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GELI2 and SPAN2

FORTRAN PROGRAMS TO CALCULATE NUCLIDE ABUNDANCES FROM MULTICHANNEL GAMMA RAY SPECTRA

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FORTRAN Programs to Calculate Nuclide Abundances from Multichannel Gamma Ray Spectra

by

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ABSTRACT

A FORTRAN computer program incorporating a second difference peak search was developed to calculate nuclide abundances from gamma ray spectra on magnetic tape without applying iterative fitting techniques. Peak areas are obtained by summing counts above a statistically justified cubic or linear equation background, and confidence limits are determined for all analytical results.

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INTRODUCTION

Quantitative analytical interpretation of multichannel spectra involves extensive calculations which become tedious and costly when performed manually on a routine basis. A number of computer programs have been written for data reduction of high resolution spectra. These programs[1-4] normally search for significant peaks, resolve overlapping peaks if possible, calculate the net counting rate for each peak, and identify the isotopes present. The different needs of each author and the complexity of the codes make effective use of another's program difficult. At Savannah River, this work has been done by the program GELI with peak search SPAN, written by R. A. Priest[5] in 1968.

The FORTRAN computer program described in this report is intended for routine analytical calculations of 4096-channel gamma ray spectra. It was written by modifying and supplementing GELI, and by replacing the SPAN first derivative peak search with SPAN2, a much more sensitive and quicker second difference peak search. This program has the special advantages of:

- Effective detection of overlapping peaks without time-consuming iterative curve fitting.
- More accurate area calculation by improved background determination for single peaks.
- Use of peak search data in evaluation of analytical results.
- A statistical analysis of all analytical results including "less than" estimates for nondetected isotopes.
- Comment codes which identify in detail the results of all tests.

SUMMARY

The existing computer program for routine analysis of high-resolution gamma ray spectra has been substantially modified, a new peak search subroutine has been written, and computer runtime has been decreased by more than 50%. Nuclide abundances are determined by summing counts above background in a region of the spectrum defined for each peak by empirical equations relating energy and full width at half maximum to channel numbers. Backgrounds are approximated using either a linear or cubic equation, depending on statistical justification. Confidence limits are reported for all analysis results including "less than" estimates for nondetected nuclides. Peak search data are reviewed, and peaks which may interfere are listed for each nuclide.

The peak search applies five tests in its evaluation of the second difference curve to locate significant peaks, and accurately determines the peak energy from a linear channel-energy relation by fitting a Gaussian curve to the spectral data. Areas of sufficiently separated single peaks are calculated by summing counts above background, and an error analysis is provided. Five edit options control the amount of printed detail obtained from the peak search routine. These options vary from no printout at all to the extremely detailed output which includes a graph of the spectrum. Comment codes generated during the search cross reference overlapping peaks and identify all test failures.

DISCUSSION

The computer program described here consists of two parts: the main program GELI2, and the peak search subroutine SPAN2. GELI2 calculates all analytical results; SPAN2 performs peak searches on the input spectra and supplies information such as peak energies, areas, and full width at half maximum (FWHM) for user evaluation of the GELI2 analytical results. The only quantitative data from SPAN2 used by GELI2 are peak locations needed for the energy-channel calibration. The GELI2 and SPAN2 routines will, therefore, be discussed separately, as will the subroutine BKGND, which is called by both GELI2 and SPAN2 to calculate backgrounds under peaks. Examples of the program are used in the Appendix to illustrate proper form and arrangement of input data cards.

GELI2

The computer program (as shown in the GELI2 Flow Diagram of Figure 1) first calls subroutine READIT to read nuclide input information such as energy, intensity, efficiency, etc. This information is organized by the user into sets, each containing data for up to 100 nuclides of interest. Selected nuclides are then designated for analysis by identifying the set. A maximum of five nuclide sets is permitted by the DEFINE FILE statements. The CALL NINIT(IDF) statement identifies the set of nuclides (IDF) to be considered and supplies all interference information needed later in the interference calculations. After reading sample input data from cards, the 4096-channel gamma ray spectrum is read into common storage from magnetic tape for use by both GELI2 and SPAN2. A peak search is performed on each spectrum. No option has been provided to bypass the peak search because this information is necessary to evaluate effectively the analytical results.

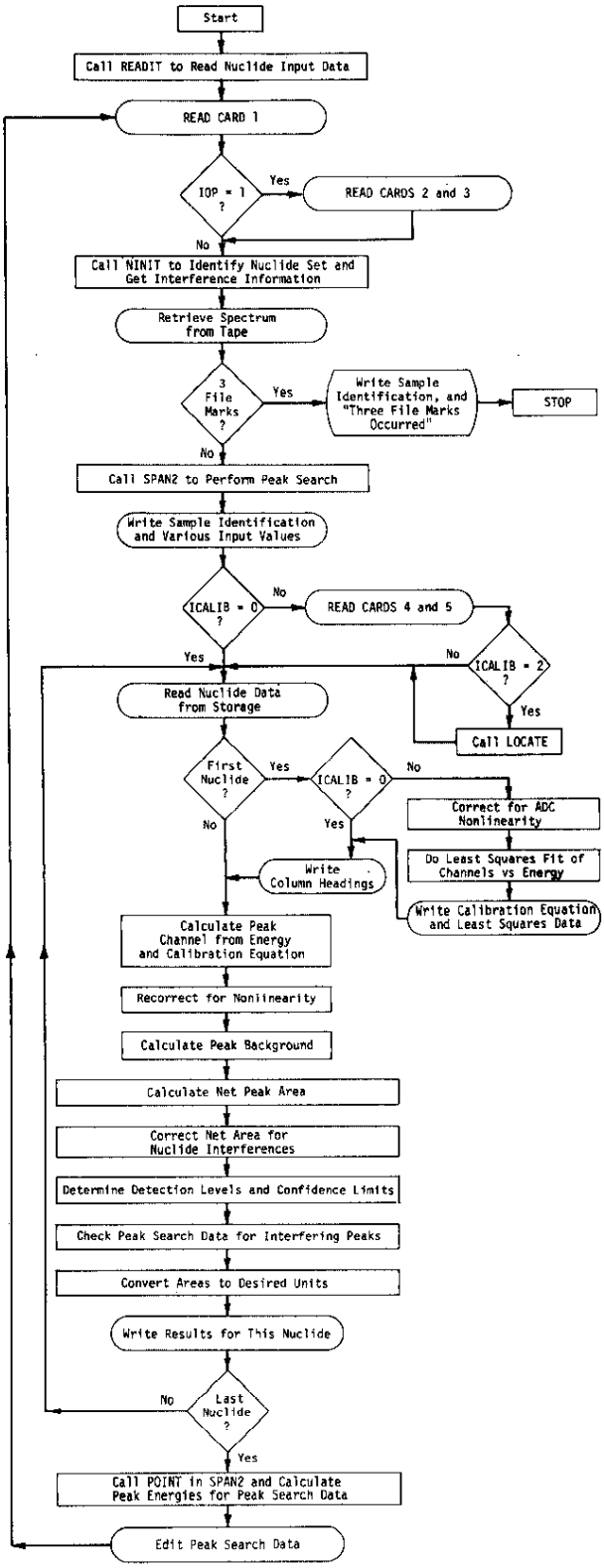

FIGURE 1. GELI2 Flow Diagram

The calibration option must be used on the first spectrum to relate channel numbers to energies. The channel numbers and associated energies for up to 25 peaks may be input on cards for this calibration. The minimum input data required for the calibration are the channel numbers for the four default energies (74.7, 661.6, 1173.2, and 1332.5 keV) supplied by the BLOCK DATA portion of the program. If accurate values for the channel numbers are not available, estimated channel numbers may be input, and precise values may be obtained from the spectral data by using the option to call subroutine LOCATE which examines the stored results of SPAN2 and locates the single peaks nearest to and within 15 channels of the estimated channels. If a peak is not found, the estimated channel number is used in the calibration.

After the channel numbers are corrected for any nonlinearity of the analog-to-digital converter, a linear least squares fit is performed on the data. The resulting equation which relates channels to energies is used by both GELI2 and SPAN2 for all subsequent channel-to-energy calculations.

Since the abundance of a given nuclide is proportional to its peak area, the accuracy of the analysis is directly dependent upon the accuracy of the peak area determination and is especially critical for small peaks. Calculation of the peak center and FWHM from the data for small peaks may also be unreliable. For this reason the peak center and FWHM are determined from appropriate equations in the GELI2 routine as follows.

The peak center is determined for area calculations in GELI2 from the known gamma ray energy using the energy-to-channel calibration equation and recorrecting for analog-to-digital converter nonlinearity. The FWHM is then calculated from the empirical equation FWHM=FWHMT + .001 (peak channel number), where FWHMT is an input estimate of the FWHM in the first quadrant of the spectrum. The gross area of the peak is obtained by summing the counts in each channel from (peak center - AFAC*FWHM) to (peak center + AFAC*FWHM). AFAC is a numerical constant (presently equal to 1.5) that controls the number of channels in the area summation. The background under the peak is described by a cubic equation fitted to the spectral data by subroutine BKGND. The background area is obtained by summing the background counts over the defined channel range. Any nuclide interference corrections are then made and the net peak area defined as

NET AREA = GROSS AREA - (BKGND AREA + INTERFERENCE AREA)

The data are then statistically evaluated at the 95% confidence level using the principles discussed by Currie.[6] The detection level is determined by comparing the net peak area with the net area above which the observed signal may reliably be recognized as detected (L_c) and with the level at which the measurement precision becomes satisfactory for quantitative determination (L_q). L_c, L_q, and the variance of the net area σ^2 are defined by the following equations when considering radioactivity.

$$L_c = 2.33\sqrt{\text{GROSS AREA} - \text{NET AREA}}$$

$$L_q = 50\left\{1 + \left[1 + \frac{\text{GROSS AREA} - \text{NET AREA}}{12.5}\right]^{\frac{1}{2}}\right\}$$

$$\sigma^2 = 2\ \text{GROSS AREA} - \text{NET AREA}$$

Table I summarizes the statistical evaluation. Note that for these calculations, interferences are considered simply as part of the background.

TABLE I

Summary of Statistical Data Evaluation

	Net Peak Area[a]		
	$\leq L_c$	$> L_c$ and $< L_q$	$\geq L_q$
Detection Level Reported	Not Detected	Qualitative	Quantitative
Confidence Limits Reported	Upper Limit Only: Peak Area + 1.645σ	Upper and Lower Limits: Peak Area ± 1.96σ	

a. L_c = net area above which the observed signal may be reliably recognized as detected. L_q = level at which area measurement precision becomes satisfactory for quantitive determination. σ = standard deviation of net peak area.

After the GELI2 routine has examined the peak search data of SPAN2 to identify all peaks in the vicinity of the peak of interest, the analytical results in terms of area are converted to the desired units using the appropriate equation of Table II; the variables used are identified in Table III. The input variable ICALC identifies the calculation option and will be discussed in the section on the use of the GELI2 program.

TABLE II

Peak Area Conversion Expressions

ICALC	Expression Defining ABUND1 or ABUN in GELI2	Units
0	DEFAULTS TO 1	
1	$\frac{AREA*DIL*100}{CT*EFF(IEFF)*XIN*EXP(-(.693*DT)/HL*1440))}$	dpm
2	$\frac{AREA*100*10^{6}}{CPMMG*WT*CT*EFF(IEFF)*XIN*EXP(-(.693*DT)/(HL*1440))}$	ppm
3	$\frac{AREA*100*HL*1440*WTMOL*10^{6}}{CT*EFF(IEFF)*XIN*.693*XSECT*FLUX*10^{-24}*6.02*10^{20}*ABISO*.01}$ *WT*EXP(-(.693*DT)/(HL*1440)	ppm
4	$\frac{AREA*100*HL*1440*WTMOL*10^{24}}{CT*EFF(IEFF)*XIN*.693*XSECT*ELMASS*ABISO*.01*6.02*10^{20}}$ *EXP(-(.693*DT)/(HL*1440)	neutron/cm^2

TABLE III

Identification of Variables

Variable or Constant	Identification	Units
ABISO	(Ratio of Isotope abundances)*100	None
ABUN	Uncertainty of ABUND1	Table II
ABUND1	Nuclide abundance or integrated flux	Table II
AREA	Net peak area or its uncertainty	counts
CPMMG	Nuclide specific activity	dpm/mg
CT	Counting time	minutes
DIL	Dilution factor	None
DT	Decay time	minutes
EFF(IEFF)	Efficiency	counts/photon
ELMASS	Element mass	mg
FLUX	Integrated flux	neutron/cm^2
HL	Half. life	days
ICALC	Input variable specifying calculation option	None
IEFF	Input variable specifying efficiency option	None
WT	Sample weight	mg
WTMOL	Molecular weight	g/mol
XIN	Intensity*100	photon/dis-integration
XSECT	Cross section	barns

The analysis results for the nuclide of interest are printed out in the form shown in Figure 2. In this output the "background" includes any nuclide interference corrections made, the "channel number" indicates the center channel for the area summation, and the "peaks from peak search" lists all peaks which occur within (2.0* SEPFAC*FWHM) channels of the calculated center channel. SEPFAC is a numerical constant (presently equal to 2.0) which defines peak separation requirements. The program then reads the next nuclide and repeats the calculations until all nuclides of the set are considered. Control is then returned to subroutine SPAN2 by the CALL POINT statement for calculation of the peak energies for the peak search data. After the peak search data are edited (Figure 3), GELI2 begins calculations on the next spectrum.

243AM,137CS,60CO SAMPLE, TAPE NA1071, FILE 1

SAMPLE WEIGHT 0.0 MILLIGRAMS DILLUTION FACTOR 0.10E 01 COUNTING TIME 6.67 MINUTES DECAY TIME 0.0 MINUTES

FLUX 0.0 NEUTRON/CM**CM ID NUMBER 1601 FILE NUMBER 1 EFFICIENCY OPT 1 CALIB OPT 2 CALCULATION OPT 1

CALIBRATION: CHANNEL NO. EQUALS -98.4 CHANNELS + 3.0687 CHANNELS PER KEV

ENERGIES	CHANNEL
74.7	131.8
661.6	1930.3
1173.2	3501.6
1332.5	3991.6

NUCLIDE	HALF LIFE DAYS	GAMMA ENERGY KEV	% GAMMA INTENS. PHO/DIS	COUNTING EFF. CT/PHOTON	CROSS SECTION BARNS	GROSS COUNTS	BKGND COUNTS	NUCLIDE	DETECT LEVEL	ELEMENT ABUNDANCE UNITS = DPM	CONF LIMITS	CHAN NO.	PEAKS FROM PEAK SEARCH
AM243	2.90E 06	74.7	75.20	7.70E-02	0.0	229098.	64576.	AM243	QUAN	0.426E 06 +/-	0.275E 04	135	135.7,
CO60	1.92E 03	1173.2	100.00	1.00E 00	0.0	67885.	5941.	CO60	QUAN	0.929E 04 +/-	0.793E 02	3502	3502.3,
CO60	1.92E 03	1332.5	100.00	1.00E 00	0.0	56436.	2175.	CO60	QUAN	0.814E 04 +/-	0.712E 02	3992	3992.3,
CS137	0.0	661.6	85.00	9.37E-03	0.0	115360.	12107.	CS137	QUAN	0.194E 07 +/-	0.132E 05	1931	1929.2,
YB169	0.0	63.1	45.00	1.00E 00	0.0	72160.	72160.	YB169	NOT DET:	LESS THAN 0.208E 03		99	88.3, 93.5
YB169	0.0	109.8	18.00	1.00E 00	0.0	92792.	92792.	YB169	NOT DET:	LESS THAN 0.591E 03		242	211.5, 224.3 227.7, 264.4
YB169	0.0	130.5	11.00	1.00E 00	0.0	35856.	35856.	YB169	NOT DET:	LESS THAN 0.601E 03		335	276.3, 334.3
YB169	0.0	177.2	22.00	1.00E 00	0.0	31631.	31631.	YB169	NOT DET:	LESS THAN 0.282E 03		448	NONE
YB169	0.0	198.0	35.00	1.00E 00	0.0	34313.	31764.	YB169	QUAL	0.109E 04 +/-	0.216E 03	511	534.0,

FIGURE 2. Typical GELI2 Analysis Output

P E A K A N A L Y S I S FILE 1

WINDOW = 5. TOLERANCE = 3 SEPFAC = 2.000 AFAC = 1.530

PEAK(CHANNEL)	COUNTS AT PEAK	ENERGY (KEV)	NET PEAK AREA (COUNTS)	REL STD DEVIATION OF AREA IN PERCENT	FULL WIDTH AT HALF MAX	COMMENT CODE
19.8	2279.	36.97	-----	-----	5.90	0.0
41.4	2750.	44.06	-----	-----	8.26	0.0
65.2	1841.	51.86	-----	-----	7.08	0.0
88.0	2852.	59.34	-----	-----	-----	20.0095
93.5	3186.	61.14	-----	-----	17.70	20.0000
135.7	34505.	74.99	-----	-----	8.26	0.0
211.6	7400.	99.87	-----	-----	7.08	0.0
224.0	11033.	103.94	-----	-----	-----	20.0232
227.7	12716.	105.15	-----	-----	15.34	20.0000
264.4	4046.	117.18	-----	-----	8.26	0.0
276.3	2273.	121.10	-----	-----	5.90	0.0
334.0	1388.	140.30	-----	-----	22.42	41.0000
347.0	1309.	144.26	-----	-----	-----	50.0334
534.0	1361.	205.52	-----	-----	4.72	0.0
547.0	2415.	209.77	-----	-----	7.08	0.0
567.0	1265.	216.31	-----	-----	15.34	41.0000
575.0	1304.	218.92	-----	-----	-----	50.0567
602.7	3547.	228.00	0.1263076E 05	2.151	8.26	0.0
649.0	1017.	243.14	-----	-----	12.98	41.0000
655.0	988.	245.11	-----	-----	-----	50.0649
753.7	3172.	277.38	0.1276943E 05	1.836	8.26	0.0
854.8	817.	310.47	-----	-----	7.08	0.0
870.0	925.	315.43	-----	-----	8.26	0.0
886.2	742.	320.71	-----	-----	8.26	0.0
926.7	1001.	333.95	0.1256918E 04	15.142	8.26	0.0
1145.0	700.	405.29	-----	-----	-----	50.1152
1147.0	701.	405.94	-----	-----	-----	50.1152
1152.0	690.	407.57	-----	-----	12.98	41.0000
1246.0	774.	438.26	-----	-----	14.16	41.0000
1254.0	756.	440.88	-----	-----	-----	50.1246
1438.0	500.	500.93	-----	-----	4.72	41.0000
1441.0	472.	501.90	-----	-----	-----	50.1438
1497.9	468.	520.46	0.0	529.396	7.08	0.0
1621.0	377.	560.61	-----	-----	-----	50.1628
1624.0	337.	561.59	-----	-----	-----	50.1628
1628.0	366.	562.90	-----	-----	15.34	41.0000
1754.5	588.	604.13	0.1689273E 04	8.090	8.26	0.0
1929.2	14802.	661.37	0.1029372E 06	0.341	8.26	0.0
2036.0	299.	695.86	-----	-----	-----	50.2042
2042.0	321.	697.82	-----	-----	11.80	41.0000
2084.0	335.	711.50	-----	-----	-----	50.2086
2086.0	295.	712.15	-----	-----	11.80	41.0000
2232.0	327.	759.69	-----	-----	-----	50.2236
2236.0	320.	760.99	-----	-----	11.80	41.0000
2300.0	332.	781.83	-----	-----	8.26	41.0000
2302.0	309.	782.48	-----	-----	-----	50.2300
2341.9	470.	795.47	0.4917031E 03	39.317	13.62	0.0
2393.0	323.	812.11	-----	-----	-----	50.2399
2399.0	379.	814.06	-----	-----	11.80	41.0000
2551.0	384.	863.54	-----	-----	-----	50.2558
2558.0	395.	865.82	-----	-----	11.80	41.0000
2674.0	422.	903.57	-----	-----	15.34	41.0000
2683.0	423.	906.50	-----	-----	-----	50.2674
2769.0	489.	934.48	-----	-----	12.98	41.0000
2776.0	484.	936.76	-----	-----	-----	50.2769
3038.0	336.	1022.02	-----	-----	15.34	41.0000
3046.0	328.	1024.62	-----	-----	-----	50.3038
3061.0	349.	1029.50	-----	-----	-----	50.3069
3069.0	351.	1032.11	-----	-----	15.34	41.0000
3419.0	178.	1146.02	-----	-----	-----	50.3425
3425.0	177.	1147.97	-----	-----	12.98	41.0000
3437.0	198.	1151.89	-----	-----	14.16	41.0000
3445.0	187.	1154.48	-----	-----	-----	50.3437
3592.3	6822.	1173.13	0.6141406E 05	0.441	13.62	0.0
3596.0	96.	1203.64	-----	-----	-----	50.3602
3602.0	92.	1205.60	-----	-----	11.80	41.0000
3656.0	68.	1223.18	-----	-----	-----	50.3663
3663.0	75.	1225.46	-----	-----	12.98	41.0000
3700.0	60.	1237.51	-----	-----	-----	50.3704
3704.0	57.	1238.81	-----	-----	11.80	41.0000
3841.0	39.	1283.44	-----	-----	-----	50.3844
3844.0	31.	1284.42	-----	-----	8.26	41.0000
3876.0	37.	1294.84	-----	-----	13.62	41.0000
3879.0	41.	1295.82	-----	-----	-----	50.3876
3992.5	5661.	1332.81	0.5392266E 05	0.448	11.80	0.0

FIGURE 3. Typical Peak Search Output

SPAN2

Subroutine SPAN2 is called by GELI2 to perform peak searches on spectral data in common storage. This routine uses a second difference method to find peaks, and locates the peak centers precisely by fitting a Gaussian curve to the spectral data. Peak shapes are thoroughly evaluated by applying tests to the second difference curve, thus making it possible to distinguish single peaks from Compton edges and multiple peaks. Peak areas are calculated for single peaks if no interfering peaks are present. The relative standard deviations of the peak areas are also determined. A comment code is generated which identifies all test failures, classifies peaks, and cross references overlapping peaks. Five editing options are available to vary the amount and detail of the printout.

