI) =HOLD	DUMV1310
GO TO 100	DUMV1320
150 RETURN	DUMV1330
END	DUMV1340
SUBROUTINE OUT2 (LABEL)	OUT20010
	OUT20020
COMMON /COM1/ LENGTH,NFIRST,NLAST,NWINDJ,DATA(8192)	OUT20030
COMMON /COM2/ MAXPKS,NPEAKS,POS(250),ENERGY(250),AREA(250),	OUT20040
1 FWHM(250),TAU(250),NPKS(250),FITLO(250),FITHI(250),NFITS	OUT20050
COMMON /COM3/ EO,ECH,FWHM0,FWMEV,TAU0,TAUMEV,SKU_01,SKU_05,	OUT20060
1 SKUH11,SKUH15,TAI11,TAI15,NSKULO,NSKUHI,NLO1,NH11,MAXIT,ITO,	OUT20070
1 EPS0,EFFS,EFMXLG,EFTERM,PKLMT,NRDR,NPRTN,NPNCH	OUT20080
COMMON /COM4/ IFIT,IPRINT,IPUNCH,IGRAPH,IFIX,MLTPLT,MXFTSZ,EPSHT,	OUT20090
1 EPSX0,EPSPW,EPSTAU,EP SA,EP SB,DIFLIN,CONST,SEP,FITABV,FITBEL,	OUT20100
1 FITCTF,FWCTF,TAUCTF,XSF	OUT20110
COMMON /COM7/ P(38),IHOLD(38),DEPRV(38),TERM(10),ALPHA1(9),	OUT20120
1 ALPHA2(9),BETA1(9),BETA2(9),BETA3(9),TAIL(9),SKULO(9),SKUHI(9),	OUT20130
1 NPRMS,NF,NFREE,NJ,IOP,T,XFIRST,BPRIME	OUT20140
COMMON /COM8/ NFRSV(250),ICNVSV(250),ITRNSV(250),VARSV(250),	OUT20150
1 HEIGHT(250),SDHT(250),SDX0(250),SDFW(250),SDTAU(250),ASV(250),	OUT20160
1 BSV(250),LFIT(252)	OUT20170
	OUT20180
	OUT20190
DIMENSION X(210),Y(210),YCAL(200),XC(201),LABEL(20)	

INTEGER FITHI,FITLO	OUT20200
INTEGER*2 NFRSV,ICNVSV,ITRNSV	OUT20210
LOGICAL*1 LFIT	OUT20220
LOGICAL*1 LABL2(20)/'FIT	OUT20230
REAL XLAB(5)/'CHANNEL NUMBER	OUT20240
1 '/'	OUT20250
REAL MEV	OUT20260
EQUIVALENCE (LDUM(1),IDUM)	OUT20270
C	OUT20280
C PRINT HEADINGS	OUT20290
C	OUT20300
WRITE (NPRTR,100) LABEL	OUT20310
100 FORMAT (1H1,25X,20A4/1H0)	OUT20320
WRITE (NPRTR,102) NFIRST,NLAST,NWINDO,PKLMT	OUT20330
102 FORMAT (' PEAK FIND SEARCH BETWEEN CHANNELS ',I4,' AND ',I4,	OUT20340
1 10X,'SMOOTHING WINDOW =',I3,10X,'PEAK LIMIT PARAMETER =',F5.1)	OUT20350
WRITE (NPRTR,104) FITCTF,FITBEL,E0,ECH,TAILI,TAILS	OUT20360
104 FORMAT ('CUTOFFS: FIT,',F7.1,7X,'FITBEL =',F4.1,7X,'ENERGY =',	OUT20370
1 F7.2,' KEV +',F9.6,' KEV PER CHANNEL',7X,'TAIL =',F6.3,' +',	OUT20380
1 F6.3,' PER MEV')	OUT20390
WRITE (NPRTR,106) FWCTF,FITABV,FWHM0,FWM0,SKULOI,SKULOS	OUT20400
106 FORMAT (11X,'FWHM,',F6.1,7X,'FITABV =',F4.1,9X,'FWHM =',F8.3,	OUT20410
1 ' +',F7.3,' PER MEV',19X,'SKULO =',F6.3,' +',F6.3,' PER MEV')	OUT20420
WRITE (NPRTR,108) TAUCTF,SEP,TAU0,TAUM0,SKUHI,SKUHI	OUT20430
108 FORMAT (11X,'TAU,',F7.1,10X,'SEP =',F4.1,10X,'TAU =',F8.3,' +',	OUT20440
1 F7.3,' PER MEV',19X,'SKUHI =',F6.3,' +',F6.3,' PER MEV'/1H-)	OUT20450
WRITE (NPRTR,110)	OUT20460
110 FORMAT (40X,'SUMMARY OF FITTING RESULTS')	OUT20470
WRITE (NPRTR,112)	OUT20480
112 FORMAT ('OFIT NPXS NFREE NPTS VAR ICNV NIT'/25X,'ENERGY',	OUT20490
1 ' HEIGHT & ERROR CENTROID & ERROR FWHM & ERROR',	OUT20500
1 ' TAU & ERROR AREA & ERROR & % ERROR')	OUT20510
C	OUT20520
C MAIN LOOP--L LABELS FITS, J LABELS PEAKS	OUT20530
C	OUT20540