Some general aspects of the peak search are discussed before describing the details of the SPAN2 routine. Consider first the shape of the second derivative of a Gaussian curve (Figure 4). The second derivative is characterized by a minimum value at the peak center, zero at the peak's two inflection points, and maxima near the peak's two tail regions. The distance between the two zero values gives a measure of the Gaussian peak width. A peak finding procedure employing the second derivative method searches the second derivative curve for the characteristic maximum-minimum-maximum shape and applies appropriate tests to confirm or reject possible peaks.

To adapt this concept to the discrete data of a gamma ray spectrum, the second derivative must be approximated. This is done using the second difference function S_i, which is evaluated at channel i, and defined by

$$S_i = N_{i-1} - 2N_i + N_{i+1}$$

where N is the number of counts in the subscripted channel. If the second difference as described above is calculated and graphed as in Figure 5 for a real peak, a noise-like signal results which does not resemble the second derivative of a Gaussian curve because of statistical fluctuations of the data.

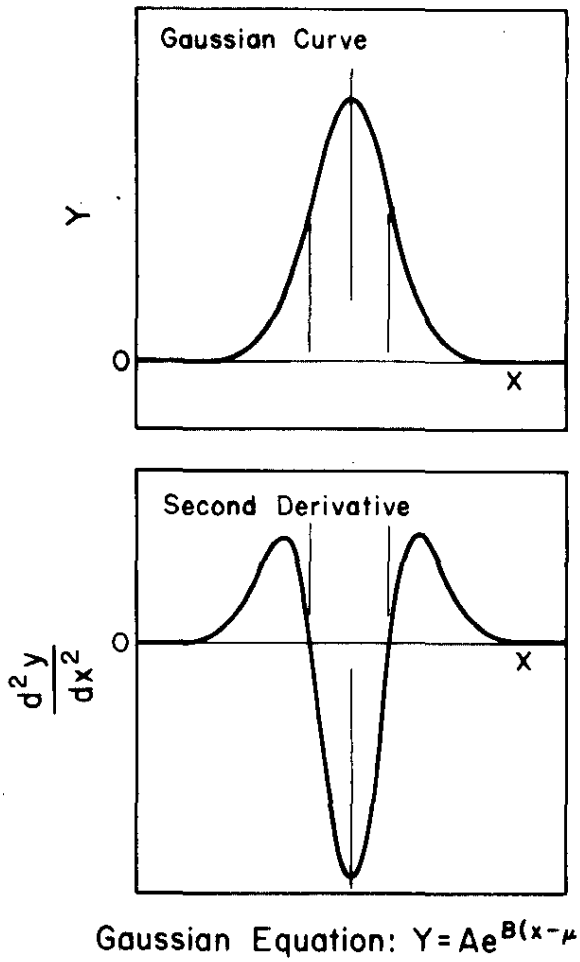

FIGURE 4. Second Derivative of Gaussian Curve

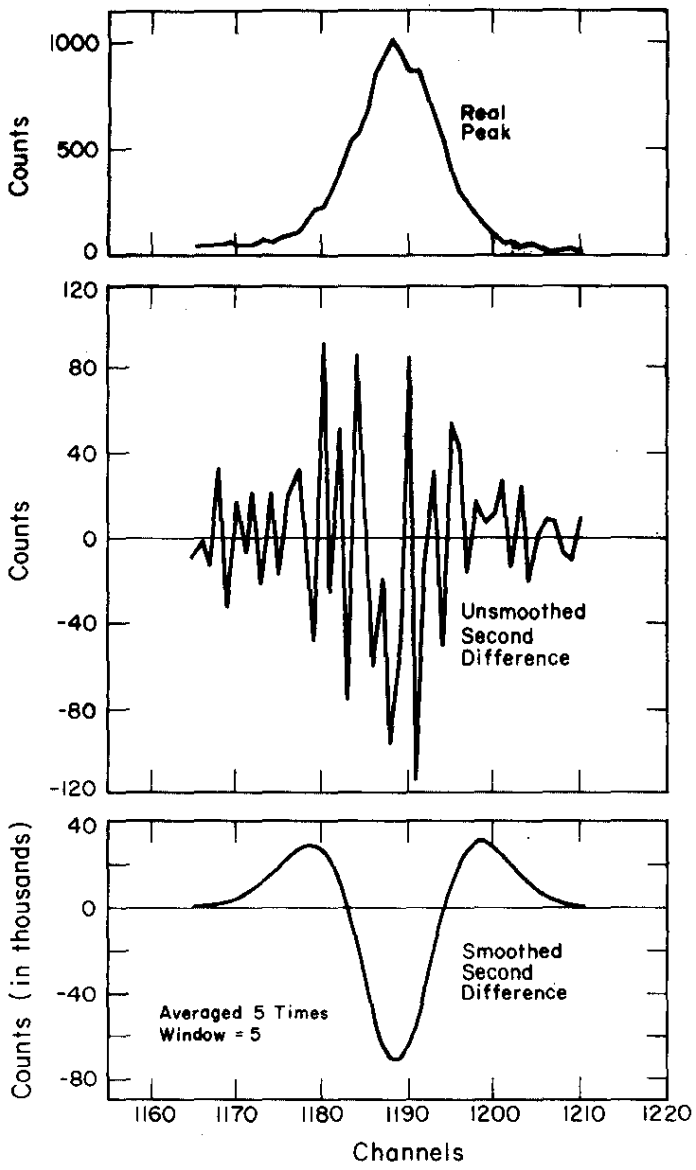

FIGURE 5. Second Differences for a Real Peak

The noiselike nature of this second difference curve, however, can be reduced by repetitive averaging of neighboring channels, as illustrated in Figure 6. Since only relative values are necessary to establish the shape of the curve, the averages are not normalized. The number of channels used in each average is called the window and is usually 3, 5, or 7. A window of 3 channels is very sensitive to narrow peaks, whereas a window of 7 channels is more sensitive to wider peaks. Mariscotti[4] has shown that peak search characteristics are optimum with a window equal to 0.6 FWHM and

								← Window →					
Second Difference	3	0	4	-3	6	5	-7	-1	4	-3	3	2	4
1st Average[a]		7	1	7	8	4	-3	-4	0	4	2	9	
2nd Average			15	16	19	9	-3	-7	0	6	15		
3rd Average				50	44	25	-1	-10	-1	21			
4th Average					119	68	14	-12	10				
5th Average						201	70	12					

a. Averages are not normalized.

FIGURE 6. Smoothing Second Difference by Averaging

five averaging steps. The smoothed second difference curve gives an excellent approximation to the second derivative, as shown in Figure 5.

The second difference followed by the averaging steps can be calculated from the spectral data in one orthogonal-polynomial type operation using the following equation if the weighting coefficients C_j are known:

$$S_i = C_o N_i + \sum_{j=1}^{j=last} C_j (N_{i-j} + N_{i+j})$$

C_j is a function of the window and the number of averaging steps, and N represents the number of counts in the subscripted channel. The subscript j has a minimum value of one for the summation, and a maximum value dependent upon the window and number of averaging steps. Weighting coefficients for five averaging steps with windows of 3, 5, 7, and 9 are given in Table IV. Since each term in the above equation is independent of the others, the standard deviation of the second difference, evaluated at channel i, is given by

$$F_i = \left\{ C_o^2 N_i + \sum_{j=1}^{j=last} C_j^2 (N_{i-j} + N_{i+j}) \right\}^{\frac{1}{2}}$$

TABLE IV

Weighting Coefficients for Calculating Smoothed Second Difference

	Weighting Coefficients C_j for Averaging 5 Times			
j	Window of 3	Window of 5	Window of 7	Window of 9
0	-12	-32	-62	-102
1	-9	-29	-59	-99
2	0	-20	-50	-90
3	+5	-5	-35	-75
4	+6	+6	-14	-54
5	+3	+13	+3	-27
6	+1	+16	+16	-4
7		+15	+25	+15
8		+10	+30	+30
9		+6	+31	+41
10		+3	+28	+48
11		+1	+21	+51
12			+15	+50
13			+10	+45
14			+6	+36
15			+3	+28
16			+1	+21
17				+15
18				+10
19				+6
20				+3
21				+1

For practical application in the computer program a simpler expression for the standard deviation of the second difference is used which requires the assumption that all values of N be replaced by N_i. The approximated value of the standard deviation is then

$$F_i \text{ approx} = \left\{ C_o^2 N_i + \sum_{j=1}^{j=last} C_j^2 (N_i + N_i) \right\}^{\frac{1}{2}}$$

$$= \left\{ \left(C_o^2 + 2 \sum_{j=1}^{j=last} C_j^2 \right) N_i \right\}^{\frac{1}{2}}$$

The term $(C_o^2 + 2 \sum C_j^2)$, evaluated for five averaging steps using windows of 3, 5, 7, and 9 has the values 448, 5220, 27342, and 95034, respectively. The approximate expression for F_i is very nearly equal to the correct value for small peaks on large backgrounds. For large peaks the approximate value exceeds the correct value, but the difference is small compared to the magnitude of the second difference at the peak center.

The peak finding portion of SPAN2 was written using a procedure similar to that of Mariscotti[4] because this procedure provides an excellent test of peak shape with a tolerance control, and because optimum smoothing parameters have been defined for this method.

This peak search begins by calculating the smoothed second difference and its standard deviation at each channel in the spectrum as shown in Figure 7. (Since data for neighboring channels are required in these calculations, S_i and F_i cannot be calculated for the 1 + 2.5(WINDOW - 1) channels at each end of the spectrum.) The data are evaluated and significant channels identified by comparing the second difference values with their standard deviations and with zero for each channel. A channel I1 is identified (Figure 7) each time the second difference becomes greater than its standard deviation; an I2, when it becomes less than its standard deviation; an I3, when it becomes less than zero; and an I5 when it becomes greater than zero. When a channel I5 is identified, all minimum values of the second difference between I3 and I5 are located, since each could possibly indicate a peak. The most negative minimum identifies the main peak and is called I4. In the case of two overlapping peaks, the second difference has two minima as shown in Figure 8.

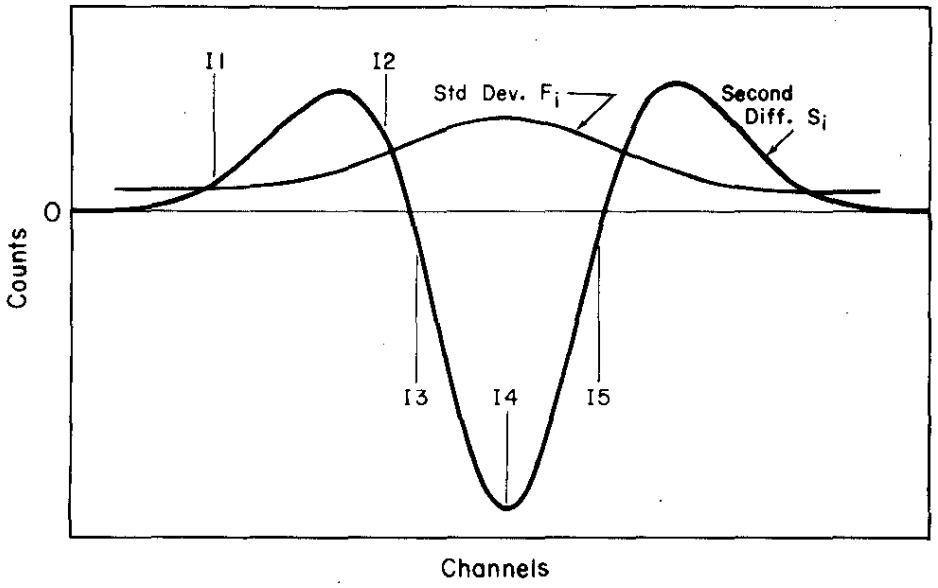

FIGURE 7. Smoothed Second Difference and Its Standard Deviation for a Single Peak

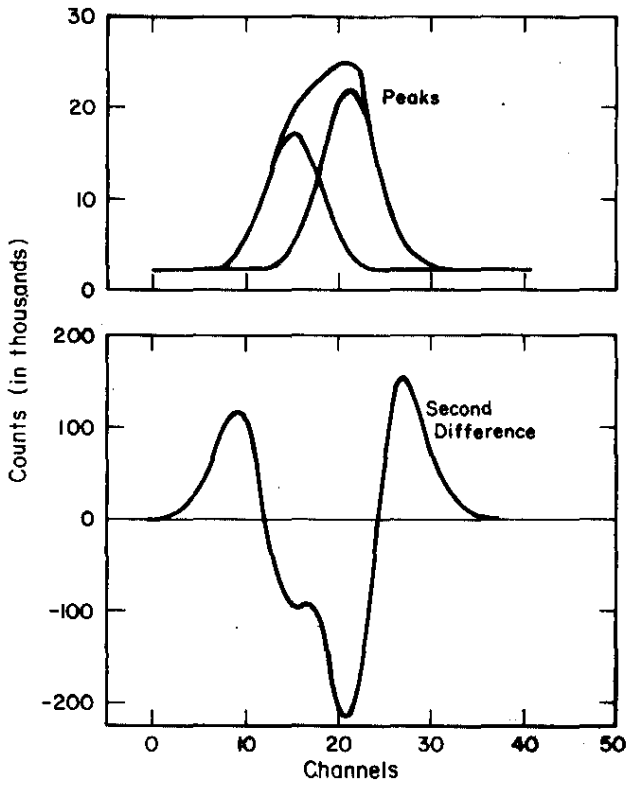

FIGURE 8. Second Difference Curve for Two Overlapping Gaussian Peaks

Five tests applied to the five significant channels for each main peak distinguish real peaks from Compton edges, statistical noise, etc. Test zero requires that channels I1-I5 be in numerically increasing order. Test one checks the significance of the second difference and requires that its absolute value be more than twice its standard deviation at channel I4. Test two defines acceptable peak widths and requires (I5-I3) to be within the range of 2 to 27 channels. Tests three and four require the number of channels between I1 and I2 and between I2 and I3 to be within a specified tolerance limit of those expected for a Gaussian peak of the same width. With the third and fourth tests, peaks can be distinguished from Compton edges because the left maximum is small or absent for an edge. The peak finding procedure can be made very selective by narrowing the acceptable range of test two and decreasing the tolerance limit.

The precise location of all single peaks is determined by fitting a Gaussian curve to the spectral data using the following technique. A Gaussian curve has the equation

$$Y = Ae^{B(X - \mu)^2}$$

where A is the height of the curve above background at the mean μ, and B is a constant dependent on the width of the Gaussian curve and equal to $(4 \ln.5)/FWHM^2$. Taking logarithms and rearranging gives the quadratic equation

$$\ln Y = [\ln A + B\mu^2] + X[-2B\mu] + X^2[B]$$

The expressions in the three brackets are numerically evaluated by performing a quadratic least squares fit of lnY and X, where Y represents the counts in channel X. By defining $R = [-2B\mu]$ and $S = [B]$, the mean for the Gaussian curve and, thus, the center for the peak are given by

$$\mu = \frac{-R}{2S}$$

The peak search subroutine SPAN2 is outlined in Figure 9. All input data are in common storage with either the calling program GELI2 or the BLOCK DATA. The window, tolerance, SEPFAC (the factor which determines acceptable peak separations) and, AFAC (the factor which determines the number of channels included in area summations) are defined in BLOCK DATA and can easily be changed. The window can assume only the values 3, 5, and 7 unless additional definitions of S_i and F_i for the new window values are included in SPAN2. The tolerance can assume any integer value. SEPFAC and AFAC should not be changed from their respective values of 2.0 and 1.5 without considering the indirect relationship between them.

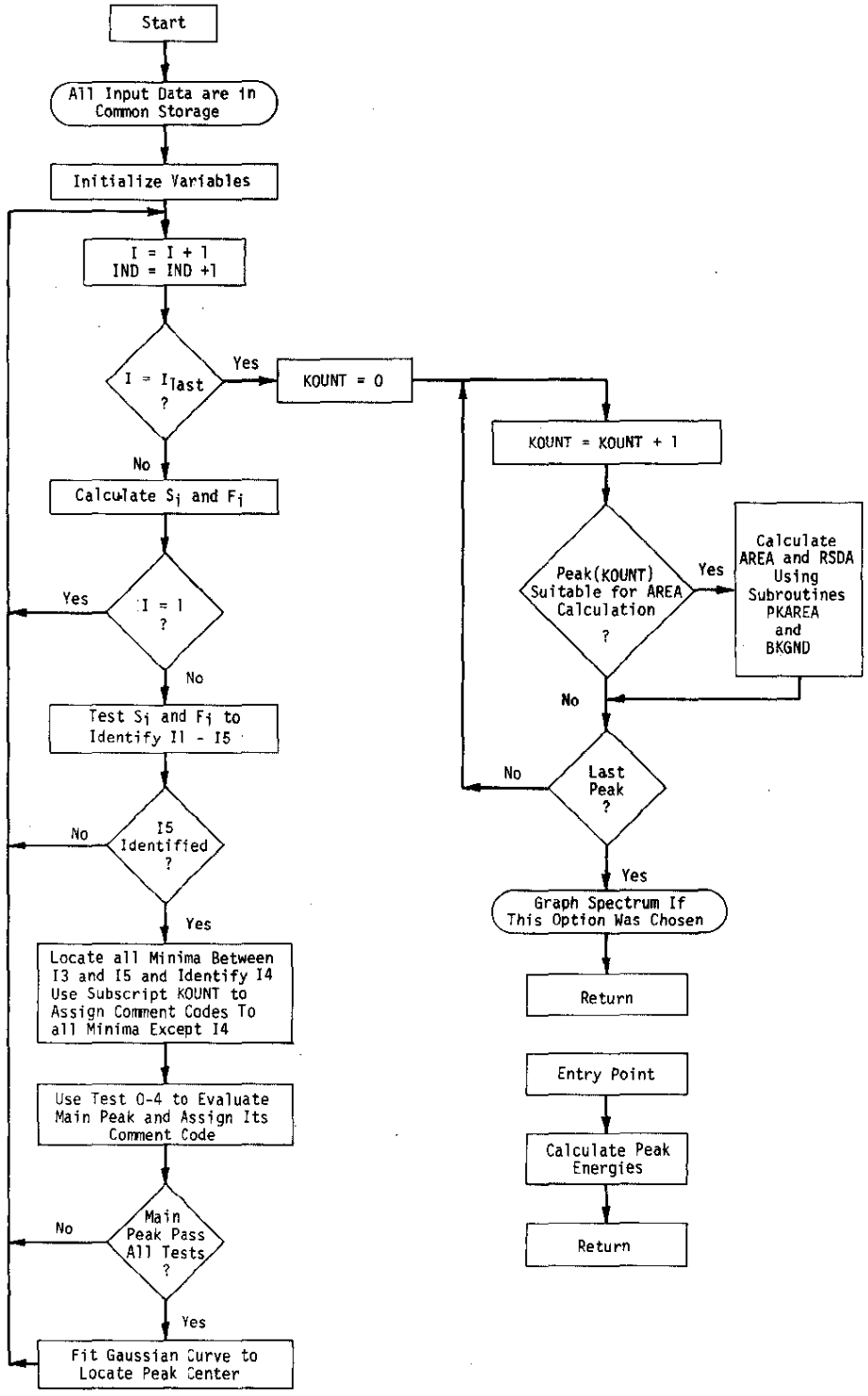

FIGURE 9. SPAN2 Flow Diagram

The variables must be properly initialized because of a dual indexing system used to conserve computer storage space. The storage location for the input spectrum TFN(I) is dimensioned 4096 so that this index correlates with channel numbers. The second difference and its standard deviation, however, each have storage locations dimensioned 300. A new index is established for these each time a new channel I1 is found such that the spectrum index (I) is related to the second difference index (IND) through I1 by the equation I = IND + I1 - 2.

After the values for the second difference and its standard deviation are calculated and channels I1 through I5 are obtained in numerically increasing order, tests zero through four are applied to the main peak at I4, and comment codes are assigned at all minima in the second difference between I3 and I5. If the curve passed all tests, the peak center is then determined for the main peak by fitting a Gaussian curve to the input data between channel MAXL, the maximum in the second difference between I2 and I3, and channel MAXR, the maximum in the second difference between I5 and (I5+I5-I3). Additional second difference data which are required to determine MAXR are calculated by temporarily setting the variable MORE equal to 1. After the peak center is calculated, the peak search is continued until the whole spectrum has been searched.

All information acquired by SPAN2 for future printout by subroutine EDIT is stored as the doubly subscripted variable PDATA in a location dimensioned 500,7. The first subscript (KOUNT) numbers all possible peaks consecutively as they are found, and the second subscript identifies the peak characteristic (peak channel, energy, etc.) which has been calculated. These data are used to evaluate peaks for area calculation by SPAN2.

Peak areas are calculated for all peaks having comment codes zero or 20 if they are sufficiently separated from other such peaks. Sufficient separation is defined by describing a region of (2*FWHM*SEPFAC) channels centered at each peak. If this region does not overlap with that of any other peak nor extend beyond either end of the spectrum, the net peak area is calculated as the sum of counts in each channel above background from channel (peak center - AFAC*FWHM) to (peak center + AFAC*FWHM) using subroutine PKAREA. FWHM is defined for each peak as FWHM = (I5-I3) $\sqrt{2 \ln 2}$. The background under the peak is described by a cubic equation fitted to the spectral data by subroutine BKGND, which is discussed later. The relative standard deviation of the net area is also calculated by PKAREA using the equation

$$RSDA = \frac{\sqrt{\text{Gross Area + Background Area}}}{\text{Gross Area - Background Area}}$$

After the last peak area is calculated and the spectrum is plotted, if this option was chosen, control goes to GELI2 and is returned to SPAN2 at ENTRY POINT for peak energy calculation at all possible peaks using the calibration equation from GELI2.

The accuracy of the area calculation was tested using synthetic data composed of various size Gaussian peaks on a quadratic background. Since the theoretical area of a Gaussian peak is given by

$$\text{THEORETICAL AREA} = A*\text{FWHM}*[\pi/4 \ln 2]^{\frac{1}{2}}$$

where A is the peak height above background, the percent difference between the calculated and theoretical areas was defined by

$$\% \text{ Diff} = \left[\frac{\text{CALC AREA} - \text{THEOR AREA}}{\text{THEOR AREA}}\right] 100$$

The data reported in Table V reflect the combined accuracy of the area calculation and the cubic background fit, and show a maximum error in the area measurements of less than 0.27% for the 12 peaks tested.

TABLE V

Accuracy of Area Calculation for Gaussian Peaks on Quadratic Background

	Percent Difference Between Calculated and Theoretical Areas[a]	
FWHM	Peak Height Above Background of 20000	Peak Height Above Background of 200
4	0.2644	0.2651
7	0.2618	0.2621
10	0.2392	0.2387
13	0.1906	0.1897
16	0.1130	0.0544
19	-0.0684	-0.0693

a. $\% \text{ Diff} = \left[\frac{\text{CALC AREA} - \text{THEOR AREA}}{\text{THEOR AREA}}\right] 100$;
Background = $110 - 0.16X - 0.00001X^2$,
where $1 \leq x \leq 500$.

An alternate PKAREA subroutine based on the method of Reber and Major,[7] in which the peak area summation was begun at the peak center channel, was written and subsequently rejected. One channel on each side of the peak was added successively, and the relative standard deviation of the area was calculated after each addition. The summation was terminated when the RSDA reached a minimum. For a Gaussian peak on a linear background, the following empirical equation derived by the author

$$\Delta E_{opt} = FWHM*EXP[-.1364\ ln\ R + .2608]$$

accurately predicts the number of channels, ΔE_{opt}, which must be summed to obtain a minimum RSDA. R is defined as the ratio of the background height to the net peak height evaluated at the mean. A simple calculation using this equation and a table of Gaussian areas show that for R greater than 0.16 the Reber-Major[7] method underestimates the area by at least 5%. The Reber-Major method of area calculation was, therefore, rejected.

Typical output of peak search data is shown in Figure 3. Comment codes are identified in Figure 10.

COMMENT CODE	EXPLANATION
0.0	SINGLE PEAK WHICH PASSED ALL TESTS.
1.0	SINGLE PEAK WHICH PASSED ALL TESTS BUT GAVE A POSITIVE B(2) IN LEAST SQUARES FIT TO LOCATE CENTER OF PEAK.
20.0	THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS. THIS MAIN PEAK PASSED ALL TESTS.
20.AAAA	THIS PEAK OVERLAPS WITH THE PEAK AT CHANNEL AAAA WHERE AAAA PASSED ALL TESTS.
21.0	THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS AND PASSED ALL TESTS BUT GAVE POSITIVE B(2) IN LEAST SQUARES.
48.CCCC	THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS. THIS PEAK FAILED TO PASS TEST 8.
50.CCCC	THIS PEAK OVERLAPS WITH THE PEAK AT CHANNEL CCCC WHERE CCCC FAILED TO PASS ALL TESTS.
60.0000	THIS SINGLE PEAK FAILED TO PASS TEST D.
80.0000	THE MAXIMUM DIMENSION OF VARIABLES S AND F WAS EXCEEDED BEFORE A NEW VALUE OF I1 WAS FOUND. ALL MINIMA IN THE SECOND DIFFERENCE OCCURRING BETWEEN I5 AND THE MAXIMUM DIMENSION ARE GIVEN COMMENT CODE 80.0000.
81.0000	NO MINIMUM WAS FOUND IN THE SECOND DIFFERENCE CURVE BETWEEN I3 AND I5.

FIGURE 10. Explanation of Comment Codes

BKGND

Subroutine BKGND and CALCIT fit cubic equation backgrounds to peak data for both GELI2 and SPAN2. The calling program defines two background regions each M channels wide centered at channels IXL and IXR as shown in Figure 11. M is an odd integer approximately equal to the FWHM and presently limited to the range 5 through 25. Channels IXL and IXR are defined as integer values by

$$IXL = \text{Peak Center} - SEPFAC*FWHM + .5$$

$$IXR = \text{Peak Center} + SEPFAC*FWHM + .5$$

The spectrum TFN, M, IXL, IXR, AND ICA, a print control variable, are input to BKGND from common storage.

Slopes and their standard errors,[8] which are determined by subroutine CALCIT for the three linear regression lines fitted individually and jointly to the two background regions, are evaluated by BKGND. If the slopes of the lines through the two background regions are statistically the same as the slope of the line through both regions, the linear equation through both background regions is used as the background equation. If one or both slopes are statistically different from that of the line through both regions, a cubic equation is fitted to the data such that at IXL and IXR this line has the same magnitudes (PL and PR) and slopes (QL and QR) as the two individual regression lines. The background in counts is given as a function of channel number I by rearrangement of Quittners equation[9] as

$$\text{Background} = I^3[TM3] + I^2[TM2] + I[TM1] + [TM0]$$

where

$$[TM3] = [(QL + QR)(IXR-IXL) + 2(PL-PR)]/(IXR-IXL)^3$$

$$[TM2] = -3IXL[TM3] + [3(PR-PL) - (QR+2QL)(IXR-IXL)]/(IXR-IXL)^2$$

$$[TM1] = QL-2IXL[TM2] - 3IXL^2[TM3]$$

$$[TM0] = PL-IXL[QL] + IXL^2[TM2] + 2IXL^3[TM3]$$

The background equation coefficients are transferred via common storage for use by the calling program. This method usually fits a cubic equation if the counting statistics are good, but gives a linear fit if the statistics are poor.

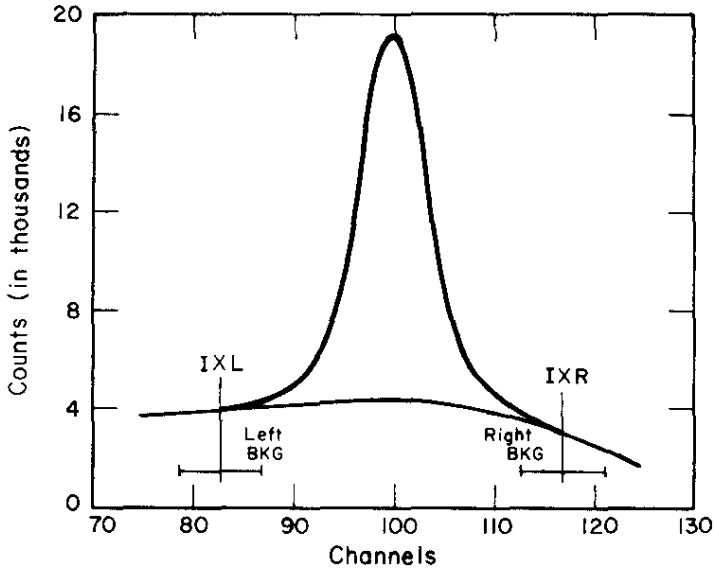

FIGURE 11. Cubic Background Fitting

The background routine was originally written without the statistical slope evaluation, and consequently a cubic equation was fitted to the data even when slopes were very uncertain. The background equations were often grossly in error if counting statistics were poor. The statistical slope evaluation incorporated in the present method greatly improves Quittner's background method and has completely eliminated this former problem, since it requires that a linear fit be used unless a higher order equation is statistically justified.

Excellent backgrounds are obtained using the statistical evaluation method (Figure 11) if no peaks interfere with the background on either side of the peak. However, if interferences are present, the slope of the interfered background, and consequently the background equation, may be in error. Although this problem should not occur for backgrounds obtained for SPAN2, the user should be aware of the possibility for GELI2 results.

USE OF PROGRAM

Tapes

Both binary and binary coded decimal (BCD) tapes are used at Savannah River to input spectra to the GELI2 program. Binary tapes are prepared using a Potter Instruments Co. Model M906II-1 Tape Transport System, and BCD tapes are prepared using a Nuclear Data, Inc., Series 2200 System Analyzer, and a Kennedy Model 1400R Tape Transport System. Both systems use 0.5-in. seven-level magnetic tapes. The Kennedy system uses a word length of 36 bits in six bit frames, even parity in the seventh level, and a packing density of 200 bits per inch. The Potter system uses a word length of 18 bits in six bit frames, odd parity in the seventh level, and a packing density of 556 bits per inch. Tagword lengths for the Kennedy and Potter systems are 36 bits (written twice before each record) and 18 bits (written once before each record), respectively.

Tape formats are as follows. The brackets enclose the format which is repeated for each spectrum.

Kennedy (BCD)	Potter (Binary)
• Reflector Spot	• Reflector Spot
• File Gap	• File Gap
• File Mark	• File Mark
[• Interrecord Gap	[• Interrecord Gap
• Tagword	• Tagword
• Tagword	
• Data for Channels 1-4096	• Data for Channels 1-4096]
• Interrecord Gap	• Interrecord Gap
• File Mark]	• File Mark
• File Mark	
• File Mark	• File Mark

Kennedy and Potter transport tapes are read in GELI2 by subroutine LFZR (I,TFN,J) and READ (I,TFN,J), respectively, as indicated by the tape option variable ICD. Binary and BCD tapes require slightly different job control language (JCL) cards. JCL cards will be discussed later. The tape number is identified in the JCL cards.

Card Arrangement for Submitting Program

The arrangement of cards for submitting data for computer calculation using GELI2 is outlined below. Cards are read in order from A through G.

A - JCL cards

B - Program (GELI2 and all subroutines)

C - JCL cards

D - Nuclide input data

E - 'ENDIT' card

F - Sample input data

G - Final card

Each section of this outline is discussed.

A - JCL Cards

JCL cards provide the computer with instructions on how to handle the program and/or data and depend on the techniques employed by the computer group. The author uses the following JCL cards at the beginning of a program:

```
//RVS13753 JOB (3753,L044,002,04,0000,,,,8477-1Y,L5365-01,T,01),          C
//              ' R V SLATES          ',MSGLEVEL=1
//STEP1 EXEC FORTHCLG,GTIME=6,GOSIZE=220K
//FORT.SYSIN DD *
```

B - Program

This section is composed of GELI2 and all subroutines.

C - JCL Cards

These JCL cards, which provide instructions to the computer and identify the tape number, depend on the techniques employed by the computer group and also on the tape transport. The JCL cards used by the author are as follows:

Kennedy Tape Transport (BCD)

```
/*
//GO.FT40F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT41F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT42F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT43F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT44F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.TAPE DD DSNAME=X,DISP=(OLD,KEEP),LABEL=(,NL),UNIT=TAPE27,
// DCB=(RECFM=U,BLKSIZE=24588,DEN=0,TRTCH=ET,BUFNO=1),
// VOLUME=SER=NA1018
//GO.SYSIN DD *
```

Potter Tape Transport (Binary)

```
/*
//GO.FT40F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT41F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT42F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT43F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.FT44F001 DD UNIT=SYSDA,DISP=(,PASS),SPACE=(68,100)
//GO.TAPE DD DUMMY
//GO.BINTAPE DD DSNAME=SAMPLE,LABEL=(,NL),UNIT=TAPE27,                  M
// DISP=(OLD,KEEP),DCB=DEN=0,VOLUME=SER=NA0018
//GO.SYSIN DD *
```

D - Nuclide Input Data

This section lists the nuclides for analysis and defines various constants for each. These data are arranged into sets, each containing information for up to 100 nuclides. Nuclides are then selected for analysis by identifying the set for each spectrum on card 1 of the sample input data. A maximum of five nuclide sets are permitted by the DEFINE FILE statements.

Two cards are required for each nuclide. The formats and identification of variables follow.

Nuclide Data Card 1	Format (A5,E14.7,F10.1,F10.2,4E10.3,A1)
Col. 1-5	SYM - Symbol identifying nuclide
Col. 6-19	HL - Nuclide half life in days
Col. 20-29	ENG - Peak energies in keV
Col. 30-39	XIN - (Peak intensity in photons per disintegration)*100
Col. 40-49	EFF(1) - Efficiency (1) in counts per photon
Col. 50-59	EFF(2) - Efficiency (2)
Col. 60-69	EFF(3) - Efficiency (3)
Col. 70-79	EFF(4) - Efficiency (4)
Col. 80	SYMBOL - This variable, which was used in Priest's original program,[5] is no longer used and should be left blank

Nuclide Data Card 2	Format (I1,F8.3,F10.2,2E11.4,I3,35X,I1)
Col. 1	BOP - This variable, which was used in Priest's original program,[5] is no longer used and should be left blank
Col. 2-9	XSECT - Nuclide cross section in barns
Col. 10-19	ABISO - (Ratio of isotope abundance)*100
Col. 20-30	ELMASS - Mass in mg of element irradiated
Col. 31-41	CPMMG - Nuclide specific activity in dpm/mg
Col. 42-44	WTMOL - Molecular weight in g/mole of element irradiated
Col. 45-79	- Not used, should be left blank
Col. 80	ND - This variable indicates the end of the nuclide set for GELI2. It must be 1 for the last nuclide of each set and left blank for all other nuclides.

Nuclide data card pairs are arranged one after another for each set. Each set, including the last set, must be followed by one blank card to indicate the end of the data set in subroutine READIT.

E - ENDIT Card

One card with ENDIT punched in the first five columns must be inserted between the nuclide data and the sample data.

F - Sample Input Data

Sample input data to GELI2 require 1, 3, or 5 cards per sample, depending on the values selected for the calibration option and the input option. The input cards required for the chosen options will be readily apparent from Figure 12, which shows a simplified flow diagram for reading input.

The first sample of every set must be used to establish the relationship between channel numbers and energies. Thus, ICALIB must be 1 or 2 for the first sample, and this requires that channel numbers or estimates be supplied on cards 4 and 5. After the channel-energy calibration, subsequent samples of the set may use the same calibration equation by setting ICALC equal to zero. GELI2 is dimensioned to accept up to 25 pairs of channel-energy data for the calibration. If energies are not supplied on cards 2 and 3 for the calibration, the four default energies are used. The five data cards will now be described in detail, using an asterisk (*) to indicate values which will not default to a usable number.