IOPT=0	OUT20550
JMAX=0	OUT20560
DO 70 L=1,NFITS	OUT20570
JMIN=JMAX+1	OUT20580
JMAX=JMAX+NPXS(L)	OUT20590
IF (.NOT. LFIT(L)) GO TO 70	OUT20600
C	OUT20610
C INITIALIZE X AND Y ARRAYS	OUT20620
C	OUT20630
12 IMIN=FITLO(L)-5	OUT20640
IF (IMIN .LT. NFIRST) IMIN=NFIRST	OUT20650
IMAX=FITHI(L)+5	OUT20660
IF (IMAX .GT. NLAST) IMAX=NLAST	OUT20670
NEXPTS=IMAX-IMIN+1	OUT20680
NPTS=FITHI(L)-FITLO(L)+1	OUT20685
X(1)=IMIN	OUT20690
Y(1)=DATA(IMIN+1)	OUT20700
IF (Y(1) .LT. 1.0) Y(1)=0.5	OUT20710
DO 14 I=2,NEXPTS	OUT20720
X(I)=X(I-1)+1.	OUT20730
Y(I)=DATA(IMIN+I)	OUT20740
IF (Y(I) .LT. 1.0) Y(I)=0.5	OUT20750
14 CONTINUE	OUT20760
XFIRST=FITLO(L)	OUT20770
C	OUT20780
C FIND PARAMETERS FROM FIT	OUT20790
C	OUT20800
NJ=NPXS(L)	OUT20810
NP=4*NJ	OUT20820
NPRMS=NP+2	OUT20830
P(NP+1)=ASV(L)	OUT20840
BFRIME=BSV(L)	OUT20850
K=1	OUT20860
DO 20 J=JMIN,JMAX	OUT20870
P(K)=HEIGHT(J)	OUT20880

P(K+1)=PCS(J)	OUT20890
P(K+2)=F WHM(J)	OUT20900
P(K+3)=TAU(J)	OUT20910
20 K=K+4	OUT20920
C	OUT20930
C FIND ALPHAS, BETAS, ETC.	OUT20940
C	OUT20950
K=1	OUT20960
DO 22 J=1,NJ	OUT20970
MEV=ENERGY(J+JMIN-1)/1000.	OUT20980
ALPHA1(J)=1.65511/P(K+2)	OUT20990
ALPHA2(J)=P(K+3)*ALPHA1(J)	OUT21000
TAIL(J)=0.0	OUT21010
SKULC(J)=SKULOI+SKULCS*MEV	OUT21020
SKUHI(J)=SKUHI I+SKUHIS*MEV	OUT21030
BETA1(J)=0.0	OUT21040
BETA2(J)=NSKULO*P(K)*SKULO(J)	OUT21050
BETA3(J)=NSKUHI*P(K)*SKUHI(J)	OUT21060
22 K=K+4	OUT21070
C	OUT21080
C FIND AREAS	OUT21090
C	OUT21100
DO 24 J=JMIN,JMAX	OUT21110
24 AREA(J)=0.	OUT21120
DO 30 I=1,NEXPTS	OUT21130
CALL FUNCT(X(I),YC)	OUT21140
DO 26 J=JMIN,JMAX	OUT21150
26 AREA(J)=AREA(J)+TERM(J-JMIN+1)	OUT21160
30 CCNTINUE	OUT21170
DO 32 J=1,NJ	OUT21180
TAIL(J)=TAIL I+TAILS*MEV	OUT21190
BETA1(J)=TAIL(J)*P(4*J-3)	OUT21200
32 CONTINUE	OUT21210
C	OUT21220
C WRITE RESULTS	OUT21230