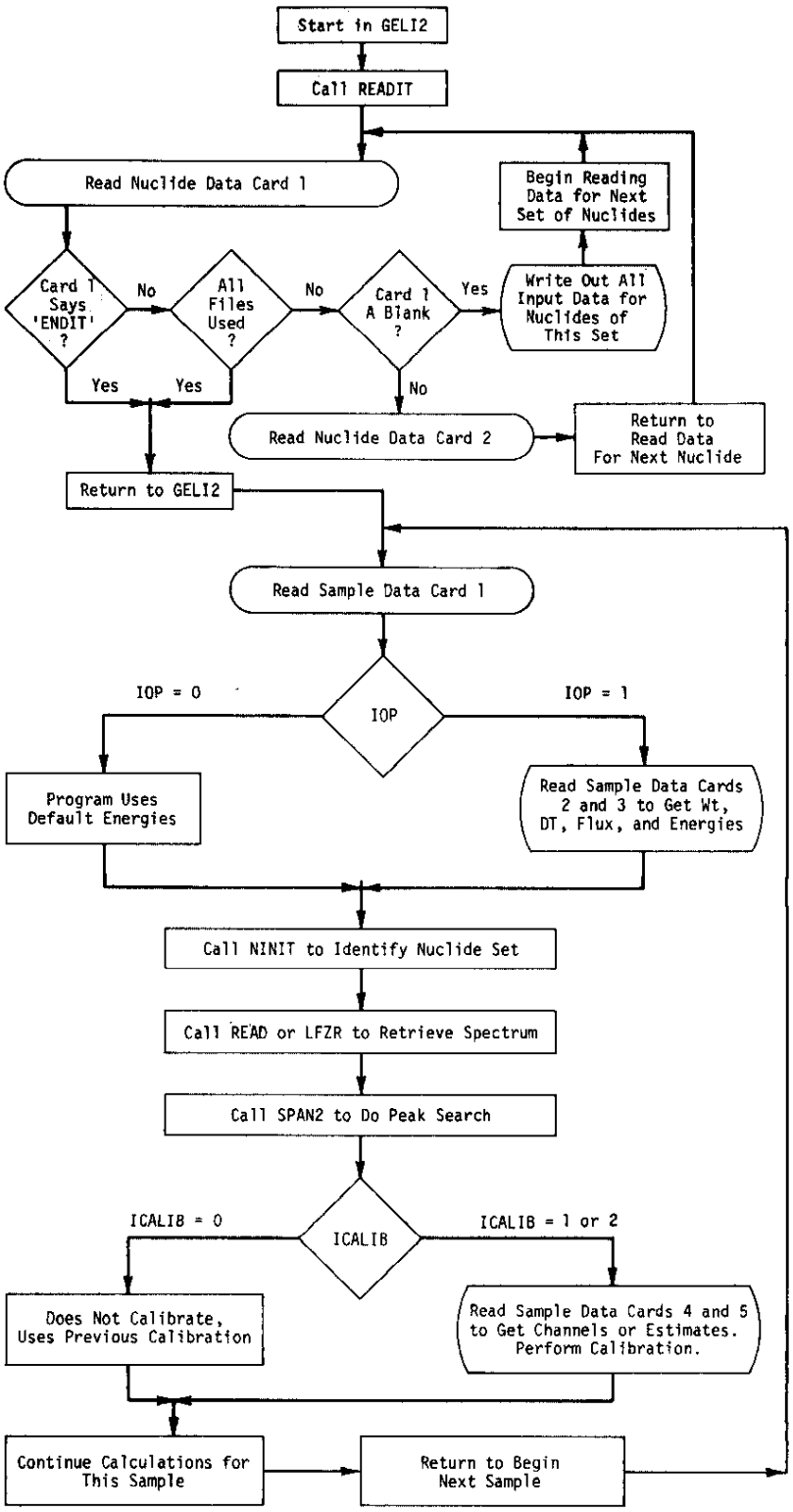

FIGURE 12. GELI2 Flow Diagram for Reading Input

Card 1 Format (I3,13A4,E9.0,F5.0,2I1,I2,4I1,F3.0)

Col. 1-3* FILE - the sequential integer location of the spectrum on the tape

Col. 4-55 SAMPL - Hollerith information describing the particular sample being considered

Col. 56-64 DIL - the sample dilution factor. Defaults to 1.0

Col. 65-69 CT - counting time in minutes; defaults to 16.66 min

Col. 70 IEFF - specifies detection efficiency (function of detector and geometry); defaults to 1.0

Col. 71 ICD - tape transport indicator

0 - Kennedy - BCD

1 - Potter - Binary; defaults to 0

Col. 72-73* IDF - Nuclide set

40 - Eu, Ce, Am, Cm, Tb, Ho, Er, Tm, Lu, Yb

41 - Rh, Cs, Ce, Pr, Eu, Zr, Nb, Am, Ru

42 - Cm, Tb

43 - Cr, Sc, Fe, Co

44 - Co, Po, Bi, Zn, Sb

Col. 74 ICALIB - calibration option

0 - uses previous calibration (not used for first sample)

1 - uses given or default energies and input channels for calibration

2 - uses given or default energies and finds exact channels from channel estimates using SPAN2 and LOCATE

Calibration option defaults to 0

Col. 75 ICALC - calculation option

1 - calculates nuclide concentration in dpm

2 - calculates ppm from dpm/mg and sample weight

3 - calculates ppm from integrated flux, cross section and sample weight

4 - calculates integrated flux from cross section, sample weight, isotope abundance, and molecular weight

Defaults to 1

Col. 76 IOP - Input option

0 - uses default energies - 74.7 keV - ^{243}Am
661.6 keV - ^{137}Cs
1173.2 keV - ^{60}Co
1332.5 keV - ^{60}Co

1 - enables user to input energies, etc. on cards 2 and 3

Col. 77 ICA - peak search print control option

0 - does not edit peak search results

1 - edits only single and overlapping peaks

2 - edits same as 1 plus all test failures

3 - edits same as 2 plus channel-by-channel details of search

4 - edits same as 3 plus graph of spectrum

Col. 78-80 FWHM - full width at half maximum to be used in GELI2 peak integration

Defaults to 7.0

Card 2 Format (2F5.0,E10.4,I5)

Col. 1-5 WT - sample weight, mg

6-10 DT - decay time, min

11-20 FLUX - integrated flux, neutron/cm^2

21-25 NET - number of energies on the next card

Card 3 Format (6F10.0)

Col. 1-10 E - the energies in keV to be used for calibration

11-20

21-30

31-40

41-50

51-60

Card 4 Format (I3)

Col. 1-3	NTOT -	the number of channels used to calibrate

Card 5 Format (6F10.0)

Col. 1-10	C -	the channels or channel estimates used to calibrate
11-20		
21-30		
31-40		
41-50		
51-60		

Sample data sets are arranged consecutively, one after another, for calculation of multiple spectra tapes.

G - Final Card

One card with /* punched in the first two columns must follow the sample data to indicate the end of cards for the job.

Computer time required for all calculations excluding the graphing option is about 15 seconds per spectrum. About 425 lines are printed per spectrum using print option ICA = 2. The appendix shows specific examples to illustrate proper form and arrangement for sample input data cards.

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APPENDIX

EXAMPLES OF CORRECT FORM AND ARRANGEMENT OF SAMPLE DATA

Correct form and arrangement of sample data cards are shown in Figure 13 for four spectra recorded using the Kennedy (BCD) tape transport system. The order in which cards are read is apparent from Figure 12. The first spectrum illustrates use of the calibration option which requires data cards 4 and 5. This spectrum of a multiple source containing ^{243}Am, ^{137}Cs, and ^{60}Co has peaks at 74.7, 661.6, 1173.2, and 1332.5 keV which are suitable for channel-energy calibration. The multiple source was counted for 25 min, and the FWHM for peaks in the first 1000 channels was estimated to be 8.5 channels. The first card identifies File 1 (col. 1-3) as the multiple source by the sample identification in columns 4-55. The dilution factor DIL (col. 56-64) is left blank causing it to default to 1.0, and counting time CT (col. 65-69) is given as 25 min. IEFF (col. 70) is left blank causing it by default to use efficiency number one from the nuclide data. The tape transport indicator ICD (col. 71) is given as zero or left blank indicating a Kennedy transport tape. The nuclides of data set 40 are designated for analysis by setting IDF (col. 72-73) equal to 40. The calibration option ICALIB (col. 74) is chosen as 2 which causes the computer to accurately locate the calibration peaks before calibration. The calculation option ICALC (col. 75) is left blank causing default to 1 which specifies that nuclide concentration in dpm be calculated. Input option IOP (col. 76) is given as zero or left blank because peak energies of the multiple source are identical to the default energies. If other energies are used, both energies and channels must be input on cards 2-5. The peak search print control option ICA (col. 77) is chosen as 1 to print only confirmed or possible peaks. The estimated FWHM of 8.5 channels is punched in column 80.

Sample data cards 2 and 3 will not be read for File 1 because IOP specifies that the default energies be used to calibrate. Sample data cards 4 and 5, however, will be required because ICALIB = 2 was chosen. Card 4 contains only a 4 in column 3 indicating that channel numbers for four peaks will be supplied on card 5. Card 5 lists the four channel estimates corresponding to the default energies.

Use of the previous calibration equation is illustrated for the second spectrum by selecting ICALIB equal zero or blank. For this spectrum, the dilution factor is 1.00E 04, counting time is changed to 15 min, and efficiency number 2 is specified in column 70.

The third spectrum illustrates the use of data cards 2 and 3. Since ICALC = 2, the analysis results will be reported in ppm, which requires that the sample weight be input on card 2. IOP must equal 1 if cards 2 and 3 are to be read. The sample weight (237.4 mg) is therefore punched in columns 1-5 of card 2. DT and FLUX are not required in the calculation, so they have been omitted. Since ICALIB equals zero, no calibration will be performed, and it is not necessary to supply energies. Card 3 in this case becomes a blank card and NET on card 2 is either blank or zero.

The fourth spectrum will be analyzed for the nuclides of set 42, and a graph of the spectrum will be printed out because ICA equals 4. The estimate of FWHM by default is 7.0 for this spectrum.

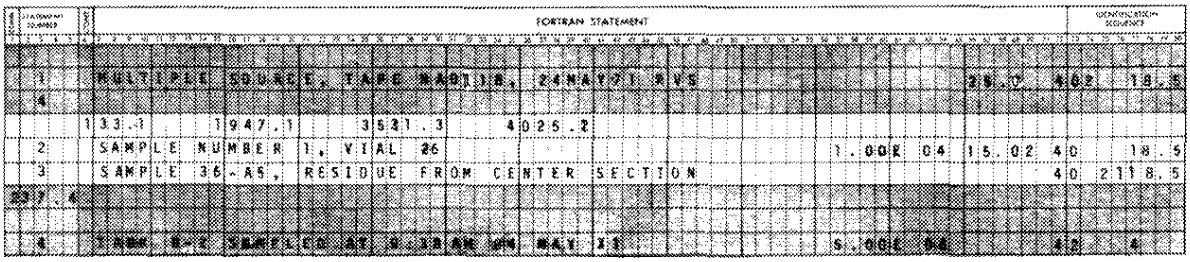

FIGURE 13. Examples of Correct Form and Arrangement of Sample Data

Separability

APPENDIX II

LISTING OF PROGRAM

```
      C     GELI2:  THIS PROGRAM CALCULATES NUCLIDE ABUNDANCES FROM GAMMA-RAY
      C     SPECTRA AND CALLS SPAN2 WHICH DOES A PEAK SEARCH ON THE DATA.
N 0002      COMMON /ARRAY/ TFN
N 0003      COMMON /BAG/ M
N 0004      COMMON /CHANEL/ C
N 0005      COMMON /DATA/ CDEL
N 0006      COMMON /ENERGY/ AA,BB
N 0007      COMMON /HELL/ IXL,IXR
N 0008      COMMON /HOME/ TM3,TM2,TM1,TM0
N 0009      COMMON /IMIT/ NT6,NT5,IP,KOUNT,WT,DT,FLUX,ID,ICALIB,ICALC,E
N 0010      COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0011      COMMON /INTERF/ NC,NI,IPT,F
N 0012      COMMON /PEDIT/ PDATA
N 0013      COMMON /SHELF/ WIND,ITCLER,SEPFAC,AFAC
N 0014      REAL *8 A,B,C(25),E(25),T,W,AA,BB,SYM,TCH,STAT,VARB
N 0015      BB = 1.0
N 0016      REAL *8 TM3,TM2,TM1,TM0
N 0017      REAL *8 DETL1/' NOT DET'/
N 0018      REAL *8 DETL2/'  QUAL  '/
N 0019      REAL *8 DETL3/'  QUAN  '/
N 0020      REAL *8 SPACES
N 0021      REAL *4 PDATA(500,7)
N 0022      REAL *4 PEAKS(30)
N 0023      REAL *4 CDIF(5),F(5,5)
N 0024      REAL *4 MASSI
N 0025      REAL *4 CDEL(5)
N 0026      INTEGER *4 FILE,CHN,WTMCL,BOP
N 0027      INTEGER *4 NFLAG(5),NI(5),IPT(5,5)
N 0028      DIMENSION B(1),STAT(3),W(25),VARB(1),T(1),EFF(4),SAMPL(15),TFN(409
           16)
N 0029      DEFINE FILE 40(100,68,L,IP),41(100,68,L,IP),42(100,68,L,IP),43(100
           1,68,L,IP),44(100,68,L,IP)
N 0030      CALL ERRSET(253,256,-1,0)
N 0031      CALL ERRSET(251,256,-1,0)
N 0032      CALL ERRSET(207,256,-1,0)
N 0033      CALL ERRSET(209,256,-1,0)
N 0034      CALL ERRSET(218,256,-1,0)
N 0035      CALL READIT
N 0036      NTOT=4
N 0037  100 CONTINUE
      C     BEGIN READING SAMPLE DATA INPUT.
N 0038      READ (NT5,550,END=480) FILE,(SAMPL(I),I=1,13),DIL,CT,IEFF,ICO,IDF,
           1ICALIB,ICALC,IOP,ICA,FWHMT
N 0039      IDIS=0
N 0040      IF (FWHMT.EQ.0.0) FWHMT=7.0
N 0042      IF (IOP.EQ.1.OR.IOP.EQ.2) READ (NT5,540) WT,DT,FLUX,NET,(E(I),I=1,
           1NET)
N 0044      IF (ICALC.EQ.0) ICALC=1
N 0046      IF (IEFF.EQ.0) IEFF=1
N 0048      IF (DIL.EQ.0.0) DIL=1.0
N 0050      IF (CT.EQ.0.0) CT=16.66
N 0052      IF (IDF.NE.0) IDF1=IDF
      C     SUBROUTINE NINIT SUPPLIES INTERFERENCE INFORMATION.
N 0054      CALL NINIT(IDF1)
      C     RETRIEVE SPECTRUM FROM TAPE.
N 0055      J=0
```

```
0056      110   IF (ICD.EQ.0) CALL LFZR(I,TFN,J)
0058            IF (ICD.EQ.1) CALL READ(I,TFN,J)
0060            IF (J.EQ.0.AND.ICD.EQ.0) CALL LFZR(I,TFN,J)
0062            IF (J.EQ.0.AND.ICD.EQ.0) CALL LFZR(I,TFN,J)
0064            IF (J.EQ.0.AND.ICD.EQ.0) CALL LFZR(I,TFN,J)
0066            IF (J.EQ.0.AND.ICD.EQ.0) CALL LFZR(I,TFN,J)
0068            IF (J.EQ.0.AND.ICD.EQ.0) CALL LFZR(I,TFN,J)
0070            IF (J.EQ.0.AND.ICD.EQ.1) CALL READ(I,TFN,J)
0072            IF (J.EQ.0.AND.ICD.EQ.1) CALL READ(I,TFN,J)
0074            IF (J.EQ.0) GO TO 120
0076            KOUNT=KOUNT+1
0077            J=0
0078            IF (FILE.EQ.0.OR.KOUNT.EQ.FILE) GO TO 130
0080            GO TO 110
0081      120   WRITE (NT6,520)
0082            WRITE (NT6,550) (SAMPL(IA),IA=1,13)
0083            WRITE (NT6,560)
          C     THIS RETURN CARD STOPS ALL CALCULATIONS IF THREE FILE MARKS OCCUR.
0084            RETURN
0085      130   IF (FILE.NE.0) ID=I
0087            IF (FILE.EQ.0.AND.ID.NE.I) GO TO 110
0089            IF (FILE.EQ.0) FILE=KOUNT
0091            ID=I
0092            CALL SPAN2
0093            WRITE (NT6,520)
0094            WRITE (NT6,550) (SAMPL(I),I=1,13)
0095            WRITE (NT6,570) WT,DIL,CT,DT
0096            WRITE (NT6,580) FLUX,ID,FILE,IEFF,ICALIB,ICALC
0097            IF (ICALIB.EQ.0) GO TO 140
          C     BEGIN CALIBRATION OPTION.
0099            READ (NT5,590,END=460) NTOT,(C(I),I=1,NTOT)
0100            IF (ICALIB.EQ.2) CALL LOCATE
0102      140   IP=1
0103            CALL CLEAR(NFLAG,5)
0104      150   FWHM=FWHMT
0105            READ (IDF1'IP) SYM,HL,ENG,XIN,EFF(1),EFF(2),EFF(3),EFF(4),SYMBOL,B
               1OP,XSECT,ABISO,ELMASS,CPMMG,WTMOL,ND
0106            FLAG=0.0
0107            IF (IP.GT.2) GO TO 180
0109            IF (ICALIB.EQ.0) GO TO 170
          C     CORRECT FOR NON-LINEARITY.
0111            DO 160 L=1,NTOT
0112      160   C(L)=C(L)-(CDEL(1)+C(L)*(CDEL(2)+C(L)*(CDEL(3)+C(L)*(CDEL(4)+C(L)*
               1CDEL(5))))
0113            CALL CLEAR(W,50)
0114            A=1.000
0115            MM=1
0116            MPL=0
          C     PERFORM LINEAR FIT FOR SAMPLE CALIBRATION.
0117            CALL LSTSQR(E,C,W,NTOT,MM,A,B,MPL,STAT,VARB,T,25)
0118            BB=B(1)
0119            AA=A
0120            WRITE (NT6,600) AA,B(1)
0121            WRITE (NT6,610) (E(I),C(I),I=1,NTOT)
0122      170   WRITE (6,630)
0123            WRITE (6,640)
```

```
 0124            IF (ICALC.EQ.1) WRITE (6,650)
 0126            IF (ICALC.EQ.2.OR.ICALC.EQ.3) WRITE (6,660)
 0128            IF (ICALC.EQ.4) WRITE (6,670)
 0130            WRITE (6,620)
 0131     180    TCH=AA+B(1)*ENG
                 C      RECORRECT FOR NON-LINEARITY.
 0132            TCH=TCH+(CDEL(1)+TCH*(CDEL(2)+TCH*(CDEL(3)+TCH*(CDEL(4)+TCH*CDEL(5
                1)))))
                 C      BEGIN AREA CALCULATION.
 0133            CHN=TCH+.5
 0134            FWHM=FWHM+TCH/1000.
                 C      DETERMINE M, THE NUMBER OF POINTS IN EACH BACKGROUND REGION.
 0135            M=FWHM+.5
 0136            IF (MOD(M,2).EQ.0.0) M=M-1
 0138            IXL=TCH-SEPFAC*FWHM+.5
 0139            IF ((TCH-SEPFAC*FWHM+1-(M/2.)).LT.1.0) GO TO 190
 0141            IXR=TCH+SEPFAC*FWHM+.5
 0142            IF ((TCH+SEPFAC*FWHM+1+(M/2.)).GE.4097.) GO TO 190
 0144            GO TO 200
 0145     190    WRITE (6,490) SYM
 0146            GO TO 470
                 C      CHANGE ICA TEMPORARILY DURING BKGND ROUTINE TO PREVENT PRINT OUT.
 0147     200    ICATEM=ICA
 0148            ICA=2
 0149            CALL BKGND
 0150            ICA=ICATEM
                 C      DETERMINE LOWER AND UPPER CHANNELS (LAL AND LAR) FOR AREA CALC'N.
 0151            LAL=TCH-AFAC*FWHM+.5
 0152            LAR=TCH+AFAC*FWHM+.5
 0153            SUM=0.0
 0154            BGSUM=0.0
 0155            DO 210 IC=LAL,LAR
 0156            SUM=SUM+TFN(IC)
 0157            BKINC=TM0+IC*(TM1+IC*(TM2+IC*TM3))
 0158            IF (BKINC.LE.0.0) BKINC=0.0
 0160     210    BGSUM=BGSUM+BKINC
 0161            DIFF=SUM-BGSUM
 0162            IF (DIFF.LE.0.0) DIFF=0.0
                 C      WHEN WE COME OUT OF THIS DO LOOP WE HAVE DETERMINED THE TOTAL AREA
                 C      OF THE PEAK (SUM) AND THE BACKGROUND AREA (BGSUM), AND HAVE
                 C      DEFINED THE NET PEAK AREA AS DIFF.  WE MUST NOW MAKE ANY NECESSARY
                 C      CORRECTIONS FOR NUCLIDE INTERFERENCES.
                 C      BEGIN NUCLIDE INTERFERENCE CALCULATION.
 0164            K=1
 0165            DO 220 N=1,NC
 0166            IF (IPT(K,N).EQ.IP-1) CDIF(N)=DIFF
 0168     220    IF (IPT(K,N).EQ.IP-1) NFLAG(N)=1
 0170            DO 240 N=1,NC
 0171            IF (NFLAG(N).EQ.0) GO TO 240
 0173            NIK=NI(N)
 0174            DO 230 K=2,NIK
 0175     230    IF (IPT(K,N).EQ.IP-1) DIFF=DIFF-CDIF(N)*F(K,N)
 0177     240    CONTINUE
 0178            IF (DIFF.LE.0.0) DIFF=0.0
                 C      AT THIS POINT, DIFF IS THE NET PEAK AREA AFTER ANY CORRECTIONS
                 C      FOR NUCLIDE INTERFERENCES HAVE BEEN MADE.  NOW REDEFINE BGSUM TO
```

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      C     INCLUDE ANY INTERFERENCES.
0180        BGSUM=SUM-DIFF
      C     NOW WE SHALL DETERMINE DETECTION LEVELS AND CALCULATE CONFIDENCE
      C     LIMITS.  NOTE THAT FOR THESE STATISTICAL CALCULATIONS, INTERFER-
      C     ENCES ARE CONSIDERED SIMPLY AS PART OF THE BACKGROUND, AND THUS
      C     THE STD DEVIATION OF THE NET PEAK AREA (SIGMA) IS DEFINED AS:
0181        SIGMA=SQRT(SUM+BGSUM)
      C     DETERMINE THE DETECTION LEVEL AND CALCULATE CONFIDENCE LIMITS ON
      C     THE INTEGRATED AREA DATA USING THE WORKING EXPRESSIONS OF TABLE II
      C     FOR PAIRED OBSERVATIONS IN L.A.CURRIE'S PAPER,ANAL CHEM, VOL 40,
      C     NO. 3, PAGE 586.
0182        $LC=2.33*(SQRT(BGSUM))
0183        $LQ=5..*(1.+(SQRT(1.+(BGSUM/12.5))))
0184        IF (DIFF.GT.$LC) GO TO 250
0186        SPACES=DETL1
      C     DETERMINE THE ONE-SIDED CONFIDENCE LIMIT.
0187        CONLIM=1.645*SIGMA
0188        GO TO 280
0189  250   IF (DIFF.GT.$LQ) GO TO 260
0191        SPACES=DETL2
0192        GO TO 270
0193  260   SPACES=DETL3
      C     DETERMINE TWO-SIDED CONFIDENCE LIMITS.
0194  270   CONLIM=1.96*SIGMA
0195        GO TO 280
0196  280   CONTINUE
      C     CHECK PEAK SEARCH DATA FOR PEAKS WHICH MAY INTERFERE.
0197        IBOT=TCH-2.0*SEPFAC*FWHM+.5
0198        IF (IBOT.LE.1) IBOT=1
0200        ITOP=TCH+2.0*SEPFAC*FWHM+.5
0201        IF (ITOP.GE.4096) ITOP=4096
      C     KFIRST AND KLAST ARE THE PEAK NUMBERS FOR THE FIRST AND LAST PEAKS
      C     BETWEEN IBOT AND ITOP FOR AREA INTERFERENCE PRINT-OUT.
      C     INITIALIZE KFIRST=1000,THEN IF KFIRST REMAINS UNCHANGED,NO
      C     INTERFERRING PEAKS WERE FOUND.
0203        KFIRST=1000
0204        IB=0
0205        DO 310 IE=1,NPD
0206        IF (PDATA(IE,1).GE.IBOT.AND.PDATA(IE,1).LE.ITOP) GO TO 290
0208        GO TO 310
0209  290   IF (PDATA(IE,3).EQ.0.0) GO TO 300
0211        IF (PDATA(IE,3).GE.20.0.AND.PDATA(IE,3).LE.20.4096) GO TO 300
0213        IF (PDATA(IE,3).GE.40.0.AND.PDATA(IE,3).LE.44.0) GO TO 300
0215        IF (PDATA(IE,3).GE.50.0.AND.PDATA(IE,3).LE.50.4096) GO TO 300
0217        IF (PDATA(IE,3).EQ.21.0) GO TO 300
0219        IF (PDATA(IE,3).EQ.1) GO TO 300
0221        GO TO 310
0222  300   IF (KFIRST.EQ.1000) KFIRST=IE
0224        KLAST=IE
0225        IB=IB+1
0226        PEAKS(IB)=PDATA(IE,1)
0227        IL=IB
0228  310   CONTINUE
      C     NOW CONVERT ANALYSIS RESULTS FROM UNITS OF AREA TO DESIRED UNITS.
0229  320   DIV=(DIFF/XIN)*100.0
0230        IF (IEFF-2) 330,340,350
```

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N 0231      330   DIV2=DIV/EFF(1)
N 0232            GO TO 370
N 0233      340   DIV2=DIV/EFF(2)
N 0234            GO TO 370
N 0235      350   IF (IEFF.EQ.4) GO TO 360
N 0237            DIV2=DIV/EFF(3)
N 0238            GO TO 370
N 0239      360   DIV2=DIV/EFF(4)
N 0240      370   DIV3=DIV2/CT
N 0241            IF (DT) 380,380,390
N 0242      380   DPMO=DIV3
N 0243            GO TO 400
N 0244      390   DPMO=DIV3/EXP(-(0.693*DT)/(HL*1440.0))
N 0245      400   IF (ICALC-2) 410,420,430
N 0246      410   ABUN=DIL*DPMO
N 0247            IF (FLAG.EQ.1.0) GO TO 450
N 0249            ABUND1=ABUN
N 0250            DPMY=DPMO
N 0251            GO TO 450
N 0252      420   ABUN=(1000000.0*DPMO)/(CPMMG*WT)
N 0253            IF (FLAG.EQ.1.0) GO TO 450
N 0255            ABUND1=ABUN
N 0256            DPMY=DPMO
N 0257            GO TO 450
N 0258      430   IF (ICALC.EQ.4) GO TO 440
N 0260            EN=DPMO*HL*1440.0/.693
N 0261            ENO=EN/((XSECT*FLUX)*10.0**(-24.0))
N 0262            MASSI=ENO*WTMOL/(6.02*10.0**20)
N 0263            ELM=MASSI/(ABISO*.01)
N 0264            ABUN=(1000000.*ELM)/WT
N 0265            IF (FLAG.EQ.1.0) GO TO 450
N 0267            ABUND1=ABUN
N 0268            DPMY=DPMO
N 0269            GO TO 450
N 0270      440   EN=DPMO*HL*1440.0/.693
N 0271            MASSI=ELMASS*ABISO*0.01
N 0272            ENO=MASSI*6.02*10.0**20/WTMOL
N 0273            FLUX=(EN/(ENO*XSECT))*10.0**(24.0)
N 0274            IF (FLAG.EQ.1.0) GO TO 450
N 0276            ABUND1=FLUX
N 0277            DPMY=DPMO
N 0278      450   DIFF=CONLIM
N 0279            IF (FLAG.EQ.1.0) GO TO 460
N 0281            FLAG=1.0
N 0282            GO TO 320
N 0283      460   IF (ICALC.EQ.4) ABUN=FLUX
N 0285            MM=IEFF
N 0286            UPABUN=ABUND1+ABUN
N 0287            WRITE (6,680) SYM,HL,ENG,XIN,EFF(MM),XSECT,SUM,BGSUM,SYM,CHN
N 0288            IF ((SUM-BGSUM).LE.$LC) WRITE (6,700) SPACES,UPABUN
N 0290            IF ((SUM-BGSUM).GT.$LC) WRITE (6,690) SPACES,ABUND1,ABUN
N 0292            IF (KFIRST.NE.1000) WRITE (6,500) (PEAKS(IB),IB=1,IL)
N 0294            IF (KFIRST.EQ.1000) WRITE (6,510)
N 0296      470   IF (ND.EQ.0) GO TO 150
N 0298            IF (ICA.GE.1.AND.IDIS.EQ.1) CALL POINT
N 0300            IF (ICA.GE.1) CALL EDIT
```