C	WRITE (NPRT,120) L,NPKS(L),NFRSV(L),NPTS,VARSV(L),ICNVSV(L),	OUT21240
	1 ITRNSV(L)	OUT21250
120	FCPMAT (1H0,I3,I5,I7,I6,1X,F6.2,I5,I6)	OUT21260
	DO 36 J=JMIN,JMAX	OUT21270
	ERAREA=SQRT((SDHT(J)/HEIGHT(J))**2+(SDFW(J)/FWHM(J))**2)	OUT21280
	SCAREA=ERAREA*AREA(J)	OUT21290
	WRITE (NPRT,122) ENERGY(J),HEIGHT(J),SDHT(J),POS(J),SDX0(J),	OUT21300
	1 FWHM(J),SDFW(J),TAU(J),SDTAU(J),AREA(J),SDAREA,ERAREA	OUT21310
122	FORMAT (25X,F6.1,F11.1,F8.1,F12.3,F7.3,F9.3,F7.3,F9.3,F7.3,	OUT21320
	1 1PE13.3,E11.3,2PF6.1)	OUT21330
	IF (IPUNCH .LT. 2) GO TO 36	OUT21340
	WRITE (NPNCH,124) POS(J),SDX0(J),AREA(J),HEIGHT(J),SDHT(J),	OUT21350
	1 FWHM(J),SDFW(J),TAU(J),SDTAU(J)	OUT21360
124	FORMAT (2F10.2,3F10.1,4F5.2)	OUT21370
	36 CONTINUE	OUT21380
C		OUT21390
C	DC GRAPHING	OUT21400
C		OUT21410
	IF (IGRAPH .EQ. 0) GO TO 70	OUT21420
38	XMIN=X(1)-AMOD(X(1),10.)	OUT21430
	IF (XSF .LT. 4.0) XSF=4.0	OUT21440
	IF (XSF .GT. 20.) XSF=20.	OUT21450
	XSIZE=(X(NEXPTS)-XMIN)/XSF	OUT21460
	XSIZE=XSIZE+0.5-AMOD(XSIZE,0.5)	OUT21470
	IF (XSIZE .LT. 5.0) XSIZE=5.0	OUT21480
	YSIZE=8.0	OUT21490
C		OUT21500
C	PUT FIT NUMBER INTO POSITIONS 5,6, AND 7 OF LABEL2	OUT21510
C		OUT21520
	IDUM=L/100+240	OUT21530
	LABEL2(5)=LDUM(4)	OUT21540
	IDUM=MOD(L/10,10)+240	OUT21550
	LABEL2(6)=LDUM(4)	OUT21560
	IDUM=MOD(L,10)+240	OUT21570
		OUT21580