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0302              IF (ND.EQ.1) GO TO 100
0304      480     STOP
          C
0305      490     FORMAT (' ',A5,5X,'CHANNEL DATA OUTSIDE THE 4096 CHANNEL RANGE IS
                 1 REQUIRED FOR THIS CALCULATION.')
0306      500     FORMAT ('+',119X,F6.1,',',F6.1/(120X,F6.1,',',F6.1))
0307      510     FORMAT ('+',122X,'NONE')
0308      520     FORMAT (1H1)
0309      530     FORMAT (I3,13A4,E9.0,F5.0,2I1,I2,4I1,F3.0)
0310      540     FORMAT (2F5.0,E10.4,I5/(6F10.0))
0311      550     FORMAT (1H-,13A4)
0312      560     FORMAT (1H1,'THREE CONSECUTIVE TAPE MARKS HAVE BEEN ENCOUNTERED ON
                 1TAPE, CHANNEL ID NOT POSSIBLE')
0313      570     FORMAT (1H-,'SAMPLE WEIGHT ',F10.2,' MILLIGRAMS','   DILLUTION FAC
                 1TOR ',E9.2,'  COUNTING TIME ',F10.2,' MINUTES    DECAY TIME',F10.2
                 2,' MINUTES')
0314      580     FORMAT (1H0,'FLUX ',E10.3,' NEUTRON/CM*CM          ID NUMBER ',A4,
                 1'    FILE NUMBER ',I2,'  EFFICIENCY OPT ',I1,'  CALIB OPT ',I1,'
                 2CALCULATION OPT ',I1)
0315      590     FORMAT (I3/(6F10.0))
0316      600     FORMAT (1H0,'CALIBRATION: CHANNEL NO. EQUALS ',F7.1,' CHANNELS + '
                 1,F6.4,' CHANNELS PER KEV')
0317      610     FORMAT (1H0,13X,'ENERGIES',3X,'CHANNEL'/14X,8(1H-),3X,7(1H-)//(14X
                 1,F8.1,3X,F7.1))
0318      620     FORMAT (' ',5(1H-),1X,8(1H-),2X,6(1H-),2X,6(1H-),2X,9(1H-),1X,8(1H
                 1-),1X,7(1H-),2X,7(1H-),2X,5(1H-),2X,8(1H-),2X,25(1H-),2X,4(1H-),2X
                 2,13(1H-)/)
0319      630     FORMAT (1H-,'NUCLIDE  HALF   GAMMA   % GAMMA  COUNTING   CROSS  G
                 1ROSS   BKGND   NUCLIDE  DETECT     ELEMENT       CONF       CHAN
                 2 PEAKS FROM')
0320      640     FORMAT (' ','          LIFE   ENERGY  INTENS.   EFF.     SECTION  C
                 1OUNTS  COUNTS          LEVEL     ABUNDANCE      LIMITS      NO.
                 2 PEAK SEARCH')
0321      650     FORMAT (' ','          DAYS    KEV    PHO/DIS CT/PHOTON   BARNS
                 1                                UNITS = DPM               ')
0322      660     FORMAT (' ','          DAYS    KEV    PHO/DIS CT/PHOTON   BARNS
                 1                                UNITS = PPM               ')
0323      670     FORMAT (' ','          DAYS    KEV    PHO/DIS CT/PHOTON   BARNS
                 1                                UNITS = NEUTRONS/CM*CM    ')
0324      680     FORMAT (1H0,A5,1X,1PE8.2,2X,0PF6.1,2X,F6.2,2X,1PE9.2,1X,1PE8.2,1X,
                 10PF7.3,2X,F7.0,2X,A5,39X,I4)
0325      690     FORMAT ('+',76X,A8,2X,E10.3,' +/- ',E10.3)
0326      700     FORMAT ('+',76X,A8,':  LESS THAN ',E10.3)
0327              END
```

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N 0002              SUBROUTINE BKGND
                C   THIS SUBROUTINE COMPARES THE SLOPES OF THE RIGHT AND LEFT BKG
                C   REGIONS WITH THE SLOPE OF THE LEAST SQUARES LINE THRU BOTH.
                C   IF THERE IS A STATISTICAL DIFFERENCE BETWEEN EITHER SIDE AND THE
                C   LEAST SQUARES LINE, A CUBIC EQUATION IS CALCULATED.  IF NOT, THE
                C   LINEAR LEAST SQUARES LINE IS USED AS THE BACKGROUND.
N 0003              COMMON /ARRAY/ TFN
N 0004              COMMON /BAG/ M
N 0005              COMMON /BOX/ X,Y,A,B,STERRB
N 0006              COMMON /HELL/ IXL,IXR
N 0007              COMMON /HOME/ TM3,TM2,TM1,TM0
N 0008              COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0009              REAL *8 AA,BB,SS,AAL,BBL,SSL,AAR,BBR,SSP,TM3,TM2,TM1,TM0,PL,QL,PR,
                   1QR,TERM1,TERM2,TERM3,TERM4
N 0010              REAL *8 X(60),Y(60),A,B,STERRB
N 0011              REAL *8 DELTA
N 0012              REAL *4 TFN(4096)
N 0013              INTEGER *4 FILE
N 0014              NN=(M-1.)/2.
N 0015              J=IXL-NN
N 0016              DO 100 I=1,M
N 0017              Y(I)=TFN(J)
N 0018              X(I)=J
N 0019          100 J=J+1
N 0020              J=IXR-NN
N 0021              MPM=M+M
N 0022              MP1=M+1
N 0023              DO 110 I=MP1,MPM
N 0024              Y(I)=TFN(J)
N 0025              X(I)=J
N 0026          110 J=J+1
N 0027              DO 120 I=1,MPM
N 0028          120 IF (ICA.GE.3) WRITE (6,170) I,X(I),Y(I)
N 0030              CALL CALCIT(MPM)
                C   DEFINE AA AND BB AS THE INTERCEPT AND SLOPE OF THE LSTSQR LINE
                C   THRU BKG REGIONS ON LEFT AND RIGHT OF PEAK WITH STD ERR IN SLOPE
                C   OF SS.
N 0031              AA=A
N 0032              BB=B
N 0033              SS=STERRB
N 0034              IF (ICA.GE.3) WRITE (6,180) MPM,BB,AA,SS
                C   WORK ON LEFT BKG FIRST.
N 0036              CALL CALCIT(M)
                C   DEFINE AAL AND BBL AS THE INTERCEPT AND SLOPE OF THE LSTSQR LINE
                C   THRU THE LEFT BKG REGION WITH STD ERROR IN SLOPE OF SSL.
N 0037              AAL=A
N 0038              BBL=B
N 0039              SSL=STERRB
N 0040              IF (ICA.GE.3) WRITE (6,180) M,BBL,AAL,SSL
                C   REINDEX X-Y DATA TO BEGIN WORK ON RIGHT BKG.
N 0042              J=IXR-NN
N 0043              DO 130 I=1,M
N 0044              Y(I)=TFN(J)
N 0045              X(I)=J
```

```
N 0046              IF (ICA.GE.3) WRITE (6,170) I,X(I),Y(I)
N 0048      130     J=J+1
N 0049              CALL CALCIT(M)
            C       DEFINE AAR AND BBR AS THE INTERCEPT AND SLOPE OF THE LSTSQR LINE
            C       THRU THE RIGHT BKG REGION WITH STD ERROR IN SLOPE OF SSR.
N 0050              AAR=A
N 0051              BBR=B
N 0052              SSR=STERRB
N 0053              IF (ICA.GE.3) WRITE (6,180) M,BBR,AAR,SSR
            C       EVALUATE THESE SLOPE DATA.
            C       COMPARE SLOPE FOR LEFT BKG WITH SLOPE THRU LEFT AND RIGHT BKGS .
N 0055              IF (BB.GE.BBL.AND.BBL+SSL.GE.BB.OR.BBL.GE.BB.AND.BB.GE.BBL-SSL) GO
                   1 TO 140
N 0057              GO TO 160
N 0058      140     IF (BB.GE.BBR.AND.BBR+SSR.GE.BB.OR.BBR.GE.BB.AND.BB.GE.BBR-SSR) GO
                   1 TO 150
            C       NEITHER THE SLOPE OF THE LEFT OR RIGHT BKG REGIONS WAS
            C       STATISTICALLY DIFFERENT FROM THE SLOPE THRU BOTH BKG REGIONS.
            C       THE LINEAR BKG WILL THEREFORE BE USED.
N 0060      150     TM3=0.0
N 0061              TM2=0.0
N 0062              TM1=BB
N 0063              TM0=AA
N 0064              RETURN
            C       SLOPE FOR LEFT OR RIGHT BKG REGION WAS STATISTICALLY DIFFERENT
            C       FROM THE SLOPE THRU BOTH REGIONS.  WE WILL THEREFORE FIT A CUBIC
            C       BKG USING THE EQUATION GIVEN BY QUITTNER IN ANAL CHEM, VOL 41,
            C       NO 11, PAGE 1504 REARRANGED IN THE FOLLOWING FORM.
            C       BACKGROUND = TM0+X*(TM1+X*(TM2+TM3*X))
N 0065      160     PL=AAL+IXL*BBL
N 0066              QL=BBL
N 0067              PR=AAR+IXR*BBR
N 0068              QR=BBR
            C       WRITE (6,190) PL,QL,PR,QR
N 0069              DELTA=IXR-IXL
N 0070              TERM1=(QR+QL+QL)/(-DELTA)
N 0071              TERM2=3.*(PR-PL)/(DELTA*DELTA)
N 0072              TERM3=(QL+QR)/(DELTA*DELTA)
N 0073              TERM4=(2.*(PL-PR))/(DELTA**3)
            C       WRITE (6,190) TERM1,TERM2,TERM3,TERM4
N 0074              TM3=TERM3+TERM4
N 0075              TM2=TERM1+TERM2-3.*IXL*(TERM3+TERM4)
N 0076              TM1=QL+IXL*(-2.*(TERM1+TERM2)+3.*IXL*(TERM3+TERM4))
            C       WRITE (6,200) IXL,PL,QL,TERM1,TERM2,TERM3,TERM4
N 0077              TM0=PL+IXL*(-QL+IXL*(TERM1+TERM2-IXL*(TERM3+TERM4)))
            C       WRITE (6,190) TM3,TM2,TM1,TM0
N 0078              RETURN
            C       190 FORMAT (' ',4(3X,D14.7))
            C       200 FORMAT (' ',I5,6(3X,D14.7))
            C
N 0079      170     FORMAT (' ',I5,3X,F8.2,3X,F10.2)
N 0080      180     FORMAT (' ','LST SQR LINE THRU',I4,' POINTS HAS SLOPE = ',D14.7,',
                   1  INTERCEPT = ',D14.7,',  STD ERR IN SLOPE = ',D14.7)
N 0081              END
```

```
0002              SUBROUTINE CALCIT(M)
                  C     SUBROUTINE CALCIT TAKES M PAIRS OF X-Y DATA AND CALCULATES THE
                  C     LINEAR LEAST SQUARES LINE OF SLOPE B AND INTERCEPT A.  IT THEN
                  C     CALCULATES THE STANDARD ERROR OF ESTIMATE (STDERR) AND THE
                  C     STANDARD ERROR OF THE SLOPE (STERRB) USING EQUATIONS (28) AND (69)
                  C     ON PAGES 149 AND 313 OF 'METHODS OF CORRELATION ANALYSIS' BY
                  C     MORDECAI EZEKIEL,WILEY AND SONS, NEW YORK,(1950)
0003              COMMON /BOX/ X,Y,A,B,STERRB
0004              REAL *8 X(60),Y(60),A,B,STDERR,SUMX,SUMY,SUMX2,SUMXY,SUMY2,MEANX,M
                 1EANY,RAD,R,RBAR2,SBAR,STDEVX,STERRB,ZOOM
0005              SUMX=0.0
0006              SUMY=0.0
0007              SUMX2=0.0
0008              SUMY2=0.0
0009              SUMXY=0.0
0010              DO 100 I=1,M
0011              SUMX=X(I)+SUMX
0012              SUMY=Y(I)+SUMY
0013              SUMX2=X(I)*X(I)+SUMX2
0014              SUMY2=Y(I)*Y(I)+SUMY2
0015        100   SUMXY=X(I)*Y(I)+SUMXY
0016              IF (SUMY2.EQ.0.0) GO TO 110
0018              MEANX=SUMX/M
0019              MEANY=SUMY/M
0020              B=(SUMXY-(M*MEANX*MEANY))/(SUMX2-(M*MEANX*MEANX))
0021              A=MEANY-B*MEANX
0022              RAD=(SUMX2-(M*MEANX*MEANX))*(SUMY2-(M*MEANY*MEANY))
0023              R=(SUMXY-(M*MEANX*MEANY))/(DSQRT(RAD))
0024              RBAR2=1.-(((1.-R*R)*(M-1.))/(M-2.))
0025              SBAR=DSQRT(((SUMY2-(M*MEANY*MEANY))*(1.-RBAR2))/(M-1.))
0026              STDEVX=DSQRT((SUMX2-((SUMX*SUMX)/M))/(M-1.))
0027              ZOOM=M
0028              STERRB=SBAR/(STDEVX*(DSQRT(ZOOM)))
0029              RETURN
0030        110   A=0.0
0031              B=0.0
0032              STERRB=0.0
0033              RETURN
0034              END
```

```
0002            SUBROUTINE EDIT
                C       SUBRCUTINE EDIT PRINTS OUT RESULTS OF THE PEAK SEARCH.
0003            COMMON /IMIT/ NT6,NT5,IP,KOUNT,WT,DT,FLUX,ID,ICALIB,ICALC
0004            COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPDX
0005            COMMON /PEDIT/ PDATA
0006            COMMON /SHELF/ WIND,ITOLER,SEPFAC,AFAC
0007            REAL *8 FMT(9)/'(3X,    ','F7.1,9X,','F7.0,7X,','F7.2,    ','
                1  ','       ','       ','         ','8X,F8.4)'/
0008            REAL *8 FMR(4)/'6X,D14.7',',8X,F9.3',',12X,   ','F6.2,   '/
0009            REAL *8 FMA(4)/'16X,A4  ',',13X,A4 ',',14X,   ','A4,     '/
0010            REAL *4 DASH/'----'/
0011            REAL *4 PDATA(500,7)
0012            INTEGER *4 FILE
0013            NPDX=NPDX-1
0014            NPD=1
0015            WRITE (6,110) FILE,WIND,ITOLER,SEPFAC,AFAC
0016            DO 100 NPD=1,NPDX
0017            IF (ICA.LE.1.AND.PDATA(NPD,3).GE.60..AND.PDATA(NPD,3).LE.69.) GO T
                10 100
0019            IF (PDATA(NPD,5).EQ.DASH) FMT(5)=FMA(1)
0021            IF (PDATA(NPD,5).NE.DASH) FMT(5)=FMR(1)
0023            IF (PDATA(NPD,6).EQ.DASH) FMT(6)=FMA(2)
0025            IF (PDATA(NPD,6).NE.DASH) FMT(6)=FMR(2)
0027            IF (PDATA(NPD,7).EQ.DASH) FMT(7)=FMA(3)
0029            IF (PDATA(NPD,7).NE.DASH) FMT(7)=FMR(3)
0031            IF (PDATA(NPD,7).EQ.DASH) FMT(8)=FMA(4)
0033            IF (PDATA(NPD,7).NE.DASH) FMT(8)=FMR(4)
0035            WRITE (6,FMT) PDATA(NPD,1),PDATA(NPD,2),PDATA(NPD,4),PDATA(NPD,5),
                1PDATA(NPD,6),PDATA(NPD,7),PDATA(NPD,3)
0036    100     CONTINUE
0037            RETURN
                C
0038    110     FORMAT ('1',22X,'P E A K   A N A L Y S I S',20X,'FILE',I4//' WINDO
                1W = ',F2.0,20X,'TOLERANCE = ',I2,20X,'SEPFAC = ',F5.3,20X,'AFAC =
                2',F5.3//20X,'COUNTS',8X,'ENERGY',6X,' NET PEAK AREA ',4X,'REL STD
                3DEVIATION',3X,'FULL WIDTH',7X,'COMMENT'/' PEAK(CHANNEL)',6X,'AT PE
                4AK',7X,'(KEV)',10X,'(COUNTS)',8X,'OF AREA IN PERCENT',2X,'AT HALF
                5MAX',6X,'CODE'/1X,13(1H-),6X,7(1H-),7X,6(1H-),7X,13(1H-),6X,13(1H-
                6),6X,11(1H-),6X,7(1H-)//)
0039            END
```

```
N 0002              SUBROUTINE LOCATE
                C   SUBROUTINE LOCATE IS USED IN THE CALIBRATION OPTION TO SEARCH THE
                C   PEAK SEARCH DATA AND LOCATE THE NON-OVERLAPPING PEAK (COMMENT
                C   CODE = 0) WHICH IS NEAREST TO AND WITHIN +/- 15 CHANNELS OF THE
                C   INPUT CHANNEL.  IF NO SUCH PEAK IS FOUND, THE INPUT CHANNEL IS
                C   ASSUMED CORRECT
N 0003              COMMON /CHANEL/ C
N 0004              COMMON /IMIT/ NT6,NT5,IP,KOUNT,WT,DT,FLUX,ID,ICALIB,ICALC
N 0005              COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0006              COMMON /PEDIT/ PDATA(500,7)
N 0007              REAL *8 C(25)
N 0008              REAL *4 CT(25)
N 0009              INTEGER *4 FILE
N 0010              DO 100 I=1,NTOT
N 0011          100 CT(I)=C(I)
N 0012              NPD=NPD-1
N 0013              DO 160 I=1,NTOT
N 0014              DIFF=4096.
N 0015              DO 120 N=1,NPD
N 0016              IF (ABS(PDATA(N,1)-CT(I)).LT.DIFF) GO TO 110
N 0018              GO TO 120
N 0019          110 DIFF=ABS(PDATA(N,1)-CT(I))
N 0020              JN=N
N 0021              GO TO 120
N 0022          120 CONTINUE
                C   AT THIS POINT, ALL POSSIBLE PEAKS HAVE BEEN TESTED AND PEAK
                C   NUMBER JN IS THE CLOSEST PEAK OR POSSIBLE PEAK TO CHANNEL C(I).
                C   THE VARIABLE 'SIGN' DETERMINES WHETHER TO LOOK LEFT OR RIGHT FIRST
                C   FROM THE INPUT CHANNEL.
N 0023              IF (PDATA(JN,1)-CT(I).GE.0.0) SIGN=-1.0
N 0025              IF (PDATA(JN,1)-CT(I).LT.0.0) SIGN=1.0
N 0027              DO 140 NUMB=1,3
N 0028              NUM=NUMB-1
N 0029              JTN=JN+SIGN*NUM
N 0030              IF (JTN.LT.1.OR.JTN.GT.NPD) GO TO 130
N 0032              IF (PDATA(JTN,3).EQ.0.0.AND.PDATA(JTN,1).GE.CT(I)-15..AND.PDATA(JT
                   1N,1).LE.CT(I)+15.) GO TO 150
N 0034          130 JTN=JN-SIGN*NUM
N 0035              IF (JTN.LT.1.OR.JTN.GT.NPD) GO TO 140
N 0037              IF (PDATA(JTN,3).EQ.0.0.AND.PDATA(JTN,1).GE.CT(I)-15..AND.PDATA(JT
                   1N,1).LE.CT(I)+15.) GO TO 150
N 0039          140 CONTINUE
N 0040              WRITE (6,170) C(I)
N 0041              C(I)=CT(I)
N 0042              GO TO 160
N 0043          150 C(I)=PDATA(JTN,1)
N 0044          160 CONTINUE
N 0045              NPD=NPD+1
N 0046              RETURN
                C
N 0047          170 FORMAT (' ','NO SINGLE PEAK COULD BE FOUND WITHIN PLUS OR MINUS 15
                   1 CHANNELS OF CHANNEL ',F7.2,'.')
N 0048              END
```

```
N 0002            SUBROUTINE NINIT(IDF)
          C       NINIT SUPPLIES COEFFICIENTS FOR NUCLIDE INTERFERENCE CALCULATIONS.
N 0003            COMMON /INTERF/ NC,NI,IPT,F
N 0004            REAL *4 F(5,5)
N 0005            INTEGER *4 NI(5),IPT(5,5)
N 0006            CALL CLEAR(NC,56)
N 0007            IF (IDF.EQ.40) GO TO 100
N 0009            WRITE (6,110) IDF
N 0010            RETURN
N 0011       100  F(2,1)=1.186
N 0012            F(3,1)=.295
N 0013            NI(1)=3
N 0014            IPT(1,1)=12
N 0015            IPT(2,1)=13
N 0016            IPT(3,1)=14
N 0017            NC=1
N 0018            RETURN
          C
N 0019       110  FORMAT (1H1,' NO NUCLIDE INTERFERENCES EXIST FOR THIS DATA SET'/'
                 1EXECUTION CONTINUING')
N 0020            END
```

```
N 0002            SUBROUTINE PKAREA(KCNTR)
                  C     THIS ROUTINE CALCULATES AREAS BY SUMMING CHANNELS BETWEEN MEAN
                  C     PLUS AND MINUS AFAC*FWHM.  IT REQUIRES THAT BKG ALWAYS BE POSITIVE
                  C     BUT PERMITS BACKGROUND TO EXCEED THE COUNTS IN THAT CHANNEL.  IF
                  C     THE FINAL AREA(KCNTR) IS NEGATIVE, IT SETS IT EQUAL TO ZERO.
N 0003            COMMON /ARRAY/ TFN
N 0004            COMMON /HOME/ TM3,TM2,TM1,TM0
N 0005            COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0006            COMMON /PEDIT/ PDATA
N 0007            COMMON /SHELF/ WIND,ITOLER,SEPFAC,AFAC
N 0008            EQUIVALENCE (PDATA(1,1),PKCNTR(1))
N 0009            EQUIVALENCE (PDATA(1,2),COUNTS(1))
N 0010            EQUIVALENCE (PDATA(1,3),COMCOD(1))
N 0011            EQUIVALENCE (PDATA(1,4),ENG(1))
N 0012            EQUIVALENCE (PDATA(1,5),AREA(1))
N 0013            EQUIVALENCE (PDATA(1,6),RSDA(1))
N 0014            EQUIVALENCE (PDATA(1,7),FWHM(1))
N 0015            REAL *8 RMEAN
N 0016            REAL *8 TM3,TM2,TM1,TM0
N 0017            REAL *4 PDATA(500,7)
N 0018            REAL *4 PKCNTR(500),COUNTS(500),COMCOD(500),ENG(500),AREA(500),RSD
                 1A(500),FWHM(500)
N 0019            REAL *4 TFN(4096)
N 0020            INTEGER *4 FILE
                  C     THE CARD IAR = DEFINES THE NUMBER OF CHANNELS TO BE SUMMED.
N 0021            IAR=PKCNTR(KCNTR)+AFAC*FWHM(KCNTR)
N 0022            MEAN=PKCNTR(KCNTR)+.5
N 0023            RMEAN=MEAN
N 0024            I=0
N 0025            SUMTFN=TFN(MEAN)
N 0026            BKG=TM0+RMEAN*(TM1+RMEAN*(TM2+RMEAN*TM3))
N 0027            IF (BKG.LT.0.0) BKG=0.0
N 0029            SUMBKG=BKG
N 0030            IF (SUMTFN-SUMBKG.GT.0.0) GO TO 100
                  C     GIVE THE COMPUTER SOME LARGE ARBITRARY VALUE FOR RSDA(KCNTR)
                  C     TO USE FOR COMPARISONS.
N 0032            RSDA(KCNTR)=999.
                  C     GIVE THE COMPUTER A LARGE ARBITRARY VALUE FOR XRSDA TO SATISFY
                  C     THE EQUATION RSDA(KCNTR) = XRSDA
N 0033            XRSDA=999.
N 0034            IF (ICA.GE.3) WRITE (6,150) I,RMEAN,TFN(MEAN),BKG,SUMTFN,SUMBKG
N 0036            GO TO 110
N 0037      100   RSDA(KCNTR)=((SQRT(TFN(MEAN)+BKG))*100.)/(TFN(MEAN)-BKG)
N 0038            IF (ICA.GE.3) WRITE (6,150) I,RMEAN,TFN(MEAN),BKG,SUMTFN,SUMBKG,RS
                 1DA(KCNTR)
N 0040      110   MEND=IAR-MEAN
N 0041            DO 140 I=1,MEND
N 0042            XCHANL=RMEAN-I
N 0043            XTFNL=TFN(MEAN-I)
N 0044            XBKGL=TM0+(RMEAN-I)*(TM1+(RMEAN-I)*(TM2+(RMEAN-I)*TM3))
N 0045            IF (XBKGL.LT.0.0) XBKGL=0.0
N 0047            XCHANR=RMEAN+I
N 0048            XTFNR=TFN(MEAN+I)
N 0049            XBKGR=TM0+(RMEAN+I)*(TM1+(RMEAN+I)*(TM2+(RMEAN+I)*TM3))
```

```
N 0050              IF (XBKGR.LT.0.0) XBKGR=0.0
N 0052              XSTFN=SUMTFN+XTFNL+XTFNR
N 0053              XSBKG=SUMBKG+XBKGL+XBKGR
N 0054              XAREA=XSTFN-XSBKG
N 0055              IF (XAREA.GT.0.0) GO TO 120
N 0057              GO TO 130
N 0058        120   XRSDA=((SQRT(XSTFN+XSBKG))*100.)/XAREA
N 0059        130   CONTINUE
N 0060              SUMTFN=XSTFN
N 0061              SUMBKG=XSBKG
N 0062              AREA(KCNTR)=XAREA
N 0063              RSDA(KCNTR)=XRSDA
N 0064              XAFAC=I/FWHM(KCNTR)
N 0065              IF (ICA.GE.3) WRITE (6,150) I,XCHANL,XTFNL,XBKGL
N 0067              IF (ICA.GE.3) WRITE (6,150) I,XCHANR,XTFNR,XBKGR,SUMTFN,SUMBKG,AR
                   1A(KCNTR),RSDA(KCNTR),XAFAC
N 0069        140   CONTINUE
N 0070              IF (AREA(KCNTR).LT.0.0) AREA(KCNTR)=0.0
N 0072              RETURN
                    C
N 0073        150   FORMAT (' ',I4,8(2X,D14.7))
N 0074              END
```

```
N 0002            SUBROUTINE PLOTIT
                  C     THIS ROUTINE GRAPHS TFN(I) AGAINST CHANNEL NUMBERS IN 100 CHANNEL
                  C     INTERVALS BEGINNING WITH CHANNEL A AND STOPPING WITH CHANNEL Z.
N 0003            COMMON /ARRAY/ TFN
N 0004            COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0005            REAL *4 TFN(4096),X(110),Y(110)
N 0006            INTEGER *4 FILE
N 0007            INTEGER *4 NSCL(5)/1,0,-1,0,-1/
N 0008            A=0.0
N 0009            Z=4096.0
N 0010            CHLF=A
N 0011            IF (CHLF.LT.100.0) CHLF=1.0
N 0013      100   ICHLF=CHLF
N 0014            IF (CHLF.EQ.1.0) CHRT=100.0
N 0016            IF (CHLF.GE.100.0) CHRT=CHLF+100.0
N 0018            ICHRT=CHRT
N 0019            J=0
N 0020            DO 110 I=ICHLF,ICHRT
N 0021            J=J+1
N 0022            X(J)=I
N 0023      110   Y(J)=TFN(I)
N 0024            YMAX=Y(1)
N 0025            DO 120 J=2,100
N 0026      120   IF (Y(J).GT.YMAX) YMAX=Y(J)
N 0028            IF (YMAX.LT.1000.0) GO TO 130
N 0030            IF (YMAX.GE.1000.0.AND.YMAX.LT.10000.0) GO TO 140
N 0032            IF (YMAX.GE.10000.0) YMAX=100000.0
N 0034            GO TO 150
N 0035      130   YMAX=1000.0
N 0036            GO TO 150
N 0037      140   YMAX=10000.0
N 0038      150   WRITE (6,180)
N 0039            LOGICAL *1 GRAPH(101,101)
N 0040            CALL PLOT1(NSCL,10,10,10,10)
N 0041            CALL PLOT2(GRAPH,YMAX,0.0,-CHLF,-CHRT)
N 0042            DO 160 J=1,100
N 0043      160   CALL PLOT3('*',Y(J),-X(J),1)
N 0044            CALL PLOT4(60,'                    CHANNEL NUMBER WITH SIGN CHANGED TO
                 1 NEGATIVE')
N 0045            WRITE (6,190) FILE
N 0046            CHLF=CHRT
N 0047            IF (CHLF.GT.Z) GO TO 170
N 0049            GO TO 100
N 0050      170   RETURN
                  C
N 0051      180   FORMAT ('1')
N 0052      190   FORMAT ('0',15X,'COUNTS FOR FILE ',I3)
N 0053            END
```

```
N 0002              SUBROUTINE READIT
                C   SUBROUTINE READIT READS THE NUCLIDE INFORMATION AND STORES IT IN
                C   THE APPROPRIATE REGION DETERMINED BY THE DEFINE FILE STATEMENTS.
                C   THE NUCLIDE DATA SET MUST END WITH AN 'ENDIT' CARD IN WHICH
                C   'ENDIT' IS PUNCHED IN THE FIRST FIVE COLUMNS.
N 0003              COMMON /IMIT/ NT6,NT5,IP,KOUNT,WT,DT,FLUX,ID,ICALIB,ICALC
N 0004              REAL *8 ENDIT/'ENDIT   '/
N 0005              REAL *8 SYM,BLK/' '/
N 0006              REAL *4 EFF(4)
N 0007              DEFINE FILE 40(100,68,L,IP),41(100,68,L,IP),42(100,68,L,IP),43(100
                   1,68,L,IP),44(100,68,L,IP)
N 0008              NX=39
N 0009      100     NX=NX+1
N 0010              IP=1
N 0011      110     READ (5,150) SYM,HL,ENG,XIN,EFF(1),EFF(2),EFF(3),EFF(4),SYMBOL
N 0012              IF (SYM.EQ.ENDIT.OR.NX.EQ.45) GO TO 140
N 0014              NP=IP
N 0015              IF (SYM.EQ.BLK) GO TO 120
N 0017              READ (5,160) BOP,XSECT,ABISO,ELMASS,CPMMG,WTMOL,ND
N 0018              WRITE (NX'IP) SYM,HL,ENG,XIN,EFF(1),EFF(2),EFF(3),EFF(4),SYMBOL,BO
                   1P,XSECT,ABISO,ELMASS,CPMMG,WTMOL,ND
N 0019              GO TO 110
N 0020      120     IP=1
N 0021      130     READ (NX'IP) SYM,HL,ENG,XIN,EFF(1),EFF(2),EFF(3),EFF(4),SYMBOL,BOP
                   1,XSECT,ABISO,ELMASS,CPMMG,WTMOL,ND
N 0022              WRITE (6,170) SYM,HL,ENG,XIN,EFF(1),EFF(2),EFF(3),EFF(4),SYMBOL
N 0023              WRITE (6,180) BOP,XSECT,ABISO,ELMASS,CPMMG,WTMOL,ND
N 0024              IF (IP.EQ.NP) GO TO 100
N 0026              GO TO 130
N 0027      140     RETURN
                C
N 0028      150     FORMAT (A5,E14.7,F10.1,F10.2,4E10.3,A1)
N 0029      160     FORMAT (I1,F8.3,F10.2,2E11.4,I3,35X,I1)
N 0030      170     FORMAT (1H-,A5,E14.7,F10.1,F10.2,4E10.3,A1)
N 0031      180     FORMAT (1HC,I1,F8.3,F10.2,2E11.4,I3,35X,I1)
N 0032              END
```

```
N 0002            SUBROUTINE SPAN2
                  C     SUBROUTINE SPAN2 TAKES 4096 CHANNELS OF DATA (TFN) FROM COMMON
                  C     STORAGE AND SEARCHES FOR PEAKS USING A SECOND DIFFERENCE METHOD
                  C     ESSENTIALLY LIKE MARISCOTTI'S.  (SEE AS REF: M.A.MARISCOTTI, NUCL.
                  C     INST. AND METH. 50(1967)309.)  THE SECOND DIFFERENCE S AND ITS STD
                  C     DEVIATION F ARE REINDEXED EACH TIME A NEW I1 IS FOUND.  THE AMOUNT
                  C     OF INFORMATION PRINTED OUT DURING THE SEARCH IS CONTROLLED BY THE
                  C     EDIT OPTION VARIABLE ICA (IN COMMON STORAGE) AS FOLLOWS:
                  C     ICA                PRINT OUT
                  C      0          DOES NOT EDIT PEAK SEARCH RESULTS.
                  C      1          EDITS ONLY SINGLE AND OVERLAPPING PEAKS.
                  C      2          EDITS SAME AS 1 + ALL TEST FAILURES.
                  C      3          EDITS SAME AS 2 + CHANNEL BY CHANNEL DETAILS OF SEARCH.
                  C      4          EDITS SAME AS 3 + GRAPH OF 4096 CHANNEL SPECTRUM.
                  C     THE FOLLOWING IS AN EXPLANATION OF COMMENT CODES GENERATED BY SPAN
                  C     COMMENT            EXPLANATION
                  C     CODE
                  C      0.0      SINGLE PEAK WHICH PASSED ALL TESTS.
                  C      1.0      SINGLE PEAK WHICH PASSED ALL TESTS BUT GAVE A POSITIVE
                  C               B(2) IN LEAST SQUARES FIT TO LOCATE CENTER OF PEAK.
                  C     20.0      THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS.
                  C               THIS MAIN PEAK PASSED ALL TESTS.
                  C     20.AAAA   THIS PEAK OVERLAPS WITH THE PEAK AT CHANNEL AAAA WHERE
                  C               AAAA PASSED ALL TESTS.
                  C     21.0      THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS AND
                  C               PASSED ALL TESTS BUT GAVE POSITIVE B(2) IN LEAST SQUARES.
                  C     4B.CCCC   THIS IS THE MAIN PEAK OF TWO OR MORE OVERLAPPING PEAKS,
                  C               THIS PEAK FAILED TO PASS TEST B.
                  C     50.CCCC   THIS PEAK OVERLAPS WITH THE PEAK AT CHANNEL CCCC WHERE
                  C               CCCC FAILED TO PASS ALL TESTS.
                  C     6D.CCCC   THIS SINGLE PEAK FAILED TO PASS TEST D.
                  C     80.0000   THE MAXIMUM DIMENSION OF VARIABLES S AND F WAS EXCEEDED
                  C               BEFORE A NEW VALUE OF I1 WAS FOUND.  ALL MINIMA IN THE
                  C               SECOND DIFFERENCE OCCURRING BETWEEN I5 AND THE MAXIMUM
                  C               DIMENSION ARE GIVEN COMMENT CODE 80.0000.
                  C     81.0000   NO MINIMUM WAS FOUND IN THE SECOND DIFFERENCE CURVE
                  C               BETWEEN I3 AND I5.
                  C     THE VARIOUS TEST (0-4) ARE DESCRIBED IN THE BODY OF THIS ROUTINE.
                  C     BEGIN CALCULATION OF THE SMOOTHED SECOND DIFFERENCE S AND ITS
                  C     APPROXIMATED STANDARD DEVIATION F.
N 0003            COMMON /ARRAY/ TFN
N 0004            COMMON /BAG/ M
N 0005            COMMON /DATA/ CDEL
N 0006            COMMON /ENERGY/ AA,BB
N 0007            COMMON /HELL/ IXL,IXR
N 0008            COMMON /HOME/ TM3,TM2,TM1,TM0
N 0009            COMMON /INDEX/ NTOT,FILE,ICA,IDIS,NPD
N 0010            COMMON /PEDIT/ PDATA
N 0011            COMMON /SHELF/ WIND,ITOLER,SEPFAC,AFAC
N 0012            REAL *8 AA,BB
N 0013            REAL *8 CH(50,2),$LNTFN(50),W(50),A,B(2),STAT(3),VARB(2),T(2)
N 0014            REAL *8 TM3,TM2,TM1,TM0
N 0015            REAL *4 CDEL(5)
N 0016            REAL *4 DASH/'----'/
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N 0017            REAL *4 PDATA(500,7)
N 0018            REAL *4 PKCNTR(500),COUNTS(500),COMCOD(500),ENG(500),AREA(500),RSD
                 1A(500),FWHM(500)
N 0019            REAL *4 S(300),F(300)
N 0020            REAL *4 TFN(4096)
N 0021            INTEGER *4 FILE
N 0022            EQUIVALENCE (PDATA(1,1),PKCNTR(1))
N 0023            EQUIVALENCE (PDATA(1,2),COUNTS(1))
N 0024            EQUIVALENCE (PDATA(1,3),COMCOD(1))
N 0025            EQUIVALENCE (PDATA(1,4),ENG(1))
N 0026            EQUIVALENCE (PDATA(1,5),AREA(1))
N 0027            EQUIVALENCE (PDATA(1,6),RSDA(1))
N 0028            EQUIVALENCE (PDATA(1,7),FWHM(1))
N 0029            EQUIVALENCE (KOUNT,NPD)
                  C     AFAC IS A FACTOR WHICH DETERMINES THE NUMBER OF CHANNELS INCLUDED
                  C     IN AREA SUMMATIONS.
                  C     SEPFAX IS THE FACTOR WHICH DETERMINES ACCEPTABLE PEAK SEPARATIONS.
                  C     ITOLER IS MARISCOTTI'S TOLERANCE DEFINED ON PAGE 316 OF HIS PAPER.
                  C     WIND IS MARISCOTTI'S WINDOW,W, DEFINED ON PAGE 319 OF HIS PAPER.
                  C     IWIND IS A FUNCTION WHICH STOPS SEARCH AT CHANNEL 4096.
N 0030            IWIND=1.+((5.*(WIND-1.))/2.)
                  C     KOUNT IS THE INDEX WHICH COUNTS THE PEAKS.
N 0031            KOUNT=0
                  C     MORE IS A VARIABLE WHICH PERMITS CALCULATION OF MORE SECOND
                  C     DIFFERENCE DATA FOR LOCATION OF PEAK CENTER IF MORE = 1.
N 0032            MORE=0
N 0033            IF (ICA.GE.3) WRITE (6,870) FILE
N 0035            IF (WIND.EQ.3.0) GO TO 100
N 0037            IF (WIND.EQ.5.0) GO TO 110
N 0039            IF (WIND.EQ.7.0) GO TO 120
N 0041       100  I=8
N 0042            GO TO 130
N 0043       110  I=13
N 0044            GO TO 130
N 0045       120  I=18
N 0046            GO TO 130
                  C     INITIALIZE THE VARIABLES I1 THRU I5.
N 0047       130  I1=I+1
N 0048            I2=I+2
N 0049            I3=I+3
N 0050            I4=99
N 0051            I5=99
N 0052            INDI1=I1-I1+2
N 0053            INDI2=I2-I1+2
N 0054            INDI3=I3-I1+2
N 0055            IND=1
N 0056       140  IF (WIND.EQ.3.0) GO TO 150
N 0058            IF (WIND.EQ.5.0) GO TO 160
N 0060            IF (WIND.EQ.7.0) GO TO 170
N 0062       150  S(IND)=1.*(TFN(I-6)+TFN(I+6))+3.*(TFN(I-5)+TFN(I+5))+6.*(TFN(I-4)+
                 1TFN(I+4))+5.*(TFN(I-3)+TFN(I+3))-9.*(TFN(I-1)+TFN(I+1))-12.*TFN(I)
N 0063            F(IND)=SQRT(448.*(TFN(I)))
                  C     TO PREVENT DIVIDING BY ZERO, LET S = 0.0000001
N 0064            IF (S(IND).EQ.0.0) S(IND)=.0000001
N 0066            IF (ICA.GE.3) WRITE (6,880) I,TFN(I),S(IND),F(IND)
N 0068            IF (MORE.EQ.1) GO TO 610
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N 0070                IF (IND.EQ.1) GO TO 180
N 0072                GO TO 240
N 0073          160   S(IND)=1.*(TFN(I-11)+TFN(I+11))+3.*(TFN(I-10)+TFN(I+10))+6.*(TFN(I
                1-9)+TFN(I+9))+10.*(TFN(I-8)+TFN(I+8))+15.*(TFN(I-7)+TFN(I+7))+16.*
                2(TFN(I-6)+TFN(I+6))+13.*(TFN(I-5)+TFN(I+5))+6.*(TFN(I-4)+TFN(I+4))
                3-5.*(TFN(I-3)+TFN(I+3))-20.*(TFN(I-2)+TFN(I+2))-29.*(TFN(I-1)+TFN(
                4I+1))-32.*TFN(I)
N 0074                F(IND)=SQRT(5220.*(TFN(I)))
                C     TO PREVENT DIVIDING BY ZERO, LET S(I) = .0000001
N 0075                IF (S(IND).EQ.0.0) S(IND)=.0000001
N 0077                IF (ICA.GE.3) WRITE (6,880) I,TFN(I),S(IND),F(IND)
N 0079                IF (MORE.EQ.1) GO TO 610
N 0081                IF (IND.EQ.1) GO TO 180
N 0083                GO TO 240
N 0084          170   S(IND)=1.*(TFN(I-16)+TFN(I+16))+3.*(TFN(I-15)+TFN(I+15))+6.*(TFN(I
                1-14)+TFN(I+14))+10.*(TFN(I-13)+TFN(I+13))+15.*(TFN(I-12)+TFN(I+12)
                2)+21.*(TFN(I-11)+TFN(I+11))+28.*(TFN(I-10)+TFN(I+10))+31.*(TFN(I-9
                3)+TFN(I+9))+30.*(TFN(I-8)+TFN(I+8))+25.*(TFN(I-7)+TFN(I+7))+16.*(T
                4FN(I-6)+TFN(I+6))+3.*(TFN(I-5)+TFN(I+5))-14.*(TFN(I-4)+TFN(I+4))-3
                55.*(TFN(I-3)+TFN(I+3))-50.*(TFN(I-2)+TFN(I+2))-59.*(TFN(I-1)+TFN(I
                6+1))-62.*TFN(I)
N 0085                F(IND)=SQRT(27342.*(TFN(I)))
N 0086                IF (S(IND).EQ.3.0) S(IND)=.0000001
                C     TO PREVENT DIVIDING BY ZERO, LET S(I) = .0000001
N 0088                IF (ICA.GE.3) WRITE (6,880) I,TFN(I),S(IND),F(IND)
N 0090                IF (MORE.EQ.1) GO TO 610
N 0092                IF (IND.EQ.1) GO TO 180
N 0094                GO TO 240
N 0095          180   IND=IND+1
N 0096                I=I+1
N 0097                IF (I.GE.4096-IWIND) GO TO 720
N 0099                IF (IND.GE.300) GO TO 190
N 0101                GO TO 140
N 0102          190   DO 230 IND=IND15,298
N 0103                IF (S(IND).GE.0.0) GO TO 230
N 0105                IF (S(IND).LT.S(IND-1).AND.S(IND).LT.S(IND+1)) GO TO 200
N 0107                IF (IND.EQ.298) GO TO 230
N 0109                IF (S(IND).LT.S(IND-1).AND.S(IND).EQ.S(IND+1).AND.S(IND).LT.S(IND+
                12)) GO TO 200
N 0111                GO TO 230
N 0112          200   KOUNT=KOUNT+1
N 0113                IF (KOUNT.GE.500) GO TO 210
N 0115                GO TO 220
N 0116          210   WRITE (6,890)
N 0117                GO TO 720
N 0118          220   I=IND+I1-2
N 0119                PKCNTR(KOUNT)=I
N 0120                ENG(KOUNT)=((PKCNTR(KOUNT)-(CDEL(1)+PKCNTR(KOUNT)*(CDEL(2)+PKCNTR(
                1KOUNT)*(CDEL(3)+PKCNTR(KOUNT)*(CDEL(4)+PKCNTR(KOUNT)*CDEL(5))))))-
                2AA)/BB
N 0121                COUNTS(KOUNT)=TFN(I)
N 0122                FWHM(KOUNT)=DASH
N 0123                COMCOD(KOUNT)=80.0
N 0124          230   CONTINUE
N 0125                S(1)=S(298)
N 0126                F(1)=F(298)
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N 0127              S(2)=S(299)
N 0128              F(2)=F(299)
N 0129              I=299+I1-2
N 0130              IND=2
N 0131              I1=I
N 0132              INDI1=2
N 0133              GO TO 180
                C   BEGIN THE SEARCH FOR VARIABLES I1 THRU I5.
N 0134          240 IF (S(IND).GT.F(IND)) GO TO 260
N 0136              IF (S(IND).GT.0.0) GO TO 270
N 0138              M=3
N 0139          250 IF (S(IND-1).GT.F(IND-1)) GO TO 280
N 0141              IF (S(IND-1).GT.0.0) GO TO 310
N 0143              IF (M.EQ.3) GO TO 180
N 0145              I5=I-1
N 0146              INDI5=IND-1
N 0147              INDZ=IND-1
N 0148              GO TO 340
N 0149          260 M=1
N 0150              GO TO 250
N 0151          270 M=2
N 0152              GO TO 250
N 0153          280 IF (M.EQ.1) GO TO 180
N 0155              IF (M.EQ.2) GO TO 290
N 0157              IF (M.EQ.3) GO TO 300
N 0159          290 I2=I-1