	LABL 2(7)=LDUM(4)	OUT21590
C		OUT21600
C	SET LP GRAPH ARRAYS	OUT21610
C		OUT21620
	YMN=1.E8	OUT21630
	YMX=1.	OUT21640
	DO 40 I=1,NEXPTS	OUT21650
	Y(I)=SQRT(Y(I))	OUT21660
	IF (Y(I) .LT. YMN) YMN=Y(I)	OUT21670
	IF (Y(I) .GT. YMX) YMX=Y(I)	OUT21680
40	CONTINUE	OUT21690
	XC(I)=FITLO(L)	OUT21710
	DO 42 I=1,NPTS	OUT21720
	CALL FUNCT(XC(I),YC)	OUT21730
	YC=SQRT(ABS(YC))	OUT21740
	IF (YC .LT. YMN) YMN=YC	OUT21750
	IF (YC .GT. YMX) YMX=YC	OUT21760
	YCAL(I)=YC	OUT21770
	XC(I+1)=XC(I)+1.0	OUT21780
42	CONTINUE	OUT21790
C		OUT21800
C	FIND Y SCALE FACTOR AND SYMBOL SIZE	OUT21810
C		OUT21820
	YMN=YMN-.5	OUT21830
	YSF=(YMX-YMN)/(YSIZE-1.0)	OUT21840
	IYSF=ALOG(YSF)+1.0	OUT21850
	IF (IYSF .GT. 6) GO TO 70	OUT21860
	GO TO (50,52,54,56,58,60),IYSF	OUT21870
	YSF=1.0	OUT21880
	GC TC 62	OUT21890
50	YSF=YSF+C.5-AMOD(YSF,0.5)	OUT21900
	GC TO 62	OUT21910
52	YSF=YSF+1.0-AMOD(YSF,1.0)	OUT21920
	GC TO 62	OUT21930
54	YSF=YSF+2.0-AMOD(YSF,2.0)	OUT21940

GO TO 62	OUT21950
56 YSF=YSF+5.0-AMOD(YSF,5.0)	OUT21960
GO TO 66	OUT21970
58 YSF=YSF+20.-AMOD(YSF,20.)	OUT21980
GO TO 66	OUT21990
60 YSF=YSF+50.-AMOD(YSF,50.)	OUT22000
GO TO 66	OUT22010
C	OUT22020
62 YFIR=YMN-AMOD(YMN,YSF)	OUT22030
SIZE=1.0/YSF	OUT22040
CALL ORIGIN(SIZE,0.5)	OUT22050
CALL GRAPH(NEXPTS,X,Y,13,7,XSIZE,YSIZE,XSF,XMIN,YSF,YFIR,XLAB,	OUT22060
1 YLAB,LABEL,LABL2)	OUT22070
GO TO 68	OUT22080
66 CALL ORIGIN(0.08,0.5)	OUT22090
YFIR=YMN-AMOD(YMN,YSF)	OUT22100
CALL GRAPH(NEXPTS,X,Y,2,7,XSIZE,YSIZE,XSF,XMIN,YSF,YFIR,XLAB,	OUT22110
1 YLAB,LABEL,LABL2)	OUT22120
68 CALL GRAPH(NPTS,XC,YCAL,2,2,0.,YSIZE,XSF,XMIN,YSF,YFIR,0,0,0,0)	OUT22130
70 CONTINUE	OUT22140
C	OUT22150
C END OF MAIN LOOP	OUT22160
C	OUT22170
WRITE (NPRTR,126)	OUT22180
126 FORMAT ('-EXPLANATION OF ICONV: 2 - Q INCREASED ON LAST ITERATION	OUT22190
1'/24X,'3 - Q DECREASED BY LESS THAN EPS3'/24X,'4 - ERROR MATRIX WA	OUT22200
1S SINGULAR'/24X,'5 - CONVERGED NORMALLY'/24X,'6 - DID NOT CONVERGE	OUT22210
1 IN MAXIT ITERATIONS'/1H0)	OUT22220
RETURN	OUT22230
END	OUT22240
INSERT MAIN	
OVERLAY ONE	
INSERT INPUT	
OVERLAY ONE	
INSERT PKFIND	

INSERT OUT1
 OVERLAY ONE
INSERT FUNCT
INSERT COM6
INSERT COM7
INSERT CCM8
 OVERLAY TWO
INSERT FKFIT
INSERT NLLS
INSERT CUMNV
 OVERLAY TWO
INSERT OUT2