N 0160              INDI2=IND-1
N 0161              GO TO 180
N 0162          300 I3=I
N 0163              INDI3=IND
N 0164              GO TO 290
N 0165          310 IF (M.EQ.1) GO TO 320
N 0167              IF (M.EQ.2) GO TO 180
N 0169              IF (M.EQ.3) GO TO 330
N 0171          320 I1=I
N 0172              INDI1=2
N 0173              S(1)=S(IND-1)
N 0174              F(1)=F(IND-1)
N 0175              S(2)=S(IND)
N 0176              F(2)=F(IND)
N 0177              IND=2
N 0178              GO TO 180
N 0179          330 I3=I
N 0180              INDI3=IND
N 0181              GO TO 180
                C   COMPUTE THE MINIMA BETWEEN I3 AND I5.  IF THERE IS ONLY ONE
                C   MINIMUM, LET IT BE CALLED I4.
N 0182          340 KOUNTA=KOUNT+1
N 0183              DO 380 IND=INDI3,INDI5
N 0184              IF (S(IND).LT.S(IND-1).AND.S(IND).LT.S(IND+1)) GO TO 350
N 0186              IF (IND.EQ.INDZ) GO TO 380
N 0188              IF (S(IND).LT.S(IND-1).AND.S(IND).EQ.S(IND+1).AND.S(IND).LT.S(IND+
                   12)) GO TO 350
N 0190              GO TO 380
N 0191          350 KOUNT=KOUNT+1
N 0192              IF (KOUNT.GE.500) GO TO 210
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N 0194                I=IND+I1-2
N 0195                PKCNTR(KOUNT)=I
N 0196                FWHM(KOUNT)=DASH
N 0197                RSDA(KOUNT)=DASH
N 0198                AREA(KOUNT)=DASH
N 0199                ENG(KOUNT)=((PKCNTR(KOUNT)-(CDEL(1)+PKCNTR(KOUNT)*(CDEL(2)+PKCNTR(
                     1KOUNT)*(CDEL(3)+PKCNTR(KOUNT)*(CDEL(4)+PKCNTR(KOUNT)*CDEL(5))))))-
                     2AA)/BB
N 0200                IF (ICA.GE.3) WRITE (6,900) KOUNT,I,I3,I5
N 0202                COUNTS(KOUNT)=TEN(I)
N 0203                IF (KOUNT.EQ.KOUNTA) GO TO 360
N 0205                GO TO 370
N 0206           360  LRGPK=IND
N 0207                KOUNTL=KOUNT
N 0208                GO TO 380
N 0209           370  IF (S(LRGPK).GT.S(IND)) GO TO 360
N 0211                GO TO 380
N 0212           380  CONTINUE
N 0213                IF (KOUNTA-1.EQ.KOUNT) GO TO 390
N 0215                GO TO 400
N 0216           390  KOUNT=KOUNT+1
N 0217                IF (KOUNT.GE.500) GO TO 210
N 0219                COMCOD(KOUNT)=81.
N 0220                IF (ICA.GE.3) WRITE (6,910) KOUNT,I3,I5
N 0222                PKCNTR(KOUNT)=(I3+I5)/2.
N 0223                FWHM(KOUNT)=DASH
N 0224                ENG(KOUNT)=((PKCNTR(KOUNT)-(CDEL(1)+PKCNTR(KOUNT)*(CDEL(2)+PKCNTR(
                     1KOUNT)*(CDEL(3)+PKCNTR(KOUNT)*(CDEL(4)+PKCNTR(KOUNT)*CDEL(5))))))-
                     2AA)/BB
N 0225                COUNTS(KOUNT)=TEN(PKCNTR(KOUNT))
N 0226                AREA(KOUNT)=DASH
N 0227                RSDA(KOUNT)=DASH
N 0228                I=I5+1
N 0229                IND=I-I1+2
N 0230                GO TO 180
N 0231           400  I=I5+1
N 0232                IND=I-I1+2
N 0233                KOUNTZ=KOUNT
N 0234                I4=LRGPK
N 0235                I4CHAN=I4+I1-2
                 C    IF PEAK IS A SINGLE PEAK GO TO 410.
N 0236                IF (KOUNTA.EQ.KOUNTZ) GO TO 410
                 C    IF THIS IS A MULTIPLE PEAK GO TO 470.
N 0238                GO TO 470
N 0239           410  N1=I5-I3+1
N 0240                N2=(-.5*(N1+ITOLER)*(F(I4)/S(I4)))+.5
N 0241                N3=((N1-ITOLER)*(1.0-(2.0*(F(I4)/S(I4)))))+.5
N 0242                FWHM(KOUNT)=1.18*(I5-I3)
                 C    TEST CONDITIONS DEFINING NUMERICAL RELATIONSHIP OF CHANNEL NUMBERS
                 C    FOR I1 THROUGH I5.  CALL THIS TEST CONDITION NUMBER ZERO.
N 0243                IF (I1.LE.I2.AND.I2.LE.I3.AND.I3+1.LT.I5) GO TO 420
N 0245                COMCOD(KOUNT)=60.
N 0246                IF (ICA.GE.3) WRITE (6,920) I1,I2,I3,I4CHAN,I5
N 0248                GO TO 180
                 C    TEST MARISCOTTI'S CONDITION NUMBER ONE.
N 0249           420  TEST1A=ABS(S(I4))
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N 0250              TEST1B=2.0*F(I4)
N 0251              IF (TEST1A.GT.TEST1B) GO TO 430
N 0253              IF (ICA.GE.3) WRITE (6,930) I4CHAN
N 0255              COMCOD(KOUNT)=61.
N 0256              GO TO 180
                C   TEST OUR CONDITION NUMBER TWO INSTEAD OF MARISCOTTI'S NUMBER TWO.
N 0257      430     IF (N1.GE.3.AND.N1.LE.28) GO TO 440
N 0259              IF (ICA.GE.3) WRITE (6,940) I4CHAN,I5,I3,N1
N 0261              COMCOD(KOUNT)=62.
N 0262              GO TO 180
                C   TEST MARISCOTTI'S CONDITION NUMBER THREE.
N 0263      440     ITEST3=I3-I2-1
N 0264              IF (ITEST3.LE.N2.AND.N2.GE.1) GO TO 450
N 0266              IF (ITEST3.LE.1.AND.N2.EQ.0) GO TO 450
N 0268              IF (ICA.GE.3) WRITE (6,950) N2,I2,I3
N 0270              COMCOD(KOUNT)=63.
N 0271              GO TO 180
                C   TEST MARISCOTTI'S CONDITION NUMBER FOUR.
N 0272      450     ITEST4=I2-I1+1
N 0273              IF (ITEST4.GE.N3) GO TO 460
N 0275              IF (ICA.GE.3) WRITE (6,960) N3,I2,I1
N 0277              COMCOD(KOUNT)=64.
N 0278              GO TO 180
N 0279      460     IF (ICA.GE.3) WRITE (6,970) I4CHAN,ITOLER,N1,N2,N3,I1,I2,I3,I4CHAN
                   1,I5
N 0281              COMCOD(KOUNT)=0.0
N 0282              GO TO 580
N 0283      470     N1=I5-I3+1
N 0284              N2=(-.5*(N1+ITOLER)*(F(I4)/S(I4)))+.5
N 0285              N3=((N1-ITOLER)*(1.0-(2.0*(F(I4)/S(I4)))))+.5
N 0286              FWHM(KOUNTL)=1.13*(I5-I3)
                C   TEST CONDITIONS DEFINING NUMERICAL RELATIONSHIP OF CHANNEL NUMBERS
                C   FOR I1 THROUGH I5.  CALL THIS TEST CONDITION NUMBER ZERO.
N 0287              IF (I1.LE.I2.AND.I2.LE.I3.AND.I3+1.LT.I5) GO TO 480
N 0289              COMCOD(KOUNTL)=40.
N 0290              IF (ICA.GE.3) WRITE (6,920) I1,I2,I3,I4CHAN,I5
N 0292              GO TO 530
                C   TEST MARISCOTTI'S CONDITION NUMBER ONE.
N 0293      480     TEST1A=ABS(S(I4))
N 0294              TEST1B=2.0*F(I4)
N 0295              IF (TEST1A.GT.TEST1B) GO TO 490
N 0297              COMCOD(KOUNTL)=41.
N 0298              IF (ICA.GE.3) WRITE (6,930) I4CHAN
N 0300              GO TO 530
                C   TEST OUR CONDITION NUMBER TWO INSTEAD OF MARISCOTTI'S NUMBER TWO.
N 0301      490     IF (N1.GE.3.AND.N1.LE.28) GO TO 500
N 0303              COMCOD(KOUNTL)=42.
N 0304              IF (ICA.GE.3) WRITE (6,940) I4CHAN,I5,I3,N1
N 0306              GO TO 530
                C   TEST MARISCOTTI'S CONDITION NUMBER THREE.
N 0307      500     ITEST3=I3-I2-1
N 0308              IF (ITEST3.LE.N2.AND.N2.GE.1) GO TO 510
N 0310              IF (ITEST3.LE.1.AND.N2.EQ.0) GO TO 510
N 0312              COMCOD(KOUNTL)=43.
N 0313              IF (ICA.GE.3) WRITE (6,950) N2,I2,I3
N 0315              GO TO 530
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                C     TEST MARISCOTTI'S CONDITION NUMBER FOUR.
N 0316          510   ITEST4=I2-I1+1
N 0317                IF (ITEST4.GE.N3) GO TO 520
N 0319                COMCOD(KOUNTL)=44.
N 0320                IF (ICA.GE.3) WRITE (6,960) N3,I2,I1
N 0322                GO TO 530
N 0323          520   COMCOD(KOUNTL)=20.0
N 0324                IF (ICA.GE.3) WRITE (6,970) I4CHAN,ITOLER,N1,N2,N3,I1,I2,I3,I4CHAN
                     1,I5
N 0326                GO TO 530
N 0327          530   CONTINUE
N 0328                IF (COMCOD(KOUNTL).EQ.20.) GO TO 540
N 0330                IF (COMCOD(KOUNTL).NE.20.0) GO TO 560
N 0332          540   DO 550 KOUNT=KOUNTA,KOUNTZ
N 0333                IF (KOUNT.EQ.KOUNTL) GO TO 550
N 0335                COMCOD(KOUNT)=(200000.+LRGPK+I1-2.00)/10000.
N 0336                FWHM(KOUNT)=DASH
N 0337          550   CONTINUE
N 0338                I=I5+1
N 0339                IND=I-I1+2
N 0340                KOUNT=KOUNTL
N 0341                GO TO 580
N 0342          560   DO 570 KOUNT=KOUNTA,KOUNTZ
N 0343                IF (KOUNT.EQ.KOUNTL) GO TO 570
N 0345                COMCOD(KOUNT)=(500000.+LRGPK+I1-2.00)/10000.
N 0346                FWHM(KOUNT)=DASH
N 0347          570   CONTINUE
N 0348                KOUNT=KOUNTZ
N 0349                I=I5+1
N 0350                IND=I-I1+2
N 0351                GO TO 180
                C     FIT A GAUSSIAN CURVE TO THE POINTS BETWEEN THE MAXIMUM IN S ON
                C     THE LEFT (MAXL) AND THE MAXIMUM ON THE RIGHT (MAXR) OF THE PEAK
                C     CENTER.  CALCULATE THE PEAK CENTER FROM THESE DATA.  LET ILSQ
                C     COUNT CHANNELS STARTING WITH MAXL = 1.  LET KOUNT BE THE INDEX
                C     WHICH COUNTS THE PEAKS.
N 0352          580   CONTINUE
N 0353                INDI1$=INDI1+1
N 0354                INDI5$=INDI5+1
N 0355                INDZZ=INDI5+INDI5-INDI3
N 0356                INDBB=INDI3+INDI3-INDI5
N 0357                IF (INDI1$.GT.INDBB) INDBB=INDI1$
N 0359                MORE=1
N 0360                MAXL=INDBB-1
N 0361                DO 600 IND=INDBB,INDI2
N 0362                IF (S(IND).GT.S(MAXL)) GO TO 590
N 0364                GO TO 600
N 0365          590   MAXL=IND
N 0366          600   CONTINUE
N 0367                IMAXL=MAXL+I1-2
N 0368                I=I5+1
N 0369                IND=I-I1+2
N 0370                GO TO 180
N 0371          610   IF (I.LE.INDZZ+I1-2) GO TO 180
N 0373                MORE=0
N 0374                GO TO 620
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N 0375      620   MAXR=INDI5
N 0376            DO 640 IND=INDI5$,INDZZ
N 0377            IF (S(IND).GT.S(MAXR)) GO TO 630
N 0379            GO TO 640
N 0380      630   MAXR=IND
N 0381      640   CONTINUE
N 0382            IMAXR=MAXR+I1-2
N 0383            ILSQ=0
N 0384            L=IMAXR-IMAXL+1
N 0385            DO 670 I=IMAXL,IMAXR
N 0386            ILSQ=ILSQ+1
N 0387            CH(ILSQ,1)=I
N 0388            IF (TFN(I).EQ.0.0) GO TO 650
N 0390            GO TO 660
N 0391      650   $LNTFN(ILSQ)=-40.
N 0392            GO TO 670
N 0393      660   $LNTFN(ILSQ)=ALOG(TFN(I))
N 0394      670   CONTINUE
N 0395            CALL CLEAR(W,100)
N 0396            A=1.0D0
N 0397            CALL LSTSQR(CH,$LNTFN,W,L,2,A,B,1,STAT,VARB,T,50)
N 0398            IF (ICA.GE.3) WRITE (6,980) B(2),B(1),A
N 0400            IF (B(2).GE.0.0.AND.COMCOD(KOUNT).EQ.0.0) GO TO 680
N 0402            IF (B(2).GE.0.0.AND.COMCOD(KOUNT).EQ.20.0) GO TO 700
N 0404            GO TO 710
N 0405      680   COMCOD(KOUNT)=1.0
N 0406      690   FWHM(KOUNT)=1.18*(I5-I3)
N 0407            I=I5+1
N 0408            IND=I-I1+2
N 0409            KOUNT=KOUNTZ
N 0410            GO TO 180
N 0411      700   COMCOD(KOUNT)=21.00
N 0412            GO TO 690
N 0413      710   PKCNTR(KOUNT)=(-.5*B(1))/B(2)
N 0414            ENG(KOUNT)=((PKCNTR(KOUNT)-(CDEL(1)+PKCNTR(KOUNT)*(CDEL(2)+PKCNTR(
                 1KOUNT)*(CDEL(3)+PKCNTR(KOUNT)*(CDEL(4)+PKCNTR(KOUNT)*CDEL(5))))))-
                 2AA)/BB
N 0415            IF (ICA.GE.3) WRITE (6,990) KOUNT,PKCNTR(KOUNT)
N 0417            I=I5+1
N 0418            IND=I-I1+2
N 0419            KOUNT=KOUNTZ
N 0420            GO TO 180
N 0421      720   CONTINUE
            C     BEGIN EVALUATION OF PEAK CENTER AND FWHM DATA TO FIND SINGLE PEAKS
            C     SUFFICIENTLY SEPARATED FROM NEIGHBORING PEAKS TO PERMIT AREA CALC.
N 0422            $LOL=1.0
N 0423            JSTART=1
N 0424            NUMPK=1
N 0425            KOUNT=0
N 0426      730   KOUNT=KOUNT+1
N 0427            IF (KOUNT.GT.KOUNTZ) GO TO 780
N 0429            IF (COMCOD(KOUNT).EQ.0.0.OR.COMCOD(KOUNT).EQ.20.) GO TO 740
N 0431            GO TO 730
N 0432      740   IF (NUMPK.EQ.1) GO TO 750
N 0434            GO TO 760
N 0435      750   KCNTR=KOUNT
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N 0436              NUMPK=2
N 0437              GO TO 730
N 0438        760   KRGHT=KOUNT
N 0439              IF (JSTART.EQ.1) GO TO 770
N 0441              GO TO 780
N 0442        770   JSTART=2
N 0443              GO TO 790
N 0444        780   $LOL=PKCNTR(KLEFT)+SEPFAC*FWHM(KLEFT)
N 0445        790   COLL=PKCNTR(KCNTR)-SEPFAC*FWHM(KCNTR)
N 0446              COLR=PKCNTR(KCNTR)+SEPFAC*FWHM(KCNTR)
N 0447              IF (KOUNT.GT.KOUNTZ) RCL=4096.
N 0449              IF (KOUNT.GT.KOUNTZ) GO TO 800
N 0451              ROL=PKCNTR(KRGHT)-SEPFAC*FWHM(KRGHT)
N 0452        800   IF ($LOL.GT.COLL.OR.COLR.GT.ROL) GO TO 810
N 0454              GO TO 820
N 0455        810   AREA(KCNTR)=DASH
N 0456              GO TO 840
              C     BEGIN AREA CALCULATION.
              C     IXL AND IXR ARE THE CHANNEL NUMBERS FOR THE LEFT AND RIGHT POINTS
              C     THRU WHICH THE BACKGROUND IS FITTED.
N 0457        820   IXL=PKCNTR(KCNTR)-SEPFAC*FWHM(KCNTR)+.5
N 0458              IXR=PKCNTR(KCNTR)+SEPFAC*FWHM(KCNTR)+.5
              C     DETERMINE M, THE NUMBER OF POINTS TO BE USED IN SMOOTHING.
N 0459              M=25
N 0460              IF (FWHM(KCNTR).LT.5.) M=5
N 0462              DO 830 N=2,11
N 0463              MS=N+N+1
N 0464        830   IF (FWHM(KCNTR).GE.MS.AND.FWHM(KCNTR).LT.MS+2) M=MS
N 0466              IF (ICA.GE.3) WRITE (6,1000) PKCNTR(KCNTR),M
N 0468              CALL BKGND
N 0469              IF (ICA.GE.3) WRITE (6,1010) TM3,TM2,TM1,TM0
N 0471              CALL PKAREA(KCNTR)
              C     END AREA CALCULATION.
N 0472        840   KLEFT=KCNTR
N 0473              KCNTR=KRGHT
N 0474              IF (KOUNT.LE.KOUNTZ) GO TO 730
N 0476              IF (KOUNT.GT.KOUNTZ) GO TO 850
N 0478        850   IF (ICA.GE.3) WRITE (6,1020) FILE
              C     CALL EDIT HERE IF IMMEDIATE EDIT OF PEAK SEARCH IS DESIRED.  NOTE
              C     HOWEVER THAT ENERGIES WILL BE INCORRECT UNTIL AA AND BB (WHICH
              C     ARE DETERMINED IN THE MAIN GELI2 ROUTINE) ARE DEFINED.
N 0480              IF (ICA.GE.4) CALL PLOTIT
N 0482              IDIS=1
N 0483              RETURN
N 0484              ENTRY POINT
N 0485              NED=NPD-1
N 0486              DO 860 I=1,NED
N 0487              P1=PDATA(I,1)
N 0488        860   PDATA(I,4)=((P1-(CDEL(1)+P1*(CDEL(2)+P1*(CDEL(3)+P1*(CDEL(4)+P1*CD
                    1EL(5))))))-AA)/BB
N 0489              RETURN
              C
N 0490        870   FORMAT ('1',5X,'BEGIN DETAILED PRINT OUT OF PEAK SEARCH FOR FILE '
                    1,I3,'.'//)
N 0491        880   FORMAT (' ',I10,3X,F10.1,3X,D14.7,3X,D14.7)
N 0492        890   FORMAT (' ','THE NUMBER OF PEAKS TESTED HAS EXCEEDED THE NUMBER PE
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     1RMITTED BY THE DIMENSION STATEMENT.'/' PEAK SEARCH IS DISCONTINUED
     2.  PRINT OUT OF PEAK ANALYSIS FOLLOWS.')
N 0493    900  FORMAT (' ',I4,'.',5X,'A MINIMUM IN THE SECOND DIFFERENCE OCCURRED
     1 AT CHANNEL ',I4,' BETWEEN I3 = CHANNEL ',I4,' AND I5 = CHANNEL ',
     2I4,'.')
N 0494    910  FORMAT (' ',I4,'.',5X,'NO MINIMUM IN THE SECOND DIFFERENCE WAS FOU
     1ND BETWEEN I3 = CHANNEL ',I4,' AND I5 = CHANNEL ',I4,'.')
N 0495    920  FORMAT (' ','THE ZEROTH CONDITION TEST FAILED.'/' I1 = ',I4,',  I2
     1 = ',I4,',  I3 = ',I4,',  I4 = ',I4,',  I5 = ',I4,'.')
N 0496    930  FORMAT (' ','THE FIRST TEST CONDITION FAILED FOR I4 = ',I4,'.')
N 0497    940  FORMAT (' ','THE SECOND TEST CONDITION FAILED FOR I4 = ',I4,'.  I5
     1 = ',I4,',  I3 = ',I4,'  N1 = ',I4,'.')
N 0498    950  FORMAT (' ','THE THIRD TEST CONDITION FAILED:  N2 = ',I4,',  I2 =
     1',I4,',  I3 = ',I4,'.')
N 0499    960  FORMAT (' ','THE FOURTH TEST CONDITION FAILED:  N3 = ',I4,',  I2 =
     1 ',I4,',  I1 = ',I4,'.')
N 0500    970  FORMAT (' ','ALL TEST CONDITIONS WERE MET FOR THE TESTS AT MINIMUM
     1 CHANNEL = ',I4,'.      TOLERANCE = ',I2,/' N1 = ',I4,',  N2 = ',I4
     2,',  N3 = ',I4,',  I1 = ',I4,',  I2 = ',I4,',  I3 = ',I4,',  I4 =
     3',I4,',  I5 = ',I4,'.')
N 0501    980  FORMAT (' ','B(2) = ',D14.7,5X,'B(1) = ',D14.7,5X,'A = ',D14.7)
N 0502    990  FORMAT (' ',I4,'.',5X,'LEAST SQUARES FIT FOR THIS PEAK LOCATES THE
     1 CENTER AT',F10.4)
N 0503   1000  FORMAT (' ','M FOR PEAK AT ',F6.1,' = ',I2,'.')
N 0504   1010  FORMAT (' ','TM3 = ',D14.7,5X,'TM2 = ',D14.7,5X,'TM1 = ',D14.7,5X,
     1'TM0 = ',D14.7)
N 0505   1020  FORMAT ('0',5X,'END DETAILED PRINTOUT OF PEAK SEARCH FOR FILE ',I3
     1,'.')
N 0506        END
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N 0002            BLOCK DATA
N 0003            COMMON /DATA/ CDEL
N 0004            COMMON /IMIT/ NT6,NT5,IP,KOUNT,WT,DT,FLUX,ID,ICALIB,ICALC,E
N 0005            COMMON /SHELF/ WIND,ITOLER,SEPFAC,AFAC
N 0006            REAL *8 E(25)/74.7,661.6,1173.2,1332.5,21*0./
N 0007            REAL *4 CDEL(5)/.48625E01,-.71069E-02,.23778E-05,-.90127E-10,-.307
                 105E-13/
N 0008            REAL *4 WIND/5./,SEPFAC/2./,AFAC/1.5/
N 0009            REAL *4 WT/0.0/,DT/0.0/,FLUX/0.0/
N 0010            INTEGER *4 NT6/6/,NT5/5/,KOUNT/0/,ID/0/,IP/1/,ICALIB/1/,ICALC/1/
N 0011            INTEGER *4 ITOLER/3/
N 0012            END
